



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:31 PM BST

PDB ID : 1O1D  
EMDB ID: : EMD-1001  
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM  
TOMOGRAMS OF INSECT FLIGHT MUSCLE  
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.  
Deposited on : 2002-11-18  
Resolution : 70.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

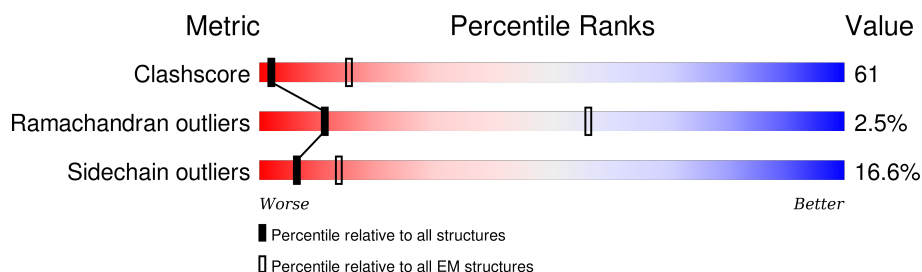
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 70.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













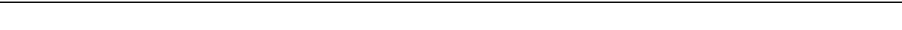

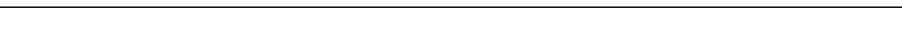
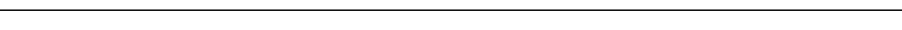
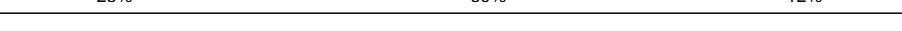


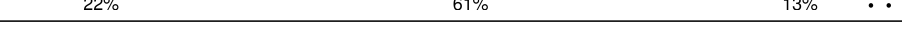
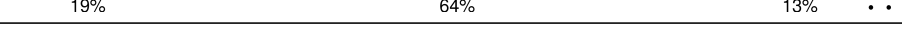




| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 840    | 25% 52% 20% .    |
| 1   | D     | 840    | 26% 52% 18% .    |
| 1   | G     | 840    | 25% 52% 19% .    |
| 1   | J     | 840    | 26% 50% 19% .    |
| 1   | M     | 840    | 25% 51% 20% .    |
| 1   | P     | 840    | 26% 51% 20% .    |
| 2   | B     | 145    | 65% 26% 6% .     |
| 2   | E     | 145    | 64% 27% 6% .     |
| 2   | H     | 145    | 63% 28% 6% .     |

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| Mol | Chain | Length | Quality of chain                                                                                    |
|-----|-------|--------|-----------------------------------------------------------------------------------------------------|
| 2   | K     | 145    |  63% 27% 6% .     |
| 2   | N     | 145    |  66% 26% 6% .     |
| 2   | Q     | 145    |  66% 26% 6% .     |
| 3   | C     | 147    |  61% 37% .        |
| 3   | F     | 147    |  60% 38% .        |
| 3   | I     | 147    |  60% 38% .        |
| 3   | L     | 147    |  60% 38% .        |
| 3   | O     | 147    |  60% 37% .        |
| 3   | R     | 147    |  59% 38% .        |
| 4   | 0     | 375    |  57% 32% 8% ..    |
| 4   | 1     | 375    |  59% 31% 7% ..    |
| 4   | 2     | 375    |  54% 36% 8% ..    |
| 4   | 3     | 375    |  27% 57% 11% .. |
| 4   | 4     | 375    |  25% 59% 12% .. |
| 4   | 5     | 375    |  24% 60% 12% .. |
| 4   | 7     | 375    |  26% 58% 12% .. |
| 4   | 8     | 375    |  22% 61% 13% .. |
| 4   | 9     | 375    |  19% 64% 13% .. |
| 4   | V     | 375    |  51% 37% 9% ..  |
| 4   | W     | 375    |  55% 35% 8% ..  |
| 4   | X     | 375    |  61% 29% 7% ..  |
| 4   | Y     | 375    |  62% 29% 7% ..  |
| 4   | Z     | 375    |  57% 32% 8% ..  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1   | MLY  | A     | 505 | -         | -        | X       | -                |
| 1   | MLY  | A     | 553 | -         | -        | X       | -                |
| 1   | MLY  | A     | 764 | -         | -        | X       | -                |
| 1   | MLY  | A     | 768 | -         | -        | X       | -                |
| 1   | MLY  | A     | 782 | -         | -        | X       | -                |
| 1   | MLY  | A     | 839 | -         | -        | X       | -                |
| 1   | MLY  | D     | 553 | -         | -        | X       | -                |
| 1   | MLY  | D     | 764 | -         | -        | X       | -                |
| 1   | MLY  | D     | 768 | -         | -        | X       | -                |
| 1   | MLY  | D     | 782 | -         | -        | X       | -                |
| 1   | MLY  | G     | 553 | -         | -        | X       | -                |
| 1   | MLY  | G     | 764 | -         | -        | X       | -                |
| 1   | MLY  | G     | 768 | -         | -        | X       | -                |
| 1   | MLY  | G     | 84  | -         | -        | X       | -                |
| 1   | MLY  | J     | 505 | -         | -        | X       | -                |
| 1   | MLY  | J     | 553 | -         | -        | X       | -                |
| 1   | MLY  | J     | 839 | -         | -        | X       | -                |
| 1   | MLY  | J     | 84  | -         | -        | X       | -                |
| 1   | MLY  | M     | 35  | -         | -        | X       | -                |
| 1   | MLY  | M     | 505 | -         | -        | X       | -                |
| 1   | MLY  | M     | 553 | -         | -        | X       | -                |
| 1   | MLY  | M     | 782 | -         | -        | X       | -                |
| 1   | MLY  | M     | 839 | -         | -        | X       | -                |
| 1   | MLY  | M     | 84  | -         | -        | X       | -                |
| 1   | MLY  | P     | 764 | -         | -        | X       | -                |
| 1   | MLY  | P     | 839 | -         | -        | X       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 94966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SKELETAL MUSCLE MYOSIN II.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | D     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | G     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | J     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | M     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |
| 1   | P     | 840      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6797  | 4382 | 1135 | 1243 | 37 |         |       |

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | E     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | H     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | K     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | N     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |
| 2   | Q     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1127  | 717 | 177 | 227 | 6 |         |       |

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | C     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | F     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | I     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | L     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | O     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |
| 3   | R     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 698 | 188 | 230 | 7 |         |       |

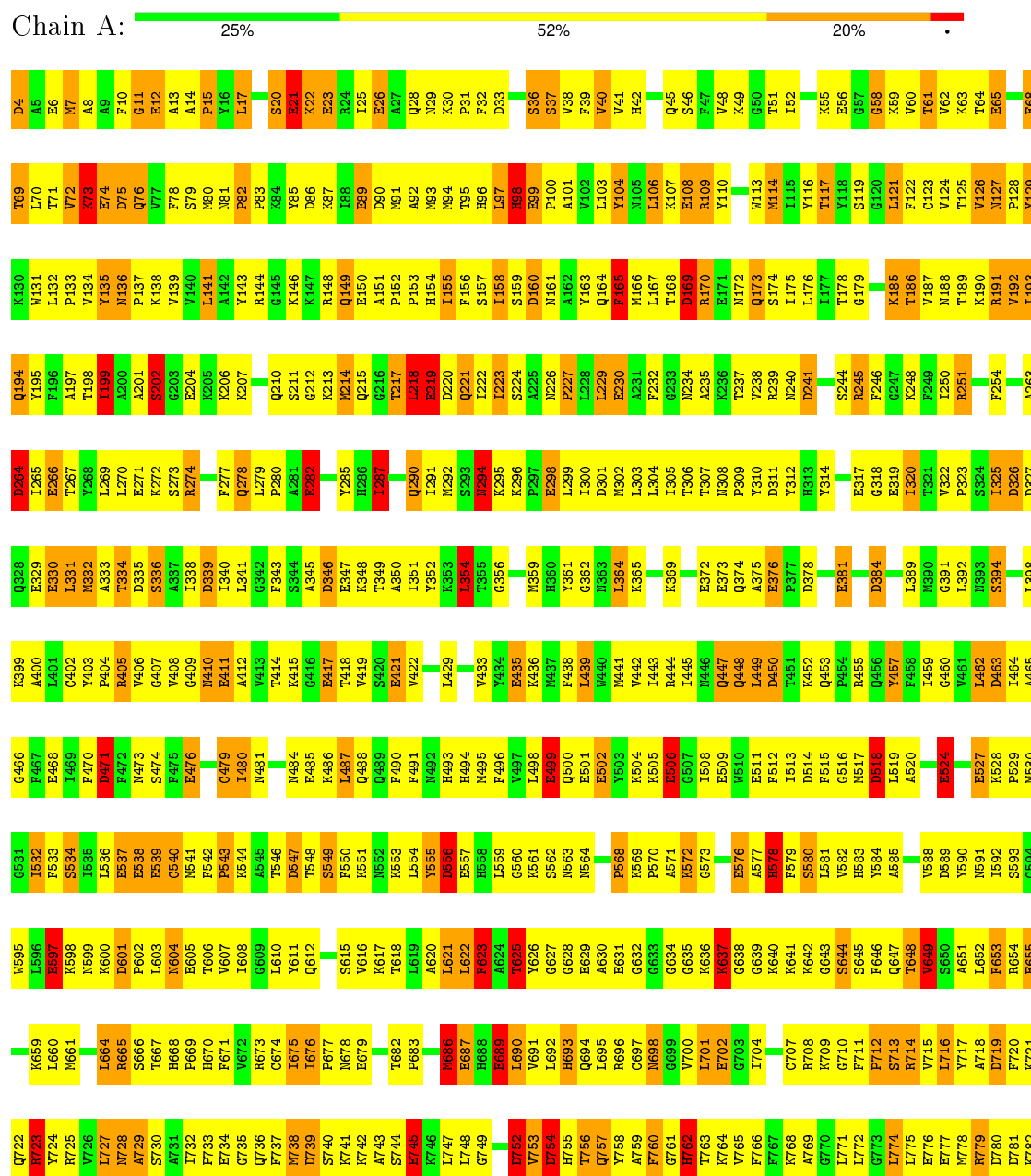
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 0     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 1     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 2     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 3     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 4     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 5     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 7     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 8     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | 9     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | V     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | W     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | X     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | Y     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |
| 4   | Z     | 372      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2906  | 1836 | 489 | 561 | 20 |         |       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

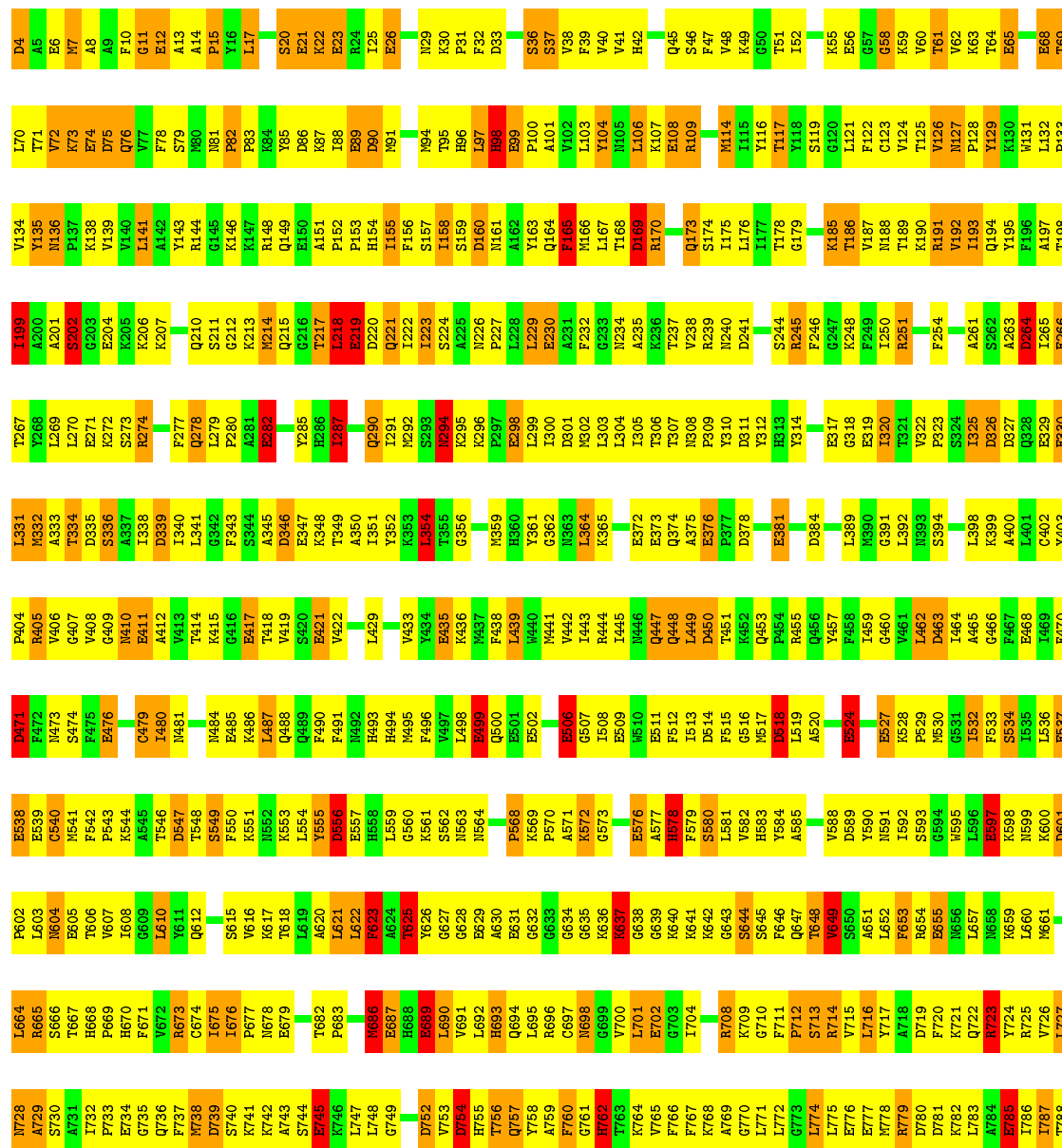
#### • Molecule 1: SKELETAL MUSCLE MYOSIN II





## • Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain D: 26% 52% 18%



## • Molecule 1: SKELETAL MUSCLE MYOSIN II

Chain G: 25% 52% 19%

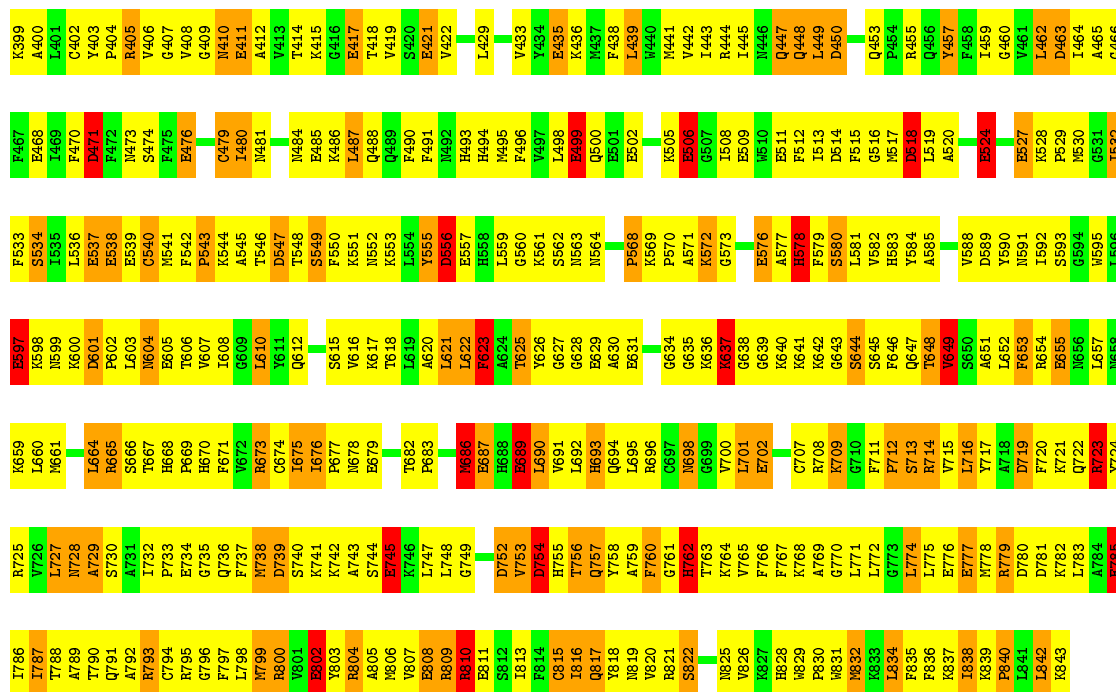




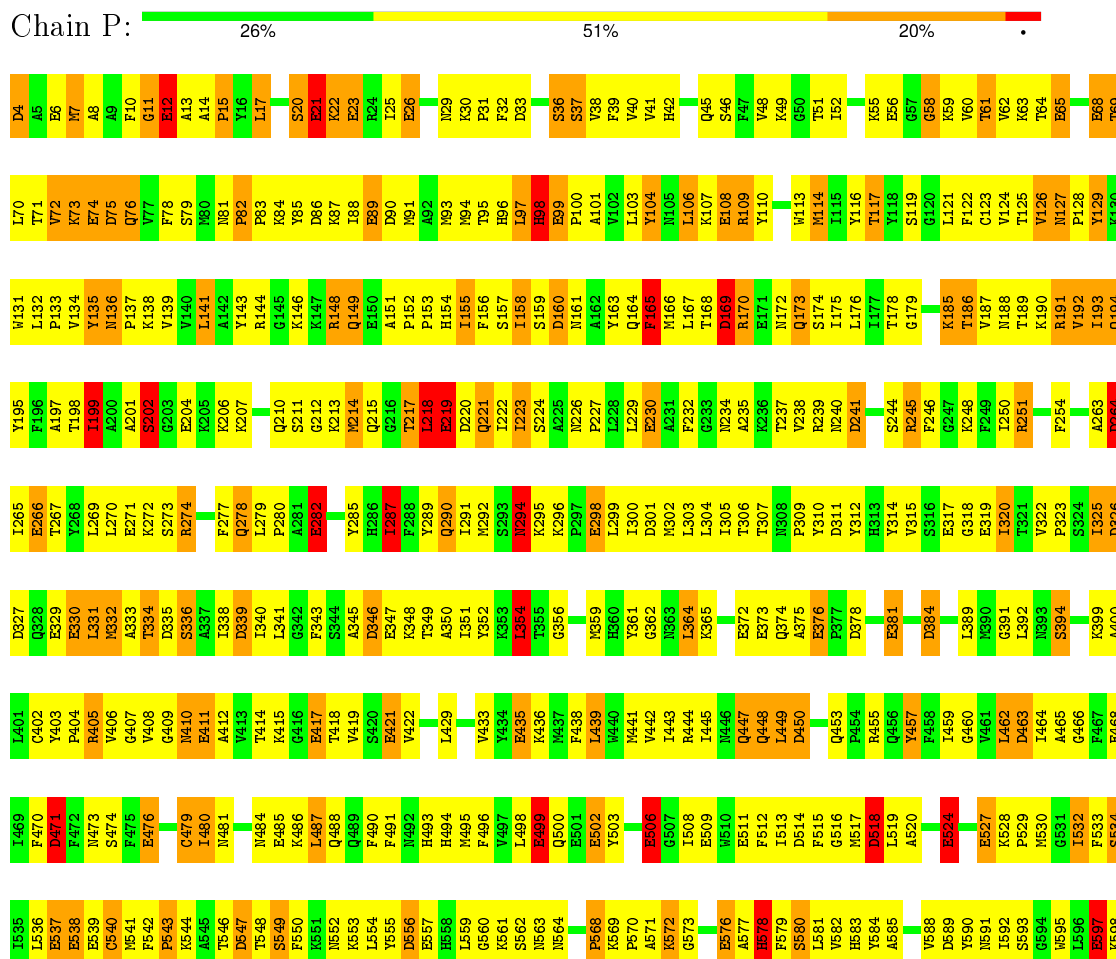
Chain J:  26% 50% 19% .

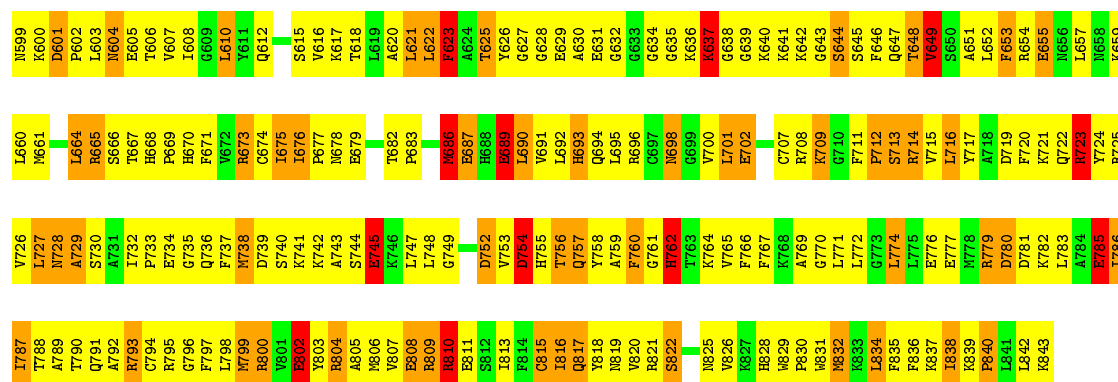






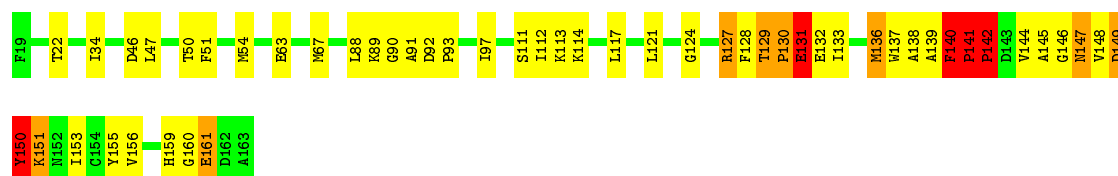
## • Molecule 1: SKELETAL MUSCLE MYOSIN II





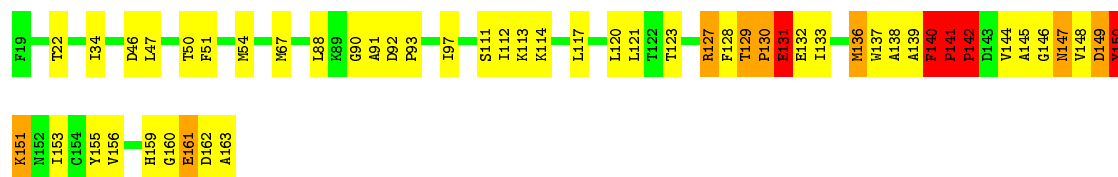
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain B: 65% 26% 6%



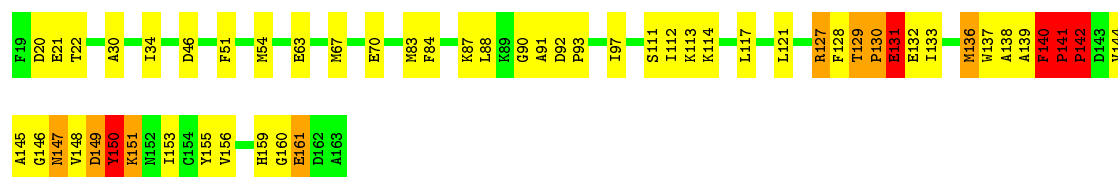
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain E: 64% 27% 6%



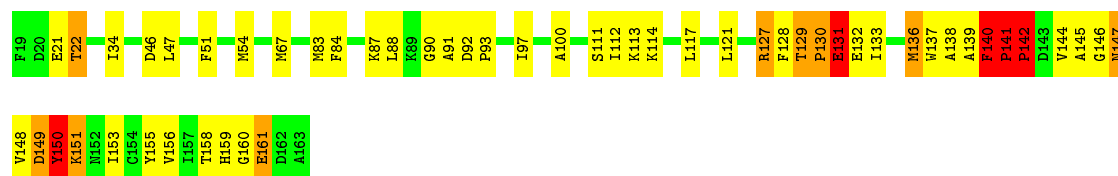
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Chain H: 63% 28% 6%

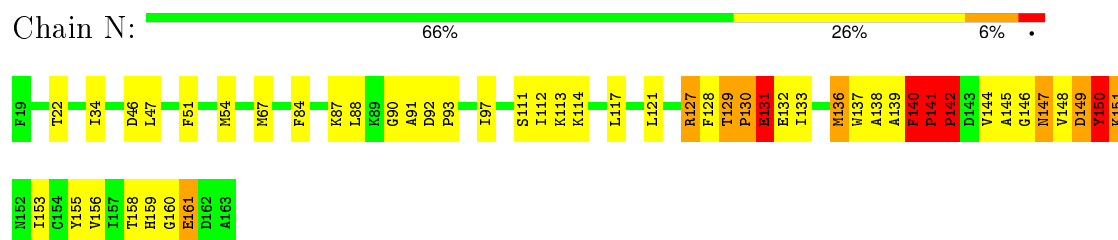


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

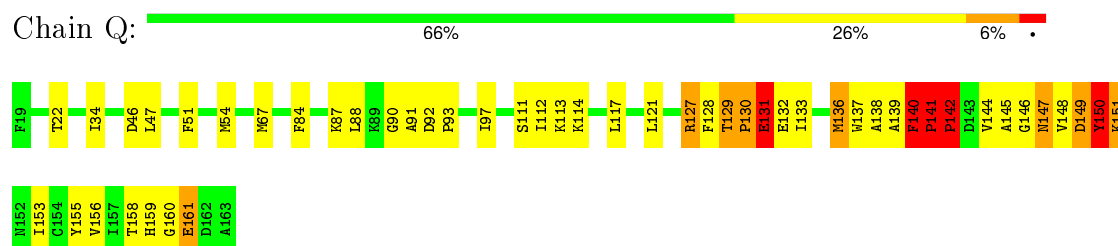
Chain K: 63% 27% 6%



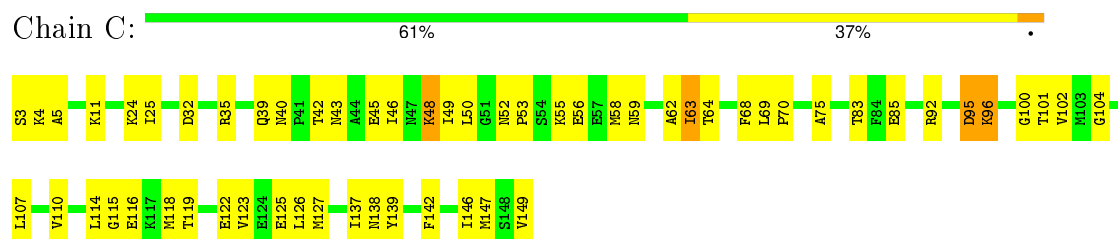
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



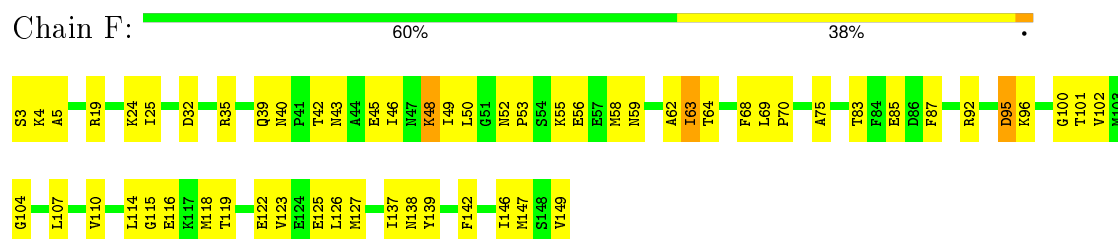
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



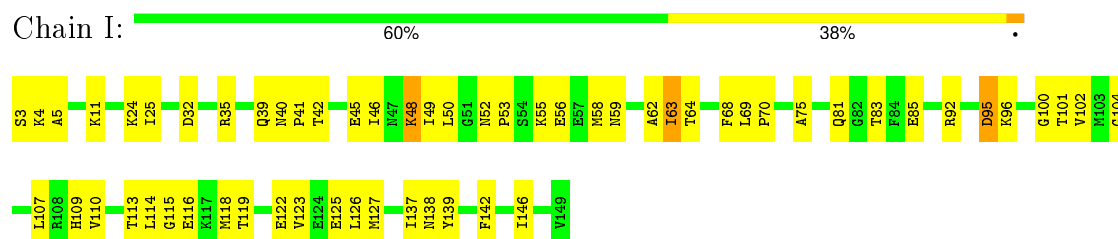
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



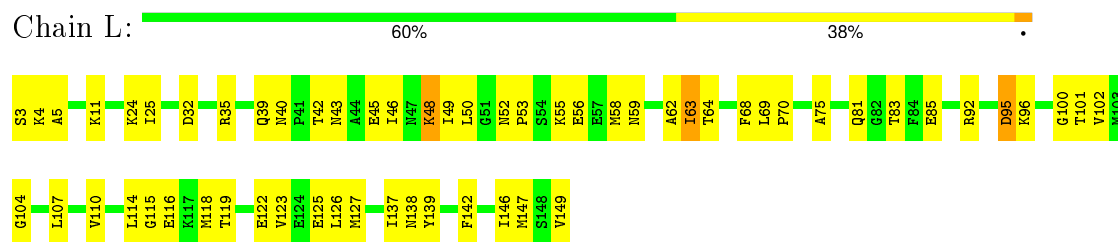
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



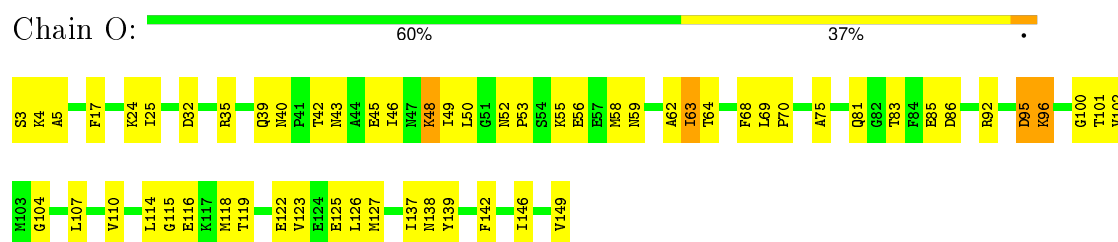
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



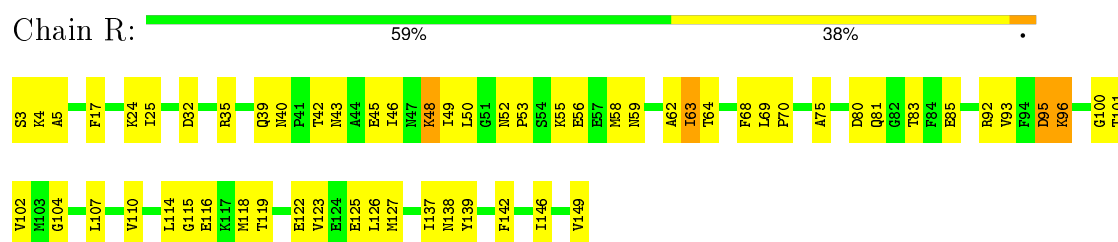
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



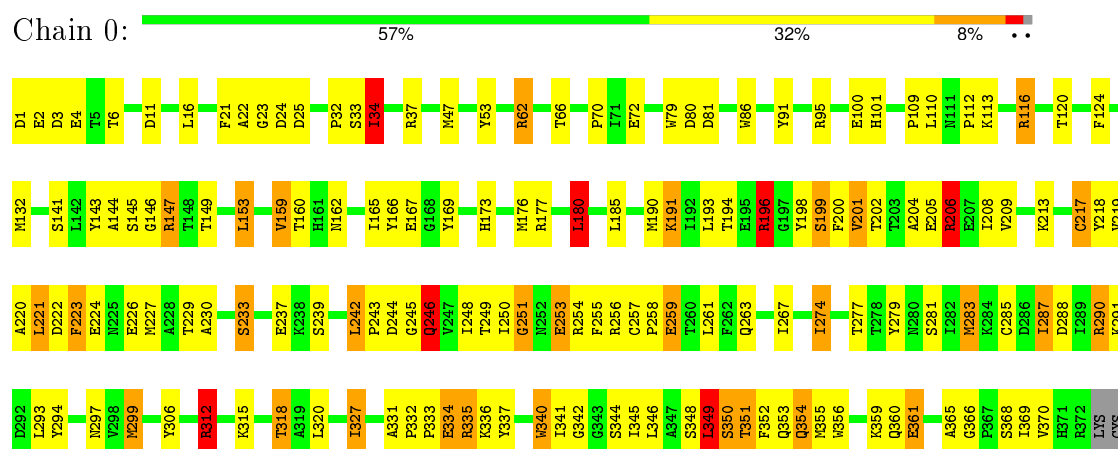
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



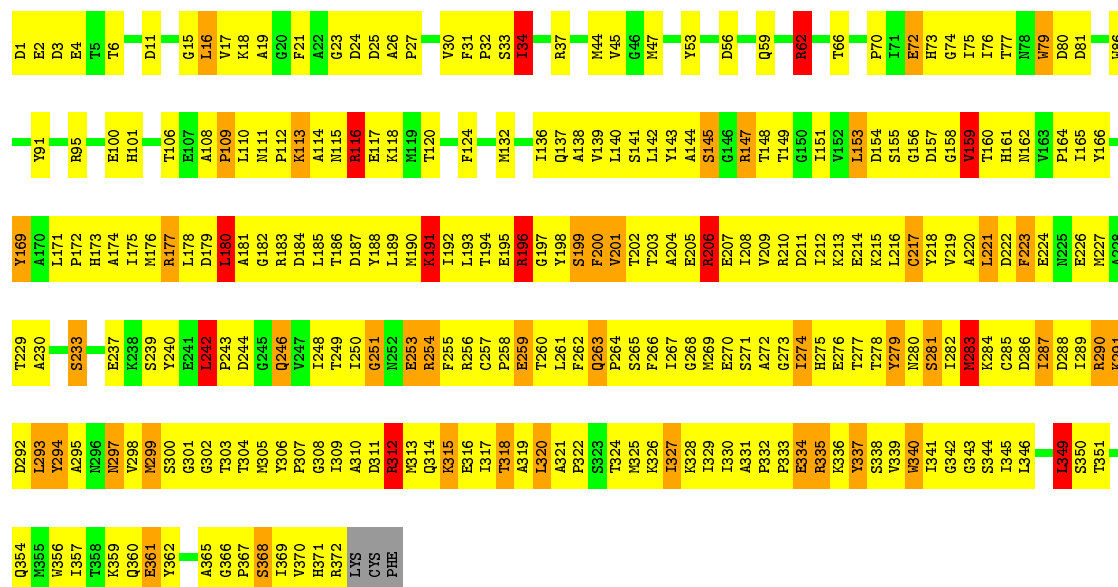
• Molecule 4: SKELETAL MUSCLE ACTIN



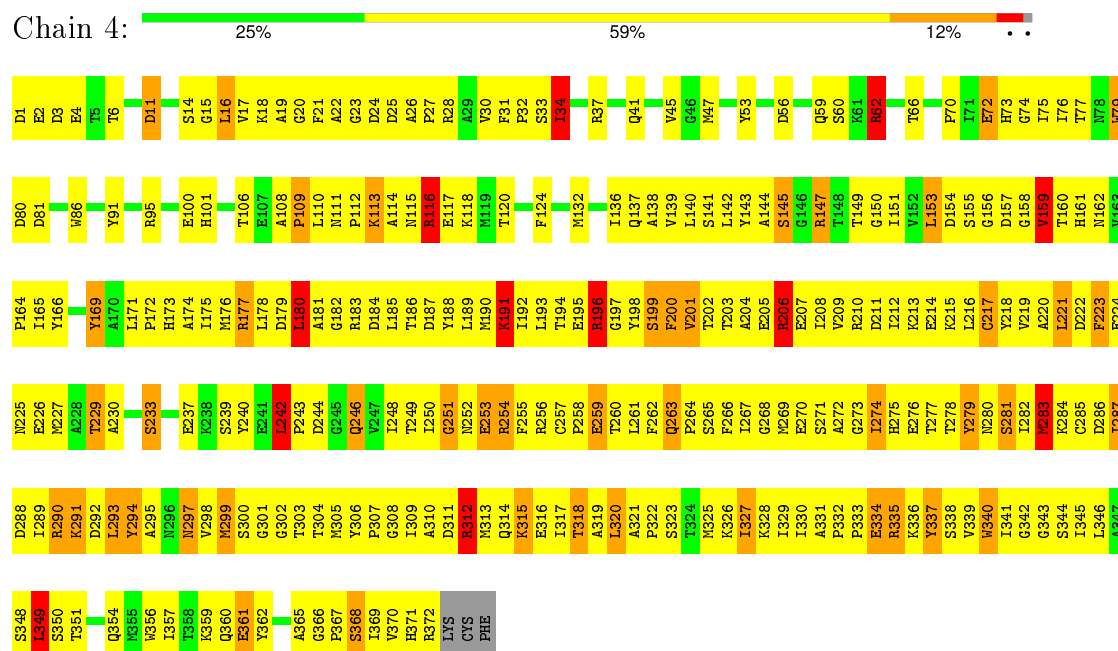
PHE

• Molecule 4: SKELETAL MUSCLE ACTIN

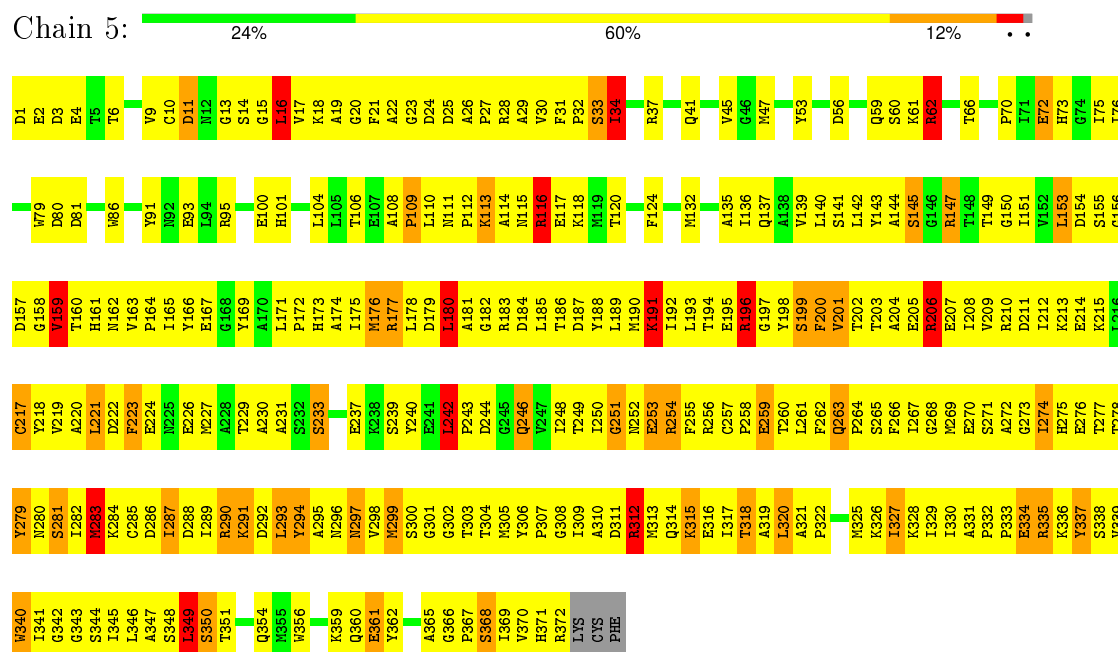




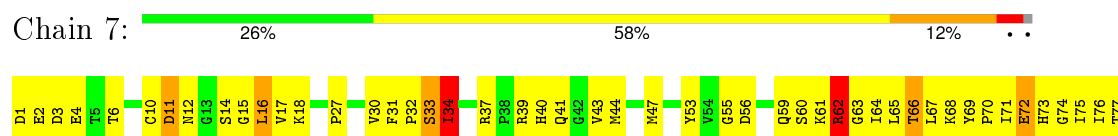
- Molecule 4: SKELETAL MUSCLE ACTIN

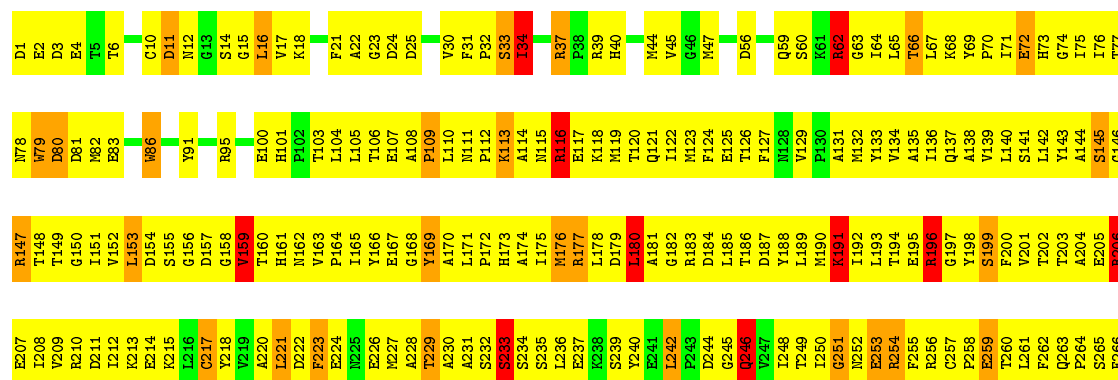


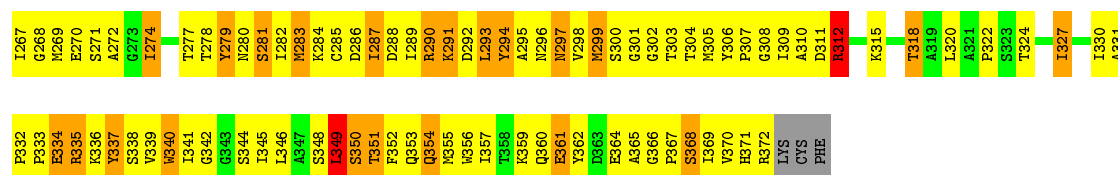
- Molecule 4: SKELETAL MUSCLE ACTIN



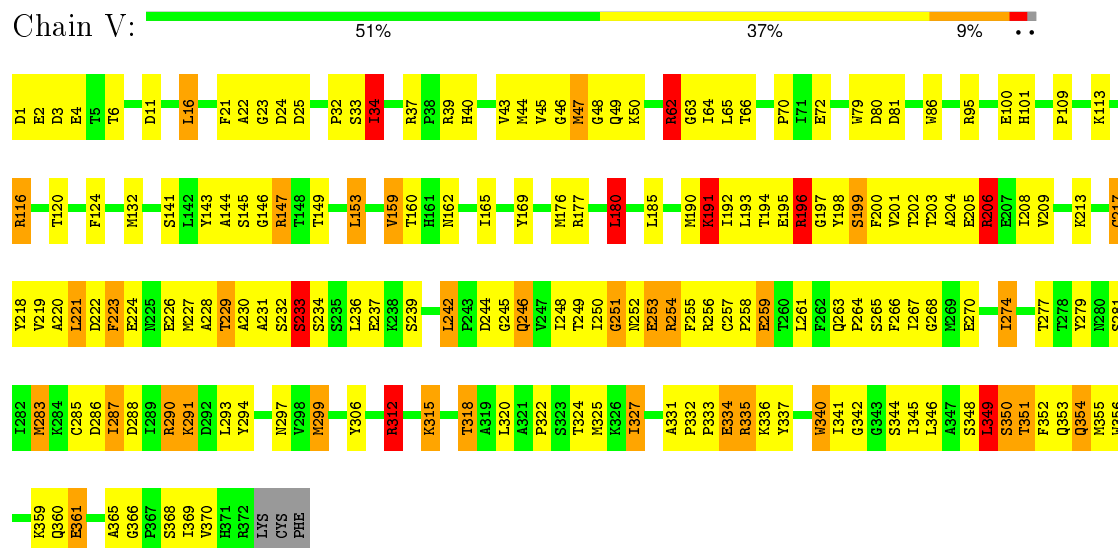
- Molecule 4: SKELETAL MUSCLE ACTIN



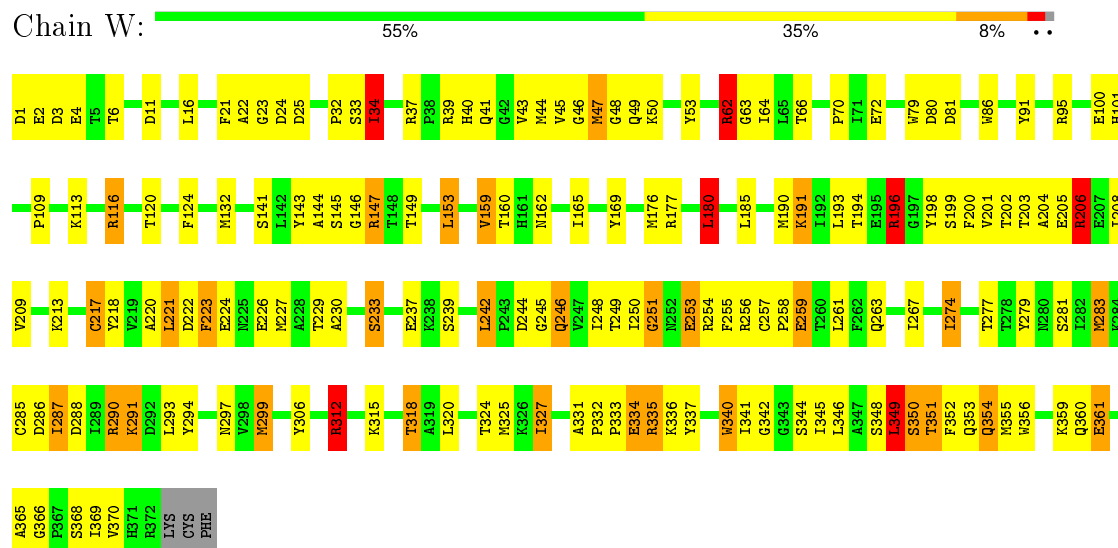




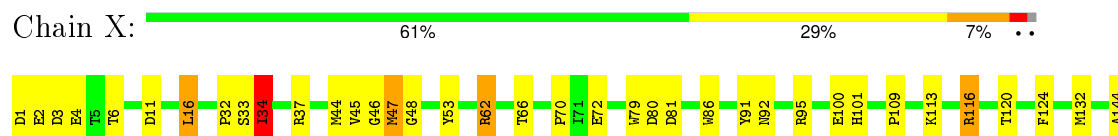
• Molecule 4: SKELETAL MUSCLE ACTIN

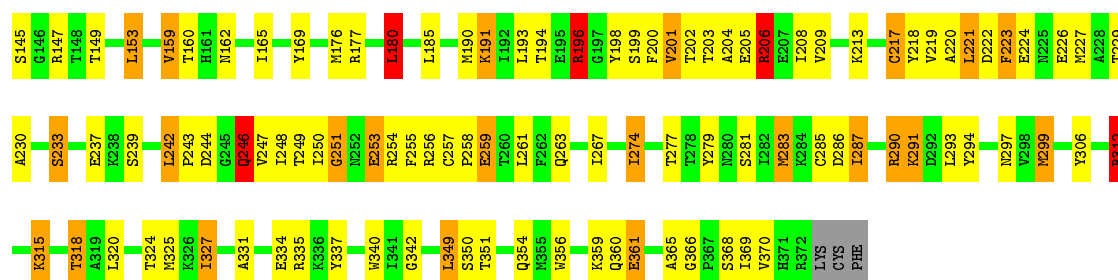


• Molecule 4: SKELETAL MUSCLE ACTIN



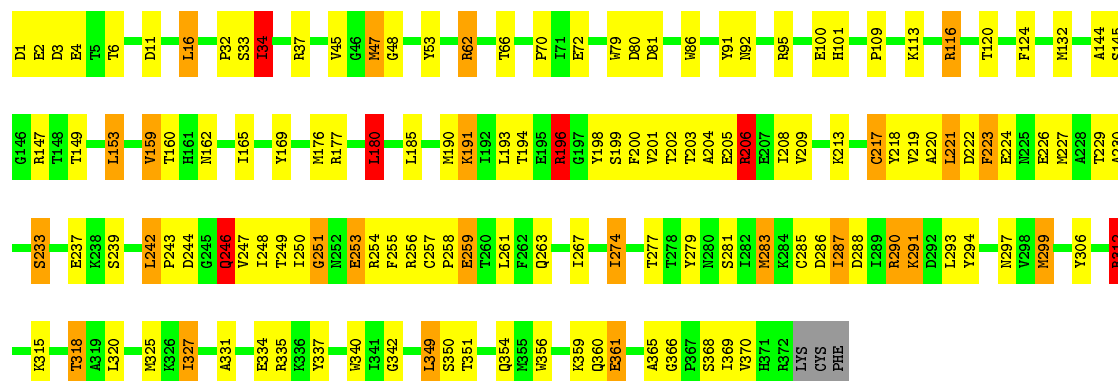
• Molecule 4: SKELETAL MUSCLE ACTIN





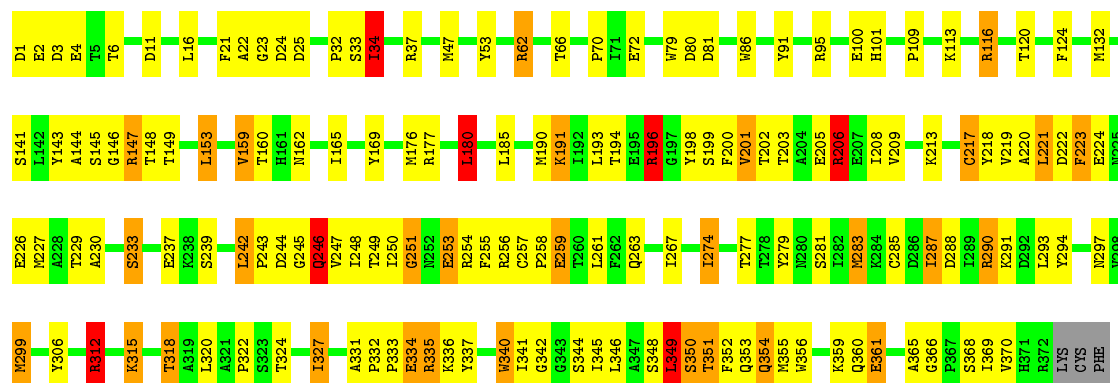
• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Y: 62% 29% 7% ..



• Molecule 4: SKELETAL MUSCLE ACTIN

Chain Z: 57% 32% 8% ..



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| Reconstruction method                | TOMOGRAPHY          | Depositor |
| Imposed symmetry                     | POINT, Not provided | Depositor |
| Number of images                     | Not provided        | Depositor |
| Resolution determination method      | Not provided        | Depositor |
| CTF correction method                | Not provided        | Depositor |
| Microscope                           | Not provided        | Depositor |
| Voltage (kV)                         | Not provided        | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | Not provided        | Depositor |
| Minimum defocus (nm)                 | Not provided        | Depositor |
| Maximum defocus (nm)                 | Not provided        | Depositor |
| Magnification                        | Not provided        | Depositor |
| Image detector                       | KODAK S0163 FILM    | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >2        | RMSZ        | # Z  >2         |
| 1   | A     | 1.77         | 67/6448 (1.0%) | 1.82        | 118/8729 (1.4%) |
| 1   | D     | 1.77         | 63/6448 (1.0%) | 1.82        | 117/8729 (1.3%) |
| 1   | G     | 1.78         | 67/6449 (1.0%) | 1.83        | 118/8732 (1.4%) |
| 1   | J     | 1.77         | 68/6449 (1.1%) | 1.87        | 117/8732 (1.3%) |
| 1   | M     | 1.78         | 66/6446 (1.0%) | 1.83        | 118/8723 (1.4%) |
| 1   | P     | 1.81         | 67/6448 (1.0%) | 1.87        | 122/8729 (1.4%) |
| 2   | B     | 1.22         | 10/1148 (0.9%) | 1.61        | 16/1548 (1.0%)  |
| 2   | E     | 1.22         | 10/1148 (0.9%) | 1.62        | 16/1548 (1.0%)  |
| 2   | H     | 1.22         | 10/1148 (0.9%) | 1.62        | 17/1548 (1.1%)  |
| 2   | K     | 1.22         | 10/1148 (0.9%) | 1.61        | 16/1548 (1.0%)  |
| 2   | N     | 1.22         | 10/1148 (0.9%) | 1.62        | 16/1548 (1.0%)  |
| 2   | Q     | 1.22         | 10/1148 (0.9%) | 1.61        | 16/1548 (1.0%)  |
| 3   | C     | 0.80         | 0/1136         | 0.95        | 4/1525 (0.3%)   |
| 3   | F     | 0.80         | 0/1136         | 0.95        | 4/1525 (0.3%)   |
| 3   | I     | 0.80         | 0/1136         | 0.94        | 4/1525 (0.3%)   |
| 3   | L     | 0.79         | 0/1136         | 0.94        | 4/1525 (0.3%)   |
| 3   | O     | 0.79         | 0/1136         | 0.95        | 4/1525 (0.3%)   |
| 3   | R     | 0.79         | 0/1136         | 0.94        | 4/1525 (0.3%)   |
| 4   | 0     | 0.89         | 1/2968 (0.0%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | 1     | 0.89         | 1/2968 (0.0%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | 2     | 0.89         | 1/2968 (0.0%)  | 1.64        | 52/4023 (1.3%)  |
| 4   | 3     | 0.89         | 2/2968 (0.1%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | 4     | 0.89         | 2/2968 (0.1%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | 5     | 0.89         | 2/2968 (0.1%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | 7     | 0.89         | 1/2968 (0.0%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | 8     | 0.89         | 2/2968 (0.1%)  | 1.64        | 52/4023 (1.3%)  |
| 4   | 9     | 0.89         | 2/2968 (0.1%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | V     | 0.89         | 2/2968 (0.1%)  | 1.64        | 50/4023 (1.2%)  |
| 4   | W     | 0.89         | 2/2968 (0.1%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | X     | 0.89         | 2/2968 (0.1%)  | 1.64        | 52/4023 (1.3%)  |
| 4   | Y     | 0.89         | 2/2968 (0.1%)  | 1.64        | 51/4023 (1.3%)  |
| 4   | Z     | 0.89         | 2/2968 (0.1%)  | 1.64        | 52/4023 (1.3%)  |

| Mol | Chain | Bond lengths |                  | Bond angles |                    |
|-----|-------|--------------|------------------|-------------|--------------------|
|     |       | RMSZ         | # Z  >2          | RMSZ        | # Z  >2            |
| All | All   | 1.35         | 482/93944 (0.5%) | 1.69        | 1548/127134 (1.2%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 4                   |
| 1   | D     | 1                   | 4                   |
| 1   | G     | 1                   | 4                   |
| 1   | J     | 1                   | 6                   |
| 1   | M     | 1                   | 6                   |
| 1   | P     | 1                   | 6                   |
| 2   | B     | 0                   | 3                   |
| 2   | E     | 0                   | 3                   |
| 2   | H     | 0                   | 3                   |
| 2   | K     | 0                   | 3                   |
| 2   | N     | 0                   | 3                   |
| 2   | Q     | 0                   | 3                   |
| 3   | C     | 0                   | 2                   |
| 3   | F     | 0                   | 2                   |
| 3   | I     | 0                   | 2                   |
| 3   | L     | 0                   | 2                   |
| 3   | O     | 0                   | 2                   |
| 3   | R     | 0                   | 2                   |
| 4   | 0     | 0                   | 1                   |
| 4   | 1     | 0                   | 1                   |
| 4   | 2     | 0                   | 1                   |
| 4   | 3     | 0                   | 1                   |
| 4   | 4     | 0                   | 1                   |
| 4   | 5     | 0                   | 1                   |
| 4   | 7     | 0                   | 1                   |
| 4   | 8     | 0                   | 1                   |
| 4   | 9     | 0                   | 1                   |
| 4   | V     | 0                   | 1                   |
| 4   | W     | 0                   | 1                   |
| 4   | X     | 0                   | 1                   |
| 4   | Y     | 0                   | 1                   |
| 4   | Z     | 0                   | 1                   |
| All | All   | 6                   | 74                  |

All (482) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | J     | 649 | VAL  | CB-CG1 | 53.30  | 2.64        | 1.52     |
| 1   | G     | 649 | VAL  | CB-CG1 | 53.30  | 2.64        | 1.52     |
| 1   | M     | 649 | VAL  | CB-CG1 | 53.28  | 2.64        | 1.52     |
| 1   | P     | 649 | VAL  | CB-CG1 | 53.28  | 2.64        | 1.52     |
| 1   | D     | 649 | VAL  | CB-CG1 | 53.20  | 2.64        | 1.52     |
| 1   | A     | 649 | VAL  | CB-CG1 | 53.18  | 2.64        | 1.52     |
| 1   | D     | 623 | PHE  | CB-CG  | 48.13  | 2.33        | 1.51     |
| 1   | A     | 623 | PHE  | CB-CG  | 48.12  | 2.33        | 1.51     |
| 1   | M     | 623 | PHE  | CB-CG  | 48.10  | 2.33        | 1.51     |
| 1   | J     | 623 | PHE  | CB-CG  | 48.10  | 2.33        | 1.51     |
| 1   | G     | 623 | PHE  | CB-CG  | 48.09  | 2.33        | 1.51     |
| 1   | P     | 623 | PHE  | CB-CG  | 48.06  | 2.33        | 1.51     |
| 1   | A     | 649 | VAL  | CB-CG2 | 46.30  | 2.50        | 1.52     |
| 1   | G     | 649 | VAL  | CB-CG2 | 46.19  | 2.49        | 1.52     |
| 1   | M     | 649 | VAL  | CB-CG2 | 46.16  | 2.49        | 1.52     |
| 1   | J     | 649 | VAL  | CB-CG2 | 46.16  | 2.49        | 1.52     |
| 1   | P     | 649 | VAL  | CB-CG2 | 46.14  | 2.49        | 1.52     |
| 1   | D     | 649 | VAL  | CB-CG2 | 46.13  | 2.49        | 1.52     |
| 1   | A     | 648 | THR  | CB-OG1 | 34.40  | 2.12        | 1.43     |
| 1   | D     | 648 | THR  | CB-OG1 | 34.38  | 2.12        | 1.43     |
| 1   | G     | 648 | THR  | CB-OG1 | 34.35  | 2.12        | 1.43     |
| 1   | P     | 648 | THR  | CB-OG1 | 34.35  | 2.12        | 1.43     |
| 1   | M     | 648 | THR  | CB-OG1 | 34.33  | 2.12        | 1.43     |
| 1   | J     | 648 | THR  | CB-OG1 | 34.32  | 2.11        | 1.43     |
| 1   | P     | 648 | THR  | CB-CG2 | -30.71 | 0.51        | 1.52     |
| 1   | M     | 648 | THR  | CB-CG2 | -30.70 | 0.51        | 1.52     |
| 1   | J     | 648 | THR  | CB-CG2 | -30.70 | 0.51        | 1.52     |
| 1   | A     | 648 | THR  | CB-CG2 | -30.70 | 0.51        | 1.52     |
| 1   | D     | 648 | THR  | CB-CG2 | -30.67 | 0.51        | 1.52     |
| 1   | G     | 648 | THR  | CB-CG2 | -30.64 | 0.51        | 1.52     |
| 1   | P     | 786 | ILE  | C-N    | 24.14  | 1.89        | 1.34     |
| 1   | P     | 785 | GLU  | C-N    | 20.47  | 1.81        | 1.34     |
| 1   | M     | 637 | LYS  | C-N    | -15.08 | 1.05        | 1.33     |
| 1   | P     | 637 | LYS  | C-N    | -15.01 | 1.06        | 1.33     |
| 1   | D     | 637 | LYS  | C-N    | -14.98 | 1.06        | 1.33     |
| 1   | J     | 637 | LYS  | C-N    | -14.97 | 1.06        | 1.33     |
| 1   | G     | 637 | LYS  | C-N    | -14.88 | 1.06        | 1.33     |
| 1   | A     | 637 | LYS  | C-N    | -14.80 | 1.06        | 1.33     |
| 1   | M     | 709 | LYS  | C-N    | -13.65 | 1.08        | 1.33     |
| 1   | G     | 649 | VAL  | C-N    | -13.53 | 1.02        | 1.34     |
| 1   | A     | 649 | VAL  | C-N    | -13.53 | 1.02        | 1.34     |
| 1   | P     | 649 | VAL  | C-N    | -13.46 | 1.03        | 1.34     |
| 1   | D     | 649 | VAL  | C-N    | -13.43 | 1.03        | 1.34     |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | N     | 150 | TYR  | CB-CG  | -13.41 | 1.31        | 1.51     |
| 2   | Q     | 150 | TYR  | CB-CG  | -13.41 | 1.31        | 1.51     |
| 1   | J     | 649 | VAL  | C-N    | -13.39 | 1.03        | 1.34     |
| 2   | H     | 150 | TYR  | CB-CG  | -13.37 | 1.31        | 1.51     |
| 1   | M     | 649 | VAL  | C-N    | -13.37 | 1.03        | 1.34     |
| 1   | G     | 709 | LYS  | C-N    | 13.35  | 1.57        | 1.33     |
| 2   | K     | 150 | TYR  | CB-CG  | -13.32 | 1.31        | 1.51     |
| 2   | E     | 150 | TYR  | CB-CG  | -13.27 | 1.31        | 1.51     |
| 2   | B     | 150 | TYR  | CB-CG  | -13.26 | 1.31        | 1.51     |
| 2   | B     | 140 | PHE  | C-N    | -13.01 | 1.09        | 1.34     |
| 2   | E     | 140 | PHE  | C-N    | -12.99 | 1.09        | 1.34     |
| 2   | Q     | 140 | PHE  | C-N    | -12.92 | 1.09        | 1.34     |
| 2   | N     | 140 | PHE  | C-N    | -12.92 | 1.09        | 1.34     |
| 2   | K     | 140 | PHE  | C-N    | -12.88 | 1.09        | 1.34     |
| 2   | H     | 140 | PHE  | C-N    | -12.80 | 1.09        | 1.34     |
| 2   | B     | 150 | TYR  | CG-CD2 | -11.38 | 1.24        | 1.39     |
| 2   | H     | 150 | TYR  | CG-CD2 | -11.31 | 1.24        | 1.39     |
| 2   | Q     | 150 | TYR  | CG-CD2 | -11.27 | 1.24        | 1.39     |
| 2   | E     | 150 | TYR  | CG-CD2 | -11.24 | 1.24        | 1.39     |
| 2   | K     | 150 | TYR  | CG-CD2 | -11.23 | 1.24        | 1.39     |
| 2   | N     | 150 | TYR  | CG-CD2 | -11.15 | 1.24        | 1.39     |
| 2   | K     | 141 | PRO  | N-CD   | -10.58 | 1.33        | 1.47     |
| 2   | B     | 141 | PRO  | N-CD   | -10.49 | 1.33        | 1.47     |
| 2   | N     | 141 | PRO  | N-CD   | -10.47 | 1.33        | 1.47     |
| 2   | E     | 141 | PRO  | N-CD   | -10.44 | 1.33        | 1.47     |
| 2   | Q     | 141 | PRO  | N-CD   | -10.39 | 1.33        | 1.47     |
| 2   | H     | 141 | PRO  | N-CD   | -10.29 | 1.33        | 1.47     |
| 1   | J     | 476 | GLU  | CD-OE1 | 8.92   | 1.35        | 1.25     |
| 1   | M     | 476 | GLU  | CD-OE1 | 8.86   | 1.35        | 1.25     |
| 1   | P     | 476 | GLU  | CD-OE1 | 8.86   | 1.35        | 1.25     |
| 1   | J     | 785 | GLU  | C-N    | 8.81   | 1.54        | 1.34     |
| 1   | D     | 476 | GLU  | CD-OE1 | 8.79   | 1.35        | 1.25     |
| 1   | G     | 476 | GLU  | CD-OE1 | 8.72   | 1.35        | 1.25     |
| 1   | M     | 622 | LEU  | C-N    | 8.70   | 1.54        | 1.34     |
| 1   | A     | 476 | GLU  | CD-OE1 | 8.69   | 1.35        | 1.25     |
| 1   | A     | 622 | LEU  | C-N    | 8.66   | 1.53        | 1.34     |
| 1   | J     | 622 | LEU  | C-N    | 8.65   | 1.53        | 1.34     |
| 1   | D     | 622 | LEU  | C-N    | 8.63   | 1.53        | 1.34     |
| 1   | P     | 622 | LEU  | C-N    | 8.63   | 1.53        | 1.34     |
| 1   | G     | 622 | LEU  | C-N    | 8.57   | 1.53        | 1.34     |
| 1   | P     | 745 | GLU  | CD-OE2 | 8.41   | 1.34        | 1.25     |
| 1   | G     | 411 | GLU  | CD-OE1 | 8.36   | 1.34        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | M     | 745 | GLU  | CD-OE2 | 8.33  | 1.34        | 1.25     |
| 1   | M     | 411 | GLU  | CD-OE1 | 8.33  | 1.34        | 1.25     |
| 1   | P     | 411 | GLU  | CD-OE1 | 8.31  | 1.34        | 1.25     |
| 1   | G     | 745 | GLU  | CD-OE2 | 8.27  | 1.34        | 1.25     |
| 1   | J     | 411 | GLU  | CD-OE1 | 8.26  | 1.34        | 1.25     |
| 2   | K     | 150 | TYR  | CA-CB  | -8.24 | 1.35        | 1.53     |
| 1   | D     | 411 | GLU  | CD-OE1 | 8.23  | 1.34        | 1.25     |
| 2   | B     | 150 | TYR  | CA-CB  | -8.22 | 1.35        | 1.53     |
| 1   | D     | 745 | GLU  | CD-OE2 | 8.20  | 1.34        | 1.25     |
| 1   | J     | 745 | GLU  | CD-OE2 | 8.19  | 1.34        | 1.25     |
| 1   | A     | 411 | GLU  | CD-OE1 | 8.16  | 1.34        | 1.25     |
| 2   | N     | 150 | TYR  | CA-CB  | -8.16 | 1.35        | 1.53     |
| 2   | H     | 150 | TYR  | CA-CB  | -8.15 | 1.36        | 1.53     |
| 2   | Q     | 150 | TYR  | CA-CB  | -8.14 | 1.36        | 1.53     |
| 1   | A     | 745 | GLU  | CD-OE2 | 8.09  | 1.34        | 1.25     |
| 1   | A     | 381 | GLU  | CD-OE1 | 8.03  | 1.34        | 1.25     |
| 2   | E     | 150 | TYR  | CA-CB  | -8.02 | 1.36        | 1.53     |
| 1   | G     | 108 | GLU  | CD-OE1 | 7.97  | 1.34        | 1.25     |
| 1   | M     | 108 | GLU  | CD-OE1 | 7.94  | 1.34        | 1.25     |
| 1   | P     | 108 | GLU  | CD-OE1 | 7.92  | 1.34        | 1.25     |
| 1   | J     | 108 | GLU  | CD-OE1 | 7.92  | 1.34        | 1.25     |
| 1   | A     | 108 | GLU  | CD-OE1 | 7.91  | 1.34        | 1.25     |
| 1   | G     | 381 | GLU  | CD-OE1 | 7.87  | 1.34        | 1.25     |
| 1   | M     | 381 | GLU  | CD-OE1 | 7.83  | 1.34        | 1.25     |
| 1   | D     | 381 | GLU  | CD-OE1 | 7.82  | 1.34        | 1.25     |
| 1   | M     | 202 | SER  | CB-OG  | 7.82  | 1.52        | 1.42     |
| 1   | J     | 202 | SER  | CB-OG  | 7.79  | 1.52        | 1.42     |
| 1   | J     | 381 | GLU  | CD-OE1 | 7.79  | 1.34        | 1.25     |
| 1   | P     | 381 | GLU  | CD-OE1 | 7.77  | 1.34        | 1.25     |
| 1   | P     | 202 | SER  | CB-OG  | 7.76  | 1.52        | 1.42     |
| 1   | G     | 202 | SER  | CB-OG  | 7.76  | 1.52        | 1.42     |
| 1   | D     | 202 | SER  | CB-OG  | 7.73  | 1.52        | 1.42     |
| 1   | A     | 202 | SER  | CB-OG  | 7.71  | 1.52        | 1.42     |
| 1   | D     | 108 | GLU  | CD-OE1 | 7.53  | 1.33        | 1.25     |
| 1   | G     | 689 | GLU  | CD-OE2 | 7.51  | 1.33        | 1.25     |
| 1   | D     | 689 | GLU  | CD-OE2 | 7.48  | 1.33        | 1.25     |
| 1   | A     | 689 | GLU  | CD-OE2 | 7.44  | 1.33        | 1.25     |
| 1   | A     | 23  | GLU  | CD-OE1 | 7.37  | 1.33        | 1.25     |
| 1   | M     | 689 | GLU  | CD-OE2 | 7.37  | 1.33        | 1.25     |
| 1   | J     | 689 | GLU  | CD-OE2 | 7.35  | 1.33        | 1.25     |
| 1   | D     | 23  | GLU  | CD-OE1 | 7.33  | 1.33        | 1.25     |
| 1   | P     | 689 | GLU  | CD-OE2 | 7.32  | 1.33        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | J     | 347 | GLU  | CD-OE1 | 7.32 | 1.33        | 1.25     |
| 1   | J     | 23  | GLU  | CD-OE1 | 7.27 | 1.33        | 1.25     |
| 1   | G     | 347 | GLU  | CD-OE1 | 7.25 | 1.33        | 1.25     |
| 1   | P     | 23  | GLU  | CD-OE1 | 7.24 | 1.33        | 1.25     |
| 1   | D     | 347 | GLU  | CD-OE1 | 7.21 | 1.33        | 1.25     |
| 1   | M     | 23  | GLU  | CD-OE1 | 7.21 | 1.33        | 1.25     |
| 1   | P     | 347 | GLU  | CD-OE1 | 7.20 | 1.33        | 1.25     |
| 1   | M     | 347 | GLU  | CD-OE1 | 7.18 | 1.33        | 1.25     |
| 1   | G     | 23  | GLU  | CD-OE1 | 7.17 | 1.33        | 1.25     |
| 1   | A     | 347 | GLU  | CD-OE1 | 7.17 | 1.33        | 1.25     |
| 1   | P     | 511 | GLU  | CD-OE1 | 7.12 | 1.33        | 1.25     |
| 1   | M     | 524 | GLU  | CD-OE1 | 7.08 | 1.33        | 1.25     |
| 1   | M     | 511 | GLU  | CD-OE1 | 7.08 | 1.33        | 1.25     |
| 1   | G     | 68  | GLU  | CD-OE2 | 7.07 | 1.33        | 1.25     |
| 1   | D     | 524 | GLU  | CD-OE1 | 7.06 | 1.33        | 1.25     |
| 1   | J     | 511 | GLU  | CD-OE1 | 7.06 | 1.33        | 1.25     |
| 1   | J     | 524 | GLU  | CD-OE1 | 7.04 | 1.33        | 1.25     |
| 1   | D     | 68  | GLU  | CD-OE2 | 7.04 | 1.33        | 1.25     |
| 1   | A     | 511 | GLU  | CD-OE1 | 7.02 | 1.33        | 1.25     |
| 1   | J     | 330 | GLU  | CD-OE1 | 7.01 | 1.33        | 1.25     |
| 1   | G     | 26  | GLU  | CD-OE1 | 7.00 | 1.33        | 1.25     |
| 1   | P     | 811 | GLU  | CD-OE1 | 7.00 | 1.33        | 1.25     |
| 1   | J     | 811 | GLU  | CD-OE1 | 7.00 | 1.33        | 1.25     |
| 1   | M     | 330 | GLU  | CD-OE1 | 6.98 | 1.33        | 1.25     |
| 1   | P     | 330 | GLU  | CD-OE1 | 6.96 | 1.33        | 1.25     |
| 1   | M     | 68  | GLU  | CD-OE2 | 6.96 | 1.33        | 1.25     |
| 1   | A     | 376 | GLU  | CD-OE1 | 6.95 | 1.33        | 1.25     |
| 1   | D     | 376 | GLU  | CD-OE1 | 6.95 | 1.33        | 1.25     |
| 1   | J     | 26  | GLU  | CD-OE1 | 6.94 | 1.33        | 1.25     |
| 1   | M     | 811 | GLU  | CD-OE1 | 6.94 | 1.33        | 1.25     |
| 1   | A     | 524 | GLU  | CD-OE1 | 6.94 | 1.33        | 1.25     |
| 1   | P     | 524 | GLU  | CD-OE1 | 6.94 | 1.33        | 1.25     |
| 1   | G     | 376 | GLU  | CD-OE1 | 6.93 | 1.33        | 1.25     |
| 1   | D     | 511 | GLU  | CD-OE1 | 6.93 | 1.33        | 1.25     |
| 1   | D     | 26  | GLU  | CD-OE1 | 6.92 | 1.33        | 1.25     |
| 1   | M     | 26  | GLU  | CD-OE1 | 6.91 | 1.33        | 1.25     |
| 1   | G     | 330 | GLU  | CD-OE1 | 6.89 | 1.33        | 1.25     |
| 1   | G     | 524 | GLU  | CD-OE1 | 6.89 | 1.33        | 1.25     |
| 1   | A     | 330 | GLU  | CD-OE1 | 6.87 | 1.33        | 1.25     |
| 1   | P     | 26  | GLU  | CD-OE1 | 6.87 | 1.33        | 1.25     |
| 1   | M     | 376 | GLU  | CD-OE1 | 6.86 | 1.33        | 1.25     |
| 1   | J     | 376 | GLU  | CD-OE1 | 6.85 | 1.33        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | P     | 376 | GLU  | CD-OE1  | 6.85  | 1.33        | 1.25     |
| 1   | A     | 655 | GLU  | CD-OE1  | 6.84  | 1.33        | 1.25     |
| 1   | P     | 68  | GLU  | CD-OE2  | 6.83  | 1.33        | 1.25     |
| 1   | A     | 68  | GLU  | CD-OE2  | 6.81  | 1.33        | 1.25     |
| 1   | J     | 68  | GLU  | CD-OE2  | 6.81  | 1.33        | 1.25     |
| 1   | G     | 511 | GLU  | CD-OE1  | 6.76  | 1.33        | 1.25     |
| 1   | D     | 330 | GLU  | CD-OE1  | 6.75  | 1.33        | 1.25     |
| 1   | A     | 26  | GLU  | CD-OE1  | 6.74  | 1.33        | 1.25     |
| 1   | J     | 319 | GLU  | CD-OE1  | 6.74  | 1.33        | 1.25     |
| 1   | A     | 811 | GLU  | CD-OE1  | 6.72  | 1.33        | 1.25     |
| 1   | P     | 538 | GLU  | CD-OE1  | 6.71  | 1.33        | 1.25     |
| 1   | J     | 709 | LYS  | C-N     | 6.70  | 1.45        | 1.33     |
| 1   | J     | 538 | GLU  | CD-OE1  | 6.70  | 1.33        | 1.25     |
| 1   | D     | 811 | GLU  | CD-OE1  | 6.70  | 1.33        | 1.25     |
| 1   | M     | 538 | GLU  | CD-OE1  | 6.68  | 1.32        | 1.25     |
| 1   | P     | 655 | GLU  | CD-OE1  | 6.67  | 1.32        | 1.25     |
| 1   | M     | 319 | GLU  | CD-OE1  | 6.66  | 1.32        | 1.25     |
| 1   | G     | 655 | GLU  | CD-OE1  | 6.66  | 1.32        | 1.25     |
| 1   | J     | 655 | GLU  | CD-OE1  | 6.65  | 1.32        | 1.25     |
| 1   | M     | 655 | GLU  | CD-OE1  | 6.65  | 1.32        | 1.25     |
| 1   | G     | 811 | GLU  | CD-OE1  | 6.63  | 1.32        | 1.25     |
| 1   | A     | 538 | GLU  | CD-OE1  | 6.60  | 1.32        | 1.25     |
| 1   | P     | 319 | GLU  | CD-OE1  | 6.60  | 1.32        | 1.25     |
| 1   | G     | 538 | GLU  | CD-OE1  | 6.59  | 1.32        | 1.25     |
| 1   | D     | 655 | GLU  | CD-OE1  | 6.59  | 1.32        | 1.25     |
| 1   | G     | 319 | GLU  | CD-OE1  | 6.59  | 1.32        | 1.25     |
| 1   | A     | 266 | GLU  | CD-OE2  | 6.58  | 1.32        | 1.25     |
| 2   | B     | 150 | TYR  | CD2-CE2 | -6.55 | 1.29        | 1.39     |
| 1   | G     | 785 | GLU  | C-N     | 6.55  | 1.49        | 1.34     |
| 1   | G     | 99  | GLU  | CD-OE2  | 6.54  | 1.32        | 1.25     |
| 1   | A     | 319 | GLU  | CD-OE1  | 6.54  | 1.32        | 1.25     |
| 1   | G     | 89  | GLU  | CD-OE1  | 6.54  | 1.32        | 1.25     |
| 2   | E     | 150 | TYR  | CD2-CE2 | -6.53 | 1.29        | 1.39     |
| 1   | D     | 538 | GLU  | CD-OE2  | -6.53 | 1.18        | 1.25     |
| 1   | D     | 319 | GLU  | CD-OE1  | 6.51  | 1.32        | 1.25     |
| 1   | D     | 538 | GLU  | CD-OE1  | 6.51  | 1.32        | 1.25     |
| 2   | K     | 150 | TYR  | CD2-CE2 | -6.49 | 1.29        | 1.39     |
| 1   | P     | 266 | GLU  | CD-OE2  | 6.48  | 1.32        | 1.25     |
| 1   | J     | 266 | GLU  | CD-OE2  | 6.48  | 1.32        | 1.25     |
| 1   | M     | 808 | GLU  | CD-OE1  | 6.48  | 1.32        | 1.25     |
| 1   | D     | 99  | GLU  | CD-OE2  | 6.47  | 1.32        | 1.25     |
| 2   | Q     | 150 | TYR  | CD2-CE2 | -6.47 | 1.29        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | P     | 808 | GLU  | CD-OE1  | 6.46  | 1.32        | 1.25     |
| 1   | P     | 89  | GLU  | CD-OE1  | 6.46  | 1.32        | 1.25     |
| 1   | M     | 266 | GLU  | CD-OE2  | 6.45  | 1.32        | 1.25     |
| 1   | J     | 502 | GLU  | CD-OE2  | 6.44  | 1.32        | 1.25     |
| 1   | P     | 6   | GLU  | CD-OE1  | 6.43  | 1.32        | 1.25     |
| 1   | A     | 502 | GLU  | CD-OE2  | 6.42  | 1.32        | 1.25     |
| 1   | G     | 538 | GLU  | CD-OE2  | -6.42 | 1.18        | 1.25     |
| 1   | D     | 266 | GLU  | CD-OE2  | 6.42  | 1.32        | 1.25     |
| 1   | P     | 538 | GLU  | CD-OE2  | -6.42 | 1.18        | 1.25     |
| 1   | G     | 502 | GLU  | CD-OE2  | 6.41  | 1.32        | 1.25     |
| 1   | A     | 89  | GLU  | CD-OE1  | 6.41  | 1.32        | 1.25     |
| 1   | J     | 538 | GLU  | CD-OE2  | -6.41 | 1.18        | 1.25     |
| 1   | J     | 89  | GLU  | CD-OE1  | 6.39  | 1.32        | 1.25     |
| 1   | G     | 266 | GLU  | CD-OE2  | 6.39  | 1.32        | 1.25     |
| 1   | A     | 538 | GLU  | CD-OE2  | -6.39 | 1.18        | 1.25     |
| 2   | N     | 150 | TYR  | CD2-CE2 | -6.38 | 1.29        | 1.39     |
| 2   | B     | 150 | TYR  | N-CA    | -6.38 | 1.33        | 1.46     |
| 1   | J     | 6   | GLU  | CD-OE1  | 6.38  | 1.32        | 1.25     |
| 4   | 2     | 259 | GLU  | CG-CD   | 6.38  | 1.61        | 1.51     |
| 1   | G     | 802 | GLU  | CD-OE1  | 6.37  | 1.32        | 1.25     |
| 1   | G     | 605 | GLU  | CD-OE1  | 6.37  | 1.32        | 1.25     |
| 1   | J     | 808 | GLU  | CD-OE1  | 6.37  | 1.32        | 1.25     |
| 1   | D     | 89  | GLU  | CD-OE1  | 6.36  | 1.32        | 1.25     |
| 1   | D     | 502 | GLU  | CD-OE2  | 6.36  | 1.32        | 1.25     |
| 1   | D     | 6   | GLU  | CD-OE1  | 6.35  | 1.32        | 1.25     |
| 1   | M     | 89  | GLU  | CD-OE1  | 6.34  | 1.32        | 1.25     |
| 1   | M     | 99  | GLU  | CD-OE2  | 6.34  | 1.32        | 1.25     |
| 2   | H     | 150 | TYR  | CD2-CE2 | -6.33 | 1.29        | 1.39     |
| 4   | V     | 259 | GLU  | CG-CD   | 6.33  | 1.61        | 1.51     |
| 1   | M     | 538 | GLU  | CD-OE2  | -6.33 | 1.18        | 1.25     |
| 1   | D     | 808 | GLU  | CD-OE1  | 6.32  | 1.32        | 1.25     |
| 1   | J     | 99  | GLU  | CD-OE2  | 6.32  | 1.32        | 1.25     |
| 1   | M     | 6   | GLU  | CD-OE1  | 6.32  | 1.32        | 1.25     |
| 1   | A     | 605 | GLU  | CD-OE1  | 6.30  | 1.32        | 1.25     |
| 2   | Q     | 150 | TYR  | N-CA    | -6.30 | 1.33        | 1.46     |
| 1   | G     | 6   | GLU  | CD-OE1  | 6.29  | 1.32        | 1.25     |
| 1   | P     | 99  | GLU  | CD-OE2  | 6.28  | 1.32        | 1.25     |
| 1   | G     | 808 | GLU  | CD-OE1  | 6.27  | 1.32        | 1.25     |
| 4   | 7     | 259 | GLU  | CG-CD   | 6.27  | 1.61        | 1.51     |
| 1   | M     | 502 | GLU  | CD-OE2  | 6.27  | 1.32        | 1.25     |
| 4   | 1     | 259 | GLU  | CG-CD   | 6.27  | 1.61        | 1.51     |
| 1   | P     | 502 | GLU  | CD-OE2  | 6.26  | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 802 | GLU  | CD-OE1 | 6.26  | 1.32        | 1.25     |
| 4   | 3     | 259 | GLU  | CG-CD  | 6.26  | 1.61        | 1.51     |
| 1   | A     | 808 | GLU  | CD-OE1 | 6.26  | 1.32        | 1.25     |
| 1   | P     | 605 | GLU  | CD-OE1 | 6.25  | 1.32        | 1.25     |
| 4   | W     | 259 | GLU  | CG-CD  | 6.24  | 1.61        | 1.51     |
| 4   | Y     | 259 | GLU  | CG-CD  | 6.24  | 1.61        | 1.51     |
| 1   | A     | 6   | GLU  | CD-OE1 | 6.24  | 1.32        | 1.25     |
| 4   | 4     | 259 | GLU  | CG-CD  | 6.23  | 1.61        | 1.51     |
| 1   | J     | 605 | GLU  | CD-OE1 | 6.22  | 1.32        | 1.25     |
| 1   | M     | 605 | GLU  | CD-OE1 | 6.22  | 1.32        | 1.25     |
| 1   | G     | 509 | GLU  | CD-OE1 | 6.22  | 1.32        | 1.25     |
| 2   | K     | 150 | TYR  | N-CA   | -6.22 | 1.33        | 1.46     |
| 4   | 8     | 259 | GLU  | CG-CD  | 6.22  | 1.61        | 1.51     |
| 1   | D     | 605 | GLU  | CD-OE1 | 6.22  | 1.32        | 1.25     |
| 2   | E     | 150 | TYR  | N-CA   | -6.22 | 1.33        | 1.46     |
| 2   | H     | 150 | TYR  | N-CA   | -6.20 | 1.33        | 1.46     |
| 4   | X     | 259 | GLU  | CG-CD  | 6.19  | 1.61        | 1.51     |
| 4   | 0     | 259 | GLU  | CG-CD  | 6.19  | 1.61        | 1.51     |
| 4   | 5     | 259 | GLU  | CG-CD  | 6.19  | 1.61        | 1.51     |
| 4   | 9     | 259 | GLU  | CG-CD  | 6.18  | 1.61        | 1.51     |
| 1   | A     | 99  | GLU  | CD-OE2 | 6.18  | 1.32        | 1.25     |
| 1   | P     | 802 | GLU  | CD-OE1 | 6.18  | 1.32        | 1.25     |
| 1   | P     | 329 | GLU  | CD-OE1 | 6.17  | 1.32        | 1.25     |
| 4   | Z     | 259 | GLU  | CG-CD  | 6.17  | 1.61        | 1.51     |
| 1   | D     | 802 | GLU  | CD-OE1 | 6.16  | 1.32        | 1.25     |
| 2   | N     | 150 | TYR  | N-CA   | -6.15 | 1.34        | 1.46     |
| 1   | P     | 509 | GLU  | CD-OE1 | 6.15  | 1.32        | 1.25     |
| 1   | M     | 509 | GLU  | CD-OE1 | 6.15  | 1.32        | 1.25     |
| 1   | M     | 329 | GLU  | CD-OE1 | 6.14  | 1.32        | 1.25     |
| 1   | M     | 802 | GLU  | CD-OE1 | 6.13  | 1.32        | 1.25     |
| 1   | D     | 509 | GLU  | CD-OE1 | 6.12  | 1.32        | 1.25     |
| 1   | J     | 509 | GLU  | CD-OE1 | 6.12  | 1.32        | 1.25     |
| 1   | J     | 329 | GLU  | CD-OE1 | 6.08  | 1.32        | 1.25     |
| 1   | G     | 329 | GLU  | CD-OE1 | 6.08  | 1.32        | 1.25     |
| 1   | A     | 509 | GLU  | CD-OE1 | 6.07  | 1.32        | 1.25     |
| 1   | A     | 329 | GLU  | CD-OE1 | 6.06  | 1.32        | 1.25     |
| 1   | P     | 230 | GLU  | CD-OE2 | 5.97  | 1.32        | 1.25     |
| 1   | D     | 417 | GLU  | CD-OE1 | 5.96  | 1.32        | 1.25     |
| 1   | A     | 417 | GLU  | CD-OE1 | 5.96  | 1.32        | 1.25     |
| 1   | G     | 476 | GLU  | CD-OE2 | -5.92 | 1.19        | 1.25     |
| 1   | J     | 230 | GLU  | CD-OE2 | 5.92  | 1.32        | 1.25     |
| 1   | A     | 802 | GLU  | CD-OE1 | 5.92  | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 417 | GLU  | CD-OE1 | 5.91  | 1.32        | 1.25     |
| 1   | G     | 540 | CYS  | CB-SG  | -5.91 | 1.72        | 1.81     |
| 1   | P     | 417 | GLU  | CD-OE1 | 5.90  | 1.32        | 1.25     |
| 1   | M     | 417 | GLU  | CD-OE1 | 5.88  | 1.32        | 1.25     |
| 1   | D     | 329 | GLU  | CD-OE1 | 5.88  | 1.32        | 1.25     |
| 1   | J     | 527 | GLU  | CD-OE1 | 5.87  | 1.32        | 1.25     |
| 1   | M     | 540 | CYS  | CB-SG  | -5.87 | 1.72        | 1.81     |
| 1   | P     | 540 | CYS  | CB-SG  | -5.86 | 1.72        | 1.81     |
| 1   | G     | 230 | GLU  | CD-OE2 | 5.86  | 1.32        | 1.25     |
| 1   | D     | 230 | GLU  | CD-OE2 | 5.85  | 1.32        | 1.25     |
| 1   | G     | 417 | GLU  | CD-OE1 | 5.85  | 1.32        | 1.25     |
| 1   | M     | 230 | GLU  | CD-OE2 | 5.85  | 1.32        | 1.25     |
| 1   | P     | 527 | GLU  | CD-OE1 | 5.84  | 1.32        | 1.25     |
| 1   | M     | 74  | GLU  | CD-OE2 | 5.84  | 1.32        | 1.25     |
| 1   | D     | 468 | GLU  | CD-OE1 | 5.83  | 1.32        | 1.25     |
| 1   | J     | 540 | CYS  | CB-SG  | -5.83 | 1.72        | 1.81     |
| 1   | A     | 74  | GLU  | CD-OE2 | 5.82  | 1.32        | 1.25     |
| 1   | P     | 74  | GLU  | CD-OE2 | 5.81  | 1.32        | 1.25     |
| 1   | P     | 499 | GLU  | CD-OE2 | 5.81  | 1.32        | 1.25     |
| 1   | M     | 527 | GLU  | CD-OE1 | 5.80  | 1.32        | 1.25     |
| 1   | A     | 785 | GLU  | CD-OE2 | 5.79  | 1.32        | 1.25     |
| 1   | J     | 476 | GLU  | CD-OE2 | -5.79 | 1.19        | 1.25     |
| 1   | A     | 468 | GLU  | CD-OE1 | 5.79  | 1.32        | 1.25     |
| 1   | D     | 476 | GLU  | CD-OE2 | -5.79 | 1.19        | 1.25     |
| 1   | J     | 499 | GLU  | CD-OE2 | 5.79  | 1.32        | 1.25     |
| 1   | M     | 499 | GLU  | CD-OE2 | 5.79  | 1.32        | 1.25     |
| 1   | D     | 540 | CYS  | CB-SG  | -5.78 | 1.72        | 1.81     |
| 1   | M     | 421 | GLU  | CD-OE2 | 5.78  | 1.32        | 1.25     |
| 1   | A     | 540 | CYS  | CB-SG  | -5.77 | 1.72        | 1.81     |
| 1   | G     | 218 | LEU  | CB-CG  | 5.77  | 1.69        | 1.52     |
| 1   | M     | 476 | GLU  | CD-OE2 | -5.77 | 1.19        | 1.25     |
| 1   | P     | 468 | GLU  | CD-OE1 | 5.77  | 1.31        | 1.25     |
| 1   | J     | 421 | GLU  | CD-OE2 | 5.76  | 1.31        | 1.25     |
| 1   | J     | 468 | GLU  | CD-OE1 | 5.76  | 1.31        | 1.25     |
| 1   | D     | 785 | GLU  | CD-OE2 | 5.75  | 1.31        | 1.25     |
| 1   | P     | 476 | GLU  | CD-OE2 | -5.75 | 1.19        | 1.25     |
| 1   | M     | 468 | GLU  | CD-OE1 | 5.75  | 1.31        | 1.25     |
| 1   | A     | 527 | GLU  | CD-OE1 | 5.73  | 1.31        | 1.25     |
| 1   | A     | 230 | GLU  | CD-OE2 | 5.73  | 1.31        | 1.25     |
| 1   | A     | 597 | GLU  | CD-OE1 | 5.73  | 1.31        | 1.25     |
| 1   | A     | 625 | THR  | CB-CG2 | 5.73  | 1.71        | 1.52     |
| 1   | M     | 785 | GLU  | CD-OE2 | 5.73  | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 74  | GLU  | CD-OE2 | 5.72  | 1.31        | 1.25     |
| 1   | D     | 625 | THR  | CB-CG2 | 5.71  | 1.71        | 1.52     |
| 1   | G     | 597 | GLU  | CD-OE1 | 5.71  | 1.31        | 1.25     |
| 1   | P     | 625 | THR  | CB-CG2 | 5.71  | 1.71        | 1.52     |
| 1   | J     | 74  | GLU  | CD-OE2 | 5.71  | 1.31        | 1.25     |
| 1   | D     | 687 | GLU  | CD-OE1 | 5.70  | 1.31        | 1.25     |
| 1   | J     | 625 | THR  | CB-CG2 | 5.68  | 1.71        | 1.52     |
| 1   | P     | 785 | GLU  | CD-OE2 | 5.68  | 1.31        | 1.25     |
| 1   | M     | 625 | THR  | CB-CG2 | 5.68  | 1.71        | 1.52     |
| 1   | A     | 218 | LEU  | CB-CG  | 5.68  | 1.69        | 1.52     |
| 1   | J     | 218 | LEU  | CB-CG  | 5.67  | 1.69        | 1.52     |
| 1   | J     | 785 | GLU  | CD-OE2 | 5.66  | 1.31        | 1.25     |
| 1   | G     | 625 | THR  | CB-CG2 | 5.66  | 1.71        | 1.52     |
| 1   | D     | 499 | GLU  | CD-OE2 | 5.65  | 1.31        | 1.25     |
| 1   | P     | 421 | GLU  | CD-OE2 | 5.65  | 1.31        | 1.25     |
| 1   | P     | 218 | LEU  | CB-CG  | 5.64  | 1.69        | 1.52     |
| 1   | D     | 218 | LEU  | CB-CG  | 5.64  | 1.68        | 1.52     |
| 1   | M     | 597 | GLU  | CD-OE1 | 5.64  | 1.31        | 1.25     |
| 1   | D     | 597 | GLU  | CD-OE1 | 5.63  | 1.31        | 1.25     |
| 1   | A     | 421 | GLU  | CD-OE2 | 5.62  | 1.31        | 1.25     |
| 1   | A     | 476 | GLU  | CD-OE2 | -5.62 | 1.19        | 1.25     |
| 1   | J     | 687 | GLU  | CD-OE1 | 5.62  | 1.31        | 1.25     |
| 1   | G     | 785 | GLU  | CD-OE2 | 5.61  | 1.31        | 1.25     |
| 1   | M     | 218 | LEU  | CB-CG  | 5.61  | 1.68        | 1.52     |
| 1   | P     | 687 | GLU  | CD-OE1 | 5.61  | 1.31        | 1.25     |
| 1   | J     | 373 | GLU  | CD-OE1 | 5.59  | 1.31        | 1.25     |
| 1   | D     | 74  | GLU  | CD-OE2 | 5.58  | 1.31        | 1.25     |
| 1   | G     | 687 | GLU  | CD-OE1 | 5.58  | 1.31        | 1.25     |
| 1   | G     | 527 | GLU  | CD-OE1 | 5.57  | 1.31        | 1.25     |
| 1   | P     | 597 | GLU  | CD-OE1 | 5.56  | 1.31        | 1.25     |
| 1   | J     | 597 | GLU  | CD-OE1 | 5.56  | 1.31        | 1.25     |
| 1   | G     | 468 | GLU  | CD-OE1 | 5.53  | 1.31        | 1.25     |
| 1   | G     | 373 | GLU  | CD-OE1 | 5.52  | 1.31        | 1.25     |
| 2   | H     | 150 | TYR  | CE1-CZ | 5.52  | 1.45        | 1.38     |
| 1   | M     | 687 | GLU  | CD-OE1 | 5.52  | 1.31        | 1.25     |
| 1   | A     | 499 | GLU  | CD-OE2 | 5.50  | 1.31        | 1.25     |
| 1   | D     | 527 | GLU  | CD-OE1 | 5.50  | 1.31        | 1.25     |
| 1   | G     | 421 | GLU  | CD-OE2 | 5.49  | 1.31        | 1.25     |
| 1   | P     | 373 | GLU  | CD-OE1 | 5.49  | 1.31        | 1.25     |
| 1   | A     | 777 | GLU  | CD-OE2 | 5.48  | 1.31        | 1.25     |
| 1   | M     | 373 | GLU  | CD-OE1 | 5.48  | 1.31        | 1.25     |
| 1   | A     | 373 | GLU  | CD-OE1 | 5.47  | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 777 | GLU  | CD-OE2 | 5.47  | 1.31        | 1.25     |
| 1   | D     | 421 | GLU  | CD-OE2 | 5.46  | 1.31        | 1.25     |
| 1   | G     | 499 | GLU  | CD-OE2 | 5.46  | 1.31        | 1.25     |
| 1   | D     | 373 | GLU  | CD-OE1 | 5.46  | 1.31        | 1.25     |
| 2   | E     | 150 | TYR  | CE1-CZ | 5.46  | 1.45        | 1.38     |
| 2   | Q     | 150 | TYR  | CE1-CZ | 5.46  | 1.45        | 1.38     |
| 1   | A     | 687 | GLU  | CD-OE1 | 5.45  | 1.31        | 1.25     |
| 1   | D     | 777 | GLU  | CD-OE2 | 5.45  | 1.31        | 1.25     |
| 1   | M     | 479 | CYS  | CB-SG  | -5.45 | 1.73        | 1.81     |
| 1   | P     | 777 | GLU  | CD-OE2 | 5.45  | 1.31        | 1.25     |
| 2   | B     | 150 | TYR  | CE1-CZ | 5.45  | 1.45        | 1.38     |
| 1   | G     | 479 | CYS  | CB-SG  | -5.44 | 1.73        | 1.81     |
| 1   | G     | 298 | GLU  | CD-OE2 | 5.44  | 1.31        | 1.25     |
| 2   | K     | 131 | GLU  | N-CA   | 5.44  | 1.57        | 1.46     |
| 1   | A     | 298 | GLU  | CD-OE2 | 5.43  | 1.31        | 1.25     |
| 1   | G     | 777 | GLU  | CD-OE2 | 5.43  | 1.31        | 1.25     |
| 2   | Q     | 131 | GLU  | N-CA   | 5.42  | 1.57        | 1.46     |
| 1   | P     | 298 | GLU  | CD-OE2 | 5.42  | 1.31        | 1.25     |
| 1   | D     | 218 | LEU  | C-N    | -5.41 | 1.21        | 1.34     |
| 1   | J     | 298 | GLU  | CD-OE2 | 5.40  | 1.31        | 1.25     |
| 2   | H     | 131 | GLU  | N-CA   | 5.39  | 1.57        | 1.46     |
| 2   | N     | 150 | TYR  | CE1-CZ | 5.39  | 1.45        | 1.38     |
| 1   | J     | 479 | CYS  | CB-SG  | -5.39 | 1.73        | 1.81     |
| 1   | A     | 479 | CYS  | CB-SG  | -5.38 | 1.73        | 1.81     |
| 2   | N     | 131 | GLU  | N-CA   | 5.38  | 1.57        | 1.46     |
| 1   | A     | 506 | GLU  | CD-OE2 | 5.38  | 1.31        | 1.25     |
| 1   | G     | 506 | GLU  | CD-OE2 | 5.37  | 1.31        | 1.25     |
| 2   | B     | 131 | GLU  | N-CA   | 5.37  | 1.57        | 1.46     |
| 1   | D     | 298 | GLU  | CD-OE2 | 5.37  | 1.31        | 1.25     |
| 1   | M     | 298 | GLU  | CD-OE2 | 5.36  | 1.31        | 1.25     |
| 1   | A     | 65  | GLU  | CD-OE1 | 5.36  | 1.31        | 1.25     |
| 1   | A     | 218 | LEU  | C-N    | -5.36 | 1.21        | 1.34     |
| 2   | E     | 131 | GLU  | N-CA   | 5.36  | 1.57        | 1.46     |
| 1   | M     | 777 | GLU  | CD-OE2 | 5.36  | 1.31        | 1.25     |
| 1   | M     | 218 | LEU  | C-N    | -5.35 | 1.21        | 1.34     |
| 1   | J     | 218 | LEU  | C-N    | -5.35 | 1.21        | 1.34     |
| 1   | P     | 218 | LEU  | C-N    | -5.35 | 1.21        | 1.34     |
| 2   | K     | 150 | TYR  | CE1-CZ | 5.34  | 1.45        | 1.38     |
| 1   | M     | 527 | GLU  | CD-OE2 | -5.34 | 1.19        | 1.25     |
| 1   | P     | 479 | CYS  | CB-SG  | -5.32 | 1.73        | 1.81     |
| 1   | G     | 218 | LEU  | C-N    | -5.30 | 1.21        | 1.34     |
| 1   | M     | 679 | GLU  | CD-OE2 | 5.30  | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 527 | GLU  | CD-OE2 | -5.29 | 1.19        | 1.25     |
| 2   | K     | 149 | ASP  | CB-CG  | 5.26  | 1.62        | 1.51     |
| 1   | D     | 65  | GLU  | CD-OE1 | 5.26  | 1.31        | 1.25     |
| 1   | G     | 679 | GLU  | CD-OE2 | 5.25  | 1.31        | 1.25     |
| 1   | A     | 527 | GLU  | CD-OE2 | -5.25 | 1.19        | 1.25     |
| 1   | D     | 479 | CYS  | CB-SG  | -5.25 | 1.73        | 1.81     |
| 1   | P     | 702 | GLU  | CD-OE2 | 5.24  | 1.31        | 1.25     |
| 1   | P     | 65  | GLU  | CD-OE1 | 5.23  | 1.31        | 1.25     |
| 1   | D     | 679 | GLU  | CD-OE2 | 5.23  | 1.31        | 1.25     |
| 1   | J     | 65  | GLU  | CD-OE1 | 5.23  | 1.31        | 1.25     |
| 1   | P     | 506 | GLU  | CD-OE2 | 5.22  | 1.31        | 1.25     |
| 1   | P     | 679 | GLU  | CD-OE2 | 5.20  | 1.31        | 1.25     |
| 1   | J     | 679 | GLU  | CD-OE2 | 5.18  | 1.31        | 1.25     |
| 1   | M     | 506 | GLU  | CD-OE2 | 5.18  | 1.31        | 1.25     |
| 1   | A     | 679 | GLU  | CD-OE2 | 5.17  | 1.31        | 1.25     |
| 2   | B     | 149 | ASP  | CB-CG  | 5.15  | 1.62        | 1.51     |
| 1   | A     | 697 | CYS  | CB-SG  | 5.15  | 1.91        | 1.82     |
| 1   | D     | 282 | GLU  | CD-OE1 | 5.15  | 1.31        | 1.25     |
| 1   | G     | 21  | GLU  | CD-OE2 | 5.15  | 1.31        | 1.25     |
| 1   | J     | 12  | GLU  | CD-OE2 | 5.14  | 1.31        | 1.25     |
| 2   | Q     | 149 | ASP  | CB-CG  | 5.14  | 1.62        | 1.51     |
| 1   | G     | 702 | GLU  | CD-OE2 | 5.14  | 1.31        | 1.25     |
| 1   | M     | 12  | GLU  | CD-OE2 | 5.14  | 1.31        | 1.25     |
| 1   | P     | 12  | GLU  | CD-OE2 | 5.13  | 1.31        | 1.25     |
| 1   | G     | 65  | GLU  | CD-OE1 | 5.12  | 1.31        | 1.25     |
| 1   | P     | 527 | GLU  | CD-OE2 | -5.12 | 1.20        | 1.25     |
| 2   | N     | 149 | ASP  | CB-CG  | 5.12  | 1.62        | 1.51     |
| 1   | A     | 702 | GLU  | CD-OE2 | 5.12  | 1.31        | 1.25     |
| 1   | M     | 65  | GLU  | CD-OE1 | 5.11  | 1.31        | 1.25     |
| 2   | E     | 149 | ASP  | CB-CG  | 5.11  | 1.62        | 1.51     |
| 1   | D     | 506 | GLU  | CD-OE2 | 5.10  | 1.31        | 1.25     |
| 4   | 3     | 259 | GLU  | CB-CG  | 5.09  | 1.61        | 1.52     |
| 1   | P     | 21  | GLU  | CD-OE2 | 5.09  | 1.31        | 1.25     |
| 1   | P     | 282 | GLU  | CD-OE1 | 5.09  | 1.31        | 1.25     |
| 1   | D     | 702 | GLU  | CD-OE2 | 5.08  | 1.31        | 1.25     |
| 1   | J     | 506 | GLU  | CD-OE2 | 5.08  | 1.31        | 1.25     |
| 1   | G     | 697 | CYS  | CB-SG  | 5.07  | 1.90        | 1.82     |
| 1   | G     | 282 | GLU  | CD-OE1 | 5.07  | 1.31        | 1.25     |
| 1   | J     | 702 | GLU  | CD-OE2 | 5.06  | 1.31        | 1.25     |
| 1   | M     | 282 | GLU  | CD-OE1 | 5.06  | 1.31        | 1.25     |
| 1   | A     | 21  | GLU  | CD-OE2 | 5.05  | 1.31        | 1.25     |
| 1   | A     | 282 | GLU  | CD-OE1 | 5.05  | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | M     | 702 | GLU  | CD-OE2 | 5.05 | 1.31        | 1.25     |
| 1   | M     | 150 | GLU  | CD-OE1 | 5.05 | 1.31        | 1.25     |
| 4   | 9     | 259 | GLU  | CB-CG  | 5.05 | 1.61        | 1.52     |
| 4   | Y     | 259 | GLU  | CB-CG  | 5.05 | 1.61        | 1.52     |
| 1   | D     | 697 | CYS  | CB-SG  | 5.04 | 1.90        | 1.82     |
| 1   | J     | 282 | GLU  | CD-OE1 | 5.04 | 1.31        | 1.25     |
| 1   | A     | 150 | GLU  | CD-OE1 | 5.04 | 1.31        | 1.25     |
| 1   | J     | 150 | GLU  | CD-OE1 | 5.04 | 1.31        | 1.25     |
| 4   | 8     | 259 | GLU  | CB-CG  | 5.04 | 1.61        | 1.52     |
| 1   | A     | 539 | GLU  | CD-OE1 | 5.04 | 1.31        | 1.25     |
| 2   | H     | 149 | ASP  | CB-CG  | 5.03 | 1.62        | 1.51     |
| 4   | 4     | 259 | GLU  | CB-CG  | 5.03 | 1.61        | 1.52     |
| 4   | 5     | 259 | GLU  | CB-CG  | 5.03 | 1.61        | 1.52     |
| 4   | W     | 259 | GLU  | CB-CG  | 5.02 | 1.61        | 1.52     |
| 1   | J     | 21  | GLU  | CD-OE2 | 5.02 | 1.31        | 1.25     |
| 1   | G     | 12  | GLU  | CD-OE2 | 5.01 | 1.31        | 1.25     |
| 4   | V     | 259 | GLU  | CB-CG  | 5.01 | 1.61        | 1.52     |
| 4   | X     | 259 | GLU  | CB-CG  | 5.01 | 1.61        | 1.52     |
| 4   | Z     | 259 | GLU  | CB-CG  | 5.00 | 1.61        | 1.52     |

All (1548) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | G     | 637 | LYS  | O-C-N      | -58.51 | 23.73       | 123.20   |
| 1   | D     | 637 | LYS  | O-C-N      | -58.48 | 23.79       | 123.20   |
| 1   | M     | 637 | LYS  | O-C-N      | -58.47 | 23.80       | 123.20   |
| 1   | J     | 637 | LYS  | O-C-N      | -58.45 | 23.83       | 123.20   |
| 1   | P     | 637 | LYS  | O-C-N      | -58.45 | 23.83       | 123.20   |
| 1   | A     | 637 | LYS  | O-C-N      | -58.45 | 23.84       | 123.20   |
| 1   | J     | 709 | LYS  | O-C-N      | -41.34 | 52.92       | 123.20   |
| 1   | P     | 649 | VAL  | CG1-CB-CG2 | -34.03 | 56.46       | 110.90   |
| 1   | D     | 649 | VAL  | CG1-CB-CG2 | -34.00 | 56.50       | 110.90   |
| 1   | J     | 649 | VAL  | CG1-CB-CG2 | -34.00 | 56.49       | 110.90   |
| 1   | A     | 649 | VAL  | CG1-CB-CG2 | -34.00 | 56.50       | 110.90   |
| 1   | M     | 649 | VAL  | CG1-CB-CG2 | -34.00 | 56.50       | 110.90   |
| 1   | G     | 649 | VAL  | CG1-CB-CG2 | -34.00 | 56.51       | 110.90   |
| 1   | J     | 648 | THR  | CA-CB-OG1  | -31.72 | 42.38       | 109.00   |
| 1   | A     | 648 | THR  | CA-CB-OG1  | -31.71 | 42.41       | 109.00   |
| 1   | M     | 648 | THR  | CA-CB-OG1  | -31.70 | 42.42       | 109.00   |
| 1   | P     | 648 | THR  | CA-CB-OG1  | -31.70 | 42.42       | 109.00   |
| 1   | D     | 648 | THR  | CA-CB-OG1  | -31.70 | 42.42       | 109.00   |
| 1   | G     | 648 | THR  | CA-CB-OG1  | -31.68 | 42.48       | 109.00   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | Q     | 150 | TYR  | CB-CG-CD2  | -28.69 | 103.79      | 121.00   |
| 2   | N     | 150 | TYR  | CB-CG-CD2  | -28.68 | 103.79      | 121.00   |
| 2   | H     | 150 | TYR  | CB-CG-CD2  | -28.62 | 103.83      | 121.00   |
| 2   | E     | 150 | TYR  | CB-CG-CD2  | -28.59 | 103.84      | 121.00   |
| 2   | B     | 150 | TYR  | CB-CG-CD2  | -28.59 | 103.84      | 121.00   |
| 2   | K     | 150 | TYR  | CB-CG-CD2  | -28.54 | 103.88      | 121.00   |
| 1   | G     | 649 | VAL  | CA-CB-CG1  | -28.52 | 68.11       | 110.90   |
| 1   | D     | 649 | VAL  | CA-CB-CG1  | -28.50 | 68.14       | 110.90   |
| 1   | P     | 649 | VAL  | CA-CB-CG1  | -28.50 | 68.15       | 110.90   |
| 1   | M     | 649 | VAL  | CA-CB-CG1  | -28.48 | 68.18       | 110.90   |
| 1   | J     | 649 | VAL  | CA-CB-CG1  | -28.47 | 68.19       | 110.90   |
| 1   | A     | 649 | VAL  | CA-CB-CG1  | -28.45 | 68.22       | 110.90   |
| 1   | D     | 649 | VAL  | CA-CB-CG2  | -28.18 | 68.63       | 110.90   |
| 1   | A     | 649 | VAL  | CA-CB-CG2  | -28.18 | 68.64       | 110.90   |
| 1   | P     | 649 | VAL  | CA-CB-CG2  | -28.16 | 68.65       | 110.90   |
| 1   | J     | 649 | VAL  | CA-CB-CG2  | -28.16 | 68.66       | 110.90   |
| 1   | G     | 649 | VAL  | CA-CB-CG2  | -28.16 | 68.67       | 110.90   |
| 1   | M     | 649 | VAL  | CA-CB-CG2  | -28.15 | 68.67       | 110.90   |
| 1   | P     | 785 | GLU  | O-C-N      | -27.49 | 78.72       | 122.70   |
| 1   | M     | 648 | THR  | CA-CB-CG2  | -25.61 | 76.54       | 112.40   |
| 1   | D     | 648 | THR  | CA-CB-CG2  | -25.60 | 76.56       | 112.40   |
| 1   | P     | 648 | THR  | CA-CB-CG2  | -25.57 | 76.60       | 112.40   |
| 1   | J     | 648 | THR  | CA-CB-CG2  | -25.55 | 76.63       | 112.40   |
| 1   | A     | 648 | THR  | CA-CB-CG2  | -25.50 | 76.69       | 112.40   |
| 1   | G     | 648 | THR  | CA-CB-CG2  | -25.36 | 76.89       | 112.40   |
| 2   | H     | 150 | TYR  | CG-CD2-CE2 | -20.86 | 104.61      | 121.30   |
| 2   | N     | 150 | TYR  | CG-CD2-CE2 | -20.59 | 104.83      | 121.30   |
| 2   | E     | 150 | TYR  | CG-CD2-CE2 | -20.59 | 104.83      | 121.30   |
| 2   | Q     | 150 | TYR  | CG-CD2-CE2 | -20.57 | 104.84      | 121.30   |
| 2   | K     | 150 | TYR  | CG-CD2-CE2 | -20.53 | 104.88      | 121.30   |
| 2   | B     | 150 | TYR  | CG-CD2-CE2 | -20.45 | 104.94      | 121.30   |
| 2   | Q     | 150 | TYR  | CD1-CG-CD2 | 19.51  | 139.37      | 117.90   |
| 2   | H     | 150 | TYR  | CD1-CG-CD2 | 19.50  | 139.35      | 117.90   |
| 2   | N     | 150 | TYR  | CD1-CG-CD2 | 19.48  | 139.32      | 117.90   |
| 2   | K     | 150 | TYR  | CD1-CG-CD2 | 19.47  | 139.32      | 117.90   |
| 2   | E     | 150 | TYR  | CD1-CG-CD2 | 19.46  | 139.31      | 117.90   |
| 2   | B     | 150 | TYR  | CD1-CG-CD2 | 19.45  | 139.29      | 117.90   |
| 1   | M     | 709 | LYS  | O-C-N      | -18.71 | 91.39       | 123.20   |
| 2   | H     | 150 | TYR  | CG-CD1-CE1 | -18.50 | 106.50      | 121.30   |
| 2   | E     | 150 | TYR  | CG-CD1-CE1 | -18.48 | 106.52      | 121.30   |
| 2   | K     | 150 | TYR  | CG-CD1-CE1 | -18.46 | 106.53      | 121.30   |
| 2   | N     | 150 | TYR  | CG-CD1-CE1 | -18.44 | 106.55      | 121.30   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 2   | Q     | 150 | TYR  | CG-CD1-CE1 | -18.43 | 106.55      | 121.30   |
| 2   | B     | 150 | TYR  | CG-CD1-CE1 | -18.32 | 106.64      | 121.30   |
| 1   | J     | 800 | ARG  | NE-CZ-NH2  | -16.78 | 111.91      | 120.30   |
| 1   | D     | 800 | ARG  | NE-CZ-NH2  | -16.52 | 112.04      | 120.30   |
| 1   | M     | 800 | ARG  | NE-CZ-NH2  | -16.48 | 112.06      | 120.30   |
| 1   | P     | 800 | ARG  | NE-CZ-NH2  | -16.41 | 112.09      | 120.30   |
| 1   | G     | 800 | ARG  | NE-CZ-NH2  | -16.30 | 112.15      | 120.30   |
| 1   | A     | 800 | ARG  | NE-CZ-NH2  | -16.13 | 112.23      | 120.30   |
| 1   | P     | 786 | ILE  | CA-C-N     | -14.47 | 85.37       | 117.20   |
| 1   | G     | 623 | PHE  | CB-CG-CD2  | -13.75 | 111.18      | 120.80   |
| 1   | M     | 623 | PHE  | CB-CG-CD2  | -13.71 | 111.20      | 120.80   |
| 1   | J     | 623 | PHE  | CB-CG-CD2  | -13.70 | 111.21      | 120.80   |
| 1   | A     | 623 | PHE  | CB-CG-CD2  | -13.67 | 111.23      | 120.80   |
| 1   | P     | 786 | ILE  | O-C-N      | 13.66  | 144.55      | 122.70   |
| 1   | P     | 623 | PHE  | CB-CG-CD2  | -13.64 | 111.25      | 120.80   |
| 1   | D     | 623 | PHE  | CB-CG-CD2  | -13.60 | 111.28      | 120.80   |
| 1   | J     | 623 | PHE  | CB-CG-CD1  | 12.43  | 129.50      | 120.80   |
| 1   | M     | 623 | PHE  | CB-CG-CD1  | 12.34  | 129.44      | 120.80   |
| 1   | P     | 623 | PHE  | CB-CG-CD1  | 12.34  | 129.44      | 120.80   |
| 1   | G     | 623 | PHE  | CB-CG-CD1  | 12.33  | 129.43      | 120.80   |
| 1   | A     | 623 | PHE  | CB-CG-CD1  | 12.33  | 129.43      | 120.80   |
| 1   | M     | 623 | PHE  | CA-CB-CG   | -12.27 | 84.45       | 113.90   |
| 1   | A     | 623 | PHE  | CA-CB-CG   | -12.26 | 84.47       | 113.90   |
| 1   | J     | 623 | PHE  | CA-CB-CG   | -12.26 | 84.47       | 113.90   |
| 1   | P     | 623 | PHE  | CA-CB-CG   | -12.24 | 84.51       | 113.90   |
| 1   | D     | 623 | PHE  | CA-CB-CG   | -12.21 | 84.58       | 113.90   |
| 1   | G     | 623 | PHE  | CA-CB-CG   | -12.20 | 84.63       | 113.90   |
| 1   | D     | 623 | PHE  | CB-CG-CD1  | 12.05  | 129.24      | 120.80   |
| 1   | P     | 98  | HIS  | CB-CA-C    | -11.58 | 87.24       | 110.40   |
| 1   | J     | 98  | HIS  | CB-CA-C    | -11.58 | 87.25       | 110.40   |
| 1   | M     | 98  | HIS  | CB-CA-C    | -11.57 | 87.26       | 110.40   |
| 1   | G     | 98  | HIS  | CB-CA-C    | -11.56 | 87.28       | 110.40   |
| 1   | A     | 98  | HIS  | CB-CA-C    | -11.55 | 87.30       | 110.40   |
| 1   | D     | 98  | HIS  | CB-CA-C    | -11.54 | 87.32       | 110.40   |
| 1   | G     | 709 | LYS  | O-C-N      | 10.88  | 141.71      | 123.20   |
| 1   | G     | 568 | PRO  | O-C-N      | 10.68  | 139.79      | 122.70   |
| 1   | A     | 568 | PRO  | O-C-N      | 10.67  | 139.77      | 122.70   |
| 1   | D     | 568 | PRO  | O-C-N      | 10.67  | 139.77      | 122.70   |
| 1   | P     | 568 | PRO  | O-C-N      | 10.62  | 139.70      | 122.70   |
| 1   | J     | 568 | PRO  | O-C-N      | 10.61  | 139.68      | 122.70   |
| 1   | M     | 568 | PRO  | O-C-N      | 10.60  | 139.67      | 122.70   |
| 1   | P     | 785 | GLU  | CA-C-N     | 10.49  | 140.29      | 117.20   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | G     | 709 | LYS  | CA-C-N    | -10.44 | 95.31       | 116.20   |
| 1   | P     | 785 | GLU  | C-N-CA    | -10.42 | 95.66       | 121.70   |
| 2   | E     | 141 | PRO  | CA-N-CD   | 10.28  | 126.09      | 111.70   |
| 2   | H     | 141 | PRO  | CA-N-CD   | 10.26  | 126.06      | 111.70   |
| 2   | N     | 141 | PRO  | CA-N-CD   | 10.25  | 126.05      | 111.70   |
| 2   | K     | 141 | PRO  | CA-N-CD   | 10.21  | 126.00      | 111.70   |
| 2   | Q     | 141 | PRO  | CA-N-CD   | 10.20  | 125.98      | 111.70   |
| 2   | B     | 141 | PRO  | CA-N-CD   | 10.17  | 125.94      | 111.70   |
| 1   | G     | 327 | ASP  | CB-CG-OD1 | -10.08 | 109.22      | 118.30   |
| 1   | A     | 625 | THR  | CA-CB-CG2 | -10.07 | 98.31       | 112.40   |
| 1   | G     | 625 | THR  | CA-CB-CG2 | -10.06 | 98.32       | 112.40   |
| 1   | J     | 327 | ASP  | CB-CG-OD1 | -10.05 | 109.25      | 118.30   |
| 1   | J     | 625 | THR  | CA-CB-CG2 | -10.05 | 98.33       | 112.40   |
| 1   | M     | 625 | THR  | CA-CB-CG2 | -10.05 | 98.33       | 112.40   |
| 1   | P     | 625 | THR  | CA-CB-CG2 | -10.04 | 98.35       | 112.40   |
| 1   | A     | 327 | ASP  | CB-CG-OD1 | -10.02 | 109.28      | 118.30   |
| 1   | D     | 625 | THR  | CA-CB-CG2 | -10.02 | 98.38       | 112.40   |
| 1   | M     | 327 | ASP  | CB-CG-OD1 | -10.00 | 109.30      | 118.30   |
| 1   | D     | 327 | ASP  | CB-CG-OD1 | -9.97  | 109.33      | 118.30   |
| 1   | P     | 327 | ASP  | CB-CG-OD1 | -9.95  | 109.34      | 118.30   |
| 1   | A     | 241 | ASP  | CB-CG-OD1 | -9.90  | 109.39      | 118.30   |
| 1   | G     | 241 | ASP  | CB-CG-OD1 | -9.85  | 109.44      | 118.30   |
| 1   | J     | 241 | ASP  | CB-CG-OD1 | -9.84  | 109.45      | 118.30   |
| 1   | M     | 241 | ASP  | CB-CG-OD1 | -9.80  | 109.47      | 118.30   |
| 3   | C     | 63  | ILE  | O-C-N     | 9.80   | 138.38      | 122.70   |
| 3   | I     | 63  | ILE  | O-C-N     | 9.77   | 138.33      | 122.70   |
| 1   | P     | 241 | ASP  | CB-CG-OD1 | -9.76  | 109.51      | 118.30   |
| 1   | D     | 728 | ASN  | O-C-N     | 9.75   | 138.30      | 122.70   |
| 1   | M     | 728 | ASN  | O-C-N     | 9.73   | 138.26      | 122.70   |
| 1   | D     | 241 | ASP  | CB-CG-OD1 | -9.72  | 109.55      | 118.30   |
| 3   | R     | 63  | ILE  | O-C-N     | 9.68   | 138.18      | 122.70   |
| 1   | A     | 728 | ASN  | O-C-N     | 9.67   | 138.17      | 122.70   |
| 3   | F     | 63  | ILE  | O-C-N     | 9.66   | 138.16      | 122.70   |
| 1   | P     | 728 | ASN  | O-C-N     | 9.66   | 138.16      | 122.70   |
| 3   | L     | 63  | ILE  | O-C-N     | 9.62   | 138.10      | 122.70   |
| 3   | O     | 63  | ILE  | O-C-N     | 9.62   | 138.09      | 122.70   |
| 1   | J     | 728 | ASN  | O-C-N     | 9.61   | 138.07      | 122.70   |
| 1   | G     | 728 | ASN  | O-C-N     | 9.56   | 138.00      | 122.70   |
| 1   | G     | 264 | ASP  | CB-CG-OD2 | -9.56  | 109.70      | 118.30   |
| 1   | P     | 786 | ILE  | C-N-CA    | -9.51  | 97.92       | 121.70   |
| 1   | D     | 264 | ASP  | CB-CG-OD2 | -9.48  | 109.77      | 118.30   |
| 2   | E     | 150 | TYR  | N-CA-CB   | -9.43  | 93.62       | 110.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | K     | 150 | TYR  | N-CA-CB    | -9.38 | 93.71       | 110.60   |
| 2   | N     | 150 | TYR  | N-CA-CB    | -9.38 | 93.71       | 110.60   |
| 2   | H     | 150 | TYR  | N-CA-CB    | -9.38 | 93.72       | 110.60   |
| 1   | A     | 264 | ASP  | CB-CG-OD2  | -9.37 | 109.86      | 118.30   |
| 1   | J     | 264 | ASP  | CB-CG-OD2  | -9.38 | 109.86      | 118.30   |
| 1   | P     | 264 | ASP  | CB-CG-OD2  | -9.36 | 109.88      | 118.30   |
| 2   | Q     | 150 | TYR  | N-CA-CB    | -9.34 | 93.79       | 110.60   |
| 1   | M     | 264 | ASP  | CB-CG-OD2  | -9.34 | 109.90      | 118.30   |
| 2   | B     | 150 | TYR  | N-CA-CB    | -9.30 | 93.86       | 110.60   |
| 4   | 2     | 356 | TRP  | CD1-CG-CD2 | 9.19  | 113.65      | 106.30   |
| 4   | 9     | 356 | TRP  | CD1-CG-CD2 | 9.16  | 113.62      | 106.30   |
| 4   | 0     | 356 | TRP  | CD1-CG-CD2 | 9.15  | 113.62      | 106.30   |
| 4   | Z     | 356 | TRP  | CD1-CG-CD2 | 9.15  | 113.62      | 106.30   |
| 4   | X     | 356 | TRP  | CD1-CG-CD2 | 9.14  | 113.61      | 106.30   |
| 4   | 7     | 356 | TRP  | CD1-CG-CD2 | 9.11  | 113.59      | 106.30   |
| 4   | 1     | 356 | TRP  | CD1-CG-CD2 | 9.11  | 113.59      | 106.30   |
| 4   | 8     | 356 | TRP  | CD1-CG-CD2 | 9.11  | 113.59      | 106.30   |
| 4   | Y     | 356 | TRP  | CD1-CG-CD2 | 9.07  | 113.55      | 106.30   |
| 4   | 5     | 356 | TRP  | CD1-CG-CD2 | 9.05  | 113.54      | 106.30   |
| 4   | V     | 356 | TRP  | CD1-CG-CD2 | 9.04  | 113.53      | 106.30   |
| 4   | 3     | 356 | TRP  | CD1-CG-CD2 | 9.04  | 113.53      | 106.30   |
| 4   | W     | 356 | TRP  | CD1-CG-CD2 | 9.02  | 113.52      | 106.30   |
| 1   | M     | 352 | TYR  | CB-CG-CD1  | 9.01  | 126.41      | 121.00   |
| 4   | 4     | 356 | TRP  | CD1-CG-CD2 | 8.97  | 113.48      | 106.30   |
| 1   | J     | 378 | ASP  | CB-CG-OD2  | 8.97  | 126.37      | 118.30   |
| 1   | P     | 378 | ASP  | CB-CG-OD2  | 8.96  | 126.37      | 118.30   |
| 1   | M     | 378 | ASP  | CB-CG-OD2  | 8.95  | 126.36      | 118.30   |
| 1   | P     | 352 | TYR  | CB-CG-CD1  | 8.93  | 126.36      | 121.00   |
| 1   | J     | 352 | TYR  | CB-CG-CD1  | 8.92  | 126.35      | 121.00   |
| 1   | G     | 378 | ASP  | CB-CG-OD2  | 8.89  | 126.30      | 118.30   |
| 1   | D     | 378 | ASP  | CB-CG-OD2  | 8.88  | 126.29      | 118.30   |
| 4   | 8     | 177 | ARG  | NE-CZ-NH2  | -8.82 | 115.89      | 120.30   |
| 1   | A     | 378 | ASP  | CB-CG-OD2  | 8.77  | 126.19      | 118.30   |
| 2   | K     | 138 | ALA  | O-C-N      | -8.76 | 108.69      | 122.70   |
| 2   | Q     | 138 | ALA  | O-C-N      | -8.74 | 108.71      | 122.70   |
| 2   | N     | 138 | ALA  | O-C-N      | -8.74 | 108.72      | 122.70   |
| 1   | G     | 352 | TYR  | CB-CG-CD1  | 8.72  | 126.23      | 121.00   |
| 2   | H     | 138 | ALA  | O-C-N      | -8.71 | 108.76      | 122.70   |
| 1   | A     | 352 | TYR  | CB-CG-CD1  | 8.71  | 126.23      | 121.00   |
| 1   | D     | 352 | TYR  | CB-CG-CD1  | 8.70  | 126.22      | 121.00   |
| 4   | X     | 177 | ARG  | NE-CZ-NH2  | -8.70 | 115.95      | 120.30   |
| 4   | 1     | 177 | ARG  | NE-CZ-NH2  | -8.70 | 115.95      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | E     | 138 | ALA  | O-C-N      | -8.70 | 108.78      | 122.70   |
| 2   | B     | 138 | ALA  | O-C-N      | -8.69 | 108.80      | 122.70   |
| 4   | W     | 177 | ARG  | NE-CZ-NH2  | -8.65 | 115.97      | 120.30   |
| 4   | 4     | 177 | ARG  | NE-CZ-NH2  | -8.63 | 115.99      | 120.30   |
| 4   | 0     | 177 | ARG  | NE-CZ-NH2  | -8.61 | 115.99      | 120.30   |
| 1   | P     | 601 | ASP  | CB-CG-OD1  | -8.60 | 110.56      | 118.30   |
| 4   | V     | 86  | TRP  | CD1-CG-CD2 | 8.58  | 113.16      | 106.30   |
| 4   | V     | 177 | ARG  | NE-CZ-NH2  | -8.57 | 116.02      | 120.30   |
| 4   | Y     | 177 | ARG  | NE-CZ-NH2  | -8.56 | 116.02      | 120.30   |
| 4   | 2     | 177 | ARG  | NE-CZ-NH2  | -8.55 | 116.03      | 120.30   |
| 1   | J     | 601 | ASP  | CB-CG-OD1  | -8.54 | 110.61      | 118.30   |
| 4   | 5     | 177 | ARG  | NE-CZ-NH2  | -8.53 | 116.03      | 120.30   |
| 4   | Z     | 177 | ARG  | NE-CZ-NH2  | -8.53 | 116.04      | 120.30   |
| 4   | Y     | 86  | TRP  | CD1-CG-CD2 | 8.52  | 113.12      | 106.30   |
| 1   | D     | 601 | ASP  | CB-CG-OD1  | -8.51 | 110.64      | 118.30   |
| 4   | 2     | 86  | TRP  | CD1-CG-CD2 | 8.51  | 113.11      | 106.30   |
| 4   | Z     | 86  | TRP  | CD1-CG-CD2 | 8.51  | 113.11      | 106.30   |
| 4   | X     | 86  | TRP  | CD1-CG-CD2 | 8.51  | 113.10      | 106.30   |
| 4   | 9     | 86  | TRP  | CD1-CG-CD2 | 8.49  | 113.10      | 106.30   |
| 4   | 9     | 177 | ARG  | NE-CZ-NH2  | -8.49 | 116.05      | 120.30   |
| 1   | G     | 601 | ASP  | CB-CG-OD1  | -8.49 | 110.66      | 118.30   |
| 4   | 1     | 86  | TRP  | CD1-CG-CD2 | 8.48  | 113.09      | 106.30   |
| 4   | 4     | 86  | TRP  | CD1-CG-CD2 | 8.48  | 113.08      | 106.30   |
| 4   | 3     | 177 | ARG  | NE-CZ-NH2  | -8.47 | 116.06      | 120.30   |
| 4   | W     | 86  | TRP  | CD1-CG-CD2 | 8.47  | 113.08      | 106.30   |
| 4   | 3     | 86  | TRP  | CD1-CG-CD2 | 8.47  | 113.08      | 106.30   |
| 1   | M     | 601 | ASP  | CB-CG-OD1  | -8.46 | 110.69      | 118.30   |
| 4   | 8     | 86  | TRP  | CD1-CG-CD2 | 8.45  | 113.06      | 106.30   |
| 1   | A     | 601 | ASP  | CB-CG-OD1  | -8.44 | 110.70      | 118.30   |
| 1   | M     | 33  | ASP  | CB-CG-OD1  | -8.43 | 110.72      | 118.30   |
| 4   | 7     | 86  | TRP  | CD1-CG-CD2 | 8.43  | 113.04      | 106.30   |
| 4   | 0     | 86  | TRP  | CD1-CG-CD2 | 8.40  | 113.02      | 106.30   |
| 4   | 5     | 86  | TRP  | CD1-CG-CD2 | 8.39  | 113.01      | 106.30   |
| 1   | P     | 352 | TYR  | CB-CG-CD2  | -8.38 | 115.97      | 121.00   |
| 1   | P     | 33  | ASP  | CB-CG-OD1  | -8.38 | 110.76      | 118.30   |
| 1   | J     | 33  | ASP  | CB-CG-OD1  | -8.37 | 110.77      | 118.30   |
| 1   | M     | 352 | TYR  | CB-CG-CD2  | -8.36 | 115.98      | 121.00   |
| 1   | J     | 352 | TYR  | CB-CG-CD2  | -8.36 | 115.98      | 121.00   |
| 4   | 7     | 177 | ARG  | NE-CZ-NH2  | -8.35 | 116.12      | 120.30   |
| 1   | A     | 352 | TYR  | CB-CG-CD2  | -8.32 | 116.01      | 121.00   |
| 1   | G     | 33  | ASP  | CB-CG-OD1  | -8.30 | 110.83      | 118.30   |
| 1   | A     | 33  | ASP  | CB-CG-OD1  | -8.29 | 110.83      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 33  | ASP  | CB-CG-OD1  | -8.29 | 110.84      | 118.30   |
| 1   | G     | 352 | TYR  | CB-CG-CD2  | -8.19 | 116.09      | 121.00   |
| 1   | D     | 352 | TYR  | CB-CG-CD2  | -8.12 | 116.13      | 121.00   |
| 1   | A     | 339 | ASP  | CB-CG-OD1  | -8.05 | 111.05      | 118.30   |
| 4   | 9     | 356 | TRP  | CE2-CD2-CG | -8.03 | 100.88      | 107.30   |
| 4   | 2     | 356 | TRP  | CE2-CD2-CG | -8.01 | 100.89      | 107.30   |
| 4   | Z     | 356 | TRP  | CE2-CD2-CG | -7.99 | 100.91      | 107.30   |
| 1   | G     | 339 | ASP  | CB-CG-OD1  | -7.99 | 111.11      | 118.30   |
| 4   | 3     | 356 | TRP  | CE2-CD2-CG | -7.98 | 100.92      | 107.30   |
| 4   | 8     | 356 | TRP  | CE2-CD2-CG | -7.96 | 100.93      | 107.30   |
| 4   | 0     | 356 | TRP  | CE2-CD2-CG | -7.94 | 100.95      | 107.30   |
| 1   | A     | 637 | LYS  | CA-C-N     | 7.94  | 132.07      | 116.20   |
| 1   | P     | 637 | LYS  | CA-C-N     | 7.93  | 132.07      | 116.20   |
| 4   | 7     | 356 | TRP  | CE2-CD2-CG | -7.93 | 100.95      | 107.30   |
| 4   | V     | 356 | TRP  | CE2-CD2-CG | -7.92 | 100.96      | 107.30   |
| 1   | G     | 637 | LYS  | CA-C-N     | 7.91  | 132.03      | 116.20   |
| 2   | N     | 150 | TYR  | CD1-CE1-CZ | -7.91 | 112.68      | 119.80   |
| 1   | J     | 637 | LYS  | CA-C-N     | 7.91  | 132.02      | 116.20   |
| 1   | D     | 637 | LYS  | CA-C-N     | 7.91  | 132.01      | 116.20   |
| 1   | P     | 339 | ASP  | CB-CG-OD1  | -7.91 | 111.19      | 118.30   |
| 4   | 1     | 356 | TRP  | CE2-CD2-CG | -7.91 | 100.97      | 107.30   |
| 1   | M     | 637 | LYS  | CA-C-N     | 7.90  | 132.01      | 116.20   |
| 4   | X     | 356 | TRP  | CE2-CD2-CG | -7.90 | 100.98      | 107.30   |
| 4   | Y     | 356 | TRP  | CE2-CD2-CG | -7.90 | 100.98      | 107.30   |
| 1   | D     | 339 | ASP  | CB-CG-OD1  | -7.90 | 111.19      | 118.30   |
| 1   | M     | 339 | ASP  | CB-CG-OD1  | -7.88 | 111.20      | 118.30   |
| 1   | J     | 339 | ASP  | CB-CG-OD1  | -7.87 | 111.22      | 118.30   |
| 4   | 5     | 356 | TRP  | CE2-CD2-CG | -7.87 | 101.00      | 107.30   |
| 2   | Q     | 150 | TYR  | CD1-CE1-CZ | -7.87 | 112.72      | 119.80   |
| 4   | W     | 356 | TRP  | CE2-CD2-CG | -7.85 | 101.02      | 107.30   |
| 4   | 4     | 356 | TRP  | CE2-CD2-CG | -7.84 | 101.03      | 107.30   |
| 2   | B     | 150 | TYR  | CD1-CE1-CZ | -7.83 | 112.75      | 119.80   |
| 2   | E     | 150 | TYR  | CD1-CE1-CZ | -7.83 | 112.75      | 119.80   |
| 1   | A     | 202 | SER  | CB-CA-C    | -7.79 | 95.30       | 110.10   |
| 1   | D     | 202 | SER  | CB-CA-C    | -7.78 | 95.31       | 110.10   |
| 2   | H     | 150 | TYR  | CD1-CE1-CZ | -7.77 | 112.81      | 119.80   |
| 1   | J     | 202 | SER  | CB-CA-C    | -7.75 | 95.38       | 110.10   |
| 2   | K     | 150 | TYR  | CD1-CE1-CZ | -7.75 | 112.83      | 119.80   |
| 1   | M     | 202 | SER  | CB-CA-C    | -7.74 | 95.39       | 110.10   |
| 1   | J     | 653 | PHE  | CB-CG-CD1  | -7.73 | 115.39      | 120.80   |
| 1   | G     | 202 | SER  | CB-CA-C    | -7.71 | 95.44       | 110.10   |
| 4   | 8     | 312 | ARG  | NE-CZ-NH2  | 7.71  | 124.16      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | P     | 202 | SER  | CB-CA-C    | -7.70 | 95.47       | 110.10   |
| 1   | M     | 653 | PHE  | CB-CG-CD1  | -7.69 | 115.42      | 120.80   |
| 4   | 2     | 312 | ARG  | NE-CZ-NH2  | 7.68  | 124.14      | 120.30   |
| 4   | 0     | 312 | ARG  | NE-CZ-NH2  | 7.65  | 124.13      | 120.30   |
| 4   | 9     | 312 | ARG  | NE-CZ-NH2  | 7.64  | 124.12      | 120.30   |
| 4   | V     | 86  | TRP  | CE2-CD2-CG | -7.64 | 101.19      | 107.30   |
| 1   | P     | 653 | PHE  | CB-CG-CD1  | -7.63 | 115.46      | 120.80   |
| 4   | Z     | 312 | ARG  | NE-CZ-NH2  | 7.63  | 124.11      | 120.30   |
| 1   | G     | 654 | ARG  | NE-CZ-NH1  | 7.61  | 124.11      | 120.30   |
| 1   | D     | 653 | PHE  | CB-CG-CD1  | -7.60 | 115.48      | 120.80   |
| 4   | 1     | 312 | ARG  | NE-CZ-NH2  | 7.60  | 124.10      | 120.30   |
| 4   | 4     | 86  | TRP  | CE2-CD2-CG | -7.60 | 101.22      | 107.30   |
| 4   | V     | 312 | ARG  | NE-CZ-NH2  | 7.59  | 124.10      | 120.30   |
| 4   | W     | 312 | ARG  | NE-CZ-NH2  | 7.59  | 124.10      | 120.30   |
| 4   | X     | 86  | TRP  | CE2-CD2-CG | -7.58 | 101.24      | 107.30   |
| 1   | G     | 653 | PHE  | CB-CG-CD1  | -7.58 | 115.50      | 120.80   |
| 4   | 5     | 312 | ARG  | NE-CZ-NH2  | 7.57  | 124.09      | 120.30   |
| 4   | Y     | 312 | ARG  | NE-CZ-NH2  | 7.57  | 124.09      | 120.30   |
| 4   | W     | 86  | TRP  | CE2-CD2-CG | -7.57 | 101.24      | 107.30   |
| 4   | Y     | 86  | TRP  | CE2-CD2-CG | -7.57 | 101.25      | 107.30   |
| 4   | 5     | 86  | TRP  | CE2-CD2-CG | -7.56 | 101.25      | 107.30   |
| 4   | 7     | 86  | TRP  | CE2-CD2-CG | -7.56 | 101.25      | 107.30   |
| 4   | 8     | 86  | TRP  | CE2-CD2-CG | -7.55 | 101.26      | 107.30   |
| 4   | X     | 312 | ARG  | NE-CZ-NH2  | 7.55  | 124.07      | 120.30   |
| 4   | 9     | 86  | TRP  | CE2-CD2-CG | -7.54 | 101.27      | 107.30   |
| 1   | G     | 346 | ASP  | CB-CG-OD2  | -7.54 | 111.52      | 118.30   |
| 4   | 2     | 86  | TRP  | CE2-CD2-CG | -7.53 | 101.27      | 107.30   |
| 4   | 3     | 312 | ARG  | NE-CZ-NH2  | 7.52  | 124.06      | 120.30   |
| 4   | Z     | 86  | TRP  | CE2-CD2-CG | -7.51 | 101.29      | 107.30   |
| 4   | 1     | 86  | TRP  | CE2-CD2-CG | -7.51 | 101.29      | 107.30   |
| 4   | 3     | 86  | TRP  | CE2-CD2-CG | -7.51 | 101.29      | 107.30   |
| 3   | I     | 63  | ILE  | CG1-CB-CG2 | -7.50 | 94.91       | 111.40   |
| 3   | O     | 63  | ILE  | CG1-CB-CG2 | -7.50 | 94.90       | 111.40   |
| 3   | F     | 63  | ILE  | CG1-CB-CG2 | -7.49 | 94.91       | 111.40   |
| 3   | R     | 63  | ILE  | CG1-CB-CG2 | -7.49 | 94.92       | 111.40   |
| 1   | M     | 518 | ASP  | CB-CG-OD1  | -7.49 | 111.56      | 118.30   |
| 3   | C     | 63  | ILE  | CG1-CB-CG2 | -7.49 | 94.93       | 111.40   |
| 4   | 7     | 312 | ARG  | NE-CZ-NH2  | 7.49  | 124.05      | 120.30   |
| 3   | L     | 63  | ILE  | CG1-CB-CG2 | -7.48 | 94.94       | 111.40   |
| 1   | A     | 654 | ARG  | NE-CZ-NH1  | 7.47  | 124.04      | 120.30   |
| 1   | P     | 709 | LYS  | O-C-N      | -7.46 | 110.51      | 123.20   |
| 4   | 0     | 86  | TRP  | CE2-CD2-CG | -7.46 | 101.33      | 107.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 518 | ASP  | CB-CG-OD1 | -7.45 | 111.60      | 118.30   |
| 1   | P     | 654 | ARG  | NE-CZ-NH1 | 7.44  | 124.02      | 120.30   |
| 1   | A     | 653 | PHE  | CB-CG-CD1 | -7.44 | 115.59      | 120.80   |
| 4   | 4     | 312 | ARG  | NE-CZ-NH2 | 7.44  | 124.02      | 120.30   |
| 3   | I     | 63  | ILE  | CA-C-N    | -7.42 | 100.87      | 117.20   |
| 1   | P     | 518 | ASP  | CB-CG-OD1 | -7.42 | 111.63      | 118.30   |
| 4   | X     | 254 | ARG  | NE-CZ-NH2 | -7.41 | 116.59      | 120.30   |
| 1   | D     | 654 | ARG  | NE-CZ-NH1 | 7.41  | 124.00      | 120.30   |
| 1   | G     | 518 | ASP  | CB-CG-OD1 | -7.41 | 111.64      | 118.30   |
| 1   | A     | 518 | ASP  | CB-CG-OD1 | -7.39 | 111.65      | 118.30   |
| 4   | 2     | 233 | SER  | CA-C-N    | -7.39 | 100.94      | 117.20   |
| 4   | 7     | 180 | LEU  | CA-CB-CG  | 7.38  | 132.26      | 115.30   |
| 4   | V     | 233 | SER  | CA-C-N    | -7.37 | 100.98      | 117.20   |
| 4   | X     | 233 | SER  | CA-C-N    | -7.37 | 100.98      | 117.20   |
| 1   | D     | 346 | ASP  | CB-CG-OD2 | -7.37 | 111.67      | 118.30   |
| 4   | 3     | 233 | SER  | CA-C-N    | -7.37 | 100.99      | 117.20   |
| 4   | 8     | 233 | SER  | CA-C-N    | -7.37 | 101.00      | 117.20   |
| 4   | Y     | 233 | SER  | CA-C-N    | -7.37 | 101.00      | 117.20   |
| 4   | 7     | 233 | SER  | CA-C-N    | -7.36 | 101.00      | 117.20   |
| 4   | 9     | 233 | SER  | CA-C-N    | -7.36 | 101.01      | 117.20   |
| 4   | W     | 233 | SER  | CA-C-N    | -7.36 | 101.02      | 117.20   |
| 2   | E     | 127 | ARG  | NE-CZ-NH2 | 7.35  | 123.98      | 120.30   |
| 4   | 4     | 233 | SER  | CA-C-N    | -7.35 | 101.03      | 117.20   |
| 4   | 5     | 233 | SER  | CA-C-N    | -7.35 | 101.02      | 117.20   |
| 4   | 0     | 233 | SER  | CA-C-N    | -7.35 | 101.03      | 117.20   |
| 4   | 5     | 180 | LEU  | CA-CB-CG  | 7.35  | 132.21      | 115.30   |
| 4   | X     | 180 | LEU  | CA-CB-CG  | 7.35  | 132.20      | 115.30   |
| 4   | Z     | 254 | ARG  | NE-CZ-NH2 | -7.35 | 116.63      | 120.30   |
| 4   | 0     | 180 | LEU  | CA-CB-CG  | 7.35  | 132.19      | 115.30   |
| 4   | 4     | 180 | LEU  | CA-CB-CG  | 7.34  | 132.19      | 115.30   |
| 3   | C     | 63  | ILE  | CA-C-N    | -7.34 | 101.05      | 117.20   |
| 4   | Z     | 233 | SER  | CA-C-N    | -7.34 | 101.06      | 117.20   |
| 3   | L     | 63  | ILE  | CA-C-N    | -7.33 | 101.06      | 117.20   |
| 4   | 2     | 180 | LEU  | CA-CB-CG  | 7.33  | 132.17      | 115.30   |
| 4   | 3     | 180 | LEU  | CA-CB-CG  | 7.33  | 132.17      | 115.30   |
| 4   | Z     | 180 | LEU  | CA-CB-CG  | 7.33  | 132.17      | 115.30   |
| 4   | 1     | 233 | SER  | CA-C-N    | -7.33 | 101.08      | 117.20   |
| 3   | R     | 63  | ILE  | CA-C-N    | -7.33 | 101.08      | 117.20   |
| 4   | 1     | 180 | LEU  | CA-CB-CG  | 7.33  | 132.15      | 115.30   |
| 3   | O     | 63  | ILE  | CA-C-N    | -7.33 | 101.09      | 117.20   |
| 4   | Y     | 180 | LEU  | CA-CB-CG  | 7.33  | 132.15      | 115.30   |
| 1   | A     | 346 | ASP  | CB-CG-OD2 | -7.32 | 111.71      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 654 | ARG  | NE-CZ-NH1  | 7.32  | 123.96      | 120.30   |
| 1   | P     | 346 | ASP  | CB-CG-OD2  | -7.32 | 111.71      | 118.30   |
| 4   | 8     | 180 | LEU  | CA-CB-CG   | 7.32  | 132.13      | 115.30   |
| 1   | D     | 518 | ASP  | CB-CG-OD1  | -7.31 | 111.72      | 118.30   |
| 4   | 4     | 254 | ARG  | NE-CZ-NH2  | -7.31 | 116.64      | 120.30   |
| 4   | 9     | 180 | LEU  | CA-CB-CG   | 7.31  | 132.12      | 115.30   |
| 4   | V     | 180 | LEU  | CA-CB-CG   | 7.31  | 132.12      | 115.30   |
| 4   | W     | 180 | LEU  | CA-CB-CG   | 7.30  | 132.10      | 115.30   |
| 2   | B     | 127 | ARG  | NE-CZ-NH2  | 7.29  | 123.95      | 120.30   |
| 4   | 3     | 254 | ARG  | NE-CZ-NH2  | -7.29 | 116.65      | 120.30   |
| 1   | J     | 654 | ARG  | NE-CZ-NH1  | 7.29  | 123.94      | 120.30   |
| 4   | W     | 79  | TRP  | CD1-CG-CD2 | 7.28  | 112.12      | 106.30   |
| 1   | G     | 104 | TYR  | CB-CG-CD2  | 7.28  | 125.37      | 121.00   |
| 3   | F     | 63  | ILE  | CA-C-N     | -7.27 | 101.21      | 117.20   |
| 1   | J     | 346 | ASP  | CB-CG-OD2  | -7.26 | 111.77      | 118.30   |
| 4   | Z     | 79  | TRP  | CD1-CG-CD2 | 7.25  | 112.10      | 106.30   |
| 4   | 1     | 254 | ARG  | NE-CZ-NH2  | -7.24 | 116.68      | 120.30   |
| 1   | M     | 346 | ASP  | CB-CG-OD2  | -7.24 | 111.78      | 118.30   |
| 4   | 0     | 340 | TRP  | CE2-CD2-CG | -7.23 | 101.52      | 107.30   |
| 4   | V     | 340 | TRP  | CE2-CD2-CG | -7.23 | 101.52      | 107.30   |
| 4   | 9     | 254 | ARG  | NE-CZ-NH2  | -7.23 | 116.69      | 120.30   |
| 4   | 8     | 254 | ARG  | NE-CZ-NH2  | -7.22 | 116.69      | 120.30   |
| 4   | Y     | 340 | TRP  | CE2-CD2-CG | -7.22 | 101.53      | 107.30   |
| 4   | 5     | 254 | ARG  | NE-CZ-NH2  | -7.22 | 116.69      | 120.30   |
| 4   | 9     | 340 | TRP  | CE2-CD2-CG | -7.21 | 101.53      | 107.30   |
| 4   | 7     | 79  | TRP  | CD1-CG-CD2 | 7.21  | 112.07      | 106.30   |
| 1   | M     | 104 | TYR  | CB-CG-CD2  | 7.21  | 125.33      | 121.00   |
| 4   | W     | 254 | ARG  | NE-CZ-NH2  | -7.21 | 116.70      | 120.30   |
| 4   | Y     | 254 | ARG  | NE-CZ-NH2  | -7.20 | 116.70      | 120.30   |
| 4   | 7     | 340 | TRP  | CE2-CD2-CG | -7.19 | 101.55      | 107.30   |
| 1   | A     | 104 | TYR  | CB-CG-CD2  | 7.18  | 125.31      | 121.00   |
| 4   | 8     | 79  | TRP  | CD1-CG-CD2 | 7.18  | 112.05      | 106.30   |
| 4   | 3     | 79  | TRP  | CD1-CG-CD2 | 7.18  | 112.05      | 106.30   |
| 4   | W     | 340 | TRP  | CE2-CD2-CG | -7.18 | 101.56      | 107.30   |
| 4   | 1     | 79  | TRP  | CD1-CG-CD2 | 7.18  | 112.04      | 106.30   |
| 4   | 8     | 206 | ARG  | NE-CZ-NH1  | 7.18  | 123.89      | 120.30   |
| 4   | V     | 79  | TRP  | CD1-CG-CD2 | 7.17  | 112.04      | 106.30   |
| 1   | J     | 709 | LYS  | CA-C-N     | 7.17  | 130.53      | 116.20   |
| 4   | 2     | 206 | ARG  | NE-CZ-NH1  | 7.16  | 123.88      | 120.30   |
| 4   | 4     | 79  | TRP  | CD1-CG-CD2 | 7.15  | 112.02      | 106.30   |
| 4   | 4     | 340 | TRP  | CE2-CD2-CG | -7.15 | 101.58      | 107.30   |
| 1   | A     | 148 | ARG  | NE-CZ-NH2  | -7.15 | 116.73      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Y     | 79  | TRP  | CD1-CG-CD2 | 7.14  | 112.02      | 106.30   |
| 4   | 2     | 79  | TRP  | CD1-CG-CD2 | 7.14  | 112.01      | 106.30   |
| 2   | K     | 150 | TYR  | CB-CG-CD1  | -7.14 | 116.72      | 121.00   |
| 4   | 4     | 206 | ARG  | NE-CZ-NH1  | 7.14  | 123.87      | 120.30   |
| 4   | 2     | 340 | TRP  | CE2-CD2-CG | -7.14 | 101.59      | 107.30   |
| 2   | H     | 150 | TYR  | CB-CG-CD1  | -7.14 | 116.72      | 121.00   |
| 4   | 1     | 206 | ARG  | NE-CZ-NH1  | 7.13  | 123.87      | 120.30   |
| 1   | P     | 104 | TYR  | CB-CG-CD2  | 7.13  | 125.28      | 121.00   |
| 4   | 9     | 79  | TRP  | CD1-CG-CD2 | 7.13  | 112.00      | 106.30   |
| 4   | X     | 206 | ARG  | NE-CZ-NH1  | 7.13  | 123.86      | 120.30   |
| 4   | W     | 79  | TRP  | CE2-CD2-CG | -7.12 | 101.60      | 107.30   |
| 4   | 5     | 79  | TRP  | CD1-CG-CD2 | 7.12  | 111.99      | 106.30   |
| 1   | G     | 568 | PRO  | CA-C-N     | -7.12 | 101.55      | 117.20   |
| 1   | J     | 104 | TYR  | CB-CG-CD2  | 7.11  | 125.27      | 121.00   |
| 4   | 0     | 79  | TRP  | CD1-CG-CD2 | 7.11  | 111.99      | 106.30   |
| 1   | A     | 568 | PRO  | CA-C-N     | -7.11 | 101.56      | 117.20   |
| 4   | X     | 79  | TRP  | CD1-CG-CD2 | 7.11  | 111.99      | 106.30   |
| 4   | 7     | 206 | ARG  | NE-CZ-NH1  | 7.10  | 123.85      | 120.30   |
| 4   | V     | 206 | ARG  | NE-CZ-NH1  | 7.10  | 123.85      | 120.30   |
| 2   | Q     | 150 | TYR  | CB-CG-CD1  | -7.09 | 116.74      | 121.00   |
| 4   | 2     | 254 | ARG  | NE-CZ-NH2  | -7.09 | 116.75      | 120.30   |
| 4   | 0     | 254 | ARG  | NE-CZ-NH2  | -7.08 | 116.76      | 120.30   |
| 2   | E     | 150 | TYR  | CB-CG-CD1  | -7.08 | 116.75      | 121.00   |
| 2   | K     | 127 | ARG  | NE-CZ-NH2  | 7.07  | 123.84      | 120.30   |
| 4   | Z     | 47  | MET  | CA-CB-CG   | -7.07 | 101.28      | 113.30   |
| 4   | 8     | 340 | TRP  | CE2-CD2-CG | -7.07 | 101.65      | 107.30   |
| 4   | Y     | 206 | ARG  | NE-CZ-NH1  | 7.07  | 123.83      | 120.30   |
| 1   | J     | 568 | PRO  | CA-C-N     | -7.06 | 101.67      | 117.20   |
| 1   | P     | 568 | PRO  | CA-C-N     | -7.06 | 101.67      | 117.20   |
| 1   | M     | 568 | PRO  | CA-C-N     | -7.06 | 101.67      | 117.20   |
| 4   | 7     | 254 | ARG  | NE-CZ-NH2  | -7.06 | 116.77      | 120.30   |
| 4   | 3     | 340 | TRP  | CE2-CD2-CG | -7.06 | 101.65      | 107.30   |
| 1   | D     | 568 | PRO  | CA-C-N     | -7.05 | 101.68      | 117.20   |
| 4   | 0     | 206 | ARG  | NE-CZ-NH1  | 7.05  | 123.83      | 120.30   |
| 4   | 5     | 206 | ARG  | NE-CZ-NH1  | 7.05  | 123.83      | 120.30   |
| 4   | W     | 206 | ARG  | NE-CZ-NH1  | 7.05  | 123.82      | 120.30   |
| 4   | 5     | 340 | TRP  | CE2-CD2-CG | -7.05 | 101.66      | 107.30   |
| 4   | V     | 47  | MET  | CA-CB-CG   | -7.05 | 101.32      | 113.30   |
| 4   | V     | 254 | ARG  | NE-CZ-NH2  | -7.04 | 116.78      | 120.30   |
| 2   | B     | 150 | TYR  | CB-CG-CD1  | -7.04 | 116.77      | 121.00   |
| 1   | D     | 104 | TYR  | CB-CG-CD2  | 7.04  | 125.22      | 121.00   |
| 4   | X     | 340 | TRP  | CE2-CD2-CG | -7.04 | 101.67      | 107.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 1     | 340 | TRP  | CE2-CD2-CG | -7.04 | 101.67      | 107.30   |
| 4   | 9     | 340 | TRP  | CD1-CG-CD2 | 7.04  | 111.93      | 106.30   |
| 4   | 3     | 47  | MET  | CA-CB-CG   | -7.04 | 101.34      | 113.30   |
| 4   | 3     | 206 | ARG  | NE-CZ-NH1  | 7.04  | 123.82      | 120.30   |
| 4   | Z     | 206 | ARG  | NE-CZ-NH1  | 7.03  | 123.82      | 120.30   |
| 1   | D     | 218 | LEU  | CB-CG-CD1  | 7.03  | 122.95      | 111.00   |
| 2   | N     | 127 | ARG  | NE-CZ-NH2  | 7.03  | 123.81      | 120.30   |
| 4   | W     | 47  | MET  | CA-CB-CG   | -7.03 | 101.35      | 113.30   |
| 4   | Z     | 79  | TRP  | CE2-CD2-CG | -7.03 | 101.68      | 107.30   |
| 2   | H     | 127 | ARG  | NE-CZ-NH2  | 7.03  | 123.81      | 120.30   |
| 1   | M     | 264 | ASP  | N-CA-CB    | -7.03 | 97.95       | 110.60   |
| 4   | 8     | 47  | MET  | CA-CB-CG   | -7.03 | 101.36      | 113.30   |
| 4   | 8     | 79  | TRP  | CE2-CD2-CG | -7.03 | 101.68      | 107.30   |
| 1   | A     | 217 | THR  | N-CA-CB    | 7.02  | 123.64      | 110.30   |
| 1   | P     | 264 | ASP  | N-CA-CB    | -7.02 | 97.96       | 110.60   |
| 4   | 4     | 47  | MET  | CA-CB-CG   | -7.02 | 101.36      | 113.30   |
| 4   | 9     | 47  | MET  | CA-CB-CG   | -7.02 | 101.36      | 113.30   |
| 2   | N     | 150 | TYR  | CB-CG-CD1  | -7.02 | 116.79      | 121.00   |
| 4   | 5     | 47  | MET  | CA-CB-CG   | -7.02 | 101.37      | 113.30   |
| 4   | 7     | 47  | MET  | CA-CB-CG   | -7.02 | 101.37      | 113.30   |
| 4   | 1     | 47  | MET  | CA-CB-CG   | -7.01 | 101.38      | 113.30   |
| 4   | 5     | 340 | TRP  | CD1-CG-CD2 | 7.01  | 111.91      | 106.30   |
| 4   | Y     | 47  | MET  | CA-CB-CG   | -7.01 | 101.38      | 113.30   |
| 1   | D     | 264 | ASP  | N-CA-CB    | -7.01 | 97.98       | 110.60   |
| 4   | 0     | 47  | MET  | CA-CB-CG   | -7.01 | 101.39      | 113.30   |
| 4   | 2     | 47  | MET  | CA-CB-CG   | -7.00 | 101.39      | 113.30   |
| 1   | G     | 217 | THR  | N-CA-CB    | 7.00  | 123.60      | 110.30   |
| 4   | 1     | 79  | TRP  | CE2-CD2-CG | -7.00 | 101.70      | 107.30   |
| 4   | W     | 340 | TRP  | CD1-CG-CD2 | 7.00  | 111.90      | 106.30   |
| 1   | A     | 264 | ASP  | N-CA-CB    | -7.00 | 98.01       | 110.60   |
| 1   | D     | 217 | THR  | N-CA-CB    | 6.99  | 123.59      | 110.30   |
| 1   | M     | 217 | THR  | N-CA-CB    | 6.99  | 123.59      | 110.30   |
| 1   | M     | 218 | LEU  | CB-CG-CD1  | 6.99  | 122.89      | 111.00   |
| 1   | J     | 264 | ASP  | N-CA-CB    | -6.99 | 98.02       | 110.60   |
| 4   | 0     | 340 | TRP  | CD1-CG-CD2 | 6.99  | 111.89      | 106.30   |
| 4   | 7     | 79  | TRP  | CE2-CD2-CG | -6.99 | 101.71      | 107.30   |
| 4   | X     | 47  | MET  | CA-CB-CG   | -6.99 | 101.42      | 113.30   |
| 1   | J     | 148 | ARG  | NE-CZ-NH2  | -6.98 | 116.81      | 120.30   |
| 1   | A     | 218 | LEU  | CB-CG-CD1  | 6.98  | 122.87      | 111.00   |
| 2   | Q     | 127 | ARG  | NE-CZ-NH2  | 6.98  | 123.79      | 120.30   |
| 4   | 2     | 79  | TRP  | CE2-CD2-CG | -6.98 | 101.72      | 107.30   |
| 1   | P     | 217 | THR  | N-CA-CB    | 6.98  | 123.56      | 110.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Z     | 340 | TRP  | CE2-CD2-CG | -6.98 | 101.72      | 107.30   |
| 4   | 7     | 340 | TRP  | CD1-CG-CD2 | 6.97  | 111.88      | 106.30   |
| 1   | G     | 218 | LEU  | CB-CG-CD1  | 6.97  | 122.85      | 111.00   |
| 4   | 5     | 79  | TRP  | CE2-CD2-CG | -6.97 | 101.73      | 107.30   |
| 1   | P     | 218 | LEU  | CB-CG-CD1  | 6.96  | 122.84      | 111.00   |
| 4   | Y     | 79  | TRP  | CE2-CD2-CG | -6.96 | 101.73      | 107.30   |
| 1   | J     | 218 | LEU  | CB-CG-CD1  | 6.96  | 122.84      | 111.00   |
| 4   | X     | 79  | TRP  | CE2-CD2-CG | -6.96 | 101.73      | 107.30   |
| 4   | 2     | 340 | TRP  | CD1-CG-CD2 | 6.96  | 111.86      | 106.30   |
| 1   | P     | 148 | ARG  | NE-CZ-NH2  | -6.96 | 116.82      | 120.30   |
| 1   | J     | 217 | THR  | N-CA-CB    | 6.95  | 123.51      | 110.30   |
| 1   | G     | 264 | ASP  | N-CA-CB    | -6.95 | 98.10       | 110.60   |
| 4   | V     | 79  | TRP  | CE2-CD2-CG | -6.95 | 101.74      | 107.30   |
| 1   | D     | 148 | ARG  | NE-CZ-NH2  | -6.94 | 116.83      | 120.30   |
| 4   | V     | 340 | TRP  | CD1-CG-CD2 | 6.93  | 111.85      | 106.30   |
| 4   | 3     | 79  | TRP  | CE2-CD2-CG | -6.93 | 101.75      | 107.30   |
| 4   | Y     | 340 | TRP  | CD1-CG-CD2 | 6.93  | 111.84      | 106.30   |
| 4   | 4     | 340 | TRP  | CD1-CG-CD2 | 6.92  | 111.83      | 106.30   |
| 1   | G     | 75  | ASP  | N-CA-CB    | 6.91  | 123.03      | 110.60   |
| 4   | 8     | 340 | TRP  | CD1-CG-CD2 | 6.90  | 111.82      | 106.30   |
| 1   | G     | 148 | ARG  | NE-CZ-NH2  | -6.90 | 116.85      | 120.30   |
| 4   | 9     | 79  | TRP  | CE2-CD2-CG | -6.90 | 101.78      | 107.30   |
| 4   | 0     | 79  | TRP  | CE2-CD2-CG | -6.89 | 101.79      | 107.30   |
| 4   | 4     | 79  | TRP  | CE2-CD2-CG | -6.89 | 101.79      | 107.30   |
| 1   | P     | 728 | ASN  | CA-C-N     | -6.88 | 102.05      | 117.20   |
| 1   | M     | 728 | ASN  | CA-C-N     | -6.88 | 102.06      | 117.20   |
| 1   | A     | 75  | ASP  | N-CA-CB    | 6.87  | 122.96      | 110.60   |
| 1   | J     | 75  | ASP  | N-CA-CB    | 6.87  | 122.96      | 110.60   |
| 1   | P     | 75  | ASP  | N-CA-CB    | 6.87  | 122.96      | 110.60   |
| 1   | J     | 728 | ASN  | CA-C-N     | -6.87 | 102.09      | 117.20   |
| 4   | 9     | 206 | ARG  | NE-CZ-NH1  | 6.86  | 123.73      | 120.30   |
| 1   | M     | 148 | ARG  | NE-CZ-NH2  | -6.86 | 116.87      | 120.30   |
| 1   | G     | 728 | ASN  | CA-C-N     | -6.85 | 102.12      | 117.20   |
| 1   | M     | 75  | ASP  | N-CA-CB    | 6.85  | 122.93      | 110.60   |
| 1   | D     | 728 | ASN  | CA-C-N     | -6.85 | 102.14      | 117.20   |
| 1   | A     | 728 | ASN  | CA-C-N     | -6.84 | 102.15      | 117.20   |
| 1   | G     | 450 | ASP  | CB-CG-OD2  | 6.84  | 124.46      | 118.30   |
| 1   | D     | 450 | ASP  | CB-CG-OD2  | 6.84  | 124.45      | 118.30   |
| 4   | X     | 340 | TRP  | CD1-CG-CD2 | 6.83  | 111.77      | 106.30   |
| 1   | P     | 450 | ASP  | CB-CG-OD2  | 6.82  | 124.44      | 118.30   |
| 4   | 3     | 340 | TRP  | CD1-CG-CD2 | 6.80  | 111.74      | 106.30   |
| 1   | J     | 450 | ASP  | CB-CG-OD2  | 6.80  | 124.42      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 1     | 340 | TRP  | CD1-CG-CD2 | 6.80  | 111.74      | 106.30   |
| 1   | M     | 555 | TYR  | CB-CG-CD2  | -6.79 | 116.92      | 121.00   |
| 4   | Z     | 340 | TRP  | CD1-CG-CD2 | 6.79  | 111.73      | 106.30   |
| 1   | A     | 450 | ASP  | CB-CG-OD2  | 6.79  | 124.41      | 118.30   |
| 1   | M     | 450 | ASP  | CB-CG-OD2  | 6.76  | 124.39      | 118.30   |
| 1   | P     | 555 | TYR  | CB-CG-CD2  | -6.76 | 116.94      | 121.00   |
| 1   | D     | 75  | ASP  | N-CA-CB    | 6.74  | 122.74      | 110.60   |
| 4   | Y     | 196 | ARG  | NE-CZ-NH1  | 6.69  | 123.65      | 120.30   |
| 1   | G     | 781 | ASP  | CB-CG-OD1  | -6.69 | 112.28      | 118.30   |
| 1   | G     | 756 | THR  | N-CA-CB    | -6.68 | 97.60       | 110.30   |
| 1   | M     | 756 | THR  | N-CA-CB    | -6.68 | 97.60       | 110.30   |
| 4   | X     | 196 | ARG  | NE-CZ-NH1  | 6.68  | 123.64      | 120.30   |
| 1   | M     | 219 | GLU  | N-CA-C     | -6.68 | 92.97       | 111.00   |
| 1   | P     | 756 | THR  | N-CA-CB    | -6.67 | 97.62       | 110.30   |
| 1   | J     | 75  | ASP  | CB-CG-OD2  | 6.67  | 124.30      | 118.30   |
| 1   | J     | 555 | TYR  | CB-CG-CD2  | -6.67 | 117.00      | 121.00   |
| 1   | J     | 756 | THR  | N-CA-CB    | -6.67 | 97.63       | 110.30   |
| 1   | J     | 219 | GLU  | N-CA-C     | -6.66 | 93.02       | 111.00   |
| 1   | G     | 219 | GLU  | N-CA-C     | -6.65 | 93.04       | 111.00   |
| 1   | G     | 555 | TYR  | CB-CG-CD2  | -6.65 | 117.01      | 121.00   |
| 1   | P     | 219 | GLU  | N-CA-C     | -6.64 | 93.06       | 111.00   |
| 1   | A     | 343 | PHE  | CB-CG-CD1  | 6.64  | 125.45      | 120.80   |
| 1   | A     | 75  | ASP  | CB-CG-OD2  | 6.62  | 124.26      | 118.30   |
| 1   | D     | 756 | THR  | N-CA-CB    | -6.62 | 97.72       | 110.30   |
| 1   | M     | 75  | ASP  | CB-CG-OD2  | 6.62  | 124.25      | 118.30   |
| 1   | A     | 756 | THR  | N-CA-CB    | -6.61 | 97.74       | 110.30   |
| 1   | P     | 75  | ASP  | CB-CG-OD2  | 6.61  | 124.25      | 118.30   |
| 4   | 0     | 196 | ARG  | NE-CZ-NH1  | 6.61  | 123.60      | 120.30   |
| 4   | 2     | 169 | TYR  | CB-CG-CD2  | -6.61 | 117.04      | 121.00   |
| 1   | D     | 781 | ASP  | CB-CG-OD1  | -6.60 | 112.36      | 118.30   |
| 1   | D     | 75  | ASP  | CB-CG-OD2  | 6.60  | 124.24      | 118.30   |
| 1   | A     | 781 | ASP  | CB-CG-OD1  | -6.60 | 112.36      | 118.30   |
| 1   | D     | 219 | GLU  | N-CA-C     | -6.59 | 93.20       | 111.00   |
| 1   | D     | 555 | TYR  | CB-CG-CD2  | -6.59 | 117.05      | 121.00   |
| 1   | A     | 219 | GLU  | N-CA-C     | -6.58 | 93.23       | 111.00   |
| 1   | J     | 781 | ASP  | CB-CG-OD1  | -6.57 | 112.39      | 118.30   |
| 1   | M     | 781 | ASP  | CB-CG-OD1  | -6.56 | 112.39      | 118.30   |
| 4   | X     | 169 | TYR  | CB-CG-CD2  | -6.56 | 117.07      | 121.00   |
| 1   | D     | 332 | MET  | CG-SD-CE   | -6.55 | 89.71       | 100.20   |
| 4   | 4     | 169 | TYR  | CB-CG-CD2  | -6.55 | 117.07      | 121.00   |
| 4   | 0     | 283 | MET  | CG-SD-CE   | 6.55  | 110.68      | 100.20   |
| 1   | J     | 169 | ASP  | CB-CG-OD1  | -6.55 | 112.41      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 332 | MET  | CG-SD-CE  | -6.55 | 89.72       | 100.20   |
| 1   | M     | 169 | ASP  | CB-CG-OD1 | -6.55 | 112.41      | 118.30   |
| 1   | P     | 781 | ASP  | CB-CG-OD1 | -6.54 | 112.41      | 118.30   |
| 1   | M     | 141 | LEU  | CB-CA-C   | -6.54 | 97.77       | 110.20   |
| 1   | M     | 332 | MET  | CG-SD-CE  | -6.54 | 89.74       | 100.20   |
| 4   | 8     | 283 | MET  | CG-SD-CE  | 6.54  | 110.66      | 100.20   |
| 1   | G     | 332 | MET  | CG-SD-CE  | -6.54 | 89.74       | 100.20   |
| 4   | 2     | 283 | MET  | CG-SD-CE  | 6.54  | 110.66      | 100.20   |
| 4   | 5     | 283 | MET  | CG-SD-CE  | 6.54  | 110.66      | 100.20   |
| 1   | A     | 332 | MET  | CG-SD-CE  | -6.53 | 89.75       | 100.20   |
| 4   | 3     | 283 | MET  | CG-SD-CE  | 6.53  | 110.65      | 100.20   |
| 1   | A     | 555 | TYR  | CB-CG-CD2 | -6.53 | 117.08      | 121.00   |
| 1   | P     | 332 | MET  | CG-SD-CE  | -6.53 | 89.75       | 100.20   |
| 4   | V     | 283 | MET  | CG-SD-CE  | 6.53  | 110.64      | 100.20   |
| 4   | W     | 283 | MET  | CG-SD-CE  | 6.53  | 110.64      | 100.20   |
| 4   | Y     | 283 | MET  | CG-SD-CE  | 6.53  | 110.64      | 100.20   |
| 1   | D     | 334 | THR  | CA-CB-CG2 | -6.52 | 103.27      | 112.40   |
| 4   | 9     | 196 | ARG  | NE-CZ-NH1 | 6.52  | 123.56      | 120.30   |
| 4   | 9     | 283 | MET  | CG-SD-CE  | 6.52  | 110.63      | 100.20   |
| 4   | Z     | 283 | MET  | CG-SD-CE  | 6.52  | 110.63      | 100.20   |
| 4   | 1     | 283 | MET  | CG-SD-CE  | 6.52  | 110.63      | 100.20   |
| 1   | G     | 141 | LEU  | CB-CA-C   | -6.52 | 97.82       | 110.20   |
| 4   | 7     | 283 | MET  | CG-SD-CE  | 6.51  | 110.62      | 100.20   |
| 4   | X     | 283 | MET  | CG-SD-CE  | 6.51  | 110.62      | 100.20   |
| 1   | P     | 141 | LEU  | CB-CA-C   | -6.51 | 97.83       | 110.20   |
| 2   | E     | 141 | PRO  | N-CD-CG   | -6.51 | 93.43       | 103.20   |
| 4   | 8     | 169 | TYR  | CB-CG-CD2 | -6.51 | 117.09      | 121.00   |
| 4   | W     | 169 | TYR  | CB-CG-CD2 | -6.51 | 117.09      | 121.00   |
| 4   | Z     | 169 | TYR  | CB-CG-CD2 | -6.51 | 117.09      | 121.00   |
| 4   | 7     | 169 | TYR  | CB-CG-CD2 | -6.51 | 117.09      | 121.00   |
| 1   | J     | 334 | THR  | CA-CB-CG2 | -6.51 | 103.29      | 112.40   |
| 4   | 5     | 169 | TYR  | CB-CG-CD2 | -6.51 | 117.09      | 121.00   |
| 4   | 4     | 283 | MET  | CG-SD-CE  | 6.50  | 110.61      | 100.20   |
| 1   | P     | 334 | THR  | CA-CB-CG2 | -6.50 | 103.30      | 112.40   |
| 2   | H     | 141 | PRO  | N-CD-CG   | -6.50 | 93.45       | 103.20   |
| 4   | 3     | 169 | TYR  | CB-CG-CD2 | -6.50 | 117.10      | 121.00   |
| 4   | Y     | 169 | TYR  | CB-CG-CD2 | -6.50 | 117.10      | 121.00   |
| 4   | 7     | 159 | VAL  | CB-CA-C   | -6.50 | 99.05       | 111.40   |
| 1   | G     | 589 | ASP  | CB-CG-OD1 | -6.50 | 112.45      | 118.30   |
| 1   | A     | 334 | THR  | CA-CB-CG2 | -6.50 | 103.31      | 112.40   |
| 4   | V     | 169 | TYR  | CB-CG-CD2 | -6.49 | 117.10      | 121.00   |
| 2   | N     | 141 | PRO  | N-CD-CG   | -6.49 | 93.47       | 103.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 141 | LEU  | CB-CA-C   | -6.49 | 97.87       | 110.20   |
| 1   | J     | 141 | LEU  | CB-CA-C   | -6.49 | 97.87       | 110.20   |
| 4   | X     | 159 | VAL  | CB-CA-C   | -6.49 | 99.07       | 111.40   |
| 1   | G     | 334 | THR  | CA-CB-CG2 | -6.49 | 103.32      | 112.40   |
| 4   | 9     | 169 | TYR  | CB-CG-CD2 | -6.49 | 117.11      | 121.00   |
| 4   | Y     | 159 | VAL  | CB-CA-C   | -6.48 | 99.08       | 111.40   |
| 4   | 1     | 196 | ARG  | NE-CZ-NH1 | 6.48  | 123.54      | 120.30   |
| 4   | 3     | 159 | VAL  | CB-CA-C   | -6.48 | 99.09       | 111.40   |
| 4   | 2     | 159 | VAL  | CB-CA-C   | -6.48 | 99.09       | 111.40   |
| 4   | 5     | 159 | VAL  | CB-CA-C   | -6.48 | 99.09       | 111.40   |
| 4   | V     | 159 | VAL  | CB-CA-C   | -6.48 | 99.10       | 111.40   |
| 4   | 0     | 159 | VAL  | CB-CA-C   | -6.47 | 99.10       | 111.40   |
| 1   | G     | 169 | ASP  | CB-CG-OD1 | -6.47 | 112.47      | 118.30   |
| 1   | M     | 334 | THR  | CA-CB-CG2 | -6.47 | 103.34      | 112.40   |
| 4   | 5     | 196 | ARG  | NE-CZ-NH1 | 6.47  | 123.53      | 120.30   |
| 1   | G     | 75  | ASP  | CB-CG-OD2 | 6.47  | 124.12      | 118.30   |
| 4   | 9     | 159 | VAL  | CB-CA-C   | -6.47 | 99.11       | 111.40   |
| 1   | P     | 169 | ASP  | CB-CG-OD1 | -6.46 | 112.48      | 118.30   |
| 4   | Z     | 159 | VAL  | CB-CA-C   | -6.46 | 99.12       | 111.40   |
| 4   | 8     | 159 | VAL  | CB-CA-C   | -6.46 | 99.12       | 111.40   |
| 1   | A     | 141 | LEU  | CB-CA-C   | -6.46 | 97.92       | 110.20   |
| 1   | A     | 169 | ASP  | CB-CG-OD1 | -6.46 | 112.48      | 118.30   |
| 4   | 4     | 196 | ARG  | NE-CZ-NH1 | 6.46  | 123.53      | 120.30   |
| 4   | 4     | 159 | VAL  | CB-CA-C   | -6.45 | 99.14       | 111.40   |
| 1   | M     | 129 | TYR  | CB-CG-CD2 | -6.45 | 117.13      | 121.00   |
| 4   | 1     | 159 | VAL  | CB-CA-C   | -6.45 | 99.14       | 111.40   |
| 4   | W     | 159 | VAL  | CB-CA-C   | -6.45 | 99.14       | 111.40   |
| 1   | J     | 129 | TYR  | CB-CG-CD2 | -6.45 | 117.13      | 121.00   |
| 1   | J     | 589 | ASP  | CB-CG-OD1 | -6.44 | 112.50      | 118.30   |
| 2   | Q     | 141 | PRO  | N-CD-CG   | -6.44 | 93.54       | 103.20   |
| 4   | 1     | 169 | TYR  | CB-CG-CD2 | -6.44 | 117.14      | 121.00   |
| 4   | 2     | 196 | ARG  | NE-CZ-NH1 | 6.43  | 123.52      | 120.30   |
| 4   | 3     | 196 | ARG  | NE-CZ-NH1 | 6.42  | 123.51      | 120.30   |
| 4   | 4     | 34  | ILE  | CA-CB-CG2 | -6.42 | 98.06       | 110.90   |
| 1   | A     | 589 | ASP  | CB-CG-OD1 | -6.42 | 112.53      | 118.30   |
| 1   | D     | 343 | PHE  | CB-CG-CD1 | 6.42  | 125.29      | 120.80   |
| 1   | G     | 343 | PHE  | CB-CG-CD1 | 6.42  | 125.29      | 120.80   |
| 4   | W     | 196 | ARG  | NE-CZ-NH1 | 6.42  | 123.51      | 120.30   |
| 1   | G     | 590 | TYR  | CB-CG-CD2 | 6.42  | 124.85      | 121.00   |
| 4   | 0     | 34  | ILE  | CA-CB-CG2 | -6.42 | 98.07       | 110.90   |
| 4   | 9     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.08       | 110.90   |
| 4   | 5     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.08       | 110.90   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | V     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.08       | 110.90   |
| 2   | K     | 141 | PRO  | N-CD-CG   | -6.41 | 93.59       | 103.20   |
| 4   | Z     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.09       | 110.90   |
| 4   | 2     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.09       | 110.90   |
| 4   | X     | 34  | ILE  | CA-CB-CG2 | -6.41 | 98.09       | 110.90   |
| 4   | Y     | 34  | ILE  | CA-CB-CG2 | -6.40 | 98.09       | 110.90   |
| 4   | Z     | 196 | ARG  | NE-CZ-NH1 | 6.40  | 123.50      | 120.30   |
| 4   | 1     | 34  | ILE  | CA-CB-CG2 | -6.40 | 98.10       | 110.90   |
| 4   | 3     | 34  | ILE  | CA-CB-CG2 | -6.40 | 98.10       | 110.90   |
| 1   | J     | 327 | ASP  | CB-CG-OD2 | 6.40  | 124.06      | 118.30   |
| 4   | 8     | 34  | ILE  | CA-CB-CG2 | -6.39 | 98.11       | 110.90   |
| 4   | W     | 34  | ILE  | CA-CB-CG2 | -6.39 | 98.12       | 110.90   |
| 1   | M     | 589 | ASP  | CB-CG-OD1 | -6.39 | 112.55      | 118.30   |
| 1   | P     | 129 | TYR  | CB-CG-CD2 | -6.38 | 117.17      | 121.00   |
| 4   | V     | 196 | ARG  | NE-CZ-NH1 | 6.38  | 123.49      | 120.30   |
| 4   | 7     | 196 | ARG  | NE-CZ-NH1 | 6.37  | 123.48      | 120.30   |
| 1   | D     | 129 | TYR  | CB-CG-CD2 | -6.37 | 117.18      | 121.00   |
| 4   | 0     | 169 | TYR  | CB-CG-CD2 | -6.37 | 117.18      | 121.00   |
| 4   | 7     | 34  | ILE  | CA-CB-CG2 | -6.37 | 98.17       | 110.90   |
| 1   | G     | 341 | LEU  | CB-CA-C   | 6.36  | 122.28      | 110.20   |
| 2   | B     | 141 | PRO  | N-CD-CG   | -6.36 | 93.66       | 103.20   |
| 1   | P     | 589 | ASP  | CB-CG-OD1 | -6.36 | 112.58      | 118.30   |
| 1   | A     | 341 | LEU  | CB-CA-C   | 6.35  | 122.27      | 110.20   |
| 1   | D     | 169 | ASP  | CB-CG-OD1 | -6.35 | 112.59      | 118.30   |
| 4   | 8     | 196 | ARG  | NE-CZ-NH1 | 6.33  | 123.47      | 120.30   |
| 1   | M     | 341 | LEU  | CB-CA-C   | 6.33  | 122.23      | 110.20   |
| 1   | G     | 578 | HIS  | N-CA-CB   | 6.33  | 121.99      | 110.60   |
| 1   | D     | 589 | ASP  | CB-CG-OD1 | -6.32 | 112.61      | 118.30   |
| 1   | P     | 341 | LEU  | CB-CA-C   | 6.31  | 122.19      | 110.20   |
| 4   | X     | 217 | CYS  | CA-CB-SG  | -6.31 | 102.64      | 114.00   |
| 1   | J     | 341 | LEU  | CB-CA-C   | 6.31  | 122.19      | 110.20   |
| 1   | P     | 810 | ARG  | NE-CZ-NH1 | 6.30  | 123.45      | 120.30   |
| 1   | P     | 760 | PHE  | CB-CG-CD2 | -6.30 | 116.39      | 120.80   |
| 4   | V     | 217 | CYS  | CA-CB-SG  | -6.30 | 102.66      | 114.00   |
| 4   | Z     | 217 | CYS  | CA-CB-SG  | -6.30 | 102.66      | 114.00   |
| 4   | 1     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.67      | 114.00   |
| 4   | W     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.67      | 114.00   |
| 4   | Y     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.67      | 114.00   |
| 4   | 8     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.67      | 114.00   |
| 4   | 2     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.68      | 114.00   |
| 1   | J     | 810 | ARG  | NE-CZ-NH1 | 6.29  | 123.44      | 120.30   |
| 4   | 9     | 217 | CYS  | CA-CB-SG  | -6.29 | 102.69      | 114.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 343 | PHE  | CB-CG-CD1 | 6.28  | 125.20      | 120.80   |
| 4   | 7     | 217 | CYS  | CA-CB-SG  | -6.28 | 102.69      | 114.00   |
| 1   | J     | 578 | HIS  | N-CA-CB   | 6.28  | 121.90      | 110.60   |
| 1   | P     | 578 | HIS  | N-CA-CB   | 6.28  | 121.90      | 110.60   |
| 4   | 0     | 217 | CYS  | CA-CB-SG  | -6.28 | 102.70      | 114.00   |
| 4   | 3     | 217 | CYS  | CA-CB-SG  | -6.28 | 102.70      | 114.00   |
| 1   | M     | 343 | PHE  | CB-CG-CD1 | 6.27  | 125.19      | 120.80   |
| 4   | 4     | 217 | CYS  | CA-CB-SG  | -6.27 | 102.71      | 114.00   |
| 4   | 5     | 217 | CYS  | CA-CB-SG  | -6.27 | 102.71      | 114.00   |
| 2   | Q     | 129 | THR  | CB-CA-C   | -6.27 | 94.67       | 111.60   |
| 2   | N     | 129 | THR  | CB-CA-C   | -6.27 | 94.68       | 111.60   |
| 1   | M     | 578 | HIS  | N-CA-CB   | 6.26  | 121.87      | 110.60   |
| 1   | A     | 578 | HIS  | N-CA-CB   | 6.26  | 121.86      | 110.60   |
| 1   | P     | 343 | PHE  | CB-CG-CD1 | 6.25  | 125.18      | 120.80   |
| 1   | A     | 129 | TYR  | CB-CG-CD2 | -6.25 | 117.25      | 121.00   |
| 1   | M     | 327 | ASP  | CB-CG-OD2 | 6.25  | 123.93      | 118.30   |
| 1   | D     | 578 | HIS  | N-CA-CB   | 6.25  | 121.85      | 110.60   |
| 1   | J     | 760 | PHE  | CB-CG-CD2 | -6.25 | 116.43      | 120.80   |
| 1   | M     | 760 | PHE  | CB-CG-CD2 | -6.25 | 116.43      | 120.80   |
| 1   | G     | 129 | TYR  | CB-CG-CD2 | -6.24 | 117.25      | 121.00   |
| 1   | D     | 341 | LEU  | CB-CA-C   | 6.23  | 122.03      | 110.20   |
| 2   | K     | 129 | THR  | CB-CA-C   | -6.23 | 94.79       | 111.60   |
| 1   | G     | 810 | ARG  | NE-CZ-NH1 | 6.22  | 123.41      | 120.30   |
| 1   | P     | 327 | ASP  | CB-CG-OD2 | 6.21  | 123.89      | 118.30   |
| 1   | D     | 327 | ASP  | CB-CG-OD2 | 6.20  | 123.88      | 118.30   |
| 1   | A     | 810 | ARG  | NE-CZ-NH1 | 6.20  | 123.40      | 120.30   |
| 1   | A     | 327 | ASP  | CB-CG-OD2 | 6.20  | 123.88      | 118.30   |
| 1   | A     | 463 | ASP  | CB-CG-OD2 | -6.20 | 112.72      | 118.30   |
| 1   | G     | 327 | ASP  | CB-CG-OD2 | 6.20  | 123.88      | 118.30   |
| 2   | E     | 129 | THR  | CB-CA-C   | -6.19 | 94.89       | 111.60   |
| 1   | D     | 214 | MET  | CG-SD-CE  | 6.18  | 110.10      | 100.20   |
| 1   | D     | 760 | PHE  | CB-CG-CD2 | -6.18 | 116.47      | 120.80   |
| 2   | H     | 129 | THR  | CB-CA-C   | -6.18 | 94.90       | 111.60   |
| 2   | B     | 129 | THR  | CB-CA-C   | -6.18 | 94.91       | 111.60   |
| 1   | A     | 780 | ASP  | CB-CG-OD2 | 6.18  | 123.86      | 118.30   |
| 1   | M     | 752 | ASP  | CB-CG-OD2 | 6.17  | 123.86      | 118.30   |
| 2   | K     | 141 | PRO  | N-CA-CB   | -6.17 | 95.81       | 102.60   |
| 1   | P     | 752 | ASP  | CB-CG-OD2 | 6.17  | 123.86      | 118.30   |
| 1   | M     | 698 | ASN  | CB-CA-C   | -6.17 | 98.06       | 110.40   |
| 1   | P     | 698 | ASN  | CB-CA-C   | -6.17 | 98.06       | 110.40   |
| 1   | J     | 698 | ASN  | CB-CA-C   | -6.17 | 98.07       | 110.40   |
| 1   | A     | 698 | ASN  | CB-CA-C   | -6.16 | 98.08       | 110.40   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | M     | 463 | ASP  | CB-CG-OD2 | -6.16 | 112.75      | 118.30   |
| 1   | A     | 214 | MET  | CG-SD-CE  | 6.16  | 110.06      | 100.20   |
| 1   | M     | 214 | MET  | CG-SD-CE  | 6.16  | 110.05      | 100.20   |
| 1   | P     | 214 | MET  | CG-SD-CE  | 6.16  | 110.05      | 100.20   |
| 2   | H     | 141 | PRO  | N-CA-CB   | -6.16 | 95.83       | 102.60   |
| 1   | G     | 463 | ASP  | CB-CG-OD2 | -6.16 | 112.76      | 118.30   |
| 4   | 8     | 259 | GLU  | CA-CB-CG  | 6.15  | 126.93      | 113.40   |
| 1   | J     | 214 | MET  | CG-SD-CE  | 6.15  | 110.04      | 100.20   |
| 1   | G     | 214 | MET  | CG-SD-CE  | 6.15  | 110.03      | 100.20   |
| 1   | P     | 682 | THR  | CA-CB-CG2 | -6.14 | 103.80      | 112.40   |
| 3   | R     | 58  | MET  | CG-SD-CE  | 6.14  | 110.03      | 100.20   |
| 4   | V     | 259 | GLU  | CA-CB-CG  | 6.14  | 126.92      | 113.40   |
| 4   | 0     | 259 | GLU  | CA-CB-CG  | 6.14  | 126.91      | 113.40   |
| 4   | 1     | 259 | GLU  | CA-CB-CG  | 6.14  | 126.90      | 113.40   |
| 4   | Y     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.89      | 113.40   |
| 4   | X     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.89      | 113.40   |
| 1   | G     | 104 | TYR  | CB-CG-CD1 | -6.13 | 117.32      | 121.00   |
| 1   | P     | 450 | ASP  | CB-CG-OD1 | -6.13 | 112.78      | 118.30   |
| 1   | P     | 779 | ARG  | NE-CZ-NH1 | 6.13  | 123.37      | 120.30   |
| 4   | Z     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.88      | 113.40   |
| 1   | D     | 810 | ARG  | NE-CZ-NH1 | 6.13  | 123.36      | 120.30   |
| 4   | 4     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.88      | 113.40   |
| 4   | 7     | 259 | GLU  | CA-CB-CG  | 6.13  | 126.88      | 113.40   |
| 4   | 9     | 259 | GLU  | CA-CB-CG  | 6.12  | 126.87      | 113.40   |
| 1   | D     | 104 | TYR  | CB-CG-CD1 | -6.12 | 117.33      | 121.00   |
| 1   | J     | 779 | ARG  | NE-CZ-NH1 | 6.12  | 123.36      | 120.30   |
| 2   | N     | 141 | PRO  | N-CA-CB   | -6.12 | 95.87       | 102.60   |
| 4   | 3     | 259 | GLU  | CA-CB-CG  | 6.12  | 126.86      | 113.40   |
| 3   | L     | 58  | MET  | CG-SD-CE  | 6.11  | 109.98      | 100.20   |
| 4   | 5     | 259 | GLU  | CA-CB-CG  | 6.11  | 126.85      | 113.40   |
| 4   | W     | 259 | GLU  | CA-CB-CG  | 6.11  | 126.84      | 113.40   |
| 4   | 2     | 259 | GLU  | CA-CB-CG  | 6.11  | 126.83      | 113.40   |
| 1   | M     | 590 | TYR  | CB-CG-CD2 | 6.10  | 124.66      | 121.00   |
| 1   | J     | 463 | ASP  | CB-CG-OD2 | -6.10 | 112.81      | 118.30   |
| 1   | D     | 590 | TYR  | CB-CG-CD2 | 6.10  | 124.66      | 121.00   |
| 3   | F     | 58  | MET  | CG-SD-CE  | 6.10  | 109.95      | 100.20   |
| 1   | G     | 346 | ASP  | CB-CG-OD1 | 6.10  | 123.79      | 118.30   |
| 1   | G     | 698 | ASN  | CB-CA-C   | -6.10 | 98.21       | 110.40   |
| 1   | P     | 463 | ASP  | CB-CG-OD2 | -6.10 | 112.81      | 118.30   |
| 1   | P     | 590 | TYR  | CB-CG-CD2 | 6.09  | 124.66      | 121.00   |
| 1   | D     | 698 | ASN  | CB-CA-C   | -6.09 | 98.22       | 110.40   |
| 3   | O     | 58  | MET  | CG-SD-CE  | 6.09  | 109.94      | 100.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 450 | ASP  | CB-CG-OD1 | -6.07 | 112.83      | 118.30   |
| 1   | M     | 682 | THR  | CA-CB-CG2 | -6.07 | 103.90      | 112.40   |
| 2   | Q     | 141 | PRO  | N-CA-CB   | -6.07 | 95.92       | 102.60   |
| 1   | P     | 104 | TYR  | CB-CG-CD1 | -6.07 | 117.36      | 121.00   |
| 1   | A     | 779 | ARG  | NE-CZ-NH1 | 6.07  | 123.33      | 120.30   |
| 1   | P     | 625 | THR  | CA-CB-OG1 | 6.07  | 121.74      | 109.00   |
| 4   | 7     | 16  | LEU  | CA-CB-CG  | 6.07  | 129.26      | 115.30   |
| 2   | E     | 141 | PRO  | N-CA-CB   | -6.06 | 95.93       | 102.60   |
| 4   | 7     | 349 | LEU  | CA-C-N    | -6.06 | 103.86      | 117.20   |
| 4   | Z     | 349 | LEU  | CA-C-N    | -6.06 | 103.86      | 117.20   |
| 3   | C     | 58  | MET  | CG-SD-CE  | 6.06  | 109.89      | 100.20   |
| 4   | 5     | 349 | LEU  | CA-C-N    | -6.06 | 103.87      | 117.20   |
| 4   | 1     | 349 | LEU  | CA-C-N    | -6.06 | 103.88      | 117.20   |
| 1   | M     | 104 | TYR  | CB-CG-CD1 | -6.06 | 117.37      | 121.00   |
| 4   | 9     | 349 | LEU  | CA-C-N    | -6.06 | 103.88      | 117.20   |
| 4   | 0     | 349 | LEU  | CA-C-N    | -6.05 | 103.88      | 117.20   |
| 1   | G     | 625 | THR  | CA-CB-OG1 | 6.05  | 121.71      | 109.00   |
| 4   | W     | 16  | LEU  | CA-CB-CG  | 6.05  | 129.22      | 115.30   |
| 2   | H     | 129 | THR  | CA-CB-CG2 | 6.05  | 120.87      | 112.40   |
| 1   | J     | 752 | ASP  | CB-CG-OD2 | 6.05  | 123.75      | 118.30   |
| 2   | E     | 129 | THR  | CA-CB-CG2 | 6.05  | 120.87      | 112.40   |
| 1   | M     | 810 | ARG  | NE-CZ-NH1 | 6.05  | 123.33      | 120.30   |
| 1   | M     | 625 | THR  | CA-CB-OG1 | 6.05  | 121.70      | 109.00   |
| 1   | A     | 760 | PHE  | CB-CG-CD2 | -6.05 | 116.57      | 120.80   |
| 4   | 3     | 349 | LEU  | CA-C-N    | -6.05 | 103.90      | 117.20   |
| 4   | Y     | 349 | LEU  | CA-C-N    | -6.05 | 103.90      | 117.20   |
| 3   | I     | 58  | MET  | CG-SD-CE  | 6.04  | 109.87      | 100.20   |
| 4   | 4     | 349 | LEU  | CA-C-N    | -6.04 | 103.90      | 117.20   |
| 2   | B     | 141 | PRO  | N-CA-CB   | -6.04 | 95.95       | 102.60   |
| 4   | 2     | 349 | LEU  | CA-C-N    | -6.04 | 103.91      | 117.20   |
| 4   | V     | 16  | LEU  | CA-CB-CG  | 6.04  | 129.20      | 115.30   |
| 4   | 8     | 16  | LEU  | CA-CB-CG  | 6.04  | 129.19      | 115.30   |
| 4   | 2     | 16  | LEU  | CA-CB-CG  | 6.04  | 129.19      | 115.30   |
| 4   | X     | 16  | LEU  | CA-CB-CG  | 6.04  | 129.19      | 115.30   |
| 4   | Y     | 16  | LEU  | CA-CB-CG  | 6.04  | 129.19      | 115.30   |
| 1   | D     | 625 | THR  | CA-CB-OG1 | 6.04  | 121.68      | 109.00   |
| 4   | 3     | 16  | LEU  | CA-CB-CG  | 6.04  | 129.18      | 115.30   |
| 1   | A     | 682 | THR  | CA-CB-CG2 | -6.03 | 103.95      | 112.40   |
| 1   | A     | 447 | GLN  | N-CA-CB   | 6.03  | 121.46      | 110.60   |
| 1   | J     | 682 | THR  | CA-CB-CG2 | -6.03 | 103.95      | 112.40   |
| 4   | X     | 349 | LEU  | CA-C-N    | -6.03 | 103.93      | 117.20   |
| 1   | P     | 447 | GLN  | N-CA-CB   | 6.03  | 121.45      | 110.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | Z     | 16  | LEU  | CA-CB-CG  | 6.03  | 129.17      | 115.30   |
| 1   | J     | 447 | GLN  | N-CA-CB   | 6.03  | 121.45      | 110.60   |
| 4   | 1     | 16  | LEU  | CA-CB-CG  | 6.03  | 129.16      | 115.30   |
| 4   | 4     | 16  | LEU  | CA-CB-CG  | 6.03  | 129.16      | 115.30   |
| 4   | 5     | 16  | LEU  | CA-CB-CG  | 6.03  | 129.16      | 115.30   |
| 4   | 8     | 335 | ARG  | NE-CZ-NH2 | -6.03 | 117.29      | 120.30   |
| 4   | V     | 116 | ARG  | NE-CZ-NH1 | 6.03  | 123.31      | 120.30   |
| 1   | P     | 192 | VAL  | CA-CB-CG1 | -6.03 | 101.86      | 110.90   |
| 4   | 9     | 16  | LEU  | CA-CB-CG  | 6.03  | 129.16      | 115.30   |
| 4   | V     | 349 | LEU  | CA-C-N    | -6.03 | 103.94      | 117.20   |
| 4   | W     | 349 | LEU  | CA-C-N    | -6.03 | 103.94      | 117.20   |
| 2   | B     | 129 | THR  | CA-CB-CG2 | 6.02  | 120.83      | 112.40   |
| 4   | 0     | 16  | LEU  | CA-CB-CG  | 6.02  | 129.16      | 115.30   |
| 1   | D     | 779 | ARG  | NE-CZ-NH1 | 6.02  | 123.31      | 120.30   |
| 1   | M     | 447 | GLN  | N-CA-CB   | 6.02  | 121.44      | 110.60   |
| 1   | J     | 104 | TYR  | CB-CG-CD1 | -6.02 | 117.39      | 121.00   |
| 1   | D     | 682 | THR  | CA-CB-CG2 | -6.02 | 103.98      | 112.40   |
| 4   | 8     | 349 | LEU  | CA-C-N    | -6.01 | 103.97      | 117.20   |
| 1   | J     | 625 | THR  | CA-CB-OG1 | 6.01  | 121.61      | 109.00   |
| 1   | M     | 779 | ARG  | NE-CZ-NH1 | 6.01  | 123.30      | 120.30   |
| 1   | D     | 463 | ASP  | CB-CG-OD2 | -6.00 | 112.90      | 118.30   |
| 1   | G     | 682 | THR  | CA-CB-CG2 | -6.00 | 103.99      | 112.40   |
| 1   | A     | 625 | THR  | CA-CB-OG1 | 6.00  | 121.60      | 109.00   |
| 1   | M     | 192 | VAL  | CA-CB-CG1 | -6.00 | 101.90      | 110.90   |
| 1   | D     | 754 | ASP  | CB-CG-OD2 | -6.00 | 112.90      | 118.30   |
| 1   | J     | 590 | TYR  | CB-CG-CD2 | 6.00  | 124.60      | 121.00   |
| 2   | K     | 129 | THR  | CA-CB-CG2 | 6.00  | 120.80      | 112.40   |
| 2   | Q     | 129 | THR  | CA-CB-CG2 | 6.00  | 120.80      | 112.40   |
| 4   | 9     | 335 | ARG  | NE-CZ-NH2 | -6.00 | 117.30      | 120.30   |
| 1   | A     | 104 | TYR  | CB-CG-CD1 | -6.00 | 117.40      | 121.00   |
| 4   | X     | 116 | ARG  | NE-CZ-NH1 | 5.99  | 123.30      | 120.30   |
| 4   | Z     | 254 | ARG  | NE-CZ-NH1 | 5.99  | 123.30      | 120.30   |
| 4   | V     | 335 | ARG  | NE-CZ-NH2 | -5.99 | 117.31      | 120.30   |
| 1   | D     | 378 | ASP  | CB-CG-OD1 | -5.99 | 112.91      | 118.30   |
| 1   | G     | 192 | VAL  | CA-CB-CG1 | -5.99 | 101.92      | 110.90   |
| 1   | A     | 590 | TYR  | CB-CG-CD2 | 5.98  | 124.59      | 121.00   |
| 1   | D     | 780 | ASP  | CB-CG-OD2 | 5.98  | 123.68      | 118.30   |
| 1   | G     | 447 | GLN  | N-CA-CB   | 5.98  | 121.36      | 110.60   |
| 1   | J     | 665 | ARG  | NE-CZ-NH2 | -5.97 | 117.31      | 120.30   |
| 1   | M     | 450 | ASP  | CB-CG-OD1 | -5.97 | 112.92      | 118.30   |
| 1   | G     | 760 | PHE  | CB-CG-CD2 | -5.97 | 116.62      | 120.80   |
| 1   | J     | 192 | VAL  | CA-CB-CG1 | -5.97 | 101.94      | 110.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 346 | ASP  | CB-CG-OD1  | 5.97  | 123.67      | 118.30   |
| 1   | J     | 346 | ASP  | CB-CG-OD1  | 5.97  | 123.67      | 118.30   |
| 1   | D     | 450 | ASP  | CB-CG-OD1  | -5.97 | 112.93      | 118.30   |
| 1   | D     | 192 | VAL  | CA-CB-CG1  | -5.96 | 101.96      | 110.90   |
| 1   | J     | 754 | ASP  | CB-CG-OD2  | -5.96 | 112.94      | 118.30   |
| 4   | 5     | 335 | ARG  | NE-CZ-NH2  | -5.96 | 117.32      | 120.30   |
| 1   | A     | 192 | VAL  | CA-CB-CG1  | -5.96 | 101.97      | 110.90   |
| 1   | D     | 447 | GLN  | N-CA-CB    | 5.95  | 121.31      | 110.60   |
| 1   | P     | 809 | ARG  | NE-CZ-NH2  | -5.95 | 117.33      | 120.30   |
| 4   | 4     | 335 | ARG  | NE-CZ-NH2  | -5.95 | 117.32      | 120.30   |
| 4   | W     | 79  | TRP  | CG-CD2-CE3 | 5.95  | 139.25      | 133.90   |
| 1   | A     | 754 | ASP  | CB-CG-OD2  | -5.93 | 112.96      | 118.30   |
| 1   | G     | 754 | ASP  | CB-CG-OD2  | -5.93 | 112.96      | 118.30   |
| 1   | G     | 780 | ASP  | CB-CG-OD2  | 5.93  | 123.64      | 118.30   |
| 1   | M     | 780 | ASP  | CB-CG-OD2  | 5.93  | 123.64      | 118.30   |
| 4   | Z     | 79  | TRP  | CG-CD2-CE3 | 5.93  | 139.24      | 133.90   |
| 1   | D     | 339 | ASP  | CB-CG-OD2  | 5.93  | 123.63      | 118.30   |
| 4   | X     | 335 | ARG  | NE-CZ-NH2  | -5.93 | 117.34      | 120.30   |
| 1   | D     | 738 | MET  | CG-SD-CE   | 5.92  | 109.68      | 100.20   |
| 1   | G     | 779 | ARG  | NE-CZ-NH1  | 5.92  | 123.26      | 120.30   |
| 1   | P     | 754 | ASP  | CB-CG-OD2  | -5.92 | 112.97      | 118.30   |
| 4   | 8     | 79  | TRP  | CG-CD2-CE3 | 5.92  | 139.22      | 133.90   |
| 4   | X     | 254 | ARG  | NE-CZ-NH1  | 5.91  | 123.26      | 120.30   |
| 1   | P     | 378 | ASP  | CB-CG-OD1  | -5.91 | 112.98      | 118.30   |
| 1   | J     | 378 | ASP  | CB-CG-OD1  | -5.91 | 112.98      | 118.30   |
| 1   | M     | 378 | ASP  | CB-CG-OD1  | -5.91 | 112.98      | 118.30   |
| 1   | G     | 378 | ASP  | CB-CG-OD1  | -5.90 | 112.99      | 118.30   |
| 4   | 1     | 335 | ARG  | NE-CZ-NH2  | -5.90 | 117.35      | 120.30   |
| 1   | P     | 738 | MET  | CG-SD-CE   | 5.90  | 109.64      | 100.20   |
| 1   | P     | 780 | ASP  | CB-CG-OD2  | 5.90  | 123.61      | 118.30   |
| 1   | A     | 815 | CYS  | CA-CB-SG   | -5.89 | 103.39      | 114.00   |
| 1   | G     | 339 | ASP  | CB-CG-OD2  | 5.89  | 123.60      | 118.30   |
| 2   | N     | 129 | THR  | CA-CB-CG2  | 5.89  | 120.65      | 112.40   |
| 4   | 4     | 79  | TRP  | CG-CD2-CE3 | 5.89  | 139.20      | 133.90   |
| 4   | 7     | 200 | PHE  | CA-C-N     | -5.89 | 104.24      | 117.20   |
| 4   | 1     | 79  | TRP  | CG-CD2-CE3 | 5.89  | 139.20      | 133.90   |
| 1   | G     | 752 | ASP  | CB-CG-OD2  | 5.89  | 123.60      | 118.30   |
| 1   | A     | 450 | ASP  | CB-CG-OD1  | -5.88 | 113.00      | 118.30   |
| 4   | 7     | 79  | TRP  | CG-CD2-CE3 | 5.88  | 139.20      | 133.90   |
| 1   | M     | 665 | ARG  | NE-CZ-NH2  | -5.88 | 117.36      | 120.30   |
| 4   | 2     | 200 | PHE  | CA-C-N     | -5.88 | 104.26      | 117.20   |
| 4   | 7     | 116 | ARG  | NE-CZ-NH1  | 5.88  | 123.24      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | W     | 200 | PHE  | CA-C-N     | -5.88 | 104.26      | 117.20   |
| 4   | Y     | 116 | ARG  | NE-CZ-NH1  | 5.88  | 123.24      | 120.30   |
| 4   | 3     | 200 | PHE  | CA-C-N     | -5.88 | 104.27      | 117.20   |
| 1   | A     | 378 | ASP  | CB-CG-OD1  | -5.87 | 113.01      | 118.30   |
| 1   | G     | 665 | ARG  | NE-CZ-NH2  | -5.87 | 117.37      | 120.30   |
| 1   | G     | 809 | ARG  | NE-CZ-NH2  | -5.87 | 117.36      | 120.30   |
| 4   | 3     | 116 | ARG  | NE-CZ-NH1  | 5.87  | 123.23      | 120.30   |
| 4   | Z     | 116 | ARG  | NE-CZ-NH1  | 5.87  | 123.23      | 120.30   |
| 4   | 4     | 200 | PHE  | CA-C-N     | -5.87 | 104.29      | 117.20   |
| 1   | A     | 738 | MET  | CG-SD-CE   | 5.86  | 109.58      | 100.20   |
| 4   | 0     | 200 | PHE  | CA-C-N     | -5.86 | 104.31      | 117.20   |
| 1   | G     | 738 | MET  | CG-SD-CE   | 5.86  | 109.58      | 100.20   |
| 1   | J     | 780 | ASP  | CB-CG-OD2  | 5.86  | 123.57      | 118.30   |
| 1   | P     | 665 | ARG  | NE-CZ-NH2  | -5.86 | 117.37      | 120.30   |
| 4   | 3     | 79  | TRP  | CG-CD2-CE3 | 5.86  | 139.17      | 133.90   |
| 4   | Y     | 335 | ARG  | NE-CZ-NH2  | -5.86 | 117.37      | 120.30   |
| 1   | G     | 450 | ASP  | CB-CG-OD1  | -5.86 | 113.03      | 118.30   |
| 4   | 9     | 200 | PHE  | CA-C-N     | -5.85 | 104.32      | 117.20   |
| 1   | D     | 471 | ASP  | CB-CG-OD1  | -5.85 | 113.03      | 118.30   |
| 4   | 1     | 200 | PHE  | CA-C-N     | -5.85 | 104.33      | 117.20   |
| 4   | 2     | 335 | ARG  | NE-CZ-NH2  | -5.85 | 117.37      | 120.30   |
| 4   | 8     | 200 | PHE  | CA-C-N     | -5.85 | 104.32      | 117.20   |
| 4   | Y     | 200 | PHE  | CA-C-N     | -5.85 | 104.33      | 117.20   |
| 1   | D     | 4   | ASP  | CB-CG-OD2  | 5.85  | 123.57      | 118.30   |
| 4   | X     | 200 | PHE  | CA-C-N     | -5.85 | 104.33      | 117.20   |
| 1   | A     | 752 | ASP  | CB-CG-OD2  | 5.85  | 123.56      | 118.30   |
| 1   | M     | 339 | ASP  | CB-CG-OD2  | 5.85  | 123.56      | 118.30   |
| 4   | Y     | 79  | TRP  | CG-CD2-CE3 | 5.85  | 139.16      | 133.90   |
| 1   | J     | 738 | MET  | CG-SD-CE   | 5.85  | 109.56      | 100.20   |
| 4   | Z     | 200 | PHE  | CA-C-N     | -5.85 | 104.34      | 117.20   |
| 1   | A     | 665 | ARG  | NE-CZ-NH2  | -5.85 | 117.38      | 120.30   |
| 4   | 0     | 79  | TRP  | CG-CD2-CE3 | 5.84  | 139.16      | 133.90   |
| 4   | 9     | 79  | TRP  | CG-CD2-CE3 | 5.84  | 139.16      | 133.90   |
| 1   | P     | 339 | ASP  | CB-CG-OD2  | 5.84  | 123.56      | 118.30   |
| 4   | 5     | 200 | PHE  | CA-C-N     | -5.84 | 104.35      | 117.20   |
| 4   | Z     | 335 | ARG  | NE-CZ-NH2  | -5.84 | 117.38      | 120.30   |
| 1   | P     | 815 | CYS  | CA-CB-SG   | -5.84 | 103.49      | 114.00   |
| 4   | V     | 200 | PHE  | CA-C-N     | -5.84 | 104.36      | 117.20   |
| 1   | J     | 815 | CYS  | CA-CB-SG   | -5.83 | 103.50      | 114.00   |
| 1   | M     | 754 | ASP  | CB-CG-OD2  | -5.83 | 113.05      | 118.30   |
| 4   | 5     | 79  | TRP  | CG-CD2-CE3 | 5.83  | 139.15      | 133.90   |
| 4   | 2     | 79  | TRP  | CG-CD2-CE3 | 5.83  | 139.15      | 133.90   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 9     | 254 | ARG  | NE-CZ-NH1  | 5.83  | 123.22      | 120.30   |
| 1   | J     | 471 | ASP  | CB-CG-OD1  | -5.83 | 113.05      | 118.30   |
| 1   | M     | 738 | MET  | CG-SD-CE   | 5.83  | 109.53      | 100.20   |
| 1   | D     | 556 | ASP  | CB-CG-OD1  | -5.83 | 113.06      | 118.30   |
| 4   | 1     | 254 | ARG  | NE-CZ-NH1  | 5.83  | 123.21      | 120.30   |
| 1   | P     | 346 | ASP  | CB-CG-OD1  | 5.82  | 123.54      | 118.30   |
| 1   | J     | 556 | ASP  | CB-CG-OD1  | -5.82 | 113.06      | 118.30   |
| 1   | D     | 752 | ASP  | CB-CG-OD2  | 5.82  | 123.54      | 118.30   |
| 1   | A     | 780 | ASP  | CB-CG-OD1  | -5.82 | 113.07      | 118.30   |
| 1   | G     | 556 | ASP  | CB-CG-OD1  | -5.82 | 113.07      | 118.30   |
| 4   | 0     | 95  | ARG  | CA-CB-CG   | 5.82  | 126.19      | 113.40   |
| 1   | P     | 556 | ASP  | CB-CG-OD1  | -5.81 | 113.07      | 118.30   |
| 4   | 9     | 116 | ARG  | NE-CZ-NH1  | 5.81  | 123.21      | 120.30   |
| 4   | 0     | 335 | ARG  | NE-CZ-NH2  | -5.81 | 117.40      | 120.30   |
| 4   | 4     | 95  | ARG  | CA-CB-CG   | 5.81  | 126.18      | 113.40   |
| 4   | V     | 95  | ARG  | CA-CB-CG   | 5.80  | 126.17      | 113.40   |
| 1   | M     | 815 | CYS  | CA-CB-SG   | -5.80 | 103.56      | 114.00   |
| 4   | Y     | 95  | ARG  | CA-CB-CG   | 5.80  | 126.16      | 113.40   |
| 1   | M     | 471 | ASP  | CB-CG-OD1  | -5.80 | 113.08      | 118.30   |
| 4   | 1     | 116 | ARG  | NE-CZ-NH1  | 5.80  | 123.20      | 120.30   |
| 1   | M     | 346 | ASP  | CB-CG-OD1  | 5.80  | 123.52      | 118.30   |
| 4   | X     | 79  | TRP  | CG-CD2-CE3 | 5.80  | 139.12      | 133.90   |
| 4   | 5     | 95  | ARG  | CA-CB-CG   | 5.79  | 126.15      | 113.40   |
| 4   | V     | 79  | TRP  | CG-CD2-CE3 | 5.79  | 139.12      | 133.90   |
| 4   | 3     | 335 | ARG  | NE-CZ-NH2  | -5.79 | 117.41      | 120.30   |
| 4   | 0     | 116 | ARG  | NE-CZ-NH1  | 5.79  | 123.19      | 120.30   |
| 4   | Z     | 95  | ARG  | CA-CB-CG   | 5.79  | 126.14      | 113.40   |
| 1   | P     | 471 | ASP  | CB-CG-OD1  | -5.79 | 113.09      | 118.30   |
| 1   | D     | 815 | CYS  | CA-CB-SG   | -5.78 | 103.59      | 114.00   |
| 1   | G     | 780 | ASP  | CB-CG-OD1  | -5.78 | 113.09      | 118.30   |
| 1   | M     | 556 | ASP  | CB-CG-OD1  | -5.78 | 113.09      | 118.30   |
| 4   | X     | 95  | ARG  | CA-CB-CG   | 5.78  | 126.11      | 113.40   |
| 4   | W     | 116 | ARG  | NE-CZ-NH1  | 5.78  | 123.19      | 120.30   |
| 4   | 1     | 95  | ARG  | CA-CB-CG   | 5.78  | 126.11      | 113.40   |
| 4   | 7     | 335 | ARG  | NE-CZ-NH2  | -5.77 | 117.41      | 120.30   |
| 4   | 9     | 95  | ARG  | CA-CB-CG   | 5.77  | 126.10      | 113.40   |
| 4   | 2     | 95  | ARG  | CA-CB-CG   | 5.77  | 126.10      | 113.40   |
| 4   | 7     | 95  | ARG  | CA-CB-CG   | 5.77  | 126.10      | 113.40   |
| 4   | 8     | 95  | ARG  | CA-CB-CG   | 5.77  | 126.10      | 113.40   |
| 4   | 3     | 95  | ARG  | CA-CB-CG   | 5.77  | 126.09      | 113.40   |
| 4   | 3     | 254 | ARG  | NE-CZ-NH1  | 5.76  | 123.18      | 120.30   |
| 1   | J     | 339 | ASP  | CB-CG-OD2  | 5.76  | 123.49      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | W     | 95  | ARG  | CA-CB-CG  | 5.76  | 126.08      | 113.40   |
| 1   | D     | 809 | ARG  | NE-CZ-NH2 | -5.76 | 117.42      | 120.30   |
| 1   | A     | 471 | ASP  | CB-CG-OD1 | -5.76 | 113.12      | 118.30   |
| 1   | A     | 339 | ASP  | CB-CG-OD2 | 5.76  | 123.48      | 118.30   |
| 4   | W     | 254 | ARG  | NE-CZ-NH1 | 5.76  | 123.18      | 120.30   |
| 1   | G     | 471 | ASP  | CB-CG-OD1 | -5.75 | 113.12      | 118.30   |
| 4   | 4     | 254 | ARG  | NE-CZ-NH1 | 5.75  | 123.18      | 120.30   |
| 4   | 4     | 116 | ARG  | NE-CZ-NH1 | 5.75  | 123.17      | 120.30   |
| 1   | P     | 4   | ASP  | CB-CG-OD2 | 5.75  | 123.47      | 118.30   |
| 1   | A     | 556 | ASP  | CB-CG-OD1 | -5.74 | 113.13      | 118.30   |
| 2   | H     | 149 | ASP  | N-CA-CB   | 5.74  | 120.94      | 110.60   |
| 1   | D     | 665 | ARG  | NE-CZ-NH2 | -5.74 | 117.43      | 120.30   |
| 4   | 5     | 335 | ARG  | CA-CB-CG  | 5.74  | 126.03      | 113.40   |
| 4   | 5     | 116 | ARG  | NE-CZ-NH1 | 5.74  | 123.17      | 120.30   |
| 1   | D     | 352 | TYR  | N-CA-CB   | 5.74  | 120.92      | 110.60   |
| 1   | J     | 4   | ASP  | CB-CG-OD2 | 5.74  | 123.46      | 118.30   |
| 4   | 2     | 116 | ARG  | NE-CZ-NH1 | 5.74  | 123.17      | 120.30   |
| 1   | G     | 4   | ASP  | CB-CG-OD2 | 5.73  | 123.46      | 118.30   |
| 4   | 7     | 254 | ARG  | NE-CZ-NH1 | 5.73  | 123.17      | 120.30   |
| 4   | V     | 254 | ARG  | NE-CZ-NH1 | 5.73  | 123.17      | 120.30   |
| 1   | A     | 346 | ASP  | CB-CG-OD1 | 5.73  | 123.46      | 118.30   |
| 4   | 2     | 254 | ARG  | NE-CZ-NH1 | 5.73  | 123.16      | 120.30   |
| 1   | A     | 4   | ASP  | CB-CG-OD2 | 5.72  | 123.45      | 118.30   |
| 1   | P     | 165 | PHE  | N-CA-CB   | -5.72 | 100.30      | 110.60   |
| 4   | W     | 335 | ARG  | NE-CZ-NH2 | -5.72 | 117.44      | 120.30   |
| 2   | B     | 149 | ASP  | N-CA-CB   | 5.72  | 120.90      | 110.60   |
| 4   | 4     | 335 | ARG  | CA-CB-CG  | 5.72  | 125.98      | 113.40   |
| 1   | J     | 165 | PHE  | N-CA-CB   | -5.72 | 100.31      | 110.60   |
| 4   | 5     | 254 | ARG  | NE-CZ-NH1 | 5.72  | 123.16      | 120.30   |
| 4   | Y     | 335 | ARG  | CA-CB-CG  | 5.71  | 125.97      | 113.40   |
| 4   | 8     | 254 | ARG  | NE-CZ-NH1 | 5.71  | 123.15      | 120.30   |
| 4   | X     | 335 | ARG  | CA-CB-CG  | 5.71  | 125.96      | 113.40   |
| 1   | G     | 165 | PHE  | N-CA-CB   | -5.70 | 100.33      | 110.60   |
| 2   | N     | 149 | ASP  | N-CA-CB   | 5.70  | 120.86      | 110.60   |
| 4   | Z     | 335 | ARG  | CA-CB-CG  | 5.70  | 125.95      | 113.40   |
| 4   | 2     | 335 | ARG  | CA-CB-CG  | 5.70  | 125.94      | 113.40   |
| 4   | 3     | 335 | ARG  | CA-CB-CG  | 5.70  | 125.94      | 113.40   |
| 4   | V     | 335 | ARG  | CA-CB-CG  | 5.70  | 125.94      | 113.40   |
| 4   | 8     | 335 | ARG  | CA-CB-CG  | 5.70  | 125.94      | 113.40   |
| 1   | D     | 781 | ASP  | CB-CG-OD2 | 5.70  | 123.43      | 118.30   |
| 4   | 0     | 335 | ARG  | CA-CB-CG  | 5.70  | 125.93      | 113.40   |
| 4   | 1     | 335 | ARG  | CA-CB-CG  | 5.70  | 125.93      | 113.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | W     | 335 | ARG  | CA-CB-CG   | 5.70  | 125.93      | 113.40   |
| 4   | 8     | 116 | ARG  | NE-CZ-NH1  | 5.70  | 123.15      | 120.30   |
| 4   | 7     | 335 | ARG  | CA-CB-CG   | 5.69  | 125.93      | 113.40   |
| 1   | D     | 780 | ASP  | CB-CG-OD1  | -5.69 | 113.18      | 118.30   |
| 1   | M     | 165 | PHE  | N-CA-CB    | -5.69 | 100.35      | 110.60   |
| 2   | Q     | 149 | ASP  | N-CA-CB    | 5.69  | 120.85      | 110.60   |
| 4   | 9     | 335 | ARG  | CA-CB-CG   | 5.69  | 125.92      | 113.40   |
| 1   | G     | 815 | CYS  | CA-CB-SG   | -5.68 | 103.77      | 114.00   |
| 1   | A     | 165 | PHE  | N-CA-CB    | -5.68 | 100.37      | 110.60   |
| 1   | D     | 165 | PHE  | N-CA-CB    | -5.68 | 100.37      | 110.60   |
| 4   | 0     | 254 | ARG  | NE-CZ-NH1  | 5.68  | 123.14      | 120.30   |
| 4   | Y     | 254 | ARG  | NE-CZ-NH1  | 5.68  | 123.14      | 120.30   |
| 1   | G     | 352 | TYR  | N-CA-CB    | 5.68  | 120.82      | 110.60   |
| 2   | K     | 149 | ASP  | N-CA-CB    | 5.67  | 120.81      | 110.60   |
| 1   | J     | 809 | ARG  | NE-CZ-NH2  | -5.67 | 117.47      | 120.30   |
| 1   | M     | 780 | ASP  | CB-CG-OD1  | -5.66 | 113.20      | 118.30   |
| 1   | G     | 781 | ASP  | CB-CG-OD2  | 5.65  | 123.38      | 118.30   |
| 1   | P     | 780 | ASP  | CB-CG-OD1  | -5.65 | 113.22      | 118.30   |
| 1   | J     | 693 | HIS  | CA-CB-CG   | -5.64 | 104.01      | 113.60   |
| 1   | G     | 785 | GLU  | O-C-N      | 5.64  | 131.72      | 122.70   |
| 1   | G     | 693 | HIS  | CA-CB-CG   | -5.63 | 104.02      | 113.60   |
| 1   | M     | 693 | HIS  | CA-CB-CG   | -5.63 | 104.02      | 113.60   |
| 2   | E     | 149 | ASP  | N-CA-CB    | 5.63  | 120.74      | 110.60   |
| 1   | P     | 33  | ASP  | CB-CG-OD2  | 5.63  | 123.37      | 118.30   |
| 1   | M     | 4   | ASP  | CB-CG-OD2  | 5.62  | 123.36      | 118.30   |
| 1   | J     | 780 | ASP  | CB-CG-OD1  | -5.62 | 113.24      | 118.30   |
| 4   | Y     | 113 | LYS  | CA-CB-CG   | 5.61  | 125.74      | 113.40   |
| 1   | P     | 352 | TYR  | N-CA-CB    | 5.61  | 120.69      | 110.60   |
| 4   | Z     | 356 | TRP  | CG-CD2-CE3 | 5.61  | 138.95      | 133.90   |
| 1   | J     | 352 | TYR  | N-CA-CB    | 5.60  | 120.68      | 110.60   |
| 1   | M     | 686 | MET  | N-CA-CB    | -5.60 | 100.52      | 110.60   |
| 4   | 3     | 279 | TYR  | CB-CG-CD2  | -5.60 | 117.64      | 121.00   |
| 4   | 7     | 279 | TYR  | CB-CG-CD2  | -5.60 | 117.64      | 121.00   |
| 1   | D     | 693 | HIS  | CA-CB-CG   | -5.60 | 104.09      | 113.60   |
| 4   | 0     | 294 | TYR  | CB-CG-CD2  | -5.60 | 117.64      | 121.00   |
| 4   | 2     | 279 | TYR  | CB-CG-CD2  | -5.60 | 117.64      | 121.00   |
| 4   | 2     | 356 | TRP  | CG-CD2-CE3 | 5.59  | 138.94      | 133.90   |
| 1   | P     | 693 | HIS  | CA-CB-CG   | -5.59 | 104.09      | 113.60   |
| 4   | 2     | 113 | LYS  | CA-CB-CG   | 5.59  | 125.70      | 113.40   |
| 4   | V     | 113 | LYS  | CA-CB-CG   | 5.59  | 125.70      | 113.40   |
| 1   | A     | 809 | ARG  | NE-CZ-NH2  | -5.59 | 117.50      | 120.30   |
| 4   | 9     | 294 | TYR  | CB-CG-CD2  | -5.59 | 117.65      | 121.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | Z     | 254 | ARG  | N-CA-CB    | -5.59 | 100.54      | 110.60   |
| 1   | M     | 809 | ARG  | NE-CZ-NH2  | -5.59 | 117.51      | 120.30   |
| 1   | A     | 352 | TYR  | N-CA-CB    | 5.59  | 120.66      | 110.60   |
| 4   | 3     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.68      | 113.40   |
| 4   | 1     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.68      | 113.40   |
| 4   | W     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.68      | 113.40   |
| 4   | Z     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.68      | 113.40   |
| 4   | 4     | 294 | TYR  | CB-CG-CD2  | -5.58 | 117.65      | 121.00   |
| 4   | X     | 113 | LYS  | CA-CB-CG   | 5.58  | 125.67      | 113.40   |
| 1   | A     | 781 | ASP  | CB-CG-OD2  | 5.58  | 123.32      | 118.30   |
| 1   | D     | 723 | ARG  | NE-CZ-NH1  | 5.57  | 123.09      | 120.30   |
| 4   | 0     | 113 | LYS  | CA-CB-CG   | 5.57  | 125.66      | 113.40   |
| 4   | 5     | 294 | TYR  | CB-CG-CD2  | -5.57 | 117.66      | 121.00   |
| 4   | 9     | 356 | TRP  | CG-CD2-CE3 | 5.57  | 138.92      | 133.90   |
| 4   | V     | 254 | ARG  | N-CA-CB    | -5.57 | 100.58      | 110.60   |
| 4   | 8     | 113 | LYS  | CA-CB-CG   | 5.57  | 125.64      | 113.40   |
| 4   | 1     | 11  | ASP  | CB-CG-OD1  | 5.56  | 123.31      | 118.30   |
| 4   | X     | 294 | TYR  | CB-CG-CD2  | -5.56 | 117.66      | 121.00   |
| 1   | D     | 306 | THR  | CA-CB-CG2  | -5.56 | 104.62      | 112.40   |
| 4   | 5     | 113 | LYS  | CA-CB-CG   | 5.56  | 125.63      | 113.40   |
| 1   | M     | 352 | TYR  | N-CA-CB    | 5.56  | 120.60      | 110.60   |
| 4   | 9     | 113 | LYS  | CA-CB-CG   | 5.56  | 125.63      | 113.40   |
| 4   | W     | 254 | ARG  | N-CA-CB    | -5.56 | 100.60      | 110.60   |
| 4   | 7     | 113 | LYS  | CA-CB-CG   | 5.55  | 125.62      | 113.40   |
| 4   | 7     | 294 | TYR  | CB-CG-CD2  | -5.55 | 117.67      | 121.00   |
| 1   | J     | 686 | MET  | N-CA-CB    | -5.55 | 100.61      | 110.60   |
| 1   | A     | 693 | HIS  | CA-CB-CG   | -5.55 | 104.17      | 113.60   |
| 4   | 7     | 356 | TRP  | CG-CD2-CE3 | 5.55  | 138.89      | 133.90   |
| 1   | M     | 33  | ASP  | CB-CG-OD2  | 5.55  | 123.29      | 118.30   |
| 4   | 4     | 113 | LYS  | CA-CB-CG   | 5.55  | 125.60      | 113.40   |
| 1   | D     | 752 | ASP  | CB-CA-C    | 5.54  | 121.49      | 110.40   |
| 1   | G     | 320 | ILE  | CB-CA-C    | -5.54 | 100.51      | 111.60   |
| 4   | 1     | 279 | TYR  | CB-CG-CD2  | -5.54 | 117.67      | 121.00   |
| 4   | X     | 11  | ASP  | CB-CG-OD1  | 5.54  | 123.29      | 118.30   |
| 1   | A     | 752 | ASP  | CB-CA-C    | 5.54  | 121.48      | 110.40   |
| 4   | 1     | 356 | TRP  | CG-CD2-CE3 | 5.54  | 138.89      | 133.90   |
| 4   | 1     | 294 | TYR  | CB-CG-CD2  | -5.54 | 117.68      | 121.00   |
| 4   | 2     | 294 | TYR  | CB-CG-CD2  | -5.54 | 117.68      | 121.00   |
| 4   | 0     | 254 | ARG  | N-CA-CB    | -5.54 | 100.63      | 110.60   |
| 4   | V     | 279 | TYR  | CB-CG-CD2  | -5.54 | 117.68      | 121.00   |
| 4   | 7     | 254 | ARG  | N-CA-CB    | -5.54 | 100.63      | 110.60   |
| 4   | 5     | 254 | ARG  | N-CA-CB    | -5.54 | 100.64      | 110.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 5     | 356 | TRP  | CG-CD2-CE3 | 5.54  | 138.88      | 133.90   |
| 1   | P     | 686 | MET  | N-CA-CB    | -5.53 | 100.64      | 110.60   |
| 1   | P     | 320 | ILE  | CB-CA-C    | -5.53 | 100.54      | 111.60   |
| 4   | 9     | 254 | ARG  | N-CA-CB    | -5.53 | 100.65      | 110.60   |
| 1   | D     | 384 | ASP  | CB-CG-OD1  | -5.53 | 113.33      | 118.30   |
| 4   | 3     | 254 | ARG  | N-CA-CB    | -5.53 | 100.65      | 110.60   |
| 4   | 8     | 254 | ARG  | N-CA-CB    | -5.53 | 100.65      | 110.60   |
| 4   | 8     | 294 | TYR  | CB-CG-CD2  | -5.53 | 117.68      | 121.00   |
| 4   | Y     | 279 | TYR  | CB-CG-CD2  | -5.53 | 117.68      | 121.00   |
| 4   | 8     | 356 | TRP  | CG-CD2-CE3 | 5.53  | 138.87      | 133.90   |
| 4   | Y     | 254 | ARG  | N-CA-CB    | -5.52 | 100.66      | 110.60   |
| 1   | J     | 752 | ASP  | CB-CA-C    | 5.52  | 121.44      | 110.40   |
| 4   | X     | 254 | ARG  | N-CA-CB    | -5.52 | 100.66      | 110.60   |
| 4   | 0     | 356 | TRP  | CG-CD2-CE3 | 5.52  | 138.87      | 133.90   |
| 4   | 8     | 279 | TYR  | CB-CG-CD2  | -5.52 | 117.69      | 121.00   |
| 1   | D     | 686 | MET  | N-CA-CB    | -5.52 | 100.67      | 110.60   |
| 4   | 8     | 11  | ASP  | CB-CG-OD1  | 5.52  | 123.27      | 118.30   |
| 1   | J     | 781 | ASP  | CB-CG-OD2  | 5.52  | 123.26      | 118.30   |
| 4   | W     | 294 | TYR  | CB-CG-CD2  | -5.52 | 117.69      | 121.00   |
| 1   | G     | 752 | ASP  | CB-CA-C    | 5.51  | 121.43      | 110.40   |
| 1   | P     | 752 | ASP  | CB-CA-C    | 5.51  | 121.43      | 110.40   |
| 4   | 1     | 254 | ARG  | N-CA-CB    | -5.51 | 100.68      | 110.60   |
| 1   | G     | 686 | MET  | N-CA-CB    | -5.51 | 100.69      | 110.60   |
| 1   | P     | 781 | ASP  | CB-CG-OD2  | 5.51  | 123.26      | 118.30   |
| 1   | A     | 241 | ASP  | CB-CG-OD2  | 5.51  | 123.26      | 118.30   |
| 1   | G     | 306 | THR  | CA-CB-CG2  | -5.51 | 104.69      | 112.40   |
| 4   | 2     | 147 | ARG  | NE-CZ-NH2  | -5.51 | 117.55      | 120.30   |
| 4   | 0     | 279 | TYR  | CB-CG-CD2  | -5.50 | 117.70      | 121.00   |
| 4   | V     | 294 | TYR  | CB-CG-CD2  | -5.50 | 117.70      | 121.00   |
| 1   | G     | 723 | ARG  | NE-CZ-NH1  | 5.50  | 123.05      | 120.30   |
| 1   | M     | 326 | ASP  | CB-CG-OD2  | 5.50  | 123.25      | 118.30   |
| 4   | 2     | 254 | ARG  | N-CA-CB    | -5.50 | 100.71      | 110.60   |
| 1   | M     | 547 | ASP  | CB-CG-OD2  | 5.50  | 123.25      | 118.30   |
| 1   | M     | 752 | ASP  | CB-CA-C    | 5.50  | 121.39      | 110.40   |
| 4   | X     | 356 | TRP  | CG-CD2-CE3 | 5.50  | 138.84      | 133.90   |
| 1   | A     | 686 | MET  | N-CA-CB    | -5.49 | 100.72      | 110.60   |
| 1   | M     | 781 | ASP  | CB-CG-OD2  | 5.49  | 123.24      | 118.30   |
| 1   | M     | 320 | ILE  | CB-CA-C    | -5.49 | 100.63      | 111.60   |
| 4   | 4     | 254 | ARG  | N-CA-CB    | -5.49 | 100.73      | 110.60   |
| 4   | X     | 279 | TYR  | CB-CG-CD2  | -5.49 | 117.71      | 121.00   |
| 1   | J     | 320 | ILE  | CB-CA-C    | -5.48 | 100.64      | 111.60   |
| 1   | D     | 33  | ASP  | CB-CG-OD2  | 5.48  | 123.23      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 33  | ASP  | CB-CG-OD2  | 5.47  | 123.23      | 118.30   |
| 1   | A     | 306 | THR  | CA-CB-CG2  | -5.47 | 104.73      | 112.40   |
| 4   | Y     | 294 | TYR  | CB-CG-CD2  | -5.47 | 117.72      | 121.00   |
| 1   | J     | 33  | ASP  | CB-CG-OD2  | 5.47  | 123.22      | 118.30   |
| 4   | 7     | 11  | ASP  | CB-CG-OD1  | 5.47  | 123.22      | 118.30   |
| 1   | D     | 326 | ASP  | CB-CG-OD2  | 5.47  | 123.22      | 118.30   |
| 4   | 7     | 79  | TRP  | CB-CG-CD1  | -5.47 | 119.89      | 127.00   |
| 4   | 9     | 279 | TYR  | CB-CG-CD2  | -5.47 | 117.72      | 121.00   |
| 1   | A     | 320 | ILE  | CB-CA-C    | -5.46 | 100.67      | 111.60   |
| 4   | V     | 356 | TRP  | CG-CD2-CE3 | 5.46  | 138.81      | 133.90   |
| 4   | W     | 356 | TRP  | CG-CD2-CE3 | 5.46  | 138.81      | 133.90   |
| 4   | 2     | 11  | ASP  | CB-CG-OD1  | 5.46  | 123.21      | 118.30   |
| 4   | 4     | 11  | ASP  | CB-CG-OD1  | 5.46  | 123.21      | 118.30   |
| 1   | P     | 547 | ASP  | CB-CG-OD2  | 5.45  | 123.21      | 118.30   |
| 4   | 3     | 356 | TRP  | CG-CD2-CE3 | 5.45  | 138.81      | 133.90   |
| 4   | V     | 335 | ARG  | NE-CZ-NH1  | 5.45  | 123.03      | 120.30   |
| 1   | D     | 320 | ILE  | CB-CA-C    | -5.45 | 100.70      | 111.60   |
| 1   | J     | 326 | ASP  | CB-CG-OD2  | 5.45  | 123.21      | 118.30   |
| 4   | 4     | 279 | TYR  | CB-CG-CD2  | -5.45 | 117.73      | 121.00   |
| 4   | V     | 147 | ARG  | NE-CZ-NH2  | -5.45 | 117.58      | 120.30   |
| 4   | Y     | 356 | TRP  | CG-CD2-CE3 | 5.45  | 138.80      | 133.90   |
| 4   | W     | 147 | ARG  | NE-CZ-NH2  | -5.45 | 117.58      | 120.30   |
| 1   | M     | 384 | ASP  | CB-CG-OD1  | -5.45 | 113.40      | 118.30   |
| 4   | Z     | 294 | TYR  | CB-CG-CD2  | -5.44 | 117.73      | 121.00   |
| 4   | 3     | 79  | TRP  | CB-CG-CD1  | -5.44 | 119.93      | 127.00   |
| 4   | Y     | 79  | TRP  | CB-CG-CD1  | -5.44 | 119.93      | 127.00   |
| 1   | J     | 384 | ASP  | CB-CG-OD1  | -5.43 | 113.41      | 118.30   |
| 1   | J     | 547 | ASP  | CB-CG-OD2  | 5.43  | 123.19      | 118.30   |
| 1   | P     | 343 | PHE  | CB-CG-CD2  | -5.43 | 117.00      | 120.80   |
| 4   | 5     | 279 | TYR  | CB-CG-CD2  | -5.43 | 117.74      | 121.00   |
| 4   | V     | 79  | TRP  | CB-CG-CD1  | -5.43 | 119.94      | 127.00   |
| 4   | Y     | 11  | ASP  | CB-CG-OD1  | 5.43  | 123.19      | 118.30   |
| 1   | D     | 547 | ASP  | CB-CG-OD2  | 5.43  | 123.19      | 118.30   |
| 4   | 5     | 11  | ASP  | CB-CG-OD1  | 5.43  | 123.19      | 118.30   |
| 4   | 9     | 11  | ASP  | CB-CG-OD1  | 5.43  | 123.19      | 118.30   |
| 1   | M     | 306 | THR  | CA-CB-CG2  | -5.43 | 104.80      | 112.40   |
| 4   | Y     | 147 | ARG  | NE-CZ-NH2  | -5.43 | 117.59      | 120.30   |
| 4   | 1     | 356 | TRP  | CB-CG-CD1  | -5.43 | 119.94      | 127.00   |
| 4   | 9     | 147 | ARG  | NE-CZ-NH2  | -5.43 | 117.59      | 120.30   |
| 4   | Z     | 79  | TRP  | CB-CG-CD1  | -5.43 | 119.95      | 127.00   |
| 1   | J     | 800 | ARG  | NH1-CZ-NH2 | 5.42  | 125.37      | 119.40   |
| 1   | P     | 306 | THR  | CA-CB-CG2  | -5.42 | 104.80      | 112.40   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | X     | 356 | TRP  | CB-CG-CD1  | -5.42 | 119.95      | 127.00   |
| 1   | P     | 384 | ASP  | CB-CG-OD1  | -5.42 | 113.42      | 118.30   |
| 4   | 4     | 356 | TRP  | CG-CD2-CE3 | 5.42  | 138.78      | 133.90   |
| 1   | A     | 384 | ASP  | CB-CG-OD1  | -5.42 | 113.42      | 118.30   |
| 1   | J     | 306 | THR  | CA-CB-CG2  | -5.42 | 104.81      | 112.40   |
| 4   | 0     | 11  | ASP  | CB-CG-OD1  | 5.42  | 123.18      | 118.30   |
| 4   | Z     | 279 | TYR  | CB-CG-CD2  | -5.42 | 117.75      | 121.00   |
| 4   | W     | 279 | TYR  | CB-CG-CD2  | -5.42 | 117.75      | 121.00   |
| 1   | P     | 326 | ASP  | CB-CG-OD2  | 5.42  | 123.17      | 118.30   |
| 1   | G     | 326 | ASP  | CB-CG-OD2  | 5.41  | 123.17      | 118.30   |
| 1   | M     | 343 | PHE  | CB-CG-CD2  | -5.41 | 117.01      | 120.80   |
| 4   | 0     | 356 | TRP  | CB-CG-CD1  | -5.41 | 119.96      | 127.00   |
| 4   | 3     | 11  | ASP  | CB-CG-OD1  | 5.41  | 123.17      | 118.30   |
| 4   | 9     | 79  | TRP  | CB-CG-CD1  | -5.41 | 119.96      | 127.00   |
| 1   | J     | 241 | ASP  | CB-CG-OD2  | 5.41  | 123.17      | 118.30   |
| 4   | 1     | 79  | TRP  | CB-CG-CD1  | -5.41 | 119.97      | 127.00   |
| 4   | Z     | 11  | ASP  | CB-CG-OD1  | 5.41  | 123.17      | 118.30   |
| 4   | 3     | 294 | TYR  | CB-CG-CD2  | -5.41 | 117.75      | 121.00   |
| 4   | 0     | 356 | TRP  | CG-CD1-NE1 | -5.41 | 104.69      | 110.10   |
| 4   | 7     | 356 | TRP  | CB-CG-CD1  | -5.41 | 119.97      | 127.00   |
| 4   | 8     | 335 | ARG  | NE-CZ-NH1  | 5.41  | 123.00      | 120.30   |
| 4   | Z     | 356 | TRP  | CG-CD1-NE1 | -5.40 | 104.70      | 110.10   |
| 4   | 2     | 79  | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 4   | 5     | 79  | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 4   | 2     | 356 | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 4   | 8     | 356 | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 1   | P     | 170 | ARG  | NE-CZ-NH1  | 5.40  | 123.00      | 120.30   |
| 4   | 8     | 79  | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 1   | J     | 343 | PHE  | CB-CG-CD2  | -5.40 | 117.02      | 120.80   |
| 1   | P     | 218 | LEU  | O-C-N      | 5.40  | 131.34      | 122.70   |
| 1   | P     | 723 | ARG  | NE-CZ-NH1  | 5.40  | 123.00      | 120.30   |
| 4   | Z     | 356 | TRP  | CB-CG-CD1  | -5.40 | 119.98      | 127.00   |
| 1   | D     | 241 | ASP  | CB-CG-OD2  | 5.39  | 123.16      | 118.30   |
| 4   | 9     | 356 | TRP  | CB-CG-CD1  | -5.39 | 119.99      | 127.00   |
| 4   | V     | 356 | TRP  | CB-CG-CD1  | -5.39 | 119.99      | 127.00   |
| 4   | X     | 356 | TRP  | CG-CD1-NE1 | -5.39 | 104.71      | 110.10   |
| 4   | 0     | 147 | ARG  | NE-CZ-NH2  | -5.39 | 117.60      | 120.30   |
| 4   | V     | 356 | TRP  | CG-CD1-NE1 | -5.39 | 104.71      | 110.10   |
| 4   | W     | 11  | ASP  | CB-CG-OD1  | 5.39  | 123.15      | 118.30   |
| 4   | W     | 79  | TRP  | CB-CG-CD1  | -5.39 | 119.99      | 127.00   |
| 4   | 7     | 147 | ARG  | NE-CZ-NH2  | -5.39 | 117.61      | 120.30   |
| 4   | 8     | 147 | ARG  | NE-CZ-NH2  | -5.39 | 117.61      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 5     | 356 | TRP  | CB-CG-CD1  | -5.38 | 120.00      | 127.00   |
| 1   | A     | 686 | MET  | CG-SD-CE   | -5.38 | 91.59       | 100.20   |
| 1   | G     | 601 | ASP  | CB-CG-OD2  | 5.38  | 123.14      | 118.30   |
| 4   | 3     | 356 | TRP  | CB-CG-CD1  | -5.38 | 120.00      | 127.00   |
| 4   | X     | 79  | TRP  | CB-CG-CD1  | -5.38 | 120.00      | 127.00   |
| 1   | A     | 326 | ASP  | CB-CG-OD2  | 5.38  | 123.14      | 118.30   |
| 4   | Y     | 356 | TRP  | CB-CG-CD1  | -5.38 | 120.01      | 127.00   |
| 4   | 4     | 356 | TRP  | CB-CG-CD1  | -5.38 | 120.01      | 127.00   |
| 4   | 8     | 356 | TRP  | CG-CD1-NE1 | -5.38 | 104.72      | 110.10   |
| 4   | X     | 147 | ARG  | NE-CZ-NH2  | -5.38 | 117.61      | 120.30   |
| 1   | G     | 33  | ASP  | CB-CG-OD2  | 5.37  | 123.14      | 118.30   |
| 1   | J     | 218 | LEU  | O-C-N      | 5.37  | 131.29      | 122.70   |
| 1   | P     | 686 | MET  | CG-SD-CE   | -5.37 | 91.61       | 100.20   |
| 4   | Z     | 251 | GLY  | CA-C-N     | -5.37 | 105.39      | 117.20   |
| 1   | G     | 218 | LEU  | O-C-N      | 5.37  | 131.29      | 122.70   |
| 4   | 2     | 251 | GLY  | CA-C-N     | -5.37 | 105.39      | 117.20   |
| 4   | 4     | 79  | TRP  | CB-CG-CD1  | -5.37 | 120.02      | 127.00   |
| 4   | 8     | 251 | GLY  | CA-C-N     | -5.37 | 105.39      | 117.20   |
| 4   | Y     | 356 | TRP  | CG-CD1-NE1 | -5.36 | 104.74      | 110.10   |
| 2   | B     | 136 | MET  | CG-SD-CE   | 5.36  | 108.78      | 100.20   |
| 4   | W     | 356 | TRP  | CB-CG-CD1  | -5.36 | 120.03      | 127.00   |
| 1   | G     | 343 | PHE  | CB-CG-CD2  | -5.36 | 117.05      | 120.80   |
| 4   | 9     | 356 | TRP  | CG-CD1-NE1 | -5.36 | 104.74      | 110.10   |
| 4   | 1     | 147 | ARG  | NE-CZ-NH2  | -5.36 | 117.62      | 120.30   |
| 4   | 4     | 251 | GLY  | CA-C-N     | -5.36 | 105.42      | 117.20   |
| 4   | 0     | 79  | TRP  | CB-CG-CD1  | -5.36 | 120.04      | 127.00   |
| 2   | N     | 136 | MET  | CG-SD-CE   | 5.35  | 108.77      | 100.20   |
| 1   | D     | 601 | ASP  | CB-CG-OD2  | 5.35  | 123.12      | 118.30   |
| 1   | D     | 800 | ARG  | NH1-CZ-NH2 | 5.35  | 125.29      | 119.40   |
| 1   | G     | 686 | MET  | CG-SD-CE   | -5.35 | 91.64       | 100.20   |
| 2   | K     | 136 | MET  | CG-SD-CE   | 5.35  | 108.77      | 100.20   |
| 1   | M     | 241 | ASP  | CB-CG-OD2  | 5.35  | 123.12      | 118.30   |
| 4   | V     | 251 | GLY  | CA-C-N     | -5.35 | 105.43      | 117.20   |
| 1   | M     | 686 | MET  | CG-SD-CE   | -5.35 | 91.64       | 100.20   |
| 4   | 0     | 251 | GLY  | CA-C-N     | -5.35 | 105.43      | 117.20   |
| 4   | 1     | 356 | TRP  | CG-CD1-NE1 | -5.35 | 104.75      | 110.10   |
| 4   | 4     | 356 | TRP  | CG-CD1-NE1 | -5.35 | 104.75      | 110.10   |
| 1   | M     | 218 | LEU  | O-C-N      | 5.35  | 131.26      | 122.70   |
| 4   | 5     | 251 | GLY  | CA-C-N     | -5.35 | 105.44      | 117.20   |
| 4   | 5     | 356 | TRP  | CG-CD1-NE1 | -5.35 | 104.75      | 110.10   |
| 4   | 9     | 251 | GLY  | CA-C-N     | -5.35 | 105.43      | 117.20   |
| 1   | A     | 601 | ASP  | CB-CG-OD2  | 5.34  | 123.11      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | J     | 686 | MET  | CG-SD-CE   | -5.34 | 91.65       | 100.20   |
| 4   | 3     | 251 | GLY  | CA-C-N     | -5.34 | 105.44      | 117.20   |
| 1   | J     | 170 | ARG  | NE-CZ-NH1  | 5.34  | 122.97      | 120.30   |
| 4   | 1     | 251 | GLY  | CA-C-N     | -5.34 | 105.45      | 117.20   |
| 4   | 2     | 356 | TRP  | CG-CD1-NE1 | -5.34 | 104.76      | 110.10   |
| 4   | W     | 251 | GLY  | CA-C-N     | -5.34 | 105.45      | 117.20   |
| 4   | V     | 11  | ASP  | CB-CG-OD1  | 5.33  | 123.10      | 118.30   |
| 4   | X     | 251 | GLY  | CA-C-N     | -5.33 | 105.47      | 117.20   |
| 1   | G     | 125 | THR  | CA-CB-CG2  | -5.33 | 104.94      | 112.40   |
| 4   | 7     | 356 | TRP  | CG-CD1-NE1 | -5.33 | 104.77      | 110.10   |
| 4   | 7     | 176 | MET  | CG-SD-CE   | 5.33  | 108.73      | 100.20   |
| 4   | Y     | 251 | GLY  | CA-C-N     | -5.33 | 105.47      | 117.20   |
| 2   | Q     | 136 | MET  | CG-SD-CE   | 5.33  | 108.72      | 100.20   |
| 4   | 7     | 251 | GLY  | CA-C-N     | -5.33 | 105.48      | 117.20   |
| 4   | W     | 356 | TRP  | CG-CD1-NE1 | -5.33 | 104.78      | 110.10   |
| 4   | X     | 62  | ARG  | NE-CZ-NH1  | 5.33  | 122.96      | 120.30   |
| 4   | Y     | 176 | MET  | CG-SD-CE   | 5.33  | 108.72      | 100.20   |
| 1   | D     | 686 | MET  | CG-SD-CE   | -5.32 | 91.68       | 100.20   |
| 1   | P     | 800 | ARG  | NH1-CZ-NH2 | 5.32  | 125.25      | 119.40   |
| 1   | A     | 343 | PHE  | CB-CG-CD2  | -5.32 | 117.08      | 120.80   |
| 4   | 3     | 356 | TRP  | CG-CD1-NE1 | -5.32 | 104.78      | 110.10   |
| 1   | D     | 660 | LEU  | CB-CG-CD2  | 5.32  | 120.04      | 111.00   |
| 1   | M     | 723 | ARG  | NE-CZ-NH1  | 5.32  | 122.96      | 120.30   |
| 4   | 1     | 176 | MET  | CG-SD-CE   | 5.32  | 108.71      | 100.20   |
| 1   | D     | 343 | PHE  | CB-CG-CD2  | -5.32 | 117.08      | 120.80   |
| 1   | G     | 241 | ASP  | CB-CG-OD2  | 5.32  | 123.08      | 118.30   |
| 1   | P     | 241 | ASP  | CB-CG-OD2  | 5.32  | 123.08      | 118.30   |
| 4   | 8     | 176 | MET  | CG-SD-CE   | 5.31  | 108.70      | 100.20   |
| 1   | A     | 723 | ARG  | NE-CZ-NH1  | 5.31  | 122.96      | 120.30   |
| 2   | H     | 136 | MET  | CG-SD-CE   | 5.31  | 108.70      | 100.20   |
| 4   | W     | 176 | MET  | CG-SD-CE   | 5.31  | 108.69      | 100.20   |
| 4   | 9     | 176 | MET  | CG-SD-CE   | 5.31  | 108.69      | 100.20   |
| 4   | X     | 176 | MET  | CG-SD-CE   | 5.31  | 108.69      | 100.20   |
| 4   | 0     | 176 | MET  | CG-SD-CE   | 5.31  | 108.69      | 100.20   |
| 1   | G     | 800 | ARG  | NH1-CZ-NH2 | 5.30  | 125.23      | 119.40   |
| 1   | M     | 125 | THR  | CA-CB-CG2  | -5.30 | 104.98      | 112.40   |
| 1   | P     | 601 | ASP  | CB-CG-OD2  | 5.30  | 123.07      | 118.30   |
| 4   | 2     | 176 | MET  | CG-SD-CE   | 5.30  | 108.68      | 100.20   |
| 4   | 4     | 176 | MET  | CG-SD-CE   | 5.30  | 108.68      | 100.20   |
| 4   | 5     | 147 | ARG  | NE-CZ-NH2  | -5.30 | 117.65      | 120.30   |
| 1   | J     | 660 | LEU  | CB-CG-CD2  | 5.30  | 120.01      | 111.00   |
| 1   | P     | 760 | PHE  | CB-CG-CD1  | 5.30  | 124.51      | 120.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | D     | 354 | LEU  | CB-CG-CD2  | -5.30 | 102.00      | 111.00   |
| 1   | J     | 601 | ASP  | CB-CG-OD2  | 5.30  | 123.07      | 118.30   |
| 4   | 3     | 176 | MET  | CG-SD-CE   | 5.30  | 108.67      | 100.20   |
| 1   | A     | 125 | THR  | CA-CB-CG2  | -5.29 | 104.99      | 112.40   |
| 1   | D     | 760 | PHE  | CB-CG-CD1  | 5.29  | 124.51      | 120.80   |
| 1   | P     | 4   | ASP  | CB-CG-OD1  | -5.29 | 113.53      | 118.30   |
| 2   | E     | 136 | MET  | CG-SD-CE   | 5.29  | 108.67      | 100.20   |
| 1   | A     | 547 | ASP  | CB-CG-OD2  | 5.29  | 123.06      | 118.30   |
| 1   | G     | 660 | LEU  | CB-CG-CD2  | 5.29  | 120.00      | 111.00   |
| 1   | J     | 125 | THR  | CA-CB-CG2  | -5.29 | 104.99      | 112.40   |
| 4   | V     | 176 | MET  | CG-SD-CE   | 5.29  | 108.67      | 100.20   |
| 1   | P     | 125 | THR  | CA-CB-CG2  | -5.29 | 104.99      | 112.40   |
| 1   | P     | 660 | LEU  | CB-CG-CD2  | 5.29  | 119.99      | 111.00   |
| 4   | 5     | 176 | MET  | CG-SD-CE   | 5.29  | 108.66      | 100.20   |
| 4   | 4     | 335 | ARG  | NE-CZ-NH1  | 5.29  | 122.94      | 120.30   |
| 1   | A     | 354 | LEU  | CB-CG-CD2  | -5.28 | 102.02      | 111.00   |
| 1   | G     | 354 | LEU  | CB-CG-CD2  | -5.27 | 102.03      | 111.00   |
| 1   | A     | 660 | LEU  | CB-CG-CD2  | 5.27  | 119.96      | 111.00   |
| 4   | Z     | 176 | MET  | CG-SD-CE   | 5.27  | 108.63      | 100.20   |
| 1   | D     | 125 | THR  | CA-CB-CG2  | -5.27 | 105.03      | 112.40   |
| 1   | D     | 4   | ASP  | CB-CG-OD1  | -5.26 | 113.57      | 118.30   |
| 4   | 3     | 147 | ARG  | NE-CZ-NH2  | -5.26 | 117.67      | 120.30   |
| 1   | G     | 384 | ASP  | CB-CG-OD1  | -5.25 | 113.57      | 118.30   |
| 1   | G     | 547 | ASP  | CB-CG-OD2  | 5.25  | 123.03      | 118.30   |
| 1   | J     | 354 | LEU  | CB-CG-CD2  | -5.25 | 102.08      | 111.00   |
| 4   | W     | 62  | ARG  | NE-CZ-NH1  | 5.25  | 122.92      | 120.30   |
| 1   | A     | 800 | ARG  | NH1-CZ-NH2 | 5.25  | 125.17      | 119.40   |
| 1   | M     | 601 | ASP  | CB-CG-OD2  | 5.25  | 123.02      | 118.30   |
| 4   | X     | 91  | TYR  | CB-CG-CD2  | -5.25 | 117.85      | 121.00   |
| 1   | J     | 4   | ASP  | CB-CG-OD1  | -5.25 | 113.58      | 118.30   |
| 1   | A     | 218 | LEU  | O-C-N      | 5.24  | 131.09      | 122.70   |
| 1   | P     | 354 | LEU  | CB-CG-CD2  | -5.24 | 102.09      | 111.00   |
| 1   | M     | 555 | TYR  | CB-CG-CD1  | 5.24  | 124.14      | 121.00   |
| 4   | 8     | 337 | TYR  | CB-CG-CD1  | -5.24 | 117.86      | 121.00   |
| 1   | J     | 346 | ASP  | N-CA-CB    | -5.24 | 101.18      | 110.60   |
| 1   | M     | 800 | ARG  | NH1-CZ-NH2 | 5.24  | 125.16      | 119.40   |
| 4   | V     | 62  | ARG  | NE-CZ-NH1  | 5.23  | 122.92      | 120.30   |
| 1   | M     | 660 | LEU  | CB-CG-CD2  | 5.23  | 119.89      | 111.00   |
| 1   | D     | 218 | LEU  | O-C-N      | 5.22  | 131.06      | 122.70   |
| 1   | M     | 760 | PHE  | CB-CG-CD1  | 5.22  | 124.46      | 120.80   |
| 4   | X     | 335 | ARG  | NE-CZ-NH1  | 5.22  | 122.91      | 120.30   |
| 1   | G     | 709 | LYS  | C-N-CA     | 5.22  | 133.26      | 122.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 4   | 5     | 91  | TYR  | CB-CG-CD2 | -5.22 | 117.87      | 121.00   |
| 4   | Y     | 335 | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 4   | Z     | 335 | ARG  | NE-CZ-NH1 | 5.22  | 122.91      | 120.30   |
| 1   | M     | 4   | ASP  | CB-CG-OD1 | -5.22 | 113.61      | 118.30   |
| 4   | 1     | 62  | ARG  | NE-CZ-NH1 | 5.21  | 122.91      | 120.30   |
| 4   | 4     | 62  | ARG  | NE-CZ-NH1 | 5.21  | 122.91      | 120.30   |
| 4   | 9     | 335 | ARG  | NE-CZ-NH1 | 5.21  | 122.91      | 120.30   |
| 1   | P     | 346 | ASP  | N-CA-CB   | -5.21 | 101.22      | 110.60   |
| 4   | Z     | 147 | ARG  | NE-CZ-NH2 | -5.21 | 117.69      | 120.30   |
| 1   | M     | 346 | ASP  | N-CA-CB   | -5.21 | 101.23      | 110.60   |
| 4   | 5     | 335 | ARG  | NE-CZ-NH1 | 5.21  | 122.90      | 120.30   |
| 1   | M     | 170 | ARG  | NE-CZ-NH1 | 5.20  | 122.90      | 120.30   |
| 1   | A     | 346 | ASP  | N-CA-CB   | -5.20 | 101.24      | 110.60   |
| 4   | 8     | 91  | TYR  | CB-CG-CD2 | -5.20 | 117.88      | 121.00   |
| 4   | 4     | 337 | TYR  | CB-CG-CD1 | -5.20 | 117.88      | 121.00   |
| 1   | M     | 354 | LEU  | CB-CG-CD2 | -5.20 | 102.17      | 111.00   |
| 4   | 4     | 147 | ARG  | NE-CZ-NH2 | -5.19 | 117.70      | 120.30   |
| 1   | G     | 4   | ASP  | CB-CG-OD1 | -5.19 | 113.63      | 118.30   |
| 4   | 0     | 62  | ARG  | NE-CZ-NH1 | 5.19  | 122.89      | 120.30   |
| 4   | X     | 53  | TYR  | CB-CG-CD1 | -5.19 | 117.89      | 121.00   |
| 1   | A     | 760 | PHE  | CB-CG-CD1 | 5.19  | 124.43      | 120.80   |
| 4   | 0     | 337 | TYR  | CB-CG-CD1 | -5.19 | 117.89      | 121.00   |
| 4   | Z     | 290 | ARG  | CA-C-N    | 5.18  | 128.61      | 117.20   |
| 1   | A     | 90  | ASP  | CB-CG-OD1 | -5.18 | 113.64      | 118.30   |
| 4   | 3     | 290 | ARG  | CA-C-N    | 5.18  | 128.60      | 117.20   |
| 4   | 2     | 62  | ARG  | NE-CZ-NH1 | 5.18  | 122.89      | 120.30   |
| 1   | G     | 555 | TYR  | CB-CG-CD1 | 5.18  | 124.11      | 121.00   |
| 4   | 2     | 335 | ARG  | NE-CZ-NH1 | 5.18  | 122.89      | 120.30   |
| 4   | 8     | 290 | ARG  | CA-C-N    | 5.18  | 128.59      | 117.20   |
| 1   | G     | 90  | ASP  | CB-CG-OD1 | -5.17 | 113.64      | 118.30   |
| 1   | P     | 555 | TYR  | CB-CG-CD1 | 5.17  | 124.10      | 121.00   |
| 4   | 7     | 337 | TYR  | CB-CG-CD1 | -5.17 | 117.90      | 121.00   |
| 4   | V     | 290 | ARG  | CA-C-N    | 5.17  | 128.58      | 117.20   |
| 4   | Z     | 62  | ARG  | NE-CZ-NH1 | 5.17  | 122.89      | 120.30   |
| 4   | 5     | 290 | ARG  | CA-C-N    | 5.17  | 128.56      | 117.20   |
| 1   | D     | 160 | ASP  | CB-CG-OD2 | -5.17 | 113.65      | 118.30   |
| 4   | 1     | 91  | TYR  | CB-CG-CD2 | -5.17 | 117.90      | 121.00   |
| 4   | X     | 290 | ARG  | CA-C-N    | 5.16  | 128.56      | 117.20   |
| 4   | 0     | 290 | ARG  | CA-C-N    | 5.16  | 128.56      | 117.20   |
| 4   | Y     | 290 | ARG  | CA-C-N    | 5.16  | 128.56      | 117.20   |
| 4   | Z     | 337 | TYR  | CB-CG-CD1 | -5.16 | 117.90      | 121.00   |
| 4   | 3     | 337 | TYR  | CB-CG-CD1 | -5.16 | 117.91      | 121.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 4     | 290 | ARG  | CA-C-N     | 5.16  | 128.55      | 117.20   |
| 4   | W     | 335 | ARG  | NE-CZ-NH1  | 5.16  | 122.88      | 120.30   |
| 4   | 0     | 91  | TYR  | CB-CG-CD2  | -5.15 | 117.91      | 121.00   |
| 4   | 9     | 290 | ARG  | CA-C-N     | 5.15  | 128.53      | 117.20   |
| 4   | W     | 337 | TYR  | CB-CG-CD1  | -5.15 | 117.91      | 121.00   |
| 4   | W     | 53  | TYR  | CB-CG-CD1  | -5.15 | 117.91      | 121.00   |
| 4   | 7     | 62  | ARG  | NE-CZ-NH1  | 5.15  | 122.87      | 120.30   |
| 4   | W     | 290 | ARG  | CA-C-N     | 5.15  | 128.52      | 117.20   |
| 4   | Z     | 91  | TYR  | CB-CG-CD2  | -5.15 | 117.91      | 121.00   |
| 4   | 1     | 290 | ARG  | CA-C-N     | 5.15  | 128.52      | 117.20   |
| 4   | 2     | 290 | ARG  | CA-C-N     | 5.14  | 128.52      | 117.20   |
| 4   | Y     | 62  | ARG  | NE-CZ-NH1  | 5.14  | 122.87      | 120.30   |
| 1   | A     | 160 | ASP  | CB-CG-OD2  | -5.14 | 113.67      | 118.30   |
| 1   | D     | 346 | ASP  | N-CA-CB    | -5.14 | 101.34      | 110.60   |
| 4   | 3     | 62  | ARG  | NE-CZ-NH1  | 5.14  | 122.87      | 120.30   |
| 4   | 4     | 91  | TYR  | CB-CG-CD2  | -5.14 | 117.92      | 121.00   |
| 1   | D     | 218 | LEU  | CA-CB-CG   | 5.14  | 127.12      | 115.30   |
| 4   | 0     | 335 | ARG  | NE-CZ-NH1  | 5.14  | 122.87      | 120.30   |
| 4   | 1     | 337 | TYR  | CB-CG-CD1  | -5.14 | 117.92      | 121.00   |
| 4   | 5     | 337 | TYR  | CB-CG-CD1  | -5.14 | 117.92      | 121.00   |
| 1   | D     | 576 | GLU  | CA-CB-CG   | -5.14 | 102.10      | 113.40   |
| 1   | J     | 723 | ARG  | NE-CZ-NH1  | 5.14  | 122.87      | 120.30   |
| 1   | J     | 628 | GLY  | O-C-N      | -5.14 | 114.48      | 122.70   |
| 4   | 2     | 86  | TRP  | CG-CD1-NE1 | -5.13 | 104.97      | 110.10   |
| 1   | J     | 82  | PRO  | N-CA-CB    | 5.13  | 109.46      | 103.30   |
| 4   | 3     | 91  | TYR  | CB-CG-CD2  | -5.13 | 117.92      | 121.00   |
| 1   | D     | 170 | ARG  | NE-CZ-NH1  | 5.13  | 122.86      | 120.30   |
| 1   | A     | 4   | ASP  | CB-CG-OD1  | -5.12 | 113.69      | 118.30   |
| 1   | G     | 346 | ASP  | N-CA-CB    | -5.12 | 101.38      | 110.60   |
| 4   | 2     | 337 | TYR  | CB-CG-CD1  | -5.12 | 117.93      | 121.00   |
| 4   | 7     | 91  | TYR  | CB-CG-CD2  | -5.12 | 117.93      | 121.00   |
| 4   | 7     | 290 | ARG  | CA-C-N     | 5.12  | 128.46      | 117.20   |
| 1   | A     | 555 | TYR  | CB-CG-CD1  | 5.11  | 124.07      | 121.00   |
| 1   | J     | 760 | PHE  | CB-CG-CD1  | 5.11  | 124.38      | 120.80   |
| 4   | 9     | 86  | TRP  | CG-CD1-NE1 | -5.11 | 104.99      | 110.10   |
| 1   | M     | 576 | GLU  | CA-CB-CG   | -5.11 | 102.16      | 113.40   |
| 4   | W     | 91  | TYR  | CB-CG-CD2  | -5.11 | 117.93      | 121.00   |
| 1   | D     | 628 | GLY  | O-C-N      | -5.11 | 114.53      | 122.70   |
| 1   | G     | 576 | GLU  | CA-CB-CG   | -5.11 | 102.16      | 113.40   |
| 4   | 1     | 335 | ARG  | NE-CZ-NH1  | 5.11  | 122.85      | 120.30   |
| 1   | A     | 576 | GLU  | CA-CB-CG   | -5.11 | 102.17      | 113.40   |
| 1   | G     | 760 | PHE  | CB-CG-CD1  | 5.11  | 124.37      | 120.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | M     | 628 | GLY  | O-C-N      | -5.11 | 114.53      | 122.70   |
| 1   | P     | 628 | GLY  | O-C-N      | -5.11 | 114.53      | 122.70   |
| 4   | 5     | 53  | TYR  | CB-CG-CD1  | -5.11 | 117.94      | 121.00   |
| 1   | G     | 160 | ASP  | CB-CG-OD2  | -5.10 | 113.71      | 118.30   |
| 1   | G     | 170 | ARG  | NE-CZ-NH1  | 5.10  | 122.85      | 120.30   |
| 1   | P     | 218 | LEU  | CA-CB-CG   | 5.10  | 127.04      | 115.30   |
| 4   | 4     | 53  | TYR  | CB-CG-CD1  | -5.10 | 117.94      | 121.00   |
| 4   | 7     | 62  | ARG  | CA-CB-CG   | 5.10  | 124.62      | 113.40   |
| 1   | D     | 621 | LEU  | CA-CB-CG   | -5.10 | 103.57      | 115.30   |
| 1   | J     | 576 | GLU  | CA-CB-CG   | -5.10 | 102.18      | 113.40   |
| 1   | P     | 576 | GLU  | CA-CB-CG   | -5.10 | 102.19      | 113.40   |
| 4   | 0     | 62  | ARG  | CA-CB-CG   | 5.10  | 124.61      | 113.40   |
| 4   | Z     | 86  | TRP  | CG-CD1-NE1 | -5.10 | 105.00      | 110.10   |
| 1   | P     | 82  | PRO  | N-CA-CB    | 5.09  | 109.41      | 103.30   |
| 4   | V     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.61      | 113.40   |
| 4   | W     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.61      | 113.40   |
| 4   | Z     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.61      | 113.40   |
| 4   | 1     | 53  | TYR  | CB-CG-CD1  | -5.09 | 117.94      | 121.00   |
| 1   | A     | 621 | LEU  | CA-CB-CG   | -5.09 | 103.60      | 115.30   |
| 1   | J     | 218 | LEU  | CA-CB-CG   | 5.09  | 127.00      | 115.30   |
| 4   | 1     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | 4     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | 8     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | Y     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | 2     | 53  | TYR  | CB-CG-CD1  | -5.09 | 117.95      | 121.00   |
| 4   | 9     | 62  | ARG  | CA-CB-CG   | 5.09  | 124.59      | 113.40   |
| 4   | Y     | 337 | TYR  | CB-CG-CD1  | -5.09 | 117.95      | 121.00   |
| 1   | M     | 218 | LEU  | CA-CB-CG   | 5.08  | 126.99      | 115.30   |
| 4   | 2     | 91  | TYR  | CB-CG-CD2  | -5.08 | 117.95      | 121.00   |
| 4   | X     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.58      | 113.40   |
| 1   | M     | 82  | PRO  | N-CA-CB    | 5.08  | 109.40      | 103.30   |
| 4   | 7     | 335 | ARG  | NE-CZ-NH1  | 5.08  | 122.84      | 120.30   |
| 4   | 9     | 337 | TYR  | CB-CG-CD1  | -5.08 | 117.95      | 121.00   |
| 4   | V     | 337 | TYR  | CB-CG-CD1  | -5.08 | 117.95      | 121.00   |
| 4   | 2     | 191 | LYS  | CA-C-N     | 5.08  | 128.38      | 117.20   |
| 4   | 5     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.58      | 113.40   |
| 4   | Z     | 53  | TYR  | CB-CG-CD1  | -5.08 | 117.95      | 121.00   |
| 1   | A     | 218 | LEU  | CA-CB-CG   | 5.08  | 126.98      | 115.30   |
| 4   | 2     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.57      | 113.40   |
| 4   | 5     | 191 | LYS  | CA-C-N     | 5.08  | 128.37      | 117.20   |
| 1   | A     | 235 | ALA  | N-CA-CB    | -5.08 | 103.00      | 110.10   |
| 1   | J     | 301 | ASP  | CB-CG-OD2  | 5.08  | 122.87      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | 3     | 62  | ARG  | CA-CB-CG   | 5.08  | 124.56      | 113.40   |
| 4   | 8     | 62  | ARG  | NE-CZ-NH1  | 5.08  | 122.84      | 120.30   |
| 4   | Z     | 191 | LYS  | CA-C-N     | 5.07  | 128.36      | 117.20   |
| 1   | M     | 160 | ASP  | CB-CG-OD2  | -5.07 | 113.74      | 118.30   |
| 4   | 4     | 191 | LYS  | CA-C-N     | 5.07  | 128.35      | 117.20   |
| 4   | 9     | 191 | LYS  | CA-C-N     | 5.07  | 128.35      | 117.20   |
| 4   | V     | 86  | TRP  | CG-CD1-NE1 | -5.07 | 105.03      | 110.10   |
| 1   | D     | 82  | PRO  | N-CA-CB    | 5.07  | 109.38      | 103.30   |
| 4   | W     | 191 | LYS  | CA-C-N     | 5.07  | 128.35      | 117.20   |
| 1   | J     | 160 | ASP  | CB-CG-OD2  | -5.07 | 113.74      | 118.30   |
| 4   | 7     | 53  | TYR  | CB-CG-CD1  | -5.07 | 117.96      | 121.00   |
| 4   | 7     | 191 | LYS  | CA-C-N     | 5.07  | 128.34      | 117.20   |
| 4   | 8     | 191 | LYS  | CA-C-N     | 5.07  | 128.35      | 117.20   |
| 1   | J     | 621 | LEU  | CA-CB-CG   | -5.06 | 103.65      | 115.30   |
| 4   | 3     | 335 | ARG  | NE-CZ-NH1  | 5.06  | 122.83      | 120.30   |
| 4   | X     | 191 | LYS  | CA-C-N     | 5.06  | 128.34      | 117.20   |
| 1   | P     | 160 | ASP  | CB-CG-OD2  | -5.06 | 113.75      | 118.30   |
| 4   | 1     | 191 | LYS  | CA-C-N     | 5.06  | 128.33      | 117.20   |
| 4   | Y     | 191 | LYS  | CA-C-N     | 5.06  | 128.33      | 117.20   |
| 4   | 3     | 53  | TYR  | CB-CG-CD1  | -5.06 | 117.97      | 121.00   |
| 4   | 3     | 191 | LYS  | CA-C-N     | 5.06  | 128.32      | 117.20   |
| 1   | G     | 621 | LEU  | CA-CB-CG   | -5.05 | 103.67      | 115.30   |
| 1   | M     | 621 | LEU  | CA-CB-CG   | -5.05 | 103.67      | 115.30   |
| 4   | 0     | 53  | TYR  | CB-CG-CD1  | -5.05 | 117.97      | 121.00   |
| 4   | Y     | 53  | TYR  | CB-CG-CD1  | -5.05 | 117.97      | 121.00   |
| 4   | V     | 191 | LYS  | CA-C-N     | 5.05  | 128.32      | 117.20   |
| 1   | P     | 621 | LEU  | CA-CB-CG   | -5.05 | 103.68      | 115.30   |
| 4   | Y     | 91  | TYR  | CB-CG-CD2  | -5.05 | 117.97      | 121.00   |
| 1   | M     | 90  | ASP  | CB-CG-OD1  | -5.05 | 113.76      | 118.30   |
| 4   | X     | 337 | TYR  | CB-CG-CD1  | -5.05 | 117.97      | 121.00   |
| 1   | A     | 628 | GLY  | O-C-N      | -5.05 | 114.62      | 122.70   |
| 4   | X     | 86  | TRP  | CG-CD1-NE1 | -5.05 | 105.05      | 110.10   |
| 4   | 9     | 62  | ARG  | NE-CZ-NH1  | 5.04  | 122.82      | 120.30   |
| 1   | A     | 739 | ASP  | CA-CB-CG   | -5.04 | 102.31      | 113.40   |
| 4   | 0     | 191 | LYS  | CA-C-N     | 5.04  | 128.28      | 117.20   |
| 4   | 5     | 62  | ARG  | NE-CZ-NH1  | 5.04  | 122.82      | 120.30   |
| 1   | A     | 611 | TYR  | CB-CG-CD1  | 5.04  | 124.02      | 121.00   |
| 1   | M     | 301 | ASP  | CB-CG-OD2  | 5.03  | 122.83      | 118.30   |
| 1   | G     | 628 | GLY  | O-C-N      | -5.03 | 114.65      | 122.70   |
| 1   | D     | 301 | ASP  | CB-CG-OD2  | 5.03  | 122.83      | 118.30   |
| 4   | 8     | 86  | TRP  | CG-CD1-NE1 | -5.03 | 105.07      | 110.10   |
| 4   | 9     | 91  | TYR  | CB-CG-CD2  | -5.03 | 117.98      | 121.00   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | M     | 235 | ALA  | N-CA-CB   | -5.02 | 103.07      | 110.10   |
| 1   | J     | 90  | ASP  | CB-CG-OD1 | -5.02 | 113.78      | 118.30   |
| 1   | J     | 739 | ASP  | N-CA-CB   | 5.02  | 119.64      | 110.60   |
| 1   | M     | 739 | ASP  | CA-CB-CG  | -5.02 | 102.36      | 113.40   |
| 1   | A     | 170 | ARG  | NE-CZ-NH1 | 5.02  | 122.81      | 120.30   |
| 1   | D     | 90  | ASP  | CB-CG-OD1 | -5.02 | 113.78      | 118.30   |
| 1   | G     | 218 | LEU  | CA-CB-CG  | 5.02  | 126.84      | 115.30   |
| 1   | D     | 739 | ASP  | N-CA-CB   | 5.01  | 119.63      | 110.60   |
| 1   | A     | 82  | PRO  | N-CA-CB   | 5.01  | 109.31      | 103.30   |
| 1   | G     | 739 | ASP  | N-CA-CB   | 5.01  | 119.62      | 110.60   |
| 2   | H     | 129 | THR  | N-CA-CB   | 5.01  | 119.82      | 110.30   |
| 1   | P     | 235 | ALA  | N-CA-CB   | -5.01 | 103.09      | 110.10   |
| 1   | P     | 301 | ASP  | CB-CG-OD2 | 5.01  | 122.81      | 118.30   |
| 1   | D     | 235 | ALA  | N-CA-CB   | -5.01 | 103.09      | 110.10   |
| 4   | 8     | 53  | TYR  | CB-CG-CD1 | -5.01 | 118.00      | 121.00   |
| 1   | A     | 301 | ASP  | CB-CG-OD2 | 5.00  | 122.80      | 118.30   |
| 1   | D     | 463 | ASP  | CB-CG-OD1 | 5.00  | 122.80      | 118.30   |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 648 | THR  | CB   |
| 1   | D     | 648 | THR  | CB   |
| 1   | G     | 648 | THR  | CB   |
| 1   | J     | 648 | THR  | CB   |
| 1   | M     | 648 | THR  | CB   |
| 1   | P     | 648 | THR  | CB   |

All (74) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | 0     | 62  | ARG  | Sidechain |
| 4   | 1     | 62  | ARG  | Sidechain |
| 4   | 2     | 62  | ARG  | Sidechain |
| 4   | 3     | 62  | ARG  | Sidechain |
| 4   | 4     | 62  | ARG  | Sidechain |
| 4   | 5     | 62  | ARG  | Sidechain |
| 4   | 7     | 62  | ARG  | Sidechain |
| 4   | 8     | 62  | ARG  | Sidechain |
| 4   | 9     | 62  | ARG  | Sidechain |
| 1   | A     | 623 | PHE  | Sidechain |
| 1   | A     | 637 | LYS  | Mainchain |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 1   | A     | 649 | VAL  | Mainchain         |
| 1   | A     | 98  | HIS  | Mainchain         |
| 2   | B     | 150 | TYR  | Sidechain         |
| 2   | B     | 155 | TYR  | Mainchain         |
| 2   | B     | 22  | THR  | Mainchain         |
| 3   | C     | 75  | ALA  | Mainchain         |
| 3   | C     | 85  | GLU  | Mainchain         |
| 1   | D     | 623 | PHE  | Sidechain         |
| 1   | D     | 637 | LYS  | Mainchain         |
| 1   | D     | 649 | VAL  | Mainchain         |
| 1   | D     | 98  | HIS  | Mainchain         |
| 2   | E     | 150 | TYR  | Sidechain         |
| 2   | E     | 155 | TYR  | Mainchain         |
| 2   | E     | 22  | THR  | Mainchain         |
| 3   | F     | 75  | ALA  | Mainchain         |
| 3   | F     | 85  | GLU  | Mainchain         |
| 1   | G     | 623 | PHE  | Sidechain         |
| 1   | G     | 637 | LYS  | Mainchain         |
| 1   | G     | 649 | VAL  | Mainchain         |
| 1   | G     | 98  | HIS  | Mainchain         |
| 2   | H     | 150 | TYR  | Sidechain         |
| 2   | H     | 155 | TYR  | Mainchain         |
| 2   | H     | 22  | THR  | Mainchain         |
| 3   | I     | 75  | ALA  | Mainchain         |
| 3   | I     | 85  | GLU  | Mainchain         |
| 1   | J     | 623 | PHE  | Sidechain         |
| 1   | J     | 637 | LYS  | Mainchain         |
| 1   | J     | 649 | VAL  | Mainchain         |
| 1   | J     | 709 | LYS  | Mainchain,Peptide |
| 1   | J     | 98  | HIS  | Mainchain         |
| 2   | K     | 150 | TYR  | Sidechain         |
| 2   | K     | 155 | TYR  | Mainchain         |
| 2   | K     | 22  | THR  | Mainchain         |
| 3   | L     | 75  | ALA  | Mainchain         |
| 3   | L     | 85  | GLU  | Mainchain         |
| 1   | M     | 623 | PHE  | Sidechain         |
| 1   | M     | 637 | LYS  | Mainchain         |
| 1   | M     | 649 | VAL  | Mainchain         |
| 1   | M     | 709 | LYS  | Mainchain,Peptide |
| 1   | M     | 98  | HIS  | Mainchain         |
| 2   | N     | 150 | TYR  | Sidechain         |
| 2   | N     | 155 | TYR  | Mainchain         |

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| Mol | Chain | Res | Type | Group             |
|-----|-------|-----|------|-------------------|
| 2   | N     | 22  | THR  | Mainchain         |
| 3   | O     | 75  | ALA  | Mainchain         |
| 3   | O     | 85  | GLU  | Mainchain         |
| 1   | P     | 623 | PHE  | Sidechain         |
| 1   | P     | 637 | LYS  | Mainchain         |
| 1   | P     | 649 | VAL  | Mainchain         |
| 1   | P     | 709 | LYS  | Mainchain,Peptide |
| 1   | P     | 98  | HIS  | Mainchain         |
| 2   | Q     | 150 | TYR  | Sidechain         |
| 2   | Q     | 155 | TYR  | Mainchain         |
| 2   | Q     | 22  | THR  | Mainchain         |
| 3   | R     | 75  | ALA  | Mainchain         |
| 3   | R     | 85  | GLU  | Mainchain         |
| 4   | V     | 62  | ARG  | Sidechain         |
| 4   | W     | 62  | ARG  | Sidechain         |
| 4   | X     | 62  | ARG  | Sidechain         |
| 4   | Y     | 62  | ARG  | Sidechain         |
| 4   | Z     | 62  | ARG  | Sidechain         |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 6797  | 0        | 6753     | 1539    | 19           |
| 1   | D     | 6797  | 0        | 6758     | 1519    | 21           |
| 1   | G     | 6797  | 0        | 6764     | 1543    | 0            |
| 1   | J     | 6797  | 0        | 6760     | 1449    | 0            |
| 1   | M     | 6797  | 0        | 6765     | 1504    | 0            |
| 1   | P     | 6797  | 0        | 6765     | 1493    | 0            |
| 2   | B     | 1127  | 0        | 1085     | 226     | 0            |
| 2   | E     | 1127  | 0        | 1085     | 249     | 0            |
| 2   | H     | 1127  | 0        | 1087     | 278     | 0            |
| 2   | K     | 1127  | 0        | 1088     | 282     | 0            |
| 2   | N     | 1127  | 0        | 1088     | 238     | 0            |
| 2   | Q     | 1127  | 0        | 1088     | 253     | 0            |
| 3   | C     | 1123  | 0        | 1083     | 200     | 0            |
| 3   | F     | 1123  | 0        | 1084     | 200     | 0            |
| 3   | I     | 1123  | 0        | 1082     | 211     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | L     | 1123  | 0        | 1083     | 168     | 0            |
| 3   | O     | 1123  | 0        | 1084     | 152     | 0            |
| 3   | R     | 1123  | 0        | 1084     | 238     | 0            |
| 4   | 0     | 2906  | 0        | 2855     | 404     | 0            |
| 4   | 1     | 2906  | 0        | 2858     | 259     | 76           |
| 4   | 2     | 2906  | 0        | 2864     | 173     | 574          |
| 4   | 3     | 2906  | 0        | 2863     | 178     | 3105         |
| 4   | 4     | 2906  | 0        | 2865     | 96      | 3229         |
| 4   | 5     | 2906  | 0        | 2865     | 97      | 3412         |
| 4   | 7     | 2906  | 0        | 2866     | 79      | 3158         |
| 4   | 8     | 2906  | 0        | 2857     | 317     | 3221         |
| 4   | 9     | 2906  | 0        | 2855     | 341     | 3470         |
| 4   | V     | 2906  | 0        | 2851     | 390     | 418          |
| 4   | W     | 2906  | 0        | 2851     | 382     | 89           |
| 4   | X     | 2906  | 0        | 2862     | 208     | 0            |
| 4   | Y     | 2906  | 0        | 2863     | 168     | 0            |
| 4   | Z     | 2906  | 0        | 2853     | 410     | 0            |
| All | All   | 94966 | 0        | 93614    | 11439   | 10396        |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

All (11439) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:797:PHE:CE1  | 3:L:146:ILE:HG23 | 1.26                     | 1.66              |
| 1:D:797:PHE:CE2  | 3:F:126:LEU:HD22 | 1.31                     | 1.66              |
| 1:G:797:PHE:CZ   | 3:I:146:ILE:HD12 | 1.28                     | 1.66              |
| 1:A:505:MLY:HB3  | 1:A:762:HIS:CD2  | 1.30                     | 1.65              |
| 1:D:508:ILE:HD11 | 1:D:766:PHE:CE1  | 1.24                     | 1.65              |
| 1:A:757:GLN:CG   | 1:A:771:LEU:HD11 | 1.25                     | 1.65              |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:CG1  | 1.17                     | 1.64              |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:CD1  | 1.22                     | 1.64              |
| 1:G:754:ASP:HA   | 1:G:779:ARG:CD   | 1.19                     | 1.62              |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:CD1  | 1.22                     | 1.62              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CD1  | 1.22                     | 1.62              |
| 4:X:324:THR:CG2  | 4:Z:247:VAL:H    | 1.09                     | 1.62              |
| 4:1:287:ILE:HG23 | 4:3:202:THR:CB   | 1.26                     | 1.61              |
| 1:M:817:GLN:CG   | 2:N:127:ARG:HD2  | 1.16                     | 1.61              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:CG1  | 1.17                     | 1.61              |
| 1:P:725:ARG:HE   | 1:P:733:PRO:CB   | 1.09                     | 1.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:206:LYS:CD   | 1:A:217:THR:HG23 | 1.28                     | 1.61              |
| 1:J:725:ARG:HE   | 1:J:733:PRO:CB   | 1.09                     | 1.61              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CD1  | 1.22                     | 1.61              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CG1  | 1.17                     | 1.60              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:CD1  | 1.26                     | 1.60              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:HD22 | 1.30                     | 1.60              |
| 1:D:508:ILE:CD1  | 1:D:766:PHE:CZ   | 1.75                     | 1.60              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CD1  | 1.22                     | 1.59              |
| 1:P:538:GLU:CA   | 4:O:349:LEU:CD1  | 1.79                     | 1.59              |
| 1:A:725:ARG:HE   | 1:A:733:PRO:CB   | 1.09                     | 1.59              |
| 1:G:768:MLY:CH2  | 1:G:772:LEU:HD13 | 1.15                     | 1.59              |
| 1:G:206:LYS:CD   | 1:G:217:THR:HG23 | 1.28                     | 1.59              |
| 1:J:206:LYS:CD   | 1:J:217:THR:HG23 | 1.28                     | 1.59              |
| 1:M:505:MLY:HD2  | 1:M:762:HIS:CE1  | 1.33                     | 1.59              |
| 1:J:84:MLY:CH2   | 1:J:720:PHE:HA   | 1.31                     | 1.59              |
| 1:M:538:GLU:CA   | 4:Z:349:LEU:CD1  | 1.79                     | 1.58              |
| 1:G:768:MLY:HH23 | 1:G:772:LEU:CD1  | 1.12                     | 1.58              |
| 1:J:538:GLU:CA   | 4:W:349:LEU:CD1  | 1.79                     | 1.58              |
| 1:J:797:PHE:CD1  | 3:L:146:ILE:CG2  | 1.74                     | 1.57              |
| 1:P:817:GLN:CG   | 2:Q:127:ARG:HD2  | 1.23                     | 1.57              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:CD1  | 1.22                     | 1.57              |
| 1:P:795:ARG:HH21 | 3:R:116:GLU:CB   | 0.97                     | 1.57              |
| 1:J:798:LEU:CD1  | 3:L:126:LEU:HD11 | 1.21                     | 1.57              |
| 2:N:111:SER:HB2  | 2:N:148:VAL:C    | 1.23                     | 1.57              |
| 1:G:538:GLU:CA   | 4:V:349:LEU:CD1  | 1.79                     | 1.57              |
| 1:D:538:GLU:CA   | 4:9:349:LEU:CD1  | 1.78                     | 1.57              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:CG1  | 1.17                     | 1.56              |
| 1:D:797:PHE:CD1  | 3:F:146:ILE:HG23 | 1.36                     | 1.56              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:HB   | 1.23                     | 1.56              |
| 1:G:818:TYR:CZ   | 2:H:127:ARG:NH2  | 1.70                     | 1.56              |
| 1:A:831:TRP:CZ3  | 2:B:50:THR:HG21  | 1.36                     | 1.56              |
| 1:J:792:ALA:HB2  | 3:L:42:THR:CG2   | 1.17                     | 1.56              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:CB   | 1.35                     | 1.56              |
| 1:G:725:ARG:HE   | 1:G:733:PRO:CB   | 1.09                     | 1.56              |
| 1:A:508:ILE:CD1  | 1:A:759:ALA:CB   | 1.77                     | 1.56              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:HB2  | 1.34                     | 1.56              |
| 1:M:545:ALA:HA   | 4:1:45:VAL:CG1   | 1.32                     | 1.56              |
| 1:D:206:LYS:CD   | 1:D:217:THR:HG23 | 1.28                     | 1.56              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:HD11 | 1.10                     | 1.56              |
| 1:J:530:MET:HG2  | 4:W:354:GLN:CB   | 1.36                     | 1.56              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:CG1  | 1.17                     | 1.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:206:LYS:CD   | 1:M:217:THR:HG23 | 1.28                     | 1.55              |
| 1:A:797:PHE:CZ   | 3:C:146:ILE:HD13 | 1.41                     | 1.55              |
| 1:J:84:MLY:HH11  | 1:J:720:PHE:CD1  | 1.36                     | 1.55              |
| 1:D:818:TYR:CB   | 2:E:90:GLY:HA3   | 1.10                     | 1.55              |
| 1:G:757:GLN:HG3  | 1:G:776:GLU:CG   | 1.33                     | 1.55              |
| 1:G:530:MET:HG2  | 4:V:354:GLN:CB   | 1.35                     | 1.55              |
| 4:O:205:GLU:CG   | 4:Y:287:ILE:HB   | 1.16                     | 1.55              |
| 1:P:548:THR:CG2  | 4:2:49:GLN:N     | 1.70                     | 1.55              |
| 1:A:530:MET:HG2  | 4:8:354:GLN:CB   | 1.35                     | 1.55              |
| 1:D:725:ARG:HE   | 1:D:733:PRO:CB   | 1.09                     | 1.54              |
| 1:G:757:GLN:CG   | 1:G:776:GLU:HG2  | 1.37                     | 1.54              |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:CG1  | 1.17                     | 1.54              |
| 1:P:798:LEU:CD2  | 3:R:126:LEU:HD11 | 1.34                     | 1.54              |
| 1:M:838:ILE:HD11 | 2:N:54:MET:CE    | 1.30                     | 1.54              |
| 1:J:28:GLN:CG    | 1:J:723:ARG:NH1  | 1.71                     | 1.54              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:CB   | 1.35                     | 1.54              |
| 1:J:710:GLY:CA   | 1:J:772:LEU:HD22 | 1.26                     | 1.54              |
| 1:J:710:GLY:HA2  | 1:J:772:LEU:CD2  | 1.33                     | 1.54              |
| 1:G:792:ALA:HB2  | 3:I:42:THR:CG2   | 1.32                     | 1.54              |
| 4:1:287:ILE:CG1  | 4:3:203:THR:N    | 1.67                     | 1.54              |
| 1:D:818:TYR:HB2  | 2:E:90:GLY:CA    | 1.33                     | 1.54              |
| 1:M:783:LEU:HA   | 1:M:786:ILE:CG1  | 1.31                     | 1.54              |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:CE    | 1.32                     | 1.54              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:CG2  | 1.71                     | 1.53              |
| 1:P:206:LYS:CD   | 1:P:217:THR:HG23 | 1.28                     | 1.53              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:CG   | 1.36                     | 1.53              |
| 1:P:792:ALA:HB2  | 3:R:42:THR:CG2   | 1.38                     | 1.53              |
| 1:D:530:MET:HG2  | 4:9:354:GLN:CB   | 1.35                     | 1.53              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:CG   | 1.37                     | 1.53              |
| 1:M:725:ARG:HE   | 1:M:733:PRO:CB   | 1.09                     | 1.53              |
| 1:D:791:GLN:HE22 | 3:F:115:GLY:CA   | 1.22                     | 1.53              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:CB   | 1.35                     | 1.53              |
| 1:A:538:GLU:CA   | 4:8:349:LEU:CD1  | 1.78                     | 1.53              |
| 1:G:93:MET:CE    | 1:G:764:MLY:HD3  | 1.37                     | 1.53              |
| 1:P:729:ALA:CB   | 3:R:93:VAL:HG21  | 1.15                     | 1.53              |
| 1:A:508:ILE:HD11 | 1:A:759:ALA:CB   | 1.30                     | 1.52              |
| 1:P:641:LYS:HG3  | 1:P:647:GLN:CG   | 1.37                     | 1.52              |
| 1:A:149:GLN:HB2  | 1:A:718:ALA:CB   | 1.39                     | 1.52              |
| 1:P:530:MET:HG2  | 4:O:354:GLN:CB   | 1.36                     | 1.52              |
| 1:A:505:MLY:CB   | 1:A:762:HIS:HD2  | 1.19                     | 1.51              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:CG2  | 1.40                     | 1.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:736:GLN:HA   | 1:M:743:ALA:CB   | 1.35                     | 1.51              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:CB   | 1.35                     | 1.51              |
| 1:M:530:MET:HG2  | 4:Z:354:GLN:CB   | 1.36                     | 1.51              |
| 1:D:508:ILE:CD1  | 1:D:766:PHE:CE1  | 1.80                     | 1.51              |
| 1:P:736:GLN:HA   | 1:P:743:ALA:CB   | 1.35                     | 1.51              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:CG   | 1.37                     | 1.51              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:CG   | 1.15                     | 1.51              |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:CG   | 1.38                     | 1.51              |
| 1:P:721:LYS:HG3  | 1:P:736:GLN:CG   | 1.15                     | 1.51              |
| 1:M:206:LYS:HD3  | 1:M:217:THR:CG2  | 1.40                     | 1.51              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CB   | 1.41                     | 1.50              |
| 2:Q:111:SER:HB2  | 2:Q:148:VAL:C    | 1.23                     | 1.50              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:CG   | 1.15                     | 1.50              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CB   | 1.41                     | 1.50              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CB   | 1.41                     | 1.50              |
| 1:A:795:ARG:HB3  | 3:C:35:ARG:CZ    | 1.39                     | 1.50              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:CG   | 1.37                     | 1.50              |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD1  | 1.06                     | 1.50              |
| 1:M:641:LYS:HG3  | 1:M:647:GLN:CG   | 1.37                     | 1.50              |
| 1:A:505:MLY:CD   | 1:A:762:HIS:HA   | 1.37                     | 1.50              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:HD2  | 1.09                     | 1.50              |
| 1:G:797:PHE:CZ   | 3:I:146:ILE:CD1  | 1.94                     | 1.50              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CB   | 1.42                     | 1.50              |
| 1:D:508:ILE:HD11 | 1:D:766:PHE:CZ   | 0.97                     | 1.49              |
| 4:X:324:THR:HB   | 4:Z:246:GLN:N    | 1.27                     | 1.49              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:CG2  | 1.40                     | 1.49              |
| 1:P:206:LYS:HD3  | 1:P:217:THR:CG2  | 1.40                     | 1.49              |
| 1:J:836:PHE:CE1  | 2:K:159:HIS:HA   | 1.45                     | 1.49              |
| 1:D:798:LEU:CD1  | 3:F:126:LEU:HD11 | 1.03                     | 1.49              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:CD   | 1.41                     | 1.49              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:HA   | 1.44                     | 1.49              |
| 1:M:831:TRP:CH2  | 2:N:47:LEU:CD2   | 1.96                     | 1.49              |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CG   | 1.29                     | 1.48              |
| 2:K:111:SER:HB2  | 2:K:148:VAL:C    | 1.23                     | 1.48              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:CG2  | 1.40                     | 1.48              |
| 1:M:641:LYS:CG   | 1:M:647:GLN:NE2  | 1.77                     | 1.48              |
| 4:O:243:PRO:C    | 4:Y:291:LYS:HE2  | 1.21                     | 1.48              |
| 2:B:111:SER:HB2  | 2:B:148:VAL:C    | 1.23                     | 1.48              |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CB   | 1.41                     | 1.48              |
| 1:D:768:MLY:C    | 1:D:771:LEU:HD12 | 1.01                     | 1.48              |
| 1:M:28:GLN:CB    | 1:M:723:ARG:HH12 | 1.19                     | 1.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:721:LYS:HG3  | 1:A:736:GLN:CG   | 1.15                     | 1.48              |
| 1:P:548:THR:CG2  | 4:2:49:GLN:HB2   | 1.41                     | 1.48              |
| 1:M:783:LEU:HG   | 1:M:786:ILE:CD1  | 1.40                     | 1.48              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:NE2  | 1.76                     | 1.48              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CG   | 1.30                     | 1.47              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:CE    | 1.39                     | 1.47              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:CG2  | 1.40                     | 1.47              |
| 1:G:97:LEU:CD2   | 1:G:712:PRO:HB3  | 1.43                     | 1.47              |
| 1:G:754:ASP:CA   | 1:G:779:ARG:HD2  | 1.40                     | 1.47              |
| 1:G:792:ALA:CB   | 3:I:42:THR:HG22  | 1.42                     | 1.47              |
| 4:W:324:THR:CG2  | 4:Y:247:VAL:H    | 1.24                     | 1.47              |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:CB   | 1.41                     | 1.47              |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:CG   | 1.29                     | 1.47              |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:CD   | 1.38                     | 1.46              |
| 1:M:798:LEU:CD2  | 3:O:126:LEU:HD11 | 1.45                     | 1.46              |
| 1:G:792:ALA:HB2  | 3:I:42:THR:CB    | 1.44                     | 1.46              |
| 1:D:823:PHE:CE1  | 2:E:160:GLY:HA2  | 1.47                     | 1.46              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:NE2  | 1.77                     | 1.46              |
| 1:G:556:ASP:CG   | 4:X:47:MET:CE    | 1.76                     | 1.46              |
| 1:G:538:GLU:C    | 4:V:349:LEU:CD1  | 1.84                     | 1.46              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:CD   | 1.85                     | 1.46              |
| 1:M:84:MLY:CG    | 1:M:723:ARG:HD2  | 1.42                     | 1.46              |
| 1:J:795:ARG:CB   | 3:L:35:ARG:NH1   | 1.74                     | 1.45              |
| 1:J:538:GLU:C    | 4:W:349:LEU:CD1  | 1.84                     | 1.45              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:CD   | 1.85                     | 1.45              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CG   | 1.30                     | 1.45              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CB   | 1.41                     | 1.45              |
| 1:P:795:ARG:HG2  | 3:R:118:MET:CE   | 1.45                     | 1.45              |
| 1:D:538:GLU:C    | 4:9:349:LEU:CD1  | 1.84                     | 1.45              |
| 1:M:783:LEU:HA   | 1:M:786:ILE:CD1  | 1.44                     | 1.45              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:NE2  | 1.77                     | 1.45              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:NE2  | 1.76                     | 1.45              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:CE    | 0.99                     | 1.45              |
| 4:0:287:ILE:CG2  | 4:2:203:THR:HG22 | 1.42                     | 1.45              |
| 2:E:111:SER:HB2  | 2:E:148:VAL:C    | 1.23                     | 1.45              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CG   | 1.29                     | 1.45              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:CD   | 1.85                     | 1.45              |
| 4:X:324:THR:CG2  | 4:Z:247:VAL:HG22 | 1.44                     | 1.45              |
| 1:A:538:GLU:C    | 4:8:349:LEU:CD1  | 1.84                     | 1.45              |
| 1:M:831:TRP:HH2  | 2:N:47:LEU:CD2   | 1.24                     | 1.45              |
| 4:1:287:ILE:HG12 | 4:3:202:THR:C    | 1.29                     | 1.44              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:834:LEU:CD2  | 2:B:54:MET:CE   | 1.95                     | 1.44              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CG  | 1.30                     | 1.44              |
| 1:P:538:GLU:C    | 4:0:349:LEU:CD1 | 1.84                     | 1.44              |
| 1:M:641:LYS:CD   | 1:M:647:GLN:CD  | 1.85                     | 1.44              |
| 1:P:729:ALA:CB   | 3:R:93:VAL:CG2  | 1.96                     | 1.44              |
| 1:J:505:MLY:HD2  | 1:J:762:HIS:CE1 | 1.49                     | 1.44              |
| 1:J:819:ASN:ND2  | 2:K:92:ASP:HB2  | 1.16                     | 1.44              |
| 1:M:786:ILE:HB   | 1:M:787:ILE:N   | 1.30                     | 1.44              |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:CD1 | 0.97                     | 1.43              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:CD  | 1.71                     | 1.43              |
| 4:0:205:GLU:HG3  | 4:Y:287:ILE:CB  | 1.33                     | 1.43              |
| 1:A:799:MET:SD   | 3:C:32:ASP:HB3  | 1.58                     | 1.43              |
| 1:J:795:ARG:HB3  | 3:L:35:ARG:NH1  | 1.10                     | 1.43              |
| 2:H:111:SER:HB2  | 2:H:148:VAL:C   | 1.23                     | 1.43              |
| 1:P:641:LYS:CG   | 1:P:647:GLN:NE2 | 1.76                     | 1.43              |
| 1:P:641:LYS:CD   | 1:P:647:GLN:CD  | 1.85                     | 1.43              |
| 1:D:641:LYS:CD   | 1:D:647:GLN:CD  | 1.85                     | 1.43              |
| 1:P:795:ARG:NH2  | 3:R:116:GLU:CG  | 1.81                     | 1.43              |
| 1:A:791:GLN:NE2  | 3:C:116:GLU:H   | 1.12                     | 1.43              |
| 1:G:567:LYS:NZ   | 4:X:92:ASN:HD22 | 1.17                     | 1.43              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:CE   | 1.48                     | 1.43              |
| 1:P:795:ARG:NH2  | 3:R:116:GLU:HB3 | 1.26                     | 1.42              |
| 1:P:798:LEU:HD21 | 3:R:126:LEU:CD1 | 1.48                     | 1.42              |
| 1:M:28:GLN:HB3   | 1:M:723:ARG:NH1 | 1.17                     | 1.42              |
| 4:0:112:PRO:HB3  | 4:1:196:ARG:CA  | 1.36                     | 1.42              |
| 1:A:797:PHE:CZ   | 3:C:146:ILE:CD1 | 2.01                     | 1.42              |
| 1:P:836:PHE:CE1  | 2:Q:159:HIS:HA  | 1.54                     | 1.42              |
| 1:M:795:ARG:HG2  | 3:O:118:MET:CE  | 1.48                     | 1.42              |
| 1:P:831:TRP:CH2  | 2:Q:47:LEU:CD2  | 2.02                     | 1.42              |
| 4:X:324:THR:HB   | 4:Z:245:GLY:C   | 1.37                     | 1.42              |
| 1:J:733:PRO:O    | 1:J:737:PHE:CD1 | 1.73                     | 1.42              |
| 2:N:144:VAL:CG1  | 2:N:153:ILE:CD1 | 1.99                     | 1.41              |
| 1:M:733:PRO:O    | 1:M:737:PHE:CD1 | 1.73                     | 1.41              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:CG  | 1.15                     | 1.41              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:CD1 | 1.99                     | 1.41              |
| 1:M:793:ARG:HH11 | 3:O:40:ASN:ND2  | 1.02                     | 1.41              |
| 1:P:202:SER:HA   | 1:P:207:LYS:CE  | 1.51                     | 1.41              |
| 1:A:530:MET:CG   | 4:8:354:GLN:HB2 | 1.50                     | 1.41              |
| 1:M:721:LYS:HG3  | 1:M:736:GLN:CG  | 1.15                     | 1.41              |
| 1:J:202:SER:HA   | 1:J:207:LYS:CE  | 1.51                     | 1.41              |
| 1:D:733:PRO:O    | 1:D:737:PHE:CD1 | 1.74                     | 1.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:797:PHE:CE1  | 3:F:146:ILE:HA   | 1.56                     | 1.41              |
| 1:G:791:GLN:NE2  | 3:I:115:GLY:HA3  | 1.31                     | 1.41              |
| 1:P:733:PRO:O    | 1:P:737:PHE:CD1  | 1.73                     | 1.41              |
| 1:D:530:MET:CG   | 4:9:354:GLN:HB2  | 1.50                     | 1.41              |
| 1:M:836:PHE:CE1  | 2:N:159:HIS:HA   | 1.55                     | 1.41              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:HE3   | 1.51                     | 1.41              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:CE    | 1.49                     | 1.41              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:CG   | 1.90                     | 1.41              |
| 1:D:791:GLN:NE2  | 3:F:115:GLY:HA3  | 1.33                     | 1.40              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:CD1  | 1.99                     | 1.40              |
| 1:P:798:LEU:CG   | 3:R:126:LEU:HD11 | 1.49                     | 1.40              |
| 4:0:112:PRO:HG3  | 4:1:195:GLU:C    | 1.17                     | 1.40              |
| 1:P:831:TRP:HH2  | 2:Q:47:LEU:CD2   | 1.32                     | 1.40              |
| 1:A:501:GLU:CG   | 1:A:762:HIS:ND1  | 1.85                     | 1.40              |
| 1:P:218:LEU:CB   | 1:P:221:GLN:HG3  | 1.52                     | 1.40              |
| 1:A:202:SER:HA   | 1:A:207:LYS:CE   | 1.51                     | 1.40              |
| 4:X:324:THR:HG21 | 4:Z:247:VAL:N    | 1.16                     | 1.40              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:CD1  | 1.99                     | 1.40              |
| 1:J:218:LEU:CB   | 1:J:221:GLN:HG3  | 1.52                     | 1.40              |
| 1:M:537:GLU:O    | 4:Z:349:LEU:CD1  | 1.70                     | 1.40              |
| 1:M:538:GLU:C    | 4:Z:349:LEU:CD1  | 1.84                     | 1.40              |
| 1:M:736:GLN:CA   | 1:M:743:ALA:CB   | 2.00                     | 1.40              |
| 4:3:288:ASP:CG   | 4:5:203:THR:CG2  | 1.90                     | 1.40              |
| 1:P:508:ILE:HD11 | 1:P:759:ALA:CB   | 1.49                     | 1.40              |
| 1:J:798:LEU:CD1  | 3:L:126:LEU:CD1  | 1.80                     | 1.40              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:CB   | 2.00                     | 1.39              |
| 1:G:792:ALA:HB2  | 3:I:42:THR:CA    | 1.52                     | 1.39              |
| 1:J:736:GLN:CA   | 1:J:743:ALA:CB   | 2.00                     | 1.39              |
| 1:D:537:GLU:O    | 4:9:349:LEU:CD1  | 1.70                     | 1.39              |
| 1:D:218:LEU:CB   | 1:D:221:GLN:HG3  | 1.52                     | 1.39              |
| 1:J:795:ARG:CD   | 3:L:43:ASN:OD1   | 1.69                     | 1.39              |
| 4:1:287:ILE:HG12 | 4:3:203:THR:N    | 1.25                     | 1.39              |
| 1:A:733:PRO:O    | 1:A:737:PHE:CD1  | 1.73                     | 1.39              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:CB   | 2.00                     | 1.39              |
| 1:A:831:TRP:CH2  | 2:B:34:ILE:HG23  | 1.58                     | 1.39              |
| 1:A:537:GLU:O    | 4:8:349:LEU:CD1  | 1.70                     | 1.39              |
| 1:D:202:SER:HA   | 1:D:207:LYS:CE   | 1.51                     | 1.39              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:ND1  | 1.08                     | 1.39              |
| 1:P:736:GLN:N    | 1:P:743:ALA:HB1  | 1.35                     | 1.39              |
| 1:P:537:GLU:O    | 4:0:349:LEU:CD1  | 1.70                     | 1.39              |
| 1:G:736:GLN:N    | 1:G:743:ALA:HB1  | 1.34                     | 1.39              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:290:ARG:CZ   | 4:4:202:THR:HG21 | 1.52                     | 1.39              |
| 1:G:202:SER:HA   | 1:G:207:LYS:CE   | 1.51                     | 1.39              |
| 4:X:291:LYS:CB   | 4:Z:244:ASP:HB3  | 1.49                     | 1.39              |
| 4:1:287:ILE:HG12 | 4:3:202:THR:CA   | 1.51                     | 1.39              |
| 1:P:530:MET:CG   | 4:0:354:GLN:HB2  | 1.51                     | 1.39              |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:CE   | 1.51                     | 1.38              |
| 1:A:218:LEU:CB   | 1:A:221:GLN:HG3  | 1.52                     | 1.38              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:HG2  | 1.38                     | 1.38              |
| 1:J:530:MET:CG   | 4:W:354:GLN:HB2  | 1.51                     | 1.38              |
| 1:G:792:ALA:CB   | 3:I:42:THR:CG2   | 1.96                     | 1.38              |
| 1:A:149:GLN:CB   | 1:A:718:ALA:HB3  | 1.53                     | 1.38              |
| 1:A:505:MLY:HD3  | 1:A:762:HIS:CA   | 1.51                     | 1.38              |
| 1:M:819:ASN:CA   | 2:N:90:GLY:O     | 1.72                     | 1.38              |
| 2:Q:144:VAL:CG1  | 2:Q:153:ILE:CD1  | 1.99                     | 1.38              |
| 1:M:530:MET:CG   | 4:Z:354:GLN:HB2  | 1.51                     | 1.38              |
| 1:M:736:GLN:N    | 1:M:743:ALA:HB1  | 1.35                     | 1.38              |
| 1:D:727:LEU:HB2  | 1:D:782:MLY:CH1  | 0.91                     | 1.38              |
| 1:D:724:TYR:CA   | 1:D:782:MLY:HD2  | 1.53                     | 1.38              |
| 1:D:736:GLN:N    | 1:D:743:ALA:HB1  | 1.35                     | 1.38              |
| 1:A:508:ILE:CD1  | 1:A:759:ALA:HB1  | 0.91                     | 1.38              |
| 1:J:736:GLN:CA   | 1:J:743:ALA:HB1  | 1.53                     | 1.38              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:CD1  | 1.99                     | 1.38              |
| 1:G:218:LEU:CB   | 1:G:221:GLN:HG3  | 1.51                     | 1.38              |
| 1:M:534:SER:O    | 4:Z:351:THR:CG2  | 1.64                     | 1.38              |
| 1:M:736:GLN:CA   | 1:M:743:ALA:HB1  | 1.53                     | 1.38              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:HG12 | 1.54                     | 1.38              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HG12 | 1.54                     | 1.38              |
| 1:J:795:ARG:NH2  | 3:L:116:GLU:OE1  | 1.56                     | 1.38              |
| 1:M:218:LEU:CB   | 1:M:221:GLN:HG3  | 1.52                     | 1.37              |
| 1:G:534:SER:O    | 4:V:351:THR:CG2  | 1.64                     | 1.37              |
| 1:P:736:GLN:CA   | 1:P:743:ALA:CB   | 2.00                     | 1.37              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:ND2  | 1.39                     | 1.37              |
| 4:X:291:LYS:HB3  | 4:Z:244:ASP:CB   | 1.54                     | 1.37              |
| 1:D:727:LEU:CB   | 1:D:782:MLY:HH13 | 1.43                     | 1.37              |
| 1:D:747:LEU:CD1  | 1:D:782:MLY:HH21 | 1.52                     | 1.37              |
| 1:G:537:GLU:O    | 4:V:349:LEU:CD1  | 1.71                     | 1.37              |
| 1:J:537:GLU:O    | 4:W:349:LEU:CD1  | 1.70                     | 1.37              |
| 1:D:823:PHE:HE1  | 2:E:160:GLY:CA   | 1.37                     | 1.37              |
| 2:Q:144:VAL:CG1  | 2:Q:153:ILE:CG1  | 2.03                     | 1.37              |
| 1:J:819:ASN:CG   | 2:K:92:ASP:CB    | 1.89                     | 1.37              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:CD   | 1.93                     | 1.37              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:203:THR:CG2  | 4:Z:288:ASP:OD2  | 1.72                     | 1.37              |
| 1:M:202:SER:HA   | 1:M:207:LYS:CE   | 1.51                     | 1.37              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:CG   | 1.51                     | 1.37              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:HD2  | 1.44                     | 1.37              |
| 1:G:819:ASN:CA   | 2:H:90:GLY:O     | 1.71                     | 1.37              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:CD   | 1.45                     | 1.37              |
| 4:0:287:ILE:HG21 | 4:2:203:THR:CG2  | 1.54                     | 1.37              |
| 1:D:642:LYS:HG3  | 4:9:23:GLY:N     | 1.40                     | 1.37              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:HB1  | 1.53                     | 1.36              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:CG1  | 2.03                     | 1.36              |
| 1:G:733:PRO:O    | 1:G:737:PHE:CD1  | 1.73                     | 1.36              |
| 2:N:144:VAL:CG1  | 2:N:153:ILE:CG1  | 2.03                     | 1.36              |
| 1:G:530:MET:CG   | 4:V:354:GLN:HB2  | 1.51                     | 1.36              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CD   | 1.75                     | 1.36              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:CD   | 1.93                     | 1.36              |
| 1:J:792:ALA:CB   | 3:L:42:THR:HG22  | 1.55                     | 1.36              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:CG   | 1.96                     | 1.36              |
| 1:M:817:GLN:CG   | 2:N:127:ARG:CD   | 2.04                     | 1.36              |
| 1:J:642:LYS:HG3  | 4:W:23:GLY:N     | 1.40                     | 1.36              |
| 1:M:641:LYS:HG3  | 1:M:647:GLN:CD   | 1.45                     | 1.36              |
| 1:D:85:TYR:OH    | 1:D:772:LEU:CD2  | 1.71                     | 1.36              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:O    | 1.74                     | 1.36              |
| 1:D:795:ARG:CZ   | 3:F:116:GLU:OE2  | 1.73                     | 1.36              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:CG1  | 2.03                     | 1.36              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:CG1  | 2.03                     | 1.36              |
| 1:M:793:ARG:NH1  | 3:O:40:ASN:ND2   | 1.70                     | 1.36              |
| 1:M:642:LYS:HG3  | 4:Z:23:GLY:N     | 1.40                     | 1.36              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:CG1  | 2.03                     | 1.36              |
| 1:A:736:GLN:N    | 1:A:743:ALA:HB1  | 1.35                     | 1.36              |
| 1:J:84:MLY:HH21  | 1:J:720:PHE:CA   | 1.53                     | 1.36              |
| 1:P:641:LYS:CG   | 1:P:647:GLN:CD   | 1.93                     | 1.36              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:O    | 1.74                     | 1.36              |
| 1:G:796:GLY:HA2  | 3:I:35:ARG:CD    | 1.53                     | 1.35              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:ND2  | 1.39                     | 1.35              |
| 1:P:642:LYS:HG3  | 4:0:23:GLY:N     | 1.40                     | 1.35              |
| 1:M:538:GLU:CA   | 4:Z:349:LEU:HD12 | 0.88                     | 1.35              |
| 1:G:538:GLU:CA   | 4:V:349:LEU:HD12 | 0.88                     | 1.35              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:ND2  | 1.39                     | 1.35              |
| 2:N:144:VAL:CG1  | 2:N:153:ILE:HG12 | 1.54                     | 1.35              |
| 1:G:553:MLY:CH1  | 4:X:45:VAL:HG11  | 1.54                     | 1.35              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:CB   | 2.00                     | 1.35              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:721:LYS:CG   | 1:G:736:GLN:CG   | 1.97                     | 1.35              |
| 1:D:815:CYS:SG   | 2:E:92:ASP:CG    | 2.04                     | 1.35              |
| 1:M:649:VAL:O    | 1:M:649:VAL:CG1  | 1.74                     | 1.35              |
| 1:G:642:LYS:HG3  | 4:V:23:GLY:N     | 1.39                     | 1.35              |
| 2:Q:144:VAL:CG1  | 2:Q:153:ILE:HG12 | 1.54                     | 1.35              |
| 1:P:736:GLN:CA   | 1:P:743:ALA:HB1  | 1.53                     | 1.35              |
| 1:J:721:LYS:CG   | 1:J:736:GLN:CG   | 1.97                     | 1.35              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HG12 | 1.54                     | 1.35              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:OD1  | 1.74                     | 1.35              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:CA   | 1.51                     | 1.35              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:HB1  | 1.53                     | 1.35              |
| 1:A:530:MET:HA   | 4:8:354:GLN:CG   | 1.56                     | 1.35              |
| 1:P:641:LYS:HG3  | 1:P:647:GLN:CD   | 1.45                     | 1.35              |
| 1:D:823:PHE:CE1  | 2:E:160:GLY:CA   | 2.07                     | 1.35              |
| 1:J:736:GLN:N    | 1:J:743:ALA:HB1  | 1.35                     | 1.34              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HG12 | 1.54                     | 1.34              |
| 1:A:534:SER:O    | 4:8:351:THR:CG2  | 1.64                     | 1.34              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:CD2  | 2.10                     | 1.34              |
| 1:J:538:GLU:CA   | 4:W:349:LEU:HD12 | 0.88                     | 1.34              |
| 1:D:534:SER:O    | 4:9:351:THR:CG2  | 1.64                     | 1.34              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:CD   | 1.93                     | 1.34              |
| 1:J:795:ARG:CB   | 3:L:35:ARG:HH12  | 1.33                     | 1.34              |
| 1:G:754:ASP:OD2  | 1:G:779:ARG:CB   | 1.72                     | 1.34              |
| 1:M:641:LYS:CG   | 1:M:647:GLN:CD   | 1.93                     | 1.34              |
| 1:P:629:GLU:HA   | 1:P:643:GLY:O    | 1.17                     | 1.34              |
| 4:1:203:THR:HG23 | 4:Z:288:ASP:CG   | 1.47                     | 1.34              |
| 1:M:805:ALA:O    | 1:M:809:ARG:N    | 1.61                     | 1.34              |
| 1:J:797:PHE:CD1  | 3:L:146:ILE:HG23 | 0.83                     | 1.34              |
| 2:N:117:LEU:HB2  | 2:N:147:ASN:ND2  | 1.39                     | 1.34              |
| 2:H:114:LYS:CA   | 2:H:146:GLY:O    | 1.76                     | 1.34              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:OD1  | 1.74                     | 1.34              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:HB1  | 1.53                     | 1.34              |
| 1:J:506:GLU:OE2  | 1:J:761:GLY:HA2  | 1.18                     | 1.34              |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:CD1  | 1.57                     | 1.34              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:CD   | 1.45                     | 1.34              |
| 1:M:84:MLY:HH22  | 1:M:719:ASP:O    | 1.20                     | 1.34              |
| 1:D:649:VAL:O    | 1:D:649:VAL:CG1  | 1.73                     | 1.34              |
| 1:A:791:GLN:HE22 | 3:C:116:GLU:N    | 1.25                     | 1.33              |
| 1:A:538:GLU:CA   | 4:8:349:LEU:HD12 | 0.87                     | 1.33              |
| 1:A:642:LYS:HG3  | 4:8:23:GLY:N     | 1.40                     | 1.33              |
| 1:D:795:ARG:HG2  | 3:F:118:MET:CE   | 1.56                     | 1.33              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:N:117:LEU:CD1 | 2:N:147:ASN:OD1  | 1.74                     | 1.33              |
| 1:P:538:GLU:CA  | 4:0:349:LEU:HD12 | 0.88                     | 1.33              |
| 1:D:538:GLU:CA  | 4:9:349:LEU:HD12 | 0.87                     | 1.33              |
| 1:A:641:LYS:CG  | 1:A:647:GLN:CD   | 1.93                     | 1.33              |
| 1:P:530:MET:HA  | 4:0:354:GLN:CG   | 1.56                     | 1.33              |
| 1:J:530:MET:HA  | 4:W:354:GLN:CG   | 1.56                     | 1.33              |
| 1:D:530:MET:HA  | 4:9:354:GLN:CG   | 1.56                     | 1.33              |
| 1:D:635:GLY:CA  | 4:9:334:GLU:HG2  | 1.59                     | 1.33              |
| 1:G:93:MET:CE   | 1:G:764:MLY:CD   | 2.07                     | 1.33              |
| 1:P:649:VAL:O   | 1:P:649:VAL:CG1  | 1.73                     | 1.33              |
| 1:J:649:VAL:CG1 | 1:J:649:VAL:O    | 1.74                     | 1.33              |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:CD   | 2.06                     | 1.33              |
| 1:G:818:TYR:OH  | 2:H:127:ARG:NH2  | 1.57                     | 1.33              |
| 2:B:114:LYS:CA  | 2:B:146:GLY:O    | 1.76                     | 1.33              |
| 1:J:629:GLU:HA  | 1:J:643:GLY:O    | 1.17                     | 1.33              |
| 1:J:635:GLY:CA  | 4:W:334:GLU:HG2  | 1.59                     | 1.33              |
| 1:G:530:MET:HA  | 4:V:354:GLN:CG   | 1.57                     | 1.33              |
| 2:E:117:LEU:HB2 | 2:E:147:ASN:ND2  | 1.39                     | 1.33              |
| 4:1:287:ILE:CG2 | 4:3:202:THR:CB   | 1.87                     | 1.33              |
| 1:P:635:GLY:CA  | 4:0:334:GLU:HG2  | 1.59                     | 1.33              |
| 1:M:530:MET:HA  | 4:Z:354:GLN:CG   | 1.56                     | 1.33              |
| 1:J:534:SER:O   | 4:W:351:THR:CG2  | 1.64                     | 1.33              |
| 1:A:834:LEU:CD2 | 2:B:54:MET:HE3   | 1.51                     | 1.33              |
| 4:3:288:ASP:OD2 | 4:5:203:THR:CG2  | 1.72                     | 1.33              |
| 1:D:721:LYS:CG  | 1:D:736:GLN:CD   | 1.98                     | 1.32              |
| 1:P:819:ASN:CG  | 2:Q:92:ASP:HB2   | 1.48                     | 1.32              |
| 2:E:114:LYS:CA  | 2:E:146:GLY:O    | 1.76                     | 1.32              |
| 2:E:117:LEU:CD1 | 2:E:147:ASN:OD1  | 1.74                     | 1.32              |
| 2:H:117:LEU:CD1 | 2:H:147:ASN:OD1  | 1.74                     | 1.32              |
| 1:D:721:LYS:HG2 | 1:D:736:GLN:OE1  | 1.29                     | 1.32              |
| 2:N:114:LYS:CA  | 2:N:146:GLY:O    | 1.76                     | 1.32              |
| 1:A:735:GLY:O   | 1:A:743:ALA:HB2  | 1.29                     | 1.32              |
| 1:G:721:LYS:CG  | 1:G:736:GLN:CD   | 1.98                     | 1.32              |
| 1:G:730:SER:OG  | 3:I:113:THR:CG2  | 1.75                     | 1.32              |
| 4:0:243:PRO:C   | 4:Y:291:LYS:CE   | 1.78                     | 1.32              |
| 1:J:721:LYS:CG  | 1:J:736:GLN:CD   | 1.98                     | 1.32              |
| 1:P:792:ALA:CB  | 3:R:42:THR:HG22  | 1.60                     | 1.32              |
| 1:A:831:TRP:CZ3 | 2:B:34:ILE:HG12  | 1.63                     | 1.32              |
| 1:G:725:ARG:NE  | 1:G:733:PRO:HB3  | 0.99                     | 1.32              |
| 1:M:795:ARG:CG  | 3:O:118:MET:HE3  | 1.58                     | 1.32              |
| 1:M:629:GLU:HA  | 1:M:643:GLY:O    | 1.17                     | 1.32              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:725:ARG:NE   | 1:D:733:PRO:HB3 | 1.00                     | 1.32              |
| 1:A:502:GLU:CA   | 1:A:761:GLY:HA3 | 1.57                     | 1.32              |
| 1:P:819:ASN:OD1  | 2:Q:92:ASP:N    | 1.59                     | 1.32              |
| 2:Q:117:LEU:CD1  | 2:Q:147:ASN:OD1 | 1.74                     | 1.32              |
| 4:1:287:ILE:CB   | 4:3:202:THR:HB  | 1.60                     | 1.32              |
| 1:M:548:THR:O    | 4:1:47:MET:CA   | 1.76                     | 1.32              |
| 1:D:629:GLU:HA   | 1:D:643:GLY:O   | 1.17                     | 1.32              |
| 1:P:534:SER:O    | 4:0:351:THR:CG2 | 1.64                     | 1.32              |
| 1:M:635:GLY:CA   | 4:Z:334:GLU:HG2 | 1.59                     | 1.32              |
| 1:P:785:GLU:C    | 1:P:786:ILE:N   | 1.81                     | 1.32              |
| 4:0:167:GLU:CD   | 4:2:42:GLY:HA3  | 1.50                     | 1.32              |
| 2:K:114:LYS:CA   | 2:K:146:GLY:O   | 1.76                     | 1.31              |
| 1:P:729:ALA:C    | 3:R:93:VAL:HG22 | 1.48                     | 1.31              |
| 1:J:725:ARG:NE   | 1:J:733:PRO:HB3 | 0.99                     | 1.31              |
| 2:K:121:LEU:O    | 2:K:128:PHE:CB  | 1.79                     | 1.31              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:CD  | 1.98                     | 1.31              |
| 1:A:538:GLU:O    | 4:8:349:LEU:CD1 | 1.78                     | 1.31              |
| 1:M:725:ARG:NE   | 1:M:733:PRO:HB3 | 1.00                     | 1.31              |
| 1:A:93:MET:HE2   | 1:A:715:VAL:CA  | 1.58                     | 1.31              |
| 2:Q:117:LEU:HB2  | 2:Q:147:ASN:ND2 | 1.39                     | 1.31              |
| 1:M:721:LYS:CG   | 1:M:736:GLN:CD  | 1.98                     | 1.31              |
| 1:D:724:TYR:HA   | 1:D:782:MLY:CD  | 1.43                     | 1.31              |
| 2:Q:114:LYS:CA   | 2:Q:146:GLY:O   | 1.76                     | 1.31              |
| 1:P:725:ARG:NE   | 1:P:733:PRO:HB3 | 1.00                     | 1.31              |
| 1:J:818:TYR:CE1  | 2:K:127:ARG:NH2 | 1.96                     | 1.31              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:CD  | 1.45                     | 1.31              |
| 4:W:324:THR:HG21 | 4:Y:247:VAL:N   | 0.98                     | 1.31              |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:CZ  | 1.65                     | 1.31              |
| 1:P:793:ARG:NH1  | 3:R:40:ASN:HD22 | 1.26                     | 1.31              |
| 4:0:167:GLU:OE1  | 4:2:42:GLY:CA   | 1.79                     | 1.31              |
| 1:D:599:ASN:HA   | 1:D:649:VAL:CB  | 1.60                     | 1.31              |
| 1:A:629:GLU:HA   | 1:A:643:GLY:O   | 1.17                     | 1.31              |
| 2:E:121:LEU:O    | 2:E:128:PHE:CB  | 1.79                     | 1.30              |
| 4:0:167:GLU:OE1  | 4:2:42:GLY:HA3  | 1.21                     | 1.30              |
| 1:A:635:GLY:CA   | 4:8:334:GLU:HG2 | 1.58                     | 1.30              |
| 1:G:635:GLY:CA   | 4:V:334:GLU:HG2 | 1.59                     | 1.30              |
| 1:G:629:GLU:HA   | 1:G:643:GLY:O   | 1.17                     | 1.30              |
| 1:A:817:GLN:OE1  | 2:B:127:ARG:NE  | 1.62                     | 1.30              |
| 1:P:538:GLU:O    | 4:0:349:LEU:CD1 | 1.78                     | 1.30              |
| 1:A:725:ARG:NE   | 1:A:733:PRO:HB3 | 1.00                     | 1.30              |
| 1:M:795:ARG:HB3  | 3:O:35:ARG:NH2  | 1.45                     | 1.30              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:95:THR:OG1   | 1:A:769:ALA:HA   | 1.20                     | 1.30              |
| 1:P:795:ARG:CD   | 3:R:43:ASN:OD1   | 1.79                     | 1.30              |
| 1:M:783:LEU:CG   | 1:M:786:ILE:CD1  | 2.10                     | 1.30              |
| 1:J:599:ASN:HA   | 1:J:649:VAL:CB   | 1.60                     | 1.30              |
| 1:J:792:ALA:CB   | 3:L:42:THR:CG2   | 2.08                     | 1.30              |
| 1:P:721:LYS:CG   | 1:P:736:GLN:CD   | 1.98                     | 1.30              |
| 2:B:121:LEU:O    | 2:B:128:PHE:CB   | 1.79                     | 1.30              |
| 1:D:767:PHE:O    | 1:D:771:LEU:CD1  | 1.79                     | 1.30              |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:CD2   | 1.60                     | 1.30              |
| 1:D:506:GLU:OE2  | 1:D:764:MLY:HH22 | 1.18                     | 1.30              |
| 1:A:757:GLN:CG   | 1:A:771:LEU:CD1  | 2.05                     | 1.30              |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:CD2  | 1.59                     | 1.30              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:CD   | 1.45                     | 1.30              |
| 1:D:767:PHE:C    | 1:D:771:LEU:HD11 | 1.51                     | 1.30              |
| 1:P:599:ASN:HA   | 1:P:649:VAL:CB   | 1.60                     | 1.30              |
| 1:P:819:ASN:CA   | 2:Q:90:GLY:O     | 1.79                     | 1.29              |
| 1:A:735:GLY:C    | 1:A:743:ALA:CB   | 2.01                     | 1.29              |
| 1:A:599:ASN:HA   | 1:A:649:VAL:CB   | 1.60                     | 1.29              |
| 1:P:537:GLU:C    | 4:O:349:LEU:HD13 | 1.52                     | 1.29              |
| 1:G:735:GLY:C    | 1:G:743:ALA:CB   | 2.01                     | 1.29              |
| 1:P:548:THR:HG21 | 4:2:49:GLN:N     | 0.97                     | 1.29              |
| 1:A:754:ASP:OD2  | 1:A:778:MET:HE3  | 1.28                     | 1.29              |
| 1:P:729:ALA:HB1  | 3:R:93:VAL:CG2   | 1.58                     | 1.29              |
| 1:G:735:GLY:O    | 1:G:743:ALA:HB2  | 1.29                     | 1.29              |
| 1:P:548:THR:CG2  | 4:2:49:GLN:CB    | 2.09                     | 1.29              |
| 1:G:599:ASN:HA   | 1:G:649:VAL:CB   | 1.60                     | 1.29              |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CG   | 1.61                     | 1.29              |
| 1:A:93:MET:CE    | 1:A:715:VAL:HA   | 1.59                     | 1.29              |
| 1:G:538:GLU:O    | 4:V:349:LEU:CD1  | 1.78                     | 1.29              |
| 2:Q:121:LEU:O    | 2:Q:128:PHE:CB   | 1.78                     | 1.29              |
| 1:A:831:TRP:CZ3  | 2:B:50:THR:CG2   | 2.16                     | 1.29              |
| 1:D:818:TYR:CB   | 2:E:90:GLY:CA    | 1.95                     | 1.29              |
| 1:M:795:ARG:CG   | 3:O:118:MET:CE   | 2.10                     | 1.29              |
| 1:M:735:GLY:C    | 1:M:743:ALA:CB   | 2.01                     | 1.29              |
| 1:G:93:MET:HG2   | 1:G:714:ARG:C    | 0.91                     | 1.29              |
| 1:M:599:ASN:HA   | 1:M:649:VAL:CB   | 1.60                     | 1.29              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:HB2  | 1.72                     | 1.29              |
| 1:G:537:GLU:C    | 4:V:349:LEU:HD13 | 1.53                     | 1.29              |
| 1:P:817:GLN:CG   | 2:Q:127:ARG:CD   | 2.09                     | 1.29              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:CD   | 1.53                     | 1.29              |
| 1:A:721:LYS:HG3  | 1:A:736:GLN:CD   | 1.53                     | 1.29              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:537:GLU:C    | 4:W:349:LEU:HD13 | 1.52                     | 1.29              |
| 1:M:84:MLY:HB3   | 1:M:723:ARG:NE   | 1.43                     | 1.29              |
| 1:P:805:ALA:O    | 1:P:809:ARG:N    | 1.64                     | 1.29              |
| 1:A:149:GLN:NE2  | 1:A:718:ALA:CB   | 1.96                     | 1.28              |
| 1:P:818:TYR:CE1  | 2:Q:127:ARG:NH2  | 1.98                     | 1.28              |
| 1:J:721:LYS:HG2  | 1:J:736:GLN:OE1  | 1.29                     | 1.28              |
| 1:D:795:ARG:CD   | 3:F:43:ASN:OD1   | 1.79                     | 1.28              |
| 1:J:735:GLY:C    | 1:J:743:ALA:CB   | 2.01                     | 1.28              |
| 1:P:797:PHE:CE2  | 3:R:146:ILE:HD12 | 1.68                     | 1.28              |
| 1:P:767:PHE:CD1  | 1:P:772:LEU:HD21 | 1.65                     | 1.28              |
| 1:D:735:GLY:C    | 1:D:743:ALA:CB   | 2.01                     | 1.28              |
| 2:H:121:LEU:O    | 2:H:128:PHE:CB   | 1.79                     | 1.28              |
| 1:A:795:ARG:HB3  | 3:C:35:ARG:NH1   | 1.46                     | 1.28              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:HH12  | 1.45                     | 1.28              |
| 1:P:502:GLU:OE2  | 1:P:761:GLY:HA3  | 1.33                     | 1.28              |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:CZ   | 1.67                     | 1.28              |
| 1:P:735:GLY:O    | 1:P:743:ALA:HB2  | 1.29                     | 1.28              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:CD   | 1.53                     | 1.28              |
| 1:P:215:GLN:N    | 1:P:340:ILE:HG12 | 1.19                     | 1.28              |
| 1:D:215:GLN:N    | 1:D:340:ILE:HG12 | 1.19                     | 1.28              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:HD21 | 1.64                     | 1.28              |
| 2:N:121:LEU:O    | 2:N:128:PHE:CB   | 1.79                     | 1.28              |
| 4:O:288:ASP:CB   | 4:2:63:GLY:HA3   | 1.64                     | 1.28              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:CA    | 1.63                     | 1.28              |
| 1:G:754:ASP:CA   | 1:G:779:ARG:CD   | 1.99                     | 1.27              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:CD2  | 1.64                     | 1.27              |
| 1:A:721:LYS:CG   | 1:A:736:GLN:OE1  | 1.82                     | 1.27              |
| 1:A:537:GLU:C    | 4:8:349:LEU:HD13 | 1.52                     | 1.27              |
| 1:M:797:PHE:CD1  | 3:O:149:VAL:CG1  | 2.15                     | 1.27              |
| 4:3:288:ASP:OD2  | 4:5:203:THR:HG21 | 1.14                     | 1.27              |
| 1:J:215:GLN:N    | 1:J:340:ILE:HG12 | 1.19                     | 1.27              |
| 1:A:499:GLU:OE1  | 1:A:766:PHE:HZ   | 1.08                     | 1.27              |
| 1:G:552:ASN:O    | 4:X:47:MET:SD    | 1.91                     | 1.27              |
| 4:X:324:THR:OG1  | 4:Z:246:GLN:HA   | 1.14                     | 1.27              |
| 1:P:735:GLY:C    | 1:P:743:ALA:CB   | 2.01                     | 1.27              |
| 1:M:553:MLY:HE2  | 4:1:43:VAL:CG2   | 1.63                     | 1.27              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:HB    | 1.69                     | 1.27              |
| 1:M:721:LYS:CG   | 1:M:736:GLN:CG   | 1.97                     | 1.27              |
| 1:P:506:GLU:CD   | 1:P:760:PHE:O    | 1.73                     | 1.27              |
| 1:P:534:SER:O    | 4:O:351:THR:CA   | 1.81                     | 1.27              |
| 1:D:799:MET:SD   | 3:F:32:ASP:HB3   | 1.75                     | 1.27              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:506:GLU:HB2  | 1:A:760:PHE:O    | 1.13                     | 1.27              |
| 1:P:721:LYS:CG   | 1:P:736:GLN:OE1  | 1.83                     | 1.27              |
| 1:J:721:LYS:CG   | 1:J:736:GLN:OE1  | 1.83                     | 1.27              |
| 1:J:538:GLU:O    | 4:W:349:LEU:CD1  | 1.78                     | 1.27              |
| 1:P:508:ILE:CD1  | 1:P:759:ALA:HB2  | 1.65                     | 1.27              |
| 1:D:831:TRP:CD1  | 2:E:51:PHE:HZ    | 1.52                     | 1.27              |
| 1:J:557:GLU:CA   | 4:Y:47:MET:HA    | 1.08                     | 1.27              |
| 4:O:166:TYR:CZ   | 4:2:64:ILE:HG21  | 1.69                     | 1.27              |
| 1:P:721:LYS:CG   | 1:P:736:GLN:CG   | 1.97                     | 1.27              |
| 1:P:721:LYS:HG2  | 1:P:736:GLN:OE1  | 1.29                     | 1.27              |
| 1:J:534:SER:O    | 4:W:351:THR:CA   | 1.82                     | 1.27              |
| 1:G:792:ALA:CB   | 3:I:42:THR:CA    | 2.13                     | 1.26              |
| 1:M:534:SER:O    | 4:Z:351:THR:CA   | 1.82                     | 1.26              |
| 1:M:537:GLU:C    | 4:Z:349:LEU:HD13 | 1.52                     | 1.26              |
| 1:G:721:LYS:HG2  | 1:G:736:GLN:OE1  | 1.29                     | 1.26              |
| 1:D:815:CYS:SG   | 2:E:92:ASP:HB2   | 1.73                     | 1.26              |
| 1:A:534:SER:O    | 4:8:351:THR:CA   | 1.81                     | 1.26              |
| 1:A:757:GLN:OE1  | 1:A:771:LEU:HD12 | 1.14                     | 1.26              |
| 4:1:288:ASP:OD2  | 4:3:203:THR:HG21 | 1.32                     | 1.26              |
| 1:J:84:MLY:HH11  | 1:J:720:PHE:CE1  | 1.70                     | 1.26              |
| 1:M:721:LYS:HG3  | 1:M:736:GLN:CD   | 1.54                     | 1.26              |
| 1:D:721:LYS:CG   | 1:D:736:GLN:OE1  | 1.83                     | 1.26              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:CG   | 1.95                     | 1.26              |
| 1:J:733:PRO:O    | 1:J:737:PHE:HD1  | 0.93                     | 1.26              |
| 1:J:819:ASN:CA   | 2:K:90:GLY:O     | 1.82                     | 1.26              |
| 1:J:28:GLN:CD    | 1:J:723:ARG:NH1  | 1.87                     | 1.26              |
| 1:D:534:SER:O    | 4:9:351:THR:CA   | 1.81                     | 1.26              |
| 4:3:288:ASP:CG   | 4:5:203:THR:HG23 | 1.47                     | 1.26              |
| 1:J:28:GLN:CB    | 1:J:723:ARG:NH1  | 1.97                     | 1.26              |
| 1:D:537:GLU:C    | 4:9:349:LEU:HD13 | 1.52                     | 1.26              |
| 1:P:721:LYS:HG3  | 1:P:736:GLN:CD   | 1.54                     | 1.26              |
| 1:M:538:GLU:O    | 4:Z:349:LEU:CD1  | 1.78                     | 1.26              |
| 1:M:721:LYS:CG   | 1:M:736:GLN:OE1  | 1.83                     | 1.26              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:HB   | 1.28                     | 1.26              |
| 1:A:149:GLN:OE1  | 1:A:716:LEU:HD23 | 1.11                     | 1.25              |
| 1:D:815:CYS:SG   | 2:E:92:ASP:CB    | 2.23                     | 1.25              |
| 1:M:34:ALA:CB    | 1:M:777:GLU:OE2  | 1.83                     | 1.25              |
| 1:D:797:PHE:HE2  | 3:F:126:LEU:CD2  | 1.46                     | 1.25              |
| 1:G:752:ASP:O    | 1:G:780:ASP:HA   | 1.18                     | 1.25              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:CE   | 1.49                     | 1.25              |
| 1:J:756:THR:HG21 | 1:J:776:GLU:O    | 1.32                     | 1.25              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:721:LYS:HG3  | 1:D:736:GLN:CD   | 1.53                     | 1.25              |
| 2:N:117:LEU:CD1  | 2:N:147:ASN:CG   | 2.05                     | 1.25              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:CG   | 2.05                     | 1.25              |
| 1:M:553:MLY:CG   | 4:1:43:VAL:HG21  | 1.65                     | 1.25              |
| 1:D:538:GLU:O    | 4:9:349:LEU:CD1  | 1.78                     | 1.25              |
| 1:G:721:LYS:CG   | 1:G:736:GLN:OE1  | 1.83                     | 1.25              |
| 1:A:795:ARG:CB   | 3:C:35:ARG:NH1   | 1.98                     | 1.25              |
| 1:D:831:TRP:NE1  | 2:E:51:PHE:CZ    | 2.04                     | 1.25              |
| 1:M:35:MLY:CH2   | 1:M:778:MET:HG2  | 1.65                     | 1.25              |
| 1:G:819:ASN:ND2  | 2:H:92:ASP:HB2   | 1.50                     | 1.25              |
| 1:G:733:PRO:O    | 1:G:737:PHE:HD1  | 0.93                     | 1.25              |
| 1:J:630:ALA:O    | 4:W:25:ASP:OD2   | 1.52                     | 1.25              |
| 1:D:791:GLN:CD   | 3:F:116:GLU:H    | 1.38                     | 1.25              |
| 1:A:149:GLN:HB3  | 1:A:719:ASP:N    | 1.51                     | 1.25              |
| 1:A:499:GLU:OE1  | 1:A:766:PHE:CZ   | 1.90                     | 1.25              |
| 1:G:534:SER:O    | 4:V:351:THR:CA   | 1.83                     | 1.25              |
| 4:X:324:THR:CB   | 4:Z:246:GLN:HA   | 1.66                     | 1.25              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:CG   | 2.05                     | 1.25              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:OD1  | 1.32                     | 1.25              |
| 1:P:786:ILE:C    | 1:P:787:ILE:N    | 1.89                     | 1.25              |
| 1:P:769:ALA:C    | 1:P:771:LEU:H    | 1.39                     | 1.25              |
| 1:A:757:GLN:CD   | 1:A:771:LEU:CD1  | 2.04                     | 1.24              |
| 1:M:819:ASN:CG   | 2:N:92:ASP:HB2   | 1.50                     | 1.24              |
| 1:M:817:GLN:CD   | 2:N:127:ARG:HD2  | 1.54                     | 1.24              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:CG   | 2.05                     | 1.24              |
| 1:P:733:PRO:O    | 1:P:737:PHE:HD1  | 0.92                     | 1.24              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:CG   | 2.05                     | 1.24              |
| 1:P:552:ASN:HD22 | 4:2:49:GLN:CG    | 1.49                     | 1.24              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:CG   | 2.15                     | 1.24              |
| 1:M:735:GLY:O    | 1:M:743:ALA:HB2  | 1.29                     | 1.24              |
| 1:G:97:LEU:CD2   | 1:G:712:PRO:CB   | 2.13                     | 1.24              |
| 1:G:797:PHE:CZ   | 3:I:126:LEU:HD22 | 1.70                     | 1.24              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:CD1  | 1.86                     | 1.24              |
| 1:J:817:GLN:CG   | 2:K:127:ARG:HD2  | 1.65                     | 1.24              |
| 4:0:112:PRO:CG   | 4:1:195:GLU:C    | 2.00                     | 1.24              |
| 4:9:322:PRO:CB   | 4:W:244:ASP:OD2  | 1.86                     | 1.24              |
| 1:P:630:ALA:O    | 4:0:25:ASP:OD2   | 1.52                     | 1.24              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:HD11 | 1.73                     | 1.24              |
| 4:X:324:THR:CB   | 4:Z:246:GLN:CA   | 2.15                     | 1.24              |
| 1:P:641:LYS:CD   | 1:P:647:GLN:NE2  | 1.99                     | 1.24              |
| 1:A:799:MET:SD   | 3:C:32:ASP:CB    | 2.26                     | 1.24              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:646:PHE:CE2  | 1:M:652:LEU:HD11 | 1.73                     | 1.24              |
| 4:V:324:THR:HG21 | 4:X:247:VAL:N    | 1.49                     | 1.24              |
| 1:P:724:TYR:HE1  | 1:P:776:GLU:OE2  | 1.11                     | 1.24              |
| 1:A:791:GLN:OE1  | 3:C:116:GLU:HG3  | 1.30                     | 1.24              |
| 1:D:768:MLY:O    | 1:D:771:LEU:HD12 | 1.32                     | 1.24              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:HD11 | 1.73                     | 1.24              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:NZ   | 1.52                     | 1.24              |
| 1:J:735:GLY:O    | 1:J:743:ALA:HB2  | 1.29                     | 1.24              |
| 1:P:793:ARG:HH11 | 3:R:40:ASN:ND2   | 1.31                     | 1.24              |
| 1:A:795:ARG:CD   | 3:C:43:ASN:OD1   | 1.86                     | 1.24              |
| 1:A:538:GLU:O    | 4:8:349:LEU:HD11 | 1.35                     | 1.24              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:CG   | 2.16                     | 1.24              |
| 1:M:641:LYS:CD   | 1:M:647:GLN:NE2  | 1.99                     | 1.24              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:HD11 | 1.73                     | 1.24              |
| 1:M:783:LEU:CA   | 1:M:786:ILE:HG13 | 1.66                     | 1.23              |
| 1:D:769:ALA:CA   | 1:D:771:LEU:HA   | 1.66                     | 1.23              |
| 4:0:288:ASP:CG   | 4:2:63:GLY:N     | 1.92                     | 1.23              |
| 1:D:792:ALA:HB2  | 3:F:42:THR:CG2   | 1.66                     | 1.23              |
| 4:7:322:PRO:CB   | 4:9:244:ASP:OD2  | 1.86                     | 1.23              |
| 4:V:325:MET:SD   | 4:X:244:ASP:HB2  | 1.77                     | 1.23              |
| 1:D:791:GLN:NE2  | 3:F:116:GLU:N    | 1.86                     | 1.23              |
| 1:D:813:ILE:HD13 | 2:E:128:PHE:CE1  | 1.73                     | 1.23              |
| 1:P:641:LYS:CG   | 1:P:647:GLN:CG   | 2.16                     | 1.23              |
| 1:M:629:GLU:CA   | 1:M:643:GLY:O    | 1.87                     | 1.23              |
| 1:A:95:THR:OG1   | 1:A:769:ALA:CA   | 1.85                     | 1.23              |
| 4:8:322:PRO:CB   | 4:V:244:ASP:OD2  | 1.86                     | 1.23              |
| 1:D:735:GLY:O    | 1:D:743:ALA:HB2  | 1.29                     | 1.23              |
| 1:G:557:GLU:CB   | 4:X:46:GLY:O     | 1.86                     | 1.23              |
| 1:P:729:ALA:C    | 3:R:93:VAL:CG2   | 2.07                     | 1.23              |
| 1:J:819:ASN:CG   | 2:K:92:ASP:HB2   | 1.05                     | 1.23              |
| 1:M:538:GLU:C    | 4:Z:349:LEU:HD12 | 1.48                     | 1.23              |
| 1:D:733:PRO:O    | 1:D:737:PHE:HD1  | 0.93                     | 1.23              |
| 2:Q:117:LEU:CD1  | 2:Q:147:ASN:CG   | 2.05                     | 1.23              |
| 4:X:324:THR:CB   | 4:Z:246:GLN:N    | 1.99                     | 1.23              |
| 1:P:538:GLU:C    | 4:0:349:LEU:HD12 | 1.48                     | 1.23              |
| 1:P:646:PHE:CE2  | 1:P:652:LEU:HD11 | 1.73                     | 1.23              |
| 1:A:721:LYS:HG2  | 1:A:736:GLN:OE1  | 1.29                     | 1.23              |
| 1:A:733:PRO:O    | 1:A:737:PHE:HD1  | 0.92                     | 1.23              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:HD11 | 1.73                     | 1.23              |
| 1:M:721:LYS:HG2  | 1:M:736:GLN:OE1  | 1.29                     | 1.23              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:NE2  | 1.99                     | 1.23              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:629:GLU:CA   | 1:A:643:GLY:O    | 1.87                     | 1.23              |
| 1:A:630:ALA:O    | 4:8:25:ASP:OD2   | 1.53                     | 1.23              |
| 1:G:538:GLU:O    | 4:V:349:LEU:HD11 | 1.34                     | 1.23              |
| 2:Q:121:LEU:C    | 2:Q:128:PHE:CB   | 2.07                     | 1.23              |
| 1:M:505:MLY:CD   | 1:M:762:HIS:CE1  | 2.22                     | 1.23              |
| 1:M:534:SER:O    | 4:Z:351:THR:CB   | 1.87                     | 1.23              |
| 4:W:324:THR:CG2  | 4:Y:247:VAL:N    | 1.89                     | 1.23              |
| 1:M:215:GLN:N    | 1:M:340:ILE:HG12 | 1.19                     | 1.23              |
| 1:D:795:ARG:CZ   | 3:F:116:GLU:CD   | 2.03                     | 1.22              |
| 1:A:752:ASP:OD2  | 1:A:782:MLY:HD3  | 1.36                     | 1.22              |
| 4:0:166:TYR:OH   | 4:2:64:ILE:HG21  | 1.33                     | 1.22              |
| 1:G:754:ASP:OD2  | 1:G:779:ARG:HB2  | 1.29                     | 1.22              |
| 2:B:121:LEU:C    | 2:B:128:PHE:CB   | 2.07                     | 1.22              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HD11 | 1.65                     | 1.22              |
| 1:A:534:SER:O    | 4:8:351:THR:CB   | 1.87                     | 1.22              |
| 1:M:641:LYS:CG   | 1:M:647:GLN:CG   | 2.16                     | 1.22              |
| 1:P:215:GLN:N    | 1:P:340:ILE:CG1  | 2.02                     | 1.22              |
| 1:A:215:GLN:N    | 1:A:340:ILE:CG1  | 2.02                     | 1.22              |
| 1:D:630:ALA:O    | 4:9:25:ASP:OD2   | 1.52                     | 1.22              |
| 1:M:630:ALA:O    | 4:Z:25:ASP:OD2   | 1.52                     | 1.22              |
| 1:D:797:PHE:CG   | 3:F:146:ILE:HG23 | 1.74                     | 1.22              |
| 1:D:797:PHE:CD1  | 3:F:146:ILE:CG2  | 2.21                     | 1.22              |
| 1:G:791:GLN:HE22 | 3:I:115:GLY:CA   | 1.52                     | 1.22              |
| 1:G:538:GLU:C    | 4:V:349:LEU:HD12 | 1.48                     | 1.22              |
| 1:M:548:THR:O    | 4:1:47:MET:HA    | 1.06                     | 1.22              |
| 1:P:793:ARG:NH1  | 3:R:40:ASN:ND2   | 1.87                     | 1.22              |
| 1:P:798:LEU:CD2  | 3:R:126:LEU:CD1  | 2.12                     | 1.22              |
| 1:D:641:LYS:CD   | 1:D:647:GLN:NE2  | 1.99                     | 1.22              |
| 1:G:215:GLN:N    | 1:G:340:ILE:CG1  | 2.02                     | 1.22              |
| 1:A:707:CYS:CA   | 1:A:714:ARG:NH1  | 2.03                     | 1.22              |
| 2:Q:144:VAL:CG1  | 2:Q:153:ILE:HD11 | 1.65                     | 1.22              |
| 2:E:121:LEU:C    | 2:E:128:PHE:CB   | 2.07                     | 1.22              |
| 4:1:287:ILE:CB   | 4:3:203:THR:N    | 2.00                     | 1.22              |
| 1:P:534:SER:O    | 4:0:351:THR:CB   | 1.87                     | 1.22              |
| 1:P:797:PHE:CE1  | 3:R:146:ILE:O    | 1.91                     | 1.22              |
| 1:P:798:LEU:CD1  | 3:R:126:LEU:HD11 | 1.67                     | 1.22              |
| 1:A:830:PRO:HB2  | 2:B:51:PHE:CE1   | 1.73                     | 1.22              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:CG   | 2.16                     | 1.22              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:OD1  | 1.32                     | 1.22              |
| 1:P:629:GLU:CA   | 1:P:643:GLY:O    | 1.87                     | 1.22              |
| 1:D:534:SER:O    | 4:9:351:THR:CB   | 1.88                     | 1.22              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:795:ARG:CZ   | 3:C:116:GLU:OE2  | 1.86                     | 1.22              |
| 1:G:93:MET:CB    | 1:G:714:ARG:O    | 1.88                     | 1.22              |
| 1:G:567:LYS:NZ   | 4:X:92:ASN:ND2   | 1.87                     | 1.22              |
| 4:1:203:THR:HG21 | 4:Z:288:ASP:OD2  | 1.14                     | 1.22              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CZ    | 2.26                     | 1.22              |
| 1:J:795:ARG:HB3  | 3:L:35:ARG:CZ    | 1.68                     | 1.21              |
| 1:G:752:ASP:OD1  | 1:G:780:ASP:O    | 1.58                     | 1.21              |
| 1:A:506:GLU:CB   | 1:A:760:PHE:O    | 1.88                     | 1.21              |
| 1:M:818:TYR:CE1  | 2:N:127:ARG:NH2  | 2.08                     | 1.21              |
| 1:G:629:GLU:CA   | 1:G:643:GLY:O    | 1.87                     | 1.21              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HD11 | 1.64                     | 1.21              |
| 1:D:538:GLU:C    | 4:9:349:LEU:HD12 | 1.48                     | 1.21              |
| 1:P:552:ASN:ND2  | 4:2:49:GLN:CG    | 2.03                     | 1.21              |
| 1:M:733:PRO:O    | 1:M:737:PHE:HD1  | 0.93                     | 1.21              |
| 2:B:54:MET:HA    | 2:H:21:GLU:OE1   | 1.36                     | 1.21              |
| 1:J:215:GLN:N    | 1:J:340:ILE:CG1  | 2.02                     | 1.21              |
| 2:N:121:LEU:C    | 2:N:128:PHE:CB   | 2.07                     | 1.21              |
| 1:G:817:GLN:OE1  | 2:H:127:ARG:HD2  | 1.06                     | 1.21              |
| 1:M:793:ARG:NH1  | 3:O:40:ASN:HD22  | 1.33                     | 1.21              |
| 1:A:641:LYS:CG   | 1:A:647:GLN:HG3  | 1.71                     | 1.21              |
| 1:D:215:GLN:N    | 1:D:340:ILE:CG1  | 2.02                     | 1.21              |
| 1:M:215:GLN:N    | 1:M:340:ILE:CG1  | 2.02                     | 1.21              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:CD   | 2.03                     | 1.21              |
| 1:J:534:SER:O    | 4:W:351:THR:CB   | 1.88                     | 1.21              |
| 1:M:786:ILE:CB   | 1:M:787:ILE:N    | 2.04                     | 1.21              |
| 4:3:287:ILE:HD13 | 4:5:203:THR:HB   | 1.22                     | 1.21              |
| 1:D:629:GLU:CA   | 1:D:643:GLY:O    | 1.87                     | 1.21              |
| 1:G:800:ARG:NH2  | 3:I:40:ASN:OD1   | 1.74                     | 1.21              |
| 1:A:754:ASP:OD2  | 1:A:778:MET:CE   | 1.89                     | 1.21              |
| 1:P:817:GLN:CD   | 2:Q:127:ARG:HD2  | 1.59                     | 1.21              |
| 1:G:813:ILE:CG2  | 2:H:128:PHE:CE1  | 2.22                     | 1.21              |
| 1:G:93:MET:SD    | 1:G:714:ARG:O    | 1.97                     | 1.21              |
| 1:G:788:THR:O    | 3:I:42:THR:HG21  | 1.36                     | 1.21              |
| 2:K:121:LEU:C    | 2:K:128:PHE:CB   | 2.07                     | 1.21              |
| 1:P:785:GLU:CG   | 3:R:81:GLN:HG3   | 1.69                     | 1.21              |
| 1:D:553:MLY:CE   | 4:W:45:VAL:HA    | 1.52                     | 1.21              |
| 1:D:641:LYS:CG   | 1:D:647:GLN:HG3  | 1.70                     | 1.21              |
| 1:M:834:LEU:HD13 | 2:N:51:PHE:CE1   | 1.75                     | 1.21              |
| 2:Q:117:LEU:CD1  | 2:Q:147:ASN:CB   | 2.19                     | 1.20              |
| 4:1:288:ASP:CG   | 4:3:203:THR:HG21 | 1.59                     | 1.20              |
| 2:H:121:LEU:C    | 2:H:128:PHE:CB   | 2.07                     | 1.20              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:721:LYS:CG   | 1:A:736:GLN:CG   | 1.96                     | 1.20              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:HD21 | 1.72                     | 1.20              |
| 1:G:795:ARG:HG2  | 3:I:118:MET:CE   | 1.69                     | 1.20              |
| 4:1:288:ASP:CG   | 4:3:203:THR:CG2  | 2.09                     | 1.20              |
| 1:J:629:GLU:CA   | 1:J:643:GLY:O    | 1.87                     | 1.20              |
| 1:M:783:LEU:CG   | 1:M:786:ILE:HD12 | 1.71                     | 1.20              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:HG3  | 1.71                     | 1.20              |
| 1:P:817:GLN:CB   | 2:Q:127:ARG:HD2  | 1.70                     | 1.20              |
| 1:P:795:ARG:HB3  | 3:R:35:ARG:NH2   | 1.55                     | 1.20              |
| 1:G:736:GLN:N    | 1:G:743:ALA:CB   | 2.05                     | 1.20              |
| 1:G:503:TYR:CE1  | 1:G:711:PHE:CE2  | 2.29                     | 1.20              |
| 1:M:34:ALA:HB3   | 1:M:777:GLU:OE2  | 1.35                     | 1.20              |
| 4:2:322:PRO:HB3  | 4:4:244:ASP:OD2  | 1.39                     | 1.20              |
| 1:G:534:SER:O    | 4:V:351:THR:CB   | 1.88                     | 1.20              |
| 1:P:538:GLU:OE2  | 4:0:355:MET:CE   | 1.90                     | 1.20              |
| 1:J:84:MLY:CH1   | 1:J:720:PHE:CD1  | 2.22                     | 1.20              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:CB    | 2.23                     | 1.20              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:NE2  | 1.99                     | 1.20              |
| 1:J:557:GLU:HA   | 4:Y:47:MET:C     | 1.62                     | 1.20              |
| 4:1:287:ILE:CG1  | 4:3:202:THR:CA   | 2.19                     | 1.20              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD2  | 1.70                     | 1.20              |
| 1:A:538:GLU:C    | 4:8:349:LEU:HD11 | 1.54                     | 1.20              |
| 1:J:94:MET:O     | 1:J:713:SER:CB   | 1.90                     | 1.20              |
| 1:G:783:LEU:O    | 1:G:787:ILE:N    | 1.71                     | 1.19              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:CB   | 2.19                     | 1.19              |
| 1:A:791:GLN:NE2  | 3:C:116:GLU:N    | 1.81                     | 1.19              |
| 1:P:641:LYS:CG   | 1:P:647:GLN:HG3  | 1.71                     | 1.19              |
| 1:J:795:ARG:NH2  | 3:L:116:GLU:CD   | 1.74                     | 1.19              |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:CB   | 1.54                     | 1.19              |
| 2:H:117:LEU:CD1  | 2:H:147:ASN:CB   | 2.19                     | 1.19              |
| 1:M:548:THR:O    | 4:1:47:MET:SD    | 1.99                     | 1.19              |
| 1:P:798:LEU:CD1  | 3:R:126:LEU:CD1  | 2.20                     | 1.19              |
| 1:A:797:PHE:CE2  | 3:C:146:ILE:HD12 | 1.77                     | 1.19              |
| 1:A:538:GLU:OE2  | 4:8:355:MET:CE   | 1.91                     | 1.19              |
| 4:9:322:PRO:HB2  | 4:W:244:ASP:OD2  | 1.39                     | 1.19              |
| 1:J:94:MET:O     | 1:J:713:SER:HB3  | 1.04                     | 1.19              |
| 1:D:727:LEU:CB   | 1:D:782:MLY:HH12 | 1.59                     | 1.19              |
| 1:M:505:MLY:HD2  | 1:M:762:HIS:NE2  | 1.57                     | 1.19              |
| 1:D:538:GLU:OE2  | 4:9:355:MET:CE   | 1.90                     | 1.19              |
| 1:P:552:ASN:HD21 | 4:2:49:GLN:CB    | 1.55                     | 1.19              |
| 1:M:736:GLN:N    | 1:M:743:ALA:CB   | 2.05                     | 1.19              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:215:GLN:N    | 1:G:340:ILE:HG12 | 1.19                     | 1.19              |
| 1:D:791:GLN:HE22 | 3:F:115:GLY:C    | 1.44                     | 1.19              |
| 1:D:795:ARG:HD3  | 3:F:43:ASN:OD1   | 1.35                     | 1.19              |
| 1:G:757:GLN:HG2  | 1:G:776:GLU:OE2  | 1.37                     | 1.19              |
| 1:G:538:GLU:OE2  | 4:V:355:MET:CE   | 1.90                     | 1.19              |
| 4:X:324:THR:OG1  | 4:Z:246:GLN:CA   | 1.89                     | 1.19              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:CB   | 2.19                     | 1.19              |
| 1:A:736:GLN:N    | 1:A:743:ALA:CB   | 2.05                     | 1.19              |
| 1:J:538:GLU:OE2  | 4:W:355:MET:CE   | 1.90                     | 1.19              |
| 1:M:783:LEU:CA   | 1:M:786:ILE:CG1  | 2.18                     | 1.19              |
| 1:D:726:VAL:CG1  | 1:D:785:GLU:HB3  | 1.70                     | 1.19              |
| 1:M:538:GLU:O    | 4:Z:349:LEU:HD11 | 1.35                     | 1.19              |
| 1:D:831:TRP:CE2  | 2:E:51:PHE:CZ    | 2.30                     | 1.19              |
| 1:P:721:LYS:HA   | 1:P:736:GLN:NE2  | 1.59                     | 1.18              |
| 1:D:557:GLU:H    | 4:W:48:GLY:CA    | 1.56                     | 1.18              |
| 1:A:557:GLU:H    | 4:V:48:GLY:CA    | 1.55                     | 1.18              |
| 1:A:538:GLU:C    | 4:8:349:LEU:HD12 | 1.48                     | 1.18              |
| 1:M:735:GLY:O    | 1:M:743:ALA:CB   | 1.91                     | 1.18              |
| 1:M:84:MLY:HB3   | 1:M:723:ARG:CD   | 1.73                     | 1.18              |
| 1:D:792:ALA:CB   | 3:F:42:THR:HG22  | 1.70                     | 1.18              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:CB   | 2.19                     | 1.18              |
| 1:M:538:GLU:OE2  | 4:Z:355:MET:CE   | 1.90                     | 1.18              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:HG23 | 1.41                     | 1.18              |
| 1:J:641:LYS:CG   | 1:J:647:GLN:HG3  | 1.71                     | 1.18              |
| 1:G:641:LYS:CB   | 1:G:647:GLN:NE2  | 2.07                     | 1.18              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CZ    | 1.61                     | 1.18              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:NH1   | 1.58                     | 1.18              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CE1   | 2.31                     | 1.18              |
| 2:N:117:LEU:CD1  | 2:N:147:ASN:CB   | 2.19                     | 1.18              |
| 1:P:821:ARG:NH2  | 2:Q:127:ARG:HG2  | 1.56                     | 1.18              |
| 1:J:721:LYS:HA   | 1:J:736:GLN:NE2  | 1.58                     | 1.18              |
| 1:A:817:GLN:CG   | 2:B:127:ARG:HD3  | 1.61                     | 1.18              |
| 1:M:639:GLY:HA2  | 4:Z:345:ILE:HA   | 1.26                     | 1.18              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:CD1  | 1.55                     | 1.18              |
| 1:A:795:ARG:NE   | 3:C:43:ASN:OD1   | 1.77                     | 1.18              |
| 4:0:205:GLU:HG3  | 4:Y:287:ILE:CG1  | 1.73                     | 1.18              |
| 1:M:641:LYS:CG   | 1:M:647:GLN:HG3  | 1.71                     | 1.18              |
| 1:P:834:LEU:HD13 | 2:Q:51:PHE:CE1   | 1.78                     | 1.18              |
| 1:D:735:GLY:O    | 1:D:743:ALA:CB   | 1.91                     | 1.18              |
| 1:M:817:GLN:CB   | 2:N:127:ARG:HD2  | 1.72                     | 1.18              |
| 1:J:641:LYS:CB   | 1:J:647:GLN:NE2  | 2.07                     | 1.18              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:641:LYS:CB   | 1:P:647:GLN:NE2  | 2.07                     | 1.18              |
| 1:M:641:LYS:CB   | 1:M:647:GLN:NE2  | 2.07                     | 1.18              |
| 1:G:201:ALA:O    | 1:G:202:SER:HB3  | 1.36                     | 1.18              |
| 1:D:721:LYS:HA   | 1:D:736:GLN:NE2  | 1.58                     | 1.17              |
| 1:G:796:GLY:CA   | 3:I:35:ARG:HD3   | 1.72                     | 1.17              |
| 1:G:817:GLN:OE1  | 2:H:127:ARG:CD   | 1.93                     | 1.17              |
| 1:P:538:GLU:HA   | 4:O:349:LEU:CD1  | 1.55                     | 1.17              |
| 1:J:530:MET:HE2  | 4:W:354:GLN:HG2  | 1.24                     | 1.17              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:CB    | 1.57                     | 1.17              |
| 1:A:502:GLU:HG3  | 1:A:761:GLY:N    | 1.24                     | 1.17              |
| 1:M:817:GLN:HG2  | 2:N:127:ARG:CD   | 1.65                     | 1.17              |
| 1:J:538:GLU:C    | 4:W:349:LEU:HD12 | 1.48                     | 1.17              |
| 1:D:815:CYS:SG   | 2:E:92:ASP:OD1   | 2.01                     | 1.17              |
| 1:A:553:MLY:CE   | 4:V:45:VAL:HA    | 1.52                     | 1.17              |
| 4:7:322:PRO:HB2  | 4:9:244:ASP:OD2  | 1.39                     | 1.17              |
| 1:G:819:ASN:HA   | 2:H:90:GLY:O     | 1.01                     | 1.17              |
| 1:M:530:MET:HE2  | 4:Z:354:GLN:HG2  | 1.22                     | 1.17              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:CD1  | 1.55                     | 1.17              |
| 1:P:552:ASN:ND2  | 4:2:49:GLN:CB    | 2.08                     | 1.17              |
| 1:P:548:THR:HG21 | 4:2:49:GLN:CA    | 1.75                     | 1.17              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:NE2  | 1.99                     | 1.17              |
| 4:1:203:THR:HB   | 4:Z:287:ILE:HD13 | 1.22                     | 1.17              |
| 2:E:144:VAL:CG1  | 2:E:153:ILE:HD11 | 1.64                     | 1.17              |
| 1:P:538:GLU:C    | 4:O:349:LEU:HD11 | 1.54                     | 1.17              |
| 1:P:548:THR:HG22 | 4:2:49:GLN:CB    | 1.70                     | 1.17              |
| 1:D:641:LYS:CB   | 1:D:647:GLN:NE2  | 2.07                     | 1.17              |
| 1:D:791:GLN:NE2  | 3:F:116:GLU:H    | 1.35                     | 1.17              |
| 1:D:727:LEU:CD1  | 1:D:782:MLY:CG   | 2.22                     | 1.17              |
| 1:G:792:ALA:CB   | 3:I:42:THR:HA    | 1.74                     | 1.17              |
| 1:J:735:GLY:O    | 1:J:743:ALA:CB   | 1.91                     | 1.17              |
| 1:D:538:GLU:OE2  | 4:9:355:MET:HE1  | 1.44                     | 1.17              |
| 1:G:721:LYS:HA   | 1:G:736:GLN:NE2  | 1.58                     | 1.17              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:HD11 | 1.74                     | 1.17              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HE2   | 1.24                     | 1.17              |
| 4:8:290:ARG:NH2  | 4:V:202:THR:HG23 | 1.59                     | 1.17              |
| 1:G:797:PHE:CE1  | 3:I:146:ILE:HD12 | 1.80                     | 1.16              |
| 1:M:817:GLN:CB   | 2:N:127:ARG:HH11 | 1.59                     | 1.16              |
| 1:G:553:MLY:HG3  | 4:X:45:VAL:O     | 1.01                     | 1.16              |
| 1:A:735:GLY:O    | 1:A:743:ALA:CB   | 1.91                     | 1.16              |
| 1:M:538:GLU:C    | 4:Z:349:LEU:HD11 | 1.54                     | 1.16              |
| 1:M:798:LEU:CD2  | 3:O:126:LEU:CD1  | 2.22                     | 1.16              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:641:LYS:CE   | 4:9:348:SER:O    | 1.93                     | 1.16              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:NE2  | 1.59                     | 1.16              |
| 1:J:641:LYS:CE   | 4:W:348:SER:O    | 1.93                     | 1.16              |
| 1:P:641:LYS:CE   | 4:0:348:SER:O    | 1.93                     | 1.16              |
| 1:G:201:ALA:O    | 1:G:202:SER:CB   | 1.92                     | 1.16              |
| 1:M:640:LYS:HB3  | 1:M:645:SER:OG   | 1.45                     | 1.16              |
| 4:9:290:ARG:NH2  | 4:W:202:THR:HG23 | 1.59                     | 1.16              |
| 1:G:553:MLY:CE   | 4:X:45:VAL:CB    | 2.22                     | 1.16              |
| 1:G:557:GLU:HA   | 4:X:48:GLY:N     | 1.13                     | 1.16              |
| 1:P:819:ASN:ND2  | 2:Q:92:ASP:HB2   | 1.56                     | 1.16              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:OD1  | 1.32                     | 1.16              |
| 1:J:538:GLU:C    | 4:W:349:LEU:HD11 | 1.54                     | 1.16              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:HD22 | 1.80                     | 1.16              |
| 1:P:548:THR:HG22 | 4:2:49:GLN:HB2   | 1.18                     | 1.16              |
| 1:A:553:MLY:HB3  | 4:V:46:GLY:CA    | 1.51                     | 1.16              |
| 1:A:641:LYS:CB   | 1:A:647:GLN:NE2  | 2.07                     | 1.16              |
| 1:D:767:PHE:O    | 1:D:771:LEU:HD11 | 1.01                     | 1.16              |
| 4:0:112:PRO:CB   | 4:1:196:ARG:CA   | 2.17                     | 1.16              |
| 1:D:838:ILE:HD12 | 2:E:54:MET:SD    | 1.85                     | 1.16              |
| 1:J:756:THR:C    | 1:J:776:GLU:OE1  | 1.84                     | 1.16              |
| 1:D:797:PHE:CE2  | 3:F:126:LEU:CD2  | 2.23                     | 1.16              |
| 1:G:795:ARG:CG   | 3:I:118:MET:HE1  | 1.74                     | 1.16              |
| 1:G:795:ARG:NE   | 3:I:116:GLU:HB3  | 1.60                     | 1.16              |
| 2:N:117:LEU:CD1  | 2:N:147:ASN:HB3  | 1.76                     | 1.16              |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:OD1  | 1.32                     | 1.16              |
| 1:A:215:GLN:N    | 1:A:340:ILE:HG12 | 1.20                     | 1.16              |
| 1:G:553:MLY:HE2  | 4:X:45:VAL:CB    | 1.75                     | 1.16              |
| 1:G:557:GLU:HB3  | 4:X:46:GLY:O     | 0.99                     | 1.16              |
| 2:K:117:LEU:CD1  | 2:K:147:ASN:HB3  | 1.76                     | 1.16              |
| 1:J:538:GLU:OE2  | 4:W:355:MET:HE1  | 1.44                     | 1.16              |
| 1:G:735:GLY:O    | 1:G:743:ALA:CB   | 1.91                     | 1.16              |
| 1:A:639:GLY:CA   | 4:8:345:ILE:HA   | 1.74                     | 1.16              |
| 1:M:721:LYS:HA   | 1:M:736:GLN:NE2  | 1.58                     | 1.16              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:CE    | 2.14                     | 1.16              |
| 1:J:754:ASP:CB   | 1:J:780:ASP:OD2  | 1.94                     | 1.16              |
| 1:M:215:GLN:HA   | 1:M:340:ILE:CG2  | 1.75                     | 1.16              |
| 1:G:215:GLN:HA   | 1:G:340:ILE:CG2  | 1.75                     | 1.16              |
| 4:7:290:ARG:NH2  | 4:9:202:THR:HG23 | 1.59                     | 1.16              |
| 1:A:149:GLN:NE2  | 1:A:718:ALA:HB3  | 1.52                     | 1.16              |
| 2:B:117:LEU:CD1  | 2:B:147:ASN:HB3  | 1.76                     | 1.16              |
| 1:P:796:GLY:HA2  | 3:R:35:ARG:HD3   | 1.18                     | 1.16              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:649:VAL:HA   | 1:D:649:VAL:CG2  | 1.76                     | 1.16              |
| 1:P:215:GLN:HA   | 1:P:340:ILE:CG2  | 1.75                     | 1.16              |
| 1:J:215:GLN:HA   | 1:J:340:ILE:CG2  | 1.75                     | 1.16              |
| 4:V:325:MET:SD   | 4:X:244:ASP:CB   | 2.33                     | 1.16              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:HB3   | 1.58                     | 1.16              |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:OD1  | 1.32                     | 1.15              |
| 1:G:640:LYS:HB3  | 1:G:645:SER:OG   | 1.46                     | 1.15              |
| 1:G:642:LYS:CG   | 4:V:23:GLY:N     | 2.08                     | 1.15              |
| 1:P:817:GLN:HG2  | 2:Q:127:ARG:CD   | 1.73                     | 1.15              |
| 1:P:642:LYS:CG   | 4:O:23:GLY:N     | 2.08                     | 1.15              |
| 1:J:640:LYS:HB3  | 1:J:645:SER:OG   | 1.45                     | 1.15              |
| 1:G:84:MLY:CH1   | 1:G:724:TYR:HE2  | 1.58                     | 1.15              |
| 1:M:642:LYS:CG   | 4:Z:23:GLY:N     | 2.08                     | 1.15              |
| 2:H:111:SER:CA   | 2:H:148:VAL:O    | 1.95                     | 1.15              |
| 1:P:635:GLY:HA2  | 4:O:334:GLU:HG2  | 1.16                     | 1.15              |
| 1:D:538:GLU:C    | 4:9:349:LEU:HD11 | 1.54                     | 1.15              |
| 1:M:641:LYS:HD2  | 1:M:647:GLN:NE2  | 1.59                     | 1.15              |
| 1:A:201:ALA:O    | 1:A:202:SER:HB3  | 1.35                     | 1.15              |
| 1:D:201:ALA:O    | 1:D:202:SER:HB3  | 1.36                     | 1.15              |
| 4:7:287:ILE:HG21 | 4:9:205:GLU:HG2  | 1.17                     | 1.15              |
| 2:N:121:LEU:C    | 2:N:128:PHE:HB2  | 1.67                     | 1.15              |
| 1:G:639:GLY:HA2  | 4:V:345:ILE:HA   | 1.26                     | 1.15              |
| 1:D:639:GLY:CA   | 4:9:345:ILE:HA   | 1.73                     | 1.15              |
| 1:P:548:THR:CG2  | 4:2:49:GLN:CA    | 2.24                     | 1.15              |
| 1:A:639:GLY:HA3  | 4:8:344:SER:O    | 1.47                     | 1.15              |
| 1:M:838:ILE:CD1  | 2:N:54:MET:CE    | 2.23                     | 1.15              |
| 1:A:641:LYS:CE   | 4:8:348:SER:O    | 1.93                     | 1.15              |
| 1:D:642:LYS:CG   | 4:9:23:GLY:N     | 2.08                     | 1.15              |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:HG22 | 1.21                     | 1.15              |
| 1:A:642:LYS:CG   | 4:8:23:GLY:N     | 2.09                     | 1.15              |
| 1:D:215:GLN:HA   | 1:D:340:ILE:CG2  | 1.76                     | 1.15              |
| 1:J:829:TRP:CZ3  | 2:K:87:LYS:NZ    | 2.14                     | 1.15              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:NH1  | 1.10                     | 1.15              |
| 1:P:542:PHE:HA   | 4:O:143:TYR:CE1  | 1.82                     | 1.15              |
| 1:M:639:GLY:HA3  | 4:Z:344:SER:O    | 1.46                     | 1.15              |
| 1:J:542:PHE:HA   | 4:W:143:TYR:CE1  | 1.82                     | 1.15              |
| 1:J:635:GLY:HA2  | 4:W:334:GLU:HG2  | 1.16                     | 1.15              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:NE2  | 1.59                     | 1.15              |
| 1:M:641:LYS:CE   | 4:Z:348:SER:O    | 1.93                     | 1.15              |
| 1:A:792:ALA:HB2  | 3:C:42:THR:CG2   | 1.77                     | 1.15              |
| 1:G:639:GLY:HA3  | 4:V:344:SER:O    | 1.46                     | 1.15              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:117:LEU:CD1  | 2:H:147:ASN:HB3  | 1.75                     | 1.15              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:HB3  | 1.77                     | 1.15              |
| 2:B:112:ILE:O    | 2:B:147:ASN:O    | 1.65                     | 1.15              |
| 1:P:530:MET:HE2  | 4:0:354:GLN:CG   | 1.77                     | 1.15              |
| 1:M:545:ALA:CA   | 4:1:45:VAL:CG1   | 2.24                     | 1.15              |
| 1:M:542:PHE:HA   | 4:Z:143:TYR:CE1  | 1.82                     | 1.15              |
| 1:P:795:ARG:CG   | 3:R:118:MET:HE1  | 1.75                     | 1.15              |
| 1:D:542:PHE:HA   | 4:9:143:TYR:CE1  | 1.82                     | 1.15              |
| 1:M:84:MLY:CB    | 1:M:723:ARG:HD2  | 1.75                     | 1.15              |
| 1:J:505:MLY:CD   | 1:J:762:HIS:CE1  | 2.30                     | 1.15              |
| 1:D:640:LYS:HB3  | 1:D:645:SER:OG   | 1.46                     | 1.15              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:HA   | 1.76                     | 1.15              |
| 4:0:288:ASP:HB2  | 4:2:63:GLY:CA    | 1.75                     | 1.15              |
| 1:G:832:MET:SD   | 2:H:84:PHE:HE2   | 1.69                     | 1.15              |
| 1:D:736:GLN:N    | 1:D:743:ALA:CB   | 2.05                     | 1.14              |
| 1:G:791:GLN:NE2  | 3:I:115:GLY:CA   | 2.09                     | 1.14              |
| 1:G:768:MLY:HH22 | 1:G:772:LEU:HD13 | 1.18                     | 1.14              |
| 1:A:502:GLU:CA   | 1:A:761:GLY:CA   | 2.25                     | 1.14              |
| 1:M:819:ASN:ND2  | 2:N:92:ASP:HB2   | 1.60                     | 1.14              |
| 2:N:111:SER:CA   | 2:N:148:VAL:O    | 1.95                     | 1.14              |
| 2:N:144:VAL:CG1  | 2:N:153:ILE:HD11 | 1.64                     | 1.14              |
| 1:G:556:ASP:CG   | 4:X:47:MET:HE3   | 1.44                     | 1.14              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HD11 | 1.65                     | 1.14              |
| 1:P:639:GLY:HA3  | 4:0:344:SER:O    | 1.46                     | 1.14              |
| 1:J:642:LYS:CG   | 4:W:23:GLY:N     | 2.08                     | 1.14              |
| 1:A:542:PHE:HA   | 4:8:143:TYR:CE1  | 1.82                     | 1.14              |
| 1:M:783:LEU:CG   | 1:M:786:ILE:HD11 | 1.75                     | 1.14              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:NE2  | 1.59                     | 1.14              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:NE2  | 1.58                     | 1.14              |
| 4:0:288:ASP:CG   | 4:2:63:GLY:H     | 1.46                     | 1.14              |
| 1:A:215:GLN:HA   | 1:A:340:ILE:CG2  | 1.76                     | 1.14              |
| 4:9:287:ILE:HG21 | 4:W:205:GLU:HG2  | 1.17                     | 1.14              |
| 2:Q:112:ILE:O    | 2:Q:147:ASN:O    | 1.65                     | 1.14              |
| 2:H:111:SER:CB   | 2:H:148:VAL:C    | 1.93                     | 1.14              |
| 1:G:817:GLN:NE2  | 2:H:127:ARG:HB2  | 1.62                     | 1.14              |
| 2:B:111:SER:CA   | 2:B:148:VAL:O    | 1.95                     | 1.14              |
| 1:A:721:LYS:HA   | 1:A:736:GLN:NE2  | 1.58                     | 1.14              |
| 1:A:530:MET:HE2  | 4:8:354:GLN:HG2  | 1.19                     | 1.14              |
| 1:P:641:LYS:HD2  | 1:P:647:GLN:NE2  | 1.59                     | 1.14              |
| 1:G:641:LYS:CE   | 4:V:348:SER:O    | 1.93                     | 1.14              |
| 4:X:325:MET:CE   | 4:Z:244:ASP:OD2  | 1.95                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:757:GLN:OE1  | 1:A:771:LEU:CD1  | 1.93                     | 1.14              |
| 2:N:112:ILE:O    | 2:N:147:ASN:O    | 1.65                     | 1.14              |
| 2:K:111:SER:CA   | 2:K:148:VAL:O    | 1.95                     | 1.14              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:HB3  | 1.78                     | 1.14              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:HB3  | 1.77                     | 1.14              |
| 1:D:641:LYS:NZ   | 4:9:348:SER:O    | 1.80                     | 1.14              |
| 1:A:640:LYS:HB3  | 1:A:645:SER:OG   | 1.46                     | 1.14              |
| 1:P:649:VAL:CG2  | 1:P:649:VAL:HA   | 1.76                     | 1.14              |
| 1:J:754:ASP:CA   | 1:J:780:ASP:OD2  | 1.95                     | 1.14              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:CD2  | 2.22                     | 1.14              |
| 1:G:542:PHE:HA   | 4:V:143:TYR:CE1  | 1.82                     | 1.14              |
| 2:Q:121:LEU:CA   | 2:Q:128:PHE:HB3  | 1.77                     | 1.14              |
| 1:G:819:ASN:CG   | 2:H:92:ASP:HB2   | 1.67                     | 1.14              |
| 1:J:736:GLN:N    | 1:J:743:ALA:CB   | 2.05                     | 1.14              |
| 2:K:121:LEU:C    | 2:K:128:PHE:HB2  | 1.67                     | 1.14              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:CA   | 2.30                     | 1.14              |
| 1:A:795:ARG:HB3  | 3:C:35:ARG:NH2   | 1.63                     | 1.14              |
| 1:M:84:MLY:HH21  | 1:M:720:PHE:HA   | 1.16                     | 1.14              |
| 1:G:649:VAL:HA   | 1:G:649:VAL:CG2  | 1.76                     | 1.14              |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HG13 | 1.21                     | 1.14              |
| 1:M:649:VAL:CG2  | 1:M:649:VAL:HA   | 1.76                     | 1.14              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:CG   | 1.83                     | 1.14              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:OD1  | 1.33                     | 1.14              |
| 1:P:730:SER:HB3  | 3:R:92:ARG:C     | 1.63                     | 1.14              |
| 1:G:818:TYR:CE1  | 2:H:127:ARG:NH2  | 2.14                     | 1.14              |
| 2:K:112:ILE:O    | 2:K:147:ASN:O    | 1.65                     | 1.14              |
| 1:A:817:GLN:CD   | 2:B:127:ARG:NE   | 1.85                     | 1.14              |
| 1:P:640:LYS:HB3  | 1:P:645:SER:OG   | 1.45                     | 1.14              |
| 1:J:639:GLY:HA3  | 4:W:344:SER:O    | 1.46                     | 1.14              |
| 1:D:635:GLY:HA2  | 4:9:334:GLU:HG2  | 1.16                     | 1.14              |
| 1:G:503:TYR:OH   | 1:G:711:PHE:HD2  | 1.30                     | 1.14              |
| 1:D:726:VAL:CG1  | 1:D:785:GLU:CG   | 2.24                     | 1.14              |
| 1:P:506:GLU:CG   | 1:P:760:PHE:H    | 1.58                     | 1.14              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:CB   | 1.96                     | 1.14              |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD21  | 1.17                     | 1.14              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:CB   | 2.35                     | 1.14              |
| 1:D:799:MET:SD   | 3:F:32:ASP:CB    | 2.35                     | 1.14              |
| 1:J:739:ASP:HB3  | 1:J:742:LYS:HB3  | 1.21                     | 1.14              |
| 1:P:735:GLY:O    | 1:P:743:ALA:CB   | 1.91                     | 1.13              |
| 1:M:553:MLY:CD   | 4:1:43:VAL:HG21  | 1.76                     | 1.13              |
| 1:D:538:GLU:O    | 4:9:349:LEU:HD11 | 1.35                     | 1.13              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CD1  | 1.77                     | 1.13              |
| 1:A:649:VAL:CG2  | 1:A:649:VAL:HA   | 1.76                     | 1.13              |
| 1:D:791:GLN:NE2  | 3:F:115:GLY:CA   | 1.97                     | 1.13              |
| 1:G:795:ARG:HB2  | 3:I:35:ARG:NH1   | 1.63                     | 1.13              |
| 1:G:639:GLY:CA   | 4:V:345:ILE:HA   | 1.73                     | 1.13              |
| 1:G:557:GLU:CA   | 4:X:48:GLY:N     | 1.99                     | 1.13              |
| 2:E:111:SER:CA   | 2:E:148:VAL:O    | 1.95                     | 1.13              |
| 1:P:530:MET:HE2  | 4:O:354:GLN:HG2  | 1.17                     | 1.13              |
| 1:J:541:MET:C    | 4:W:143:TYR:OH   | 1.87                     | 1.13              |
| 1:M:838:ILE:HD11 | 2:N:54:MET:HE1   | 1.15                     | 1.13              |
| 1:M:641:LYS:NZ   | 4:Z:348:SER:O    | 1.80                     | 1.13              |
| 1:P:599:ASN:OD1  | 1:P:649:VAL:CB   | 1.96                     | 1.13              |
| 4:8:322:PRO:HB2  | 4:V:244:ASP:OD2  | 1.39                     | 1.13              |
| 1:G:768:MLY:HH23 | 1:G:772:LEU:HD11 | 1.15                     | 1.13              |
| 2:Q:117:LEU:CD1  | 2:Q:147:ASN:HB3  | 1.76                     | 1.13              |
| 2:Q:111:SER:CA   | 2:Q:148:VAL:O    | 1.95                     | 1.13              |
| 1:P:795:ARG:NH2  | 3:R:116:GLU:CD   | 2.00                     | 1.13              |
| 1:P:641:LYS:CE   | 1:P:647:GLN:OE1  | 1.97                     | 1.13              |
| 4:W:324:THR:HG21 | 4:Y:246:GLN:C    | 1.61                     | 1.13              |
| 1:D:201:ALA:O    | 1:D:202:SER:CB   | 1.92                     | 1.13              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:CB   | 1.96                     | 1.13              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:CB   | 1.96                     | 1.13              |
| 1:J:756:THR:HG21 | 1:J:776:GLU:C    | 1.68                     | 1.13              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:HA2  | 1.79                     | 1.13              |
| 1:G:538:GLU:C    | 4:V:349:LEU:HD11 | 1.54                     | 1.13              |
| 1:G:541:MET:C    | 4:V:143:TYR:OH   | 1.87                     | 1.13              |
| 1:M:639:GLY:CA   | 4:Z:345:ILE:HA   | 1.73                     | 1.13              |
| 1:M:552:ASN:HB2  | 4:1:47:MET:C     | 1.60                     | 1.13              |
| 1:D:541:MET:C    | 4:9:143:TYR:OH   | 1.87                     | 1.13              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:HD3  | 1.17                     | 1.13              |
| 1:M:506:GLU:OE2  | 1:M:760:PHE:O    | 1.65                     | 1.13              |
| 1:M:201:ALA:O    | 1:M:202:SER:HB3  | 1.35                     | 1.13              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:CB   | 1.96                     | 1.13              |
| 1:P:805:ALA:HA   | 1:P:808:GLU:HB2  | 1.15                     | 1.13              |
| 1:P:829:TRP:CZ3  | 2:Q:87:LYS:NZ    | 2.16                     | 1.13              |
| 1:M:821:ARG:NH2  | 2:N:127:ARG:HG2  | 1.64                     | 1.13              |
| 1:J:819:ASN:ND2  | 2:K:92:ASP:CB    | 2.02                     | 1.13              |
| 1:M:541:MET:C    | 4:Z:143:TYR:OH   | 1.87                     | 1.13              |
| 1:P:838:ILE:CD1  | 2:Q:54:MET:CE    | 2.26                     | 1.13              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:HB3  | 1.77                     | 1.12              |
| 1:P:797:PHE:CZ   | 3:R:146:ILE:HD13 | 1.83                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:639:GLY:HA3  | 4:9:344:SER:O    | 1.46                     | 1.12              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:HG3  | 1.20                     | 1.12              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:OE1  | 1.97                     | 1.13              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:OE1  | 1.97                     | 1.13              |
| 1:A:201:ALA:O    | 1:A:202:SER:CB   | 1.92                     | 1.13              |
| 1:M:831:TRP:CH2  | 2:N:47:LEU:HD22  | 1.71                     | 1.12              |
| 1:D:712:PRO:HG2  | 1:D:771:LEU:HB2  | 1.15                     | 1.12              |
| 1:M:599:ASN:OD1  | 1:M:649:VAL:CB   | 1.96                     | 1.12              |
| 1:D:799:MET:CE   | 3:F:32:ASP:HB3   | 1.79                     | 1.12              |
| 1:G:830:PRO:HB3  | 2:H:67:MET:HE1   | 1.29                     | 1.13              |
| 3:O:48:LYS:C     | 3:O:52:ASN:ND2   | 2.03                     | 1.13              |
| 1:J:792:ALA:CA   | 3:L:42:THR:HG22  | 1.80                     | 1.12              |
| 1:D:721:LYS:HG3  | 1:D:736:GLN:HG2  | 1.25                     | 1.12              |
| 1:A:93:MET:HE1   | 1:A:715:VAL:HG13 | 1.30                     | 1.12              |
| 1:G:538:GLU:OE2  | 4:V:355:MET:HE1  | 1.50                     | 1.12              |
| 2:Q:121:LEU:C    | 2:Q:128:PHE:HB2  | 1.67                     | 1.12              |
| 2:K:111:SER:HB3  | 2:K:148:VAL:O    | 1.50                     | 1.12              |
| 1:P:552:ASN:HD22 | 4:2:49:GLN:HG3   | 1.03                     | 1.12              |
| 4:O:201:VAL:N    | 4:Y:287:ILE:HG12 | 1.43                     | 1.12              |
| 1:P:641:LYS:NZ   | 4:O:348:SER:O    | 1.80                     | 1.12              |
| 1:G:641:LYS:NZ   | 4:V:348:SER:O    | 1.80                     | 1.12              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:CG2  | 1.78                     | 1.12              |
| 1:D:724:TYR:CB   | 1:D:782:MLY:HD3  | 1.80                     | 1.12              |
| 1:D:732:ILE:HG21 | 1:D:782:MLY:CH2  | 1.80                     | 1.12              |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:CH2  | 1.79                     | 1.12              |
| 2:E:117:LEU:CD1  | 2:E:147:ASN:HB3  | 1.75                     | 1.12              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:NH1   | 1.64                     | 1.12              |
| 1:A:541:MET:C    | 4:8:143:TYR:OH   | 1.87                     | 1.12              |
| 1:P:806:MET:C    | 1:P:807:VAL:N    | 2.02                     | 1.12              |
| 1:A:800:ARG:NH2  | 3:C:40:ASN:HD21  | 1.47                     | 1.12              |
| 3:I:48:LYS:C     | 3:I:52:ASN:ND2   | 2.03                     | 1.12              |
| 3:F:48:LYS:C     | 3:F:52:ASN:ND2   | 2.03                     | 1.12              |
| 3:R:48:LYS:C     | 3:R:52:ASN:ND2   | 2.03                     | 1.12              |
| 1:G:754:ASP:CB   | 1:G:779:ARG:HD2  | 1.80                     | 1.12              |
| 1:G:755:HIS:ND1  | 1:G:779:ARG:NH1  | 1.96                     | 1.12              |
| 1:A:502:GLU:CG   | 1:A:761:GLY:N    | 1.98                     | 1.12              |
| 2:E:121:LEU:C    | 2:E:128:PHE:HB2  | 1.67                     | 1.12              |
| 2:B:111:SER:CB   | 2:B:148:VAL:C    | 1.93                     | 1.12              |
| 2:B:121:LEU:O    | 2:B:128:PHE:HB2  | 0.94                     | 1.12              |
| 1:A:530:MET:HE2  | 4:8:354:GLN:CG   | 1.80                     | 1.12              |
| 1:J:710:GLY:CA   | 1:J:772:LEU:CD2  | 2.04                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:783:LEU:HA   | 1:M:786:ILE:HD11 | 1.29                     | 1.12              |
| 1:M:641:LYS:CE   | 1:M:647:GLN:OE1  | 1.97                     | 1.12              |
| 1:M:806:MET:C    | 1:M:807:VAL:N    | 2.02                     | 1.12              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:CB   | 2.33                     | 1.12              |
| 1:M:623:PHE:CG   | 1:M:623:PHE:CB   | 2.33                     | 1.12              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:HH12  | 1.63                     | 1.12              |
| 1:A:149:GLN:OE1  | 1:A:716:LEU:CD2  | 1.97                     | 1.12              |
| 4:1:287:ILE:HG23 | 4:3:202:THR:OG1  | 1.48                     | 1.12              |
| 1:P:721:LYS:HG3  | 1:P:736:GLN:HG2  | 1.25                     | 1.12              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:CB   | 1.79                     | 1.12              |
| 1:P:541:MET:C    | 4:0:143:TYR:OH   | 1.87                     | 1.12              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD21 | 1.21                     | 1.12              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:OE1  | 1.97                     | 1.12              |
| 1:A:641:LYS:NZ   | 4:8:348:SER:O    | 1.79                     | 1.12              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:OE1  | 1.97                     | 1.12              |
| 3:C:48:LYS:C     | 3:C:52:ASN:ND2   | 2.03                     | 1.12              |
| 1:D:793:ARG:HH21 | 3:F:147:MET:CE   | 1.63                     | 1.11              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:CG   | 2.12                     | 1.11              |
| 1:J:538:GLU:O    | 4:W:349:LEU:HD11 | 1.35                     | 1.11              |
| 4:X:291:LYS:HD2  | 4:Z:243:PRO:HB2  | 1.18                     | 1.11              |
| 1:J:795:ARG:HG2  | 3:L:118:MET:HE1  | 1.33                     | 1.11              |
| 1:A:502:GLU:HA   | 1:A:761:GLY:CA   | 1.79                     | 1.11              |
| 2:N:121:LEU:CA   | 2:N:128:PHE:HB3  | 1.78                     | 1.11              |
| 2:N:111:SER:HB3  | 2:N:148:VAL:O    | 1.50                     | 1.11              |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:HB2  | 1.13                     | 1.11              |
| 1:G:649:VAL:HG12 | 1:G:649:VAL:O    | 0.94                     | 1.11              |
| 1:M:649:VAL:O    | 1:M:649:VAL:HG12 | 0.94                     | 1.11              |
| 1:M:805:ALA:HA   | 1:M:808:GLU:HB2  | 1.12                     | 1.11              |
| 2:N:121:LEU:O    | 2:N:128:PHE:HB2  | 0.93                     | 1.11              |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:HD11 | 1.21                     | 1.11              |
| 2:E:112:ILE:O    | 2:E:147:ASN:O    | 1.65                     | 1.11              |
| 2:H:112:ILE:O    | 2:H:147:ASN:O    | 1.65                     | 1.11              |
| 1:A:721:LYS:HG3  | 1:A:736:GLN:HG2  | 1.25                     | 1.11              |
| 1:P:639:GLY:CA   | 4:0:345:ILE:HA   | 1.73                     | 1.11              |
| 1:G:721:LYS:HG3  | 1:G:736:GLN:HG2  | 1.25                     | 1.11              |
| 1:A:791:GLN:CD   | 3:C:116:GLU:H    | 1.53                     | 1.11              |
| 1:J:641:LYS:NZ   | 4:W:348:SER:O    | 1.80                     | 1.11              |
| 1:P:831:TRP:HH2  | 2:Q:47:LEU:HD21  | 1.10                     | 1.11              |
| 1:M:649:VAL:HG13 | 1:M:649:VAL:HG22 | 1.21                     | 1.11              |
| 1:J:557:GLU:HA   | 4:Y:47:MET:CA    | 1.48                     | 1.11              |
| 1:P:834:LEU:HD13 | 2:Q:51:PHE:HE1   | 0.97                     | 1.11              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:P:834:LEU:CD1 | 2:Q:51:PHE:HE1   | 1.63                     | 1.11              |
| 3:F:24:LYS:CB   | 3:F:63:ILE:O     | 1.99                     | 1.11              |
| 3:R:24:LYS:CB   | 3:R:63:ILE:O     | 1.99                     | 1.11              |
| 1:J:800:ARG:NH2 | 3:L:40:ASN:OD1   | 1.83                     | 1.11              |
| 1:A:739:ASP:HB3 | 1:A:742:LYS:HB3  | 1.21                     | 1.11              |
| 1:M:783:LEU:C   | 1:M:786:ILE:HG13 | 1.71                     | 1.11              |
| 1:D:641:LYS:CE  | 1:D:647:GLN:CD   | 2.18                     | 1.11              |
| 1:M:721:LYS:HG3 | 1:M:736:GLN:HG2  | 1.25                     | 1.11              |
| 1:G:93:MET:HG3  | 1:G:714:ARG:O    | 1.50                     | 1.11              |
| 1:J:838:ILE:CD1 | 2:K:54:MET:HE1   | 1.81                     | 1.11              |
| 1:A:649:VAL:O   | 1:A:649:VAL:HG12 | 0.94                     | 1.11              |
| 4:9:290:ARG:CZ  | 4:W:202:THR:HG21 | 1.81                     | 1.11              |
| 1:D:623:PHE:CG  | 1:D:623:PHE:CB   | 2.33                     | 1.11              |
| 1:P:623:PHE:CG  | 1:P:623:PHE:CB   | 2.33                     | 1.11              |
| 1:M:739:ASP:HB3 | 1:M:742:LYS:HB3  | 1.21                     | 1.11              |
| 1:D:734:GLU:O   | 1:D:738:MET:HG2  | 1.51                     | 1.11              |
| 1:G:754:ASP:HA  | 1:G:779:ARG:NE   | 1.63                     | 1.11              |
| 1:P:797:PHE:CZ  | 3:R:146:ILE:HA   | 1.84                     | 1.11              |
| 1:A:831:TRP:CD1 | 2:B:51:PHE:CZ    | 2.38                     | 1.11              |
| 1:M:796:GLY:HA2 | 3:O:35:ARG:HD3   | 1.32                     | 1.11              |
| 1:G:707:CYS:SG  | 1:G:714:ARG:NH2  | 2.24                     | 1.11              |
| 1:D:85:TYR:OH   | 1:D:772:LEU:HD22 | 1.42                     | 1.11              |
| 1:A:799:MET:CE  | 3:C:32:ASP:HB3   | 1.79                     | 1.11              |
| 1:P:201:ALA:O   | 1:P:202:SER:CB   | 1.92                     | 1.11              |
| 4:W:325:MET:HE2 | 4:Y:244:ASP:OD2  | 1.50                     | 1.11              |
| 1:A:623:PHE:CB  | 1:A:623:PHE:CG   | 2.33                     | 1.11              |
| 1:G:792:ALA:HB3 | 3:I:42:THR:HG22  | 1.28                     | 1.10              |
| 1:M:817:GLN:HB3 | 2:N:127:ARG:NH1  | 1.64                     | 1.10              |
| 2:Q:117:LEU:HB2 | 2:Q:147:ASN:CG   | 1.70                     | 1.10              |
| 1:A:734:GLU:O   | 1:A:738:MET:HG2  | 1.51                     | 1.10              |
| 1:P:218:LEU:HB2 | 1:P:221:GLN:HG3  | 1.17                     | 1.10              |
| 1:J:641:LYS:CE  | 1:J:647:GLN:CD   | 2.18                     | 1.10              |
| 1:P:641:LYS:CE  | 1:P:647:GLN:CD   | 2.18                     | 1.10              |
| 1:G:641:LYS:HG3 | 1:G:647:GLN:HG3  | 1.21                     | 1.10              |
| 1:G:641:LYS:CE  | 1:G:647:GLN:CD   | 2.18                     | 1.10              |
| 1:P:201:ALA:O   | 1:P:202:SER:HB3  | 1.36                     | 1.10              |
| 1:J:797:PHE:HE1 | 3:L:146:ILE:HA   | 1.12                     | 1.10              |
| 1:D:727:LEU:CD1 | 1:D:782:MLY:HH12 | 1.80                     | 1.10              |
| 1:G:753:VAL:HA  | 1:G:780:ASP:OD1  | 1.47                     | 1.10              |
| 2:E:121:LEU:O   | 2:E:128:PHE:HB2  | 0.94                     | 1.10              |
| 1:P:730:SER:N   | 3:R:93:VAL:CG2   | 2.14                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:817:GLN:OE1  | 2:B:127:ARG:CZ   | 1.99                     | 1.10              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:CG   | 1.70                     | 1.10              |
| 1:P:798:LEU:CD1  | 3:R:126:LEU:HD21 | 1.81                     | 1.10              |
| 1:D:530:MET:CE   | 4:9:354:GLN:HG2  | 1.80                     | 1.10              |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:HE1   | 1.15                     | 1.10              |
| 1:M:641:LYS:CE   | 1:M:647:GLN:CD   | 2.18                     | 1.10              |
| 1:J:201:ALA:O    | 1:J:202:SER:HB3  | 1.36                     | 1.10              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:HG22 | 1.80                     | 1.10              |
| 3:L:48:LYS:C     | 3:L:52:ASN:ND2   | 2.03                     | 1.10              |
| 1:G:623:PHE:CG   | 1:G:623:PHE:CB   | 2.33                     | 1.10              |
| 1:P:739:ASP:HB3  | 1:P:742:LYS:HB3  | 1.21                     | 1.10              |
| 1:J:797:PHE:CG   | 3:L:146:ILE:HG23 | 1.85                     | 1.10              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:CG   | 1.70                     | 1.10              |
| 2:H:121:LEU:O    | 2:H:128:PHE:HB2  | 0.94                     | 1.10              |
| 1:A:831:TRP:NE1  | 2:B:51:PHE:CZ    | 2.19                     | 1.10              |
| 1:P:552:ASN:HD21 | 4:2:49:GLN:HB3   | 0.99                     | 1.10              |
| 1:D:649:VAL:HG13 | 1:D:649:VAL:HG22 | 1.21                     | 1.10              |
| 1:P:649:VAL:HG13 | 1:P:649:VAL:HG22 | 1.21                     | 1.10              |
| 1:M:834:LEU:CD1  | 2:N:51:PHE:HE1   | 1.65                     | 1.10              |
| 3:I:24:LYS:CB    | 3:I:63:ILE:O     | 1.99                     | 1.10              |
| 4:3:322:PRO:HB3  | 4:5:244:ASP:CG   | 1.72                     | 1.10              |
| 1:D:727:LEU:HD11 | 1:D:782:MLY:CG   | 1.80                     | 1.10              |
| 4:X:324:THR:CG2  | 4:Z:247:VAL:CG2  | 2.30                     | 1.10              |
| 1:M:553:MLY:CE   | 4:1:43:VAL:HG21  | 1.79                     | 1.10              |
| 1:J:530:MET:CE   | 4:W:354:GLN:HG2  | 1.80                     | 1.10              |
| 1:P:795:ARG:CZ   | 3:R:116:GLU:OE2  | 2.00                     | 1.10              |
| 1:P:641:LYS:HE3  | 1:P:647:GLN:OE1  | 1.50                     | 1.10              |
| 1:A:202:SER:CA   | 1:A:207:LYS:HE2  | 1.82                     | 1.10              |
| 1:P:724:TYR:CE1  | 1:P:776:GLU:OE2  | 2.03                     | 1.10              |
| 1:G:769:ALA:HB3  | 1:G:770:GLY:HA2  | 1.31                     | 1.10              |
| 3:C:24:LYS:CB    | 3:C:63:ILE:O     | 1.99                     | 1.10              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:CG   | 1.71                     | 1.10              |
| 2:K:121:LEU:O    | 2:K:128:PHE:HB2  | 0.94                     | 1.10              |
| 1:P:530:MET:CE   | 4:0:354:GLN:HG2  | 1.80                     | 1.10              |
| 1:P:796:GLY:HA2  | 3:R:35:ARG:CD    | 1.79                     | 1.10              |
| 1:D:530:MET:HE2  | 4:9:354:GLN:HG2  | 1.22                     | 1.10              |
| 4:2:288:ASP:H    | 4:4:203:THR:HG22 | 1.17                     | 1.10              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:OE1  | 1.50                     | 1.10              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CD   | 2.18                     | 1.10              |
| 1:G:202:SER:CA   | 1:G:207:LYS:HE2  | 1.82                     | 1.10              |
| 4:7:290:ARG:CZ   | 4:9:202:THR:HG21 | 1.81                     | 1.10              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:739:ASP:HB3  | 1:D:742:LYS:HB3  | 1.21                     | 1.10              |
| 1:D:732:ILE:CD1  | 1:D:782:MLY:HH11 | 1.82                     | 1.09              |
| 1:P:538:GLU:O    | 4:0:349:LEU:HD11 | 1.35                     | 1.09              |
| 1:P:797:PHE:CD1  | 3:R:146:ILE:O    | 2.05                     | 1.09              |
| 1:J:768:MLY:HH11 | 1:J:772:LEU:HD12 | 1.19                     | 1.09              |
| 1:M:785:GLU:C    | 1:M:786:ILE:HA   | 1.72                     | 1.09              |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:HE3   | 1.23                     | 1.09              |
| 1:M:641:LYS:HE3  | 1:M:647:GLN:OE1  | 1.50                     | 1.09              |
| 1:M:831:TRP:CH2  | 2:N:47:LEU:HD21  | 1.78                     | 1.09              |
| 1:P:831:TRP:CH2  | 2:Q:47:LEU:HD22  | 1.81                     | 1.09              |
| 1:M:202:SER:CA   | 1:M:207:LYS:HE2  | 1.82                     | 1.09              |
| 1:D:800:ARG:NH2  | 3:F:40:ASN:HD21  | 1.49                     | 1.09              |
| 4:1:244:ASP:CG   | 4:Z:322:PRO:HB3  | 1.72                     | 1.09              |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:HD3  | 1.20                     | 1.09              |
| 1:A:149:GLN:CB   | 1:A:718:ALA:CB   | 2.20                     | 1.09              |
| 1:P:783:LEU:HG   | 1:P:786:ILE:CD1  | 1.80                     | 1.09              |
| 1:P:793:ARG:HD3  | 3:R:40:ASN:ND2   | 1.65                     | 1.09              |
| 1:G:734:GLU:O    | 1:G:738:MET:HG2  | 1.51                     | 1.09              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:CD1  | 1.54                     | 1.09              |
| 1:A:530:MET:CE   | 4:8:354:GLN:HG2  | 1.80                     | 1.09              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:OE1  | 1.50                     | 1.09              |
| 1:M:831:TRP:CZ2  | 2:N:47:LEU:HD22  | 1.86                     | 1.09              |
| 4:0:287:ILE:CG2  | 4:2:203:THR:CG2  | 2.21                     | 1.09              |
| 1:J:649:VAL:HG13 | 1:J:649:VAL:HG22 | 1.21                     | 1.09              |
| 1:P:769:ALA:O    | 1:P:771:LEU:CB   | 1.99                     | 1.09              |
| 1:J:829:TRP:CZ2  | 2:K:87:LYS:HE2   | 1.86                     | 1.09              |
| 1:J:571:ALA:O    | 1:J:572:LYS:HG3  | 1.52                     | 1.09              |
| 1:D:571:ALA:O    | 1:D:572:LYS:HG3  | 1.52                     | 1.09              |
| 1:A:508:ILE:HD13 | 1:A:759:ALA:CB   | 1.60                     | 1.09              |
| 1:A:757:GLN:HB2  | 1:A:771:LEU:HD21 | 1.12                     | 1.09              |
| 2:N:117:LEU:HB2  | 2:N:147:ASN:CG   | 1.70                     | 1.09              |
| 1:G:530:MET:CE   | 4:V:354:GLN:HG2  | 1.80                     | 1.09              |
| 2:Q:121:LEU:O    | 2:Q:128:PHE:HB2  | 0.94                     | 1.09              |
| 2:H:121:LEU:C    | 2:H:128:PHE:HB2  | 1.67                     | 1.09              |
| 2:H:111:SER:HB3  | 2:H:148:VAL:O    | 1.49                     | 1.09              |
| 1:M:530:MET:CE   | 4:Z:354:GLN:HG2  | 1.80                     | 1.09              |
| 1:P:785:GLU:HG2  | 3:R:81:GLN:HG3   | 1.24                     | 1.09              |
| 1:P:795:ARG:HD2  | 3:R:43:ASN:OD1   | 1.42                     | 1.09              |
| 1:A:635:GLY:HA2  | 4:8:334:GLU:HG2  | 1.15                     | 1.09              |
| 1:M:838:ILE:HD11 | 2:N:54:MET:HE3   | 1.23                     | 1.09              |
| 1:M:641:LYS:HG3  | 1:M:647:GLN:HG3  | 1.21                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:202:SER:CA   | 1:D:207:LYS:HE2  | 1.82                     | 1.09              |
| 1:P:649:VAL:O    | 1:P:649:VAL:HG12 | 0.94                     | 1.09              |
| 1:G:830:PRO:CB   | 2:H:67:MET:HE1   | 1.81                     | 1.09              |
| 4:8:290:ARG:CZ   | 4:V:202:THR:HG21 | 1.81                     | 1.09              |
| 1:G:739:ASP:HB3  | 1:G:742:LYS:HB3  | 1.21                     | 1.09              |
| 3:L:24:LYS:CB    | 3:L:63:ILE:O     | 1.99                     | 1.09              |
| 1:D:797:PHE:CE1  | 3:F:146:ILE:CA   | 2.34                     | 1.09              |
| 1:J:734:GLU:O    | 1:J:738:MET:HG2  | 1.51                     | 1.09              |
| 1:P:639:GLY:HA2  | 4:0:345:ILE:HA   | 1.26                     | 1.09              |
| 1:J:218:LEU:HB2  | 1:J:221:GLN:HG3  | 1.17                     | 1.09              |
| 1:M:530:MET:HE2  | 4:Z:354:GLN:CG   | 1.82                     | 1.09              |
| 1:J:643:GLY:O    | 1:J:644:SER:OG   | 1.70                     | 1.09              |
| 1:G:721:LYS:HA   | 1:G:736:GLN:CD   | 1.73                     | 1.09              |
| 1:A:639:GLY:HA2  | 4:8:345:ILE:HA   | 1.26                     | 1.09              |
| 1:M:201:ALA:O    | 1:M:202:SER:CB   | 1.92                     | 1.09              |
| 1:J:649:VAL:HG12 | 1:J:649:VAL:O    | 0.94                     | 1.09              |
| 1:J:757:GLN:NE2  | 1:J:777:GLU:N    | 1.98                     | 1.09              |
| 4:2:324:THR:CB   | 4:4:243:PRO:O    | 2.01                     | 1.09              |
| 3:O:24:LYS:CB    | 3:O:63:ILE:O     | 1.99                     | 1.09              |
| 1:D:798:LEU:CD1  | 3:F:126:LEU:CD1  | 1.81                     | 1.09              |
| 1:G:530:MET:HE2  | 4:V:354:GLN:HG2  | 1.29                     | 1.09              |
| 1:A:218:LEU:HB2  | 1:A:221:GLN:HG3  | 1.17                     | 1.09              |
| 1:J:721:LYS:HG3  | 1:J:736:GLN:HG2  | 1.25                     | 1.09              |
| 1:J:639:GLY:HA2  | 4:W:345:ILE:HA   | 1.26                     | 1.09              |
| 1:M:218:LEU:HB2  | 1:M:221:GLN:HG3  | 1.17                     | 1.09              |
| 1:M:783:LEU:CA   | 1:M:786:ILE:CD1  | 2.30                     | 1.09              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:OE1  | 1.50                     | 1.09              |
| 1:D:768:MLY:CA   | 1:D:771:LEU:CD1  | 2.29                     | 1.09              |
| 1:D:85:TYR:OH    | 1:D:772:LEU:HD23 | 1.40                     | 1.09              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:CE    | 2.30                     | 1.09              |
| 1:D:649:VAL:O    | 1:D:649:VAL:HG12 | 0.94                     | 1.09              |
| 4:8:287:ILE:HG21 | 4:V:205:GLU:HG2  | 1.17                     | 1.09              |
| 1:M:571:ALA:O    | 1:M:572:LYS:HG3  | 1.52                     | 1.09              |
| 1:G:553:MLY:HE2  | 4:X:45:VAL:HB    | 1.09                     | 1.08              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:CD1  | 1.55                     | 1.08              |
| 1:P:819:ASN:HA   | 2:Q:90:GLY:O     | 0.92                     | 1.08              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:HB3  | 1.35                     | 1.08              |
| 1:M:798:LEU:HD22 | 3:O:126:LEU:HD11 | 1.27                     | 1.08              |
| 4:2:290:ARG:CZ   | 4:4:202:THR:CG2  | 2.20                     | 1.08              |
| 1:J:202:SER:CA   | 1:J:207:LYS:HE2  | 1.82                     | 1.08              |
| 4:1:203:THR:HG21 | 4:Z:288:ASP:CG   | 1.63                     | 1.08              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:571:ALA:O    | 1:P:572:LYS:HG3  | 1.52                     | 1.08              |
| 1:J:795:ARG:HD3  | 3:L:43:ASN:OD1   | 0.91                     | 1.08              |
| 1:G:795:ARG:HB2  | 3:I:35:ARG:HH12  | 1.00                     | 1.08              |
| 2:Q:121:LEU:HG   | 2:Q:128:PHE:CA   | 1.59                     | 1.08              |
| 2:Q:111:SER:OG   | 2:Q:148:VAL:O    | 1.71                     | 1.08              |
| 2:E:111:SER:CB   | 2:E:148:VAL:C    | 1.93                     | 1.08              |
| 1:M:548:THR:C    | 4:1:47:MET:SD    | 2.15                     | 1.08              |
| 1:J:639:GLY:CA   | 4:W:345:ILE:HA   | 1.73                     | 1.08              |
| 1:D:639:GLY:HA2  | 4:9:345:ILE:HA   | 1.26                     | 1.08              |
| 1:P:502:GLU:OE2  | 1:P:761:GLY:CA   | 2.00                     | 1.08              |
| 1:J:567:LYS:NZ   | 4:Y:92:ASN:HD22  | 1.50                     | 1.08              |
| 1:G:556:ASP:OD1  | 4:X:47:MET:HE3   | 1.53                     | 1.08              |
| 2:K:117:LEU:HB2  | 2:K:147:ASN:CG   | 1.70                     | 1.08              |
| 2:K:111:SER:OG   | 2:K:148:VAL:O    | 1.71                     | 1.08              |
| 1:M:638:GLY:CA   | 4:Z:341:ILE:O    | 2.01                     | 1.08              |
| 1:D:530:MET:HE2  | 4:9:354:GLN:CG   | 1.82                     | 1.08              |
| 1:D:218:LEU:HB2  | 1:D:221:GLN:HG3  | 1.17                     | 1.08              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:CD   | 1.70                     | 1.08              |
| 1:D:726:VAL:CG1  | 1:D:785:GLU:CB   | 2.30                     | 1.08              |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:HD13 | 1.09                     | 1.08              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:CZ    | 1.84                     | 1.08              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:HB   | 1.10                     | 1.08              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:CD   | 2.21                     | 1.08              |
| 1:A:817:GLN:HG3  | 2:B:127:ARG:HD3  | 1.30                     | 1.08              |
| 1:A:721:LYS:HA   | 1:A:736:GLN:CD   | 1.73                     | 1.08              |
| 1:M:792:ALA:HB2  | 3:O:42:THR:HG22  | 1.32                     | 1.08              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:HG3  | 1.21                     | 1.08              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:OE1  | 1.50                     | 1.08              |
| 1:P:202:SER:CA   | 1:P:207:LYS:HE2  | 1.82                     | 1.08              |
| 1:D:831:TRP:CD1  | 2:E:51:PHE:CZ    | 2.41                     | 1.08              |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CB   | 1.83                     | 1.08              |
| 1:D:721:LYS:HA   | 1:D:736:GLN:CD   | 1.73                     | 1.08              |
| 1:A:502:GLU:CB   | 1:A:761:GLY:HA3  | 1.51                     | 1.08              |
| 1:P:817:GLN:HB3  | 2:Q:127:ARG:HH11 | 0.99                     | 1.08              |
| 2:Q:111:SER:CB   | 2:Q:148:VAL:O    | 0.78                     | 1.08              |
| 2:E:111:SER:OG   | 2:E:148:VAL:O    | 1.71                     | 1.08              |
| 2:H:111:SER:OG   | 2:H:148:VAL:O    | 1.71                     | 1.08              |
| 2:B:111:SER:OG   | 2:B:148:VAL:O    | 1.71                     | 1.08              |
| 1:P:643:GLY:O    | 1:P:644:SER:OG   | 1.69                     | 1.08              |
| 1:G:218:LEU:HB2  | 1:G:221:GLN:HG3  | 1.17                     | 1.08              |
| 1:A:797:PHE:HE2  | 3:C:126:LEU:HD22 | 0.91                     | 1.08              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:149:GLN:HB3  | 1:P:716:LEU:HD21 | 1.14                     | 1.08              |
| 1:D:798:LEU:CG   | 3:F:126:LEU:HD11 | 1.84                     | 1.07              |
| 1:A:93:MET:HG2   | 1:A:715:VAL:HG22 | 1.25                     | 1.07              |
| 1:P:721:LYS:HA   | 1:P:736:GLN:CD   | 1.73                     | 1.07              |
| 2:B:111:SER:CB   | 2:B:148:VAL:O    | 0.78                     | 1.07              |
| 1:M:538:GLU:OE2  | 4:Z:355:MET:HE1  | 1.49                     | 1.07              |
| 1:P:798:LEU:CD1  | 3:R:126:LEU:CD2  | 2.30                     | 1.07              |
| 1:D:638:GLY:CA   | 4:9:341:ILE:O    | 2.01                     | 1.07              |
| 1:M:641:LYS:HD2  | 1:M:647:GLN:CD   | 1.70                     | 1.07              |
| 1:M:643:GLY:O    | 1:M:644:SER:OG   | 1.69                     | 1.07              |
| 1:D:800:ARG:NH2  | 3:F:40:ASN:ND2   | 2.02                     | 1.07              |
| 4:3:3:ASP:HA     | 4:3:6:THR:HB     | 1.36                     | 1.07              |
| 1:G:643:GLY:O    | 1:G:644:SER:OG   | 1.70                     | 1.07              |
| 2:E:111:SER:CB   | 2:E:148:VAL:O    | 0.78                     | 1.07              |
| 2:H:111:SER:CB   | 2:H:148:VAL:O    | 0.78                     | 1.07              |
| 2:B:121:LEU:C    | 2:B:128:PHE:HB2  | 1.67                     | 1.07              |
| 1:M:538:GLU:HA   | 4:Z:349:LEU:CD1  | 1.55                     | 1.07              |
| 1:M:541:MET:SD   | 4:Z:345:ILE:O    | 2.13                     | 1.07              |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:CG   | 1.82                     | 1.07              |
| 1:P:797:PHE:CE1  | 3:R:146:ILE:HA   | 1.88                     | 1.07              |
| 1:D:409:GLY:N    | 1:D:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:D:529:PRO:HB3  | 4:9:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:G:641:LYS:CG   | 1:G:647:GLN:CG   | 2.16                     | 1.07              |
| 1:A:836:PHE:CZ   | 2:B:160:GLY:N    | 2.21                     | 1.07              |
| 1:J:94:MET:C     | 1:J:713:SER:HB3  | 1.73                     | 1.07              |
| 1:M:95:THR:OG1   | 1:M:770:GLY:N    | 1.88                     | 1.07              |
| 1:G:72:VAL:HG13  | 1:G:76:GLN:HB3   | 1.36                     | 1.07              |
| 1:D:727:LEU:HD11 | 1:D:782:MLY:HG2  | 1.14                     | 1.07              |
| 1:D:795:ARG:CG   | 3:F:118:MET:HE3  | 1.85                     | 1.07              |
| 1:A:757:GLN:CD   | 1:A:771:LEU:HD11 | 1.65                     | 1.07              |
| 2:N:111:SER:CB   | 2:N:148:VAL:O    | 0.78                     | 1.07              |
| 1:G:529:PRO:HB3  | 4:V:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:P:817:GLN:HB3  | 2:Q:127:ARG:CD   | 1.84                     | 1.07              |
| 2:E:111:SER:HB3  | 2:E:148:VAL:O    | 1.50                     | 1.07              |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:CG2  | 1.84                     | 1.07              |
| 1:P:734:GLU:O    | 1:P:738:MET:HG2  | 1.51                     | 1.07              |
| 2:K:111:SER:CB   | 2:K:148:VAL:O    | 0.78                     | 1.07              |
| 1:P:638:GLY:CA   | 4:0:341:ILE:O    | 2.01                     | 1.07              |
| 1:J:529:PRO:HB3  | 4:W:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:J:530:MET:HE2  | 4:W:354:GLN:CG   | 1.84                     | 1.07              |
| 1:D:541:MET:SD   | 4:9:345:ILE:O    | 2.12                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:GLY:N    | 1:A:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:M:734:GLU:O    | 1:M:738:MET:HG2  | 1.51                     | 1.07              |
| 1:G:641:LYS:HB2  | 1:G:647:GLN:NE2  | 1.68                     | 1.07              |
| 1:D:712:PRO:CG   | 1:D:771:LEU:HB2  | 1.85                     | 1.07              |
| 1:M:84:MLY:HG2   | 1:M:723:ARG:HD2  | 1.24                     | 1.07              |
| 1:D:643:GLY:O    | 1:D:644:SER:OG   | 1.69                     | 1.07              |
| 1:M:35:MLY:HH21  | 1:M:778:MET:HG2  | 1.26                     | 1.07              |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:CD2  | 1.84                     | 1.07              |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:CG   | 1.57                     | 1.07              |
| 1:D:795:ARG:HH21 | 3:F:116:GLU:HB3  | 1.19                     | 1.07              |
| 1:G:638:GLY:CA   | 4:V:341:ILE:O    | 2.02                     | 1.07              |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:HG2  | 1.11                     | 1.07              |
| 1:M:409:GLY:N    | 1:M:636:LYS:HG3  | 1.69                     | 1.07              |
| 1:J:541:MET:SD   | 4:W:345:ILE:O    | 2.13                     | 1.07              |
| 1:J:638:GLY:CA   | 4:W:341:ILE:O    | 2.01                     | 1.07              |
| 1:P:548:THR:HG23 | 4:2:49:GLN:HB2   | 1.20                     | 1.07              |
| 1:A:529:PRO:HB3  | 4:8:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:P:641:LYS:HB2  | 1:P:647:GLN:NE2  | 1.68                     | 1.07              |
| 1:A:641:LYS:HB2  | 1:A:647:GLN:NE2  | 1.68                     | 1.07              |
| 1:A:643:GLY:O    | 1:A:644:SER:OG   | 1.70                     | 1.07              |
| 1:A:571:ALA:O    | 1:A:572:LYS:HG3  | 1.52                     | 1.07              |
| 4:X:3:ASP:HA     | 4:X:6:THR:HB     | 1.36                     | 1.07              |
| 1:J:798:LEU:HD11 | 3:L:126:LEU:HD12 | 1.37                     | 1.07              |
| 1:G:635:GLY:HA2  | 4:V:334:GLU:HG2  | 1.16                     | 1.07              |
| 1:P:736:GLN:N    | 1:P:743:ALA:CB   | 2.05                     | 1.07              |
| 1:A:813:ILE:HG21 | 2:B:127:ARG:HD2  | 1.19                     | 1.07              |
| 1:P:529:PRO:HB3  | 4:0:353:GLN:OE1  | 1.53                     | 1.07              |
| 1:M:635:GLY:HA2  | 4:Z:334:GLU:HG2  | 1.16                     | 1.07              |
| 1:P:795:ARG:CB   | 3:R:35:ARG:NH1   | 2.18                     | 1.07              |
| 1:P:795:ARG:CZ   | 3:R:116:GLU:HB3  | 1.84                     | 1.07              |
| 1:A:752:ASP:CG   | 1:A:782:MLY:HD3  | 1.72                     | 1.07              |
| 1:A:541:MET:SD   | 4:8:345:ILE:O    | 2.12                     | 1.07              |
| 1:A:638:GLY:CA   | 4:8:341:ILE:O    | 2.01                     | 1.07              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:CE    | 2.31                     | 1.07              |
| 1:M:834:LEU:HD13 | 2:N:51:PHE:HE1   | 0.93                     | 1.07              |
| 4:5:3:ASP:HA     | 4:5:6:THR:HB     | 1.36                     | 1.07              |
| 1:A:93:MET:CG    | 1:A:715:VAL:HG22 | 1.84                     | 1.06              |
| 1:A:768:MLY:CG   | 1:A:771:LEU:HD13 | 1.84                     | 1.06              |
| 2:N:111:SER:OG   | 2:N:148:VAL:O    | 1.71                     | 1.06              |
| 1:G:409:GLY:N    | 1:G:636:LYS:HG3  | 1.69                     | 1.06              |
| 1:J:721:LYS:HA   | 1:J:736:GLN:CD   | 1.73                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:791:GLN:HE22 | 3:R:115:GLY:HA3  | 1.15                     | 1.06              |
| 1:P:797:PHE:CE2  | 3:R:146:ILE:CD1  | 2.36                     | 1.06              |
| 1:D:576:GLU:HG2  | 1:D:577:ALA:N    | 1.66                     | 1.06              |
| 1:P:72:VAL:HG13  | 1:P:76:GLN:HB3   | 1.36                     | 1.06              |
| 1:G:754:ASP:N    | 1:G:776:GLU:OE1  | 1.88                     | 1.06              |
| 1:G:541:MET:SD   | 4:V:345:ILE:O    | 2.13                     | 1.06              |
| 1:J:28:GLN:HG2   | 1:J:723:ARG:NH1  | 1.62                     | 1.06              |
| 1:M:529:PRO:HB3  | 4:Z:353:GLN:OE1  | 1.53                     | 1.06              |
| 1:J:409:GLY:N    | 1:J:636:LYS:HG3  | 1.69                     | 1.06              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB3  | 1.35                     | 1.06              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HE1  | 1.17                     | 1.06              |
| 1:M:836:PHE:CZ   | 2:N:160:GLY:N    | 2.23                     | 1.06              |
| 1:M:721:LYS:HA   | 1:M:736:GLN:CD   | 1.73                     | 1.06              |
| 1:J:201:ALA:O    | 1:J:202:SER:CB   | 1.92                     | 1.06              |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CD   | 1.75                     | 1.06              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:CE1   | 2.37                     | 1.06              |
| 1:G:571:ALA:O    | 1:G:572:LYS:HG3  | 1.52                     | 1.06              |
| 1:J:797:PHE:CE2  | 3:L:126:LEU:HD22 | 1.90                     | 1.06              |
| 1:G:752:ASP:CG   | 1:G:780:ASP:O    | 1.92                     | 1.06              |
| 2:Q:111:SER:CB   | 2:Q:148:VAL:C    | 1.93                     | 1.06              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:OG1  | 2.03                     | 1.06              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:HG2  | 1.69                     | 1.06              |
| 2:B:111:SER:HB3  | 2:B:148:VAL:O    | 1.49                     | 1.06              |
| 1:P:641:LYS:HG3  | 1:P:647:GLN:HG3  | 1.21                     | 1.06              |
| 1:J:836:PHE:CE1  | 2:K:159:HIS:CA   | 2.39                     | 1.06              |
| 1:M:831:TRP:HH2  | 2:N:47:LEU:HD21  | 1.12                     | 1.06              |
| 1:P:769:ALA:O    | 1:P:771:LEU:HB3  | 1.55                     | 1.06              |
| 1:M:829:TRP:CZ3  | 2:N:87:LYS:NZ    | 2.23                     | 1.06              |
| 1:A:149:GLN:CG   | 1:A:718:ALA:HB3  | 1.85                     | 1.06              |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:HG11  | 1.37                     | 1.06              |
| 2:K:114:LYS:HA   | 2:K:146:GLY:O    | 0.89                     | 1.06              |
| 2:B:114:LYS:HA   | 2:B:146:GLY:O    | 0.89                     | 1.06              |
| 1:P:795:ARG:NH2  | 3:R:116:GLU:CB   | 1.76                     | 1.06              |
| 1:P:783:LEU:CG   | 1:P:786:ILE:HD11 | 1.84                     | 1.06              |
| 1:D:542:PHE:CG   | 4:9:143:TYR:HE1  | 1.73                     | 1.06              |
| 1:P:769:ALA:HB1  | 1:P:770:GLY:N    | 1.69                     | 1.06              |
| 4:2:322:PRO:HB3  | 4:4:244:ASP:CG   | 1.75                     | 1.06              |
| 1:A:72:VAL:HG13  | 1:A:76:GLN:HB3   | 1.36                     | 1.06              |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:CG   | 1.68                     | 1.06              |
| 1:A:149:GLN:CD   | 1:A:718:ALA:HB3  | 1.77                     | 1.06              |
| 1:A:768:MLY:HG2  | 1:A:771:LEU:HD13 | 1.08                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:541:MET:SD   | 4:0:345:ILE:O    | 2.13                     | 1.06              |
| 1:P:149:GLN:HG2  | 1:P:716:LEU:HD11 | 1.13                     | 1.06              |
| 1:J:829:TRP:CH2  | 2:K:84:PHE:CE1   | 2.43                     | 1.06              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CG   | 1.85                     | 1.06              |
| 1:A:97:LEU:HD22  | 1:A:712:PRO:CB   | 1.85                     | 1.05              |
| 2:N:140:PHE:O    | 2:N:141:PRO:O    | 1.75                     | 1.05              |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:HD11 | 1.21                     | 1.05              |
| 1:G:553:MLY:CE   | 4:X:45:VAL:HG12  | 1.68                     | 1.05              |
| 1:G:557:GLU:HB3  | 4:X:46:GLY:C     | 1.76                     | 1.05              |
| 1:M:542:PHE:CG   | 4:Z:143:TYR:HE1  | 1.73                     | 1.05              |
| 1:M:635:GLY:HA3  | 4:Z:341:ILE:HD13 | 1.36                     | 1.05              |
| 1:D:641:LYS:HB2  | 1:D:647:GLN:NE2  | 1.68                     | 1.05              |
| 1:G:838:ILE:HD12 | 2:H:54:MET:HE3   | 1.37                     | 1.05              |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:HH11 | 1.34                     | 1.05              |
| 1:A:149:GLN:CG   | 1:A:719:ASP:OD1  | 2.03                     | 1.05              |
| 2:Q:111:SER:HB3  | 2:Q:148:VAL:O    | 1.50                     | 1.05              |
| 2:E:114:LYS:HA   | 2:E:146:GLY:O    | 0.89                     | 1.05              |
| 2:E:140:PHE:O    | 2:E:141:PRO:O    | 1.74                     | 1.05              |
| 1:J:817:GLN:CD   | 2:K:127:ARG:HD2  | 1.76                     | 1.05              |
| 2:K:140:PHE:O    | 2:K:141:PRO:O    | 1.75                     | 1.05              |
| 1:P:530:MET:CA   | 4:0:354:GLN:HG3  | 1.87                     | 1.05              |
| 1:M:783:LEU:CD1  | 1:M:786:ILE:HD11 | 1.86                     | 1.05              |
| 1:D:641:LYS:HE3  | 4:9:348:SER:O    | 1.55                     | 1.05              |
| 1:J:641:LYS:HE3  | 4:W:348:SER:O    | 1.55                     | 1.05              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:HA3   | 1.08                     | 1.05              |
| 1:G:795:ARG:HG2  | 3:I:118:MET:HE1  | 1.08                     | 1.05              |
| 1:A:94:MET:O     | 1:A:713:SER:HB3  | 1.57                     | 1.05              |
| 2:N:114:LYS:HA   | 2:N:146:GLY:O    | 0.89                     | 1.05              |
| 2:Q:114:LYS:HA   | 2:Q:146:GLY:O    | 0.89                     | 1.05              |
| 2:E:121:LEU:C    | 2:E:128:PHE:HB3  | 1.72                     | 1.05              |
| 4:1:287:ILE:HB   | 4:3:203:THR:HG22 | 1.32                     | 1.05              |
| 2:B:121:LEU:C    | 2:B:128:PHE:HB3  | 1.72                     | 1.05              |
| 1:J:530:MET:CA   | 4:W:354:GLN:HG3  | 1.87                     | 1.05              |
| 1:J:638:GLY:HA2  | 4:W:341:ILE:O    | 1.57                     | 1.05              |
| 1:A:530:MET:CA   | 4:8:354:GLN:HG3  | 1.86                     | 1.05              |
| 1:M:798:LEU:HD21 | 3:O:126:LEU:CD1  | 1.85                     | 1.05              |
| 1:A:799:MET:SD   | 3:C:32:ASP:CA    | 2.45                     | 1.05              |
| 4:W:325:MET:CE   | 4:Y:244:ASP:OD2  | 2.04                     | 1.05              |
| 4:0:288:ASP:CB   | 4:2:63:GLY:CA    | 2.31                     | 1.05              |
| 1:J:831:TRP:CH2  | 2:K:47:LEU:HD21  | 1.90                     | 1.05              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:CB   | 1.85                     | 1.05              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:800:ARG:HH22 | 3:C:40:ASN:ND2   | 1.52                     | 1.05              |
| 1:D:72:VAL:HG13  | 1:D:76:GLN:HB3   | 1.36                     | 1.05              |
| 1:D:747:LEU:HD13 | 1:D:782:MLY:HH21 | 1.35                     | 1.05              |
| 1:G:754:ASP:OD2  | 1:G:779:ARG:HB3  | 1.53                     | 1.05              |
| 1:G:542:PHE:CG   | 4:V:143:TYR:HE1  | 1.74                     | 1.05              |
| 1:G:635:GLY:HA3  | 4:V:341:ILE:HD13 | 1.36                     | 1.05              |
| 2:H:114:LYS:HA   | 2:H:146:GLY:O    | 0.89                     | 1.05              |
| 1:P:538:GLU:OE2  | 4:O:355:MET:HE1  | 1.53                     | 1.05              |
| 1:M:530:MET:CA   | 4:Z:354:GLN:HG3  | 1.86                     | 1.05              |
| 1:P:785:GLU:HG3  | 3:R:81:GLN:OE1   | 1.57                     | 1.05              |
| 1:A:798:LEU:HD11 | 3:C:126:LEU:HD11 | 1.30                     | 1.05              |
| 1:A:635:GLY:HA3  | 4:8:341:ILE:HD13 | 1.36                     | 1.05              |
| 1:A:542:PHE:CG   | 4:8:143:TYR:HE1  | 1.73                     | 1.05              |
| 1:P:641:LYS:HE3  | 4:O:348:SER:O    | 1.55                     | 1.05              |
| 4:O:244:ASP:N    | 4:Y:291:LYS:HE3  | 1.41                     | 1.05              |
| 4:X:291:LYS:CD   | 4:Z:243:PRO:HB2  | 1.87                     | 1.05              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:HG22 | 1.09                     | 1.05              |
| 4:1:3:ASP:HA     | 4:1:6:THR:HB     | 1.36                     | 1.05              |
| 1:J:576:GLU:HG2  | 1:J:577:ALA:N    | 1.66                     | 1.05              |
| 1:J:72:VAL:HG13  | 1:J:76:GLN:HB3   | 1.36                     | 1.05              |
| 1:M:72:VAL:HG13  | 1:M:76:GLN:HB3   | 1.36                     | 1.05              |
| 1:P:409:GLY:N    | 1:P:636:LYS:HG3  | 1.69                     | 1.05              |
| 1:P:542:PHE:CG   | 4:O:143:TYR:HE1  | 1.73                     | 1.05              |
| 1:P:836:PHE:CZ   | 2:Q:160:GLY:N    | 2.24                     | 1.05              |
| 1:M:736:GLN:HA   | 1:M:743:ALA:HB3  | 1.35                     | 1.05              |
| 1:J:641:LYS:HB2  | 1:J:647:GLN:NE2  | 1.68                     | 1.05              |
| 1:G:84:MLY:HH22  | 1:G:719:ASP:O    | 1.53                     | 1.05              |
| 1:G:93:MET:HE1   | 1:G:764:MLY:CD   | 1.87                     | 1.05              |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:HH21 | 1.13                     | 1.04              |
| 1:M:819:ASN:HA   | 2:N:90:GLY:O     | 0.86                     | 1.04              |
| 1:G:553:MLY:CE   | 4:X:45:VAL:HG11  | 1.53                     | 1.04              |
| 1:P:817:GLN:CB   | 2:Q:127:ARG:HH11 | 1.68                     | 1.04              |
| 2:Q:144:VAL:HG11 | 2:Q:153:ILE:HG12 | 1.38                     | 1.04              |
| 1:P:817:GLN:HG2  | 2:Q:127:ARG:CB   | 1.86                     | 1.04              |
| 2:B:144:VAL:HG11 | 2:B:153:ILE:HG12 | 1.38                     | 1.04              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CD   | 1.77                     | 1.04              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CD   | 1.77                     | 1.04              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:CD   | 1.70                     | 1.04              |
| 1:A:599:ASN:HA   | 1:A:649:VAL:HB   | 1.05                     | 1.04              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:HB3  | 1.86                     | 1.04              |
| 1:M:817:GLN:CB   | 2:N:127:ARG:CD   | 2.34                     | 1.04              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:140:PHE:O    | 2:Q:141:PRO:O    | 1.75                     | 1.04              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:HB2  | 1.78                     | 1.04              |
| 2:B:121:LEU:HG   | 2:B:128:PHE:CA   | 1.59                     | 1.04              |
| 1:M:639:GLY:HA3  | 4:Z:344:SER:C    | 1.78                     | 1.04              |
| 1:J:542:PHE:CG   | 4:W:143:TYR:HE1  | 1.73                     | 1.04              |
| 1:D:638:GLY:HA2  | 4:9:341:ILE:O    | 1.57                     | 1.04              |
| 1:D:530:MET:CA   | 4:9:354:GLN:HG3  | 1.87                     | 1.04              |
| 1:M:97:LEU:CD2   | 1:M:712:PRO:HB3  | 1.86                     | 1.04              |
| 1:A:28:GLN:HE22  | 1:A:723:ARG:NH2  | 1.55                     | 1.04              |
| 1:G:552:ASN:O    | 4:X:47:MET:CE    | 2.05                     | 1.04              |
| 1:G:557:GLU:CB   | 4:X:46:GLY:C     | 2.26                     | 1.04              |
| 1:A:795:ARG:HD3  | 3:C:43:ASN:OD1   | 1.54                     | 1.04              |
| 1:A:538:GLU:OE2  | 4:8:355:MET:HE1  | 1.55                     | 1.04              |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:CB   | 1.87                     | 1.04              |
| 1:J:795:ARG:CD   | 3:L:43:ASN:CG    | 2.26                     | 1.04              |
| 1:G:797:PHE:CE1  | 3:I:146:ILE:CD1  | 2.39                     | 1.04              |
| 1:M:817:GLN:HB3  | 2:N:127:ARG:CD   | 1.88                     | 1.04              |
| 1:P:817:GLN:HB3  | 2:Q:127:ARG:NH1  | 1.73                     | 1.04              |
| 1:P:736:GLN:HA   | 1:P:743:ALA:HB3  | 1.35                     | 1.04              |
| 1:G:84:MLY:CD    | 1:G:723:ARG:HD2  | 1.88                     | 1.04              |
| 3:I:49:ILE:CA    | 3:I:52:ASN:HD22  | 1.70                     | 1.04              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HD11 | 1.21                     | 1.04              |
| 2:K:111:SER:CB   | 2:K:148:VAL:C    | 1.93                     | 1.04              |
| 1:P:797:PHE:CZ   | 3:R:146:ILE:CD1  | 2.40                     | 1.04              |
| 1:A:831:TRP:CD1  | 2:B:51:PHE:HZ    | 1.73                     | 1.04              |
| 1:A:797:PHE:HD1  | 3:C:146:ILE:O    | 1.38                     | 1.04              |
| 1:M:783:LEU:CA   | 1:M:786:ILE:HD11 | 1.86                     | 1.04              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CD   | 1.77                     | 1.04              |
| 4:0:244:ASP:N    | 4:Y:291:LYS:NZ   | 2.05                     | 1.04              |
| 1:D:768:MLY:CA   | 1:D:771:LEU:HD12 | 1.88                     | 1.04              |
| 4:0:110:LEU:O    | 4:1:195:GLU:HA   | 1.55                     | 1.04              |
| 4:2:324:THR:CG2  | 4:4:244:ASP:O    | 1.97                     | 1.04              |
| 3:F:49:ILE:HA    | 3:F:52:ASN:HD22  | 1.22                     | 1.04              |
| 1:J:56:GLU:HB2   | 1:J:59:MLY:HB3   | 1.40                     | 1.04              |
| 1:P:56:GLU:HB2   | 1:P:59:MLY:HB3   | 1.40                     | 1.04              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:HB3  | 1.35                     | 1.03              |
| 1:D:791:GLN:OE1  | 3:F:116:GLU:HG3  | 1.57                     | 1.03              |
| 1:G:791:GLN:OE1  | 3:I:116:GLU:HG3  | 1.58                     | 1.03              |
| 1:A:795:ARG:HD2  | 3:C:35:ARG:HH12  | 0.91                     | 1.03              |
| 1:P:576:GLU:HG2  | 1:P:577:ALA:N    | 1.66                     | 1.03              |
| 1:M:795:ARG:HE   | 3:O:118:MET:HE1  | 1.19                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CD   | 1.77                     | 1.03              |
| 1:G:503:TYR:OH   | 1:G:711:PHE:CD2  | 2.03                     | 1.03              |
| 1:G:84:MLY:HD3   | 1:G:723:ARG:HD2  | 1.34                     | 1.03              |
| 1:G:84:MLY:CH1   | 1:G:724:TYR:CE2  | 2.40                     | 1.03              |
| 4:0:204:ALA:HB3  | 4:Y:288:ASP:HB2  | 1.35                     | 1.03              |
| 4:3:288:ASP:CG   | 4:5:203:THR:HG21 | 1.63                     | 1.03              |
| 4:X:325:MET:SD   | 4:Z:244:ASP:OD2  | 2.16                     | 1.03              |
| 1:G:599:ASN:HA   | 1:G:649:VAL:HB   | 1.05                     | 1.03              |
| 1:J:95:THR:HA    | 1:J:713:SER:CB   | 1.88                     | 1.03              |
| 3:O:49:ILE:CA    | 3:O:52:ASN:HD22  | 1.71                     | 1.03              |
| 1:J:798:LEU:CG   | 3:L:126:LEU:HD11 | 1.89                     | 1.03              |
| 2:N:144:VAL:HG11 | 2:N:153:ILE:HG12 | 1.37                     | 1.03              |
| 1:G:639:GLY:N    | 4:V:345:ILE:N    | 1.94                     | 1.03              |
| 2:Q:121:LEU:C    | 2:Q:128:PHE:HB3  | 1.72                     | 1.03              |
| 2:K:144:VAL:HG11 | 2:K:153:ILE:HG12 | 1.38                     | 1.03              |
| 1:M:529:PRO:C    | 4:Z:354:GLN:HB3  | 1.77                     | 1.03              |
| 1:P:785:GLU:HG3  | 3:R:81:GLN:CD    | 1.78                     | 1.03              |
| 1:D:823:PHE:CD1  | 2:E:160:GLY:HA2  | 1.91                     | 1.03              |
| 1:D:202:SER:CA   | 1:D:207:LYS:CE   | 2.36                     | 1.03              |
| 3:I:49:ILE:HA    | 3:I:52:ASN:HD22  | 1.23                     | 1.03              |
| 3:C:49:ILE:CA    | 3:C:52:ASN:HD22  | 1.70                     | 1.03              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:N    | 1.91                     | 1.03              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:N    | 1.91                     | 1.03              |
| 1:G:56:GLU:HB2   | 1:G:59:MLY:HB3   | 1.40                     | 1.03              |
| 2:B:140:PHE:O    | 2:B:141:PRO:O    | 1.75                     | 1.03              |
| 1:J:506:GLU:OE2  | 1:J:761:GLY:CA   | 2.05                     | 1.03              |
| 1:M:638:GLY:HA2  | 4:Z:341:ILE:O    | 1.57                     | 1.03              |
| 1:P:798:LEU:HD21 | 3:R:126:LEU:HD12 | 1.33                     | 1.03              |
| 1:P:792:ALA:CB   | 3:R:42:THR:CG2   | 2.25                     | 1.03              |
| 1:A:797:PHE:CE2  | 3:C:146:ILE:CD1  | 2.39                     | 1.03              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:CD   | 1.70                     | 1.03              |
| 1:M:641:LYS:HE3  | 1:M:647:GLN:CD   | 1.77                     | 1.03              |
| 1:P:202:SER:CA   | 1:P:207:LYS:CE   | 2.36                     | 1.03              |
| 1:P:834:LEU:CD1  | 2:Q:51:PHE:CE1   | 2.39                     | 1.03              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB3  | 1.35                     | 1.03              |
| 2:H:140:PHE:O    | 2:H:141:PRO:O    | 1.75                     | 1.03              |
| 1:J:819:ASN:HA   | 2:K:90:GLY:O     | 0.86                     | 1.03              |
| 1:P:642:LYS:HG3  | 4:0:23:GLY:H     | 0.86                     | 1.03              |
| 1:A:638:GLY:HA2  | 4:8:341:ILE:O    | 1.57                     | 1.03              |
| 1:M:783:LEU:O    | 1:M:786:ILE:HG13 | 1.55                     | 1.03              |
| 1:G:93:MET:HE1   | 1:G:764:MLY:HD2  | 1.39                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:726:VAL:HG11 | 1:D:785:GLU:HB3  | 1.08                     | 1.03              |
| 1:A:642:LYS:HG3  | 4:8:23:GLY:H     | 0.87                     | 1.03              |
| 1:J:831:TRP:CH2  | 2:K:47:LEU:CD2   | 2.42                     | 1.03              |
| 4:8:290:ARG:CZ   | 4:V:202:THR:CG2  | 2.36                     | 1.03              |
| 1:M:97:LEU:HD23  | 1:M:712:PRO:HB3  | 1.36                     | 1.03              |
| 1:G:94:MET:O     | 1:G:713:SER:HB3  | 1.58                     | 1.03              |
| 4:8:3:ASP:HA     | 4:8:6:THR:HB     | 1.36                     | 1.03              |
| 2:H:150:TYR:O    | 2:H:151:LYS:CB   | 2.06                     | 1.03              |
| 1:J:800:ARG:HH22 | 3:L:40:ASN:ND2   | 1.56                     | 1.03              |
| 1:G:795:ARG:HE   | 3:I:116:GLU:CB   | 1.70                     | 1.03              |
| 1:A:149:GLN:HB2  | 1:A:718:ALA:HB1  | 1.36                     | 1.03              |
| 1:G:639:GLY:HA3  | 4:V:344:SER:C    | 1.78                     | 1.03              |
| 1:G:530:MET:CA   | 4:V:354:GLN:HG3  | 1.88                     | 1.03              |
| 1:G:638:GLY:HA2  | 4:V:341:ILE:O    | 1.58                     | 1.03              |
| 1:D:813:ILE:CG2  | 2:E:128:PHE:CE1  | 2.41                     | 1.03              |
| 4:1:288:ASP:OD2  | 4:3:203:THR:CG2  | 2.06                     | 1.03              |
| 1:P:795:ARG:HB3  | 3:R:35:ARG:CZ    | 1.87                     | 1.03              |
| 1:G:730:SER:OG   | 3:I:113:THR:HG21 | 0.86                     | 1.03              |
| 4:0:201:VAL:H    | 4:Y:287:ILE:CG1  | 1.53                     | 1.03              |
| 1:A:641:LYS:HE3  | 4:8:348:SER:O    | 1.56                     | 1.03              |
| 1:D:831:TRP:CZ3  | 2:E:34:ILE:HG23  | 1.93                     | 1.03              |
| 3:R:49:ILE:CA    | 3:R:52:ASN:HD22  | 1.71                     | 1.03              |
| 3:R:24:LYS:HG2   | 3:R:63:ILE:O     | 1.59                     | 1.03              |
| 4:7:3:ASP:HA     | 4:7:6:THR:HB     | 1.36                     | 1.03              |
| 2:N:149:ASP:OD2  | 2:N:150:TYR:N    | 1.91                     | 1.03              |
| 1:J:798:LEU:HD12 | 3:L:126:LEU:HD11 | 1.41                     | 1.02              |
| 1:D:727:LEU:CD1  | 1:D:782:MLY:HG2  | 1.87                     | 1.02              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:CB   | 2.36                     | 1.02              |
| 1:P:529:PRO:C    | 4:0:354:GLN:HB3  | 1.77                     | 1.02              |
| 1:J:541:MET:HB3  | 4:W:143:TYR:OH   | 1.59                     | 1.02              |
| 1:A:797:PHE:HE2  | 3:C:126:LEU:CD2  | 1.69                     | 1.02              |
| 1:A:639:GLY:HA3  | 4:8:344:SER:C    | 1.78                     | 1.02              |
| 1:G:93:MET:HA    | 1:G:714:ARG:H    | 0.90                     | 1.02              |
| 1:J:202:SER:CA   | 1:J:207:LYS:CE   | 2.36                     | 1.02              |
| 1:D:800:ARG:O    | 3:F:149:VAL:HG21 | 1.58                     | 1.02              |
| 4:2:3:ASP:HA     | 4:2:6:THR:HB     | 1.36                     | 1.02              |
| 1:G:642:LYS:HG3  | 4:V:23:GLY:H     | 0.85                     | 1.02              |
| 1:G:530:MET:HE2  | 4:V:354:GLN:CG   | 1.89                     | 1.02              |
| 1:P:639:GLY:HA3  | 4:0:344:SER:C    | 1.78                     | 1.02              |
| 1:J:639:GLY:HA3  | 4:W:344:SER:C    | 1.78                     | 1.02              |
| 1:D:639:GLY:HA3  | 4:9:344:SER:C    | 1.78                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:798:LEU:HD11 | 3:C:126:LEU:CG   | 1.90                     | 1.02              |
| 1:A:541:MET:HB3  | 4:8:143:TYR:OH   | 1.60                     | 1.02              |
| 1:G:93:MET:HE3   | 1:G:764:MLY:HD3  | 1.37                     | 1.02              |
| 1:M:641:LYS:CG   | 4:Z:348:SER:HB2  | 1.86                     | 1.02              |
| 1:M:599:ASN:HA   | 1:M:649:VAL:HB   | 1.05                     | 1.02              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:HD21 | 1.24                     | 1.02              |
| 1:P:599:ASN:CA   | 1:P:649:VAL:HB   | 1.89                     | 1.02              |
| 4:9:290:ARG:CZ   | 4:W:202:THR:CG2  | 2.36                     | 1.02              |
| 4:7:290:ARG:CZ   | 4:9:202:THR:CG2  | 2.36                     | 1.02              |
| 3:L:49:ILE:CA    | 3:L:52:ASN:HD22  | 1.71                     | 1.02              |
| 4:Z:3:ASP:HA     | 4:Z:6:THR:HB     | 1.36                     | 1.02              |
| 2:Q:149:ASP:OD2  | 2:Q:150:TYR:N    | 1.91                     | 1.02              |
| 2:B:149:ASP:OD2  | 2:B:150:TYR:N    | 1.91                     | 1.02              |
| 1:A:149:GLN:HE21 | 1:A:718:ALA:CB   | 1.64                     | 1.02              |
| 1:J:817:GLN:HB3  | 2:K:127:ARG:HH11 | 1.16                     | 1.02              |
| 1:P:541:MET:HB3  | 4:0:143:TYR:OH   | 1.59                     | 1.02              |
| 1:M:541:MET:HB3  | 4:Z:143:TYR:OH   | 1.60                     | 1.02              |
| 1:D:553:MLY:CB   | 4:W:46:GLY:CA    | 2.32                     | 1.02              |
| 1:A:202:SER:CA   | 1:A:207:LYS:CE   | 2.36                     | 1.02              |
| 1:D:642:LYS:HG3  | 4:9:23:GLY:H     | 0.86                     | 1.02              |
| 1:M:642:LYS:HG3  | 4:Z:23:GLY:H     | 0.86                     | 1.02              |
| 1:A:818:TYR:CB   | 2:B:90:GLY:N     | 2.22                     | 1.02              |
| 3:F:49:ILE:CA    | 3:F:52:ASN:HD22  | 1.70                     | 1.02              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:N    | 1.91                     | 1.02              |
| 4:V:3:ASP:HA     | 4:V:6:THR:HB     | 1.36                     | 1.02              |
| 4:W:3:ASP:HA     | 4:W:6:THR:HB     | 1.36                     | 1.02              |
| 1:D:798:LEU:HD13 | 3:F:126:LEU:HD11 | 1.36                     | 1.02              |
| 1:G:754:ASP:CG   | 1:G:779:ARG:HD2  | 1.79                     | 1.02              |
| 1:M:206:LYS:HD2  | 1:M:217:THR:HG23 | 1.41                     | 1.02              |
| 1:P:831:TRP:CZ2  | 2:Q:47:LEU:HD22  | 1.95                     | 1.02              |
| 1:J:599:ASN:CA   | 1:J:649:VAL:HB   | 1.89                     | 1.02              |
| 3:F:24:LYS:HG2   | 3:F:63:ILE:O     | 1.59                     | 1.02              |
| 3:C:24:LYS:HG2   | 3:C:63:ILE:O     | 1.59                     | 1.02              |
| 3:L:24:LYS:CG    | 3:L:63:ILE:O     | 2.08                     | 1.02              |
| 2:B:150:TYR:O    | 2:B:151:LYS:CB   | 2.07                     | 1.02              |
| 4:4:3:ASP:HA     | 4:4:6:THR:HB     | 1.36                     | 1.02              |
| 2:H:144:VAL:HG11 | 2:H:153:ILE:HG12 | 1.38                     | 1.02              |
| 1:M:576:GLU:HG2  | 1:M:577:ALA:H    | 0.85                     | 1.02              |
| 1:M:639:GLY:N    | 4:Z:345:ILE:N    | 1.94                     | 1.02              |
| 1:P:795:ARG:HB2  | 3:R:35:ARG:NH1   | 1.72                     | 1.02              |
| 1:M:797:PHE:CD1  | 3:O:149:VAL:HG11 | 1.91                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:93:MET:CG    | 1:G:714:ARG:O    | 0.72                     | 1.02              |
| 4:W:291:LYS:HD2  | 4:Y:243:PRO:HB2  | 1.41                     | 1.02              |
| 1:P:803:TYR:O    | 1:P:807:VAL:N    | 1.91                     | 1.02              |
| 1:P:767:PHE:CD1  | 1:P:772:LEU:CD2  | 2.43                     | 1.02              |
| 3:F:24:LYS:CG    | 3:F:63:ILE:O     | 2.08                     | 1.02              |
| 1:G:795:ARG:CA   | 3:I:118:MET:HE1  | 1.90                     | 1.01              |
| 1:A:149:GLN:NE2  | 1:A:718:ALA:HB2  | 1.71                     | 1.01              |
| 1:A:505:MLY:HD3  | 1:A:762:HIS:N    | 1.74                     | 1.01              |
| 1:A:505:MLY:CE   | 1:A:762:HIS:HA   | 1.87                     | 1.01              |
| 2:N:121:LEU:C    | 2:N:128:PHE:HB3  | 1.72                     | 1.01              |
| 1:G:93:MET:HA    | 1:G:714:ARG:N    | 1.75                     | 1.01              |
| 1:P:641:LYS:HE3  | 1:P:647:GLN:CD   | 1.77                     | 1.01              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:HG3  | 1.21                     | 1.01              |
| 1:M:641:LYS:HB2  | 1:M:647:GLN:NE2  | 1.68                     | 1.01              |
| 1:A:642:LYS:HD3  | 4:8:340:TRP:CZ3  | 1.95                     | 1.01              |
| 1:A:642:LYS:HD3  | 4:8:340:TRP:CH2  | 1.95                     | 1.01              |
| 1:P:599:ASN:HA   | 1:P:649:VAL:HB   | 1.05                     | 1.01              |
| 3:C:24:LYS:CG    | 3:C:63:ILE:O     | 2.08                     | 1.01              |
| 1:G:576:GLU:HG2  | 1:G:577:ALA:H    | 0.85                     | 1.01              |
| 4:0:3:ASP:HA     | 4:0:6:THR:HB     | 1.36                     | 1.01              |
| 4:Y:3:ASP:HA     | 4:Y:6:THR:HB     | 1.36                     | 1.01              |
| 1:J:98:HIS:HB3   | 1:J:100:PRO:HD2  | 1.42                     | 1.01              |
| 4:1:322:PRO:HB3  | 4:3:244:ASP:CB   | 1.90                     | 1.01              |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CE1  | 1.88                     | 1.01              |
| 1:P:817:GLN:CB   | 2:Q:127:ARG:CD   | 2.34                     | 1.01              |
| 1:G:819:ASN:CG   | 2:H:90:GLY:O     | 1.97                     | 1.01              |
| 2:K:121:LEU:CB   | 2:K:128:PHE:HB3  | 1.69                     | 1.01              |
| 2:K:144:VAL:HG13 | 2:K:153:ILE:HD11 | 1.21                     | 1.01              |
| 1:P:635:GLY:HA3  | 4:0:341:ILE:HD13 | 1.36                     | 1.01              |
| 1:D:553:MLY:HB3  | 4:W:46:GLY:CA    | 1.51                     | 1.01              |
| 1:A:797:PHE:CD1  | 3:C:146:ILE:O    | 2.12                     | 1.01              |
| 1:A:639:GLY:N    | 4:8:345:ILE:N    | 1.94                     | 1.01              |
| 1:M:795:ARG:NE   | 3:O:118:MET:HE1  | 1.73                     | 1.01              |
| 1:P:641:LYS:CG   | 4:0:348:SER:HB2  | 1.86                     | 1.01              |
| 1:A:599:ASN:CA   | 1:A:649:VAL:HB   | 1.89                     | 1.01              |
| 1:D:599:ASN:CA   | 1:D:649:VAL:HB   | 1.89                     | 1.01              |
| 4:7:290:ARG:NH2  | 4:9:202:THR:CG2  | 2.23                     | 1.01              |
| 3:R:24:LYS:CG    | 3:R:63:ILE:O     | 2.08                     | 1.01              |
| 3:L:49:ILE:HA    | 3:L:52:ASN:HD22  | 1.23                     | 1.01              |
| 1:D:732:ILE:CD1  | 1:D:782:MLY:CH1  | 2.38                     | 1.01              |
| 1:M:817:GLN:HG2  | 2:N:127:ARG:HD2  | 1.19                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:144:VAL:HG11 | 2:E:153:ILE:HG12 | 1.38                     | 1.01              |
| 1:P:638:GLY:HA2  | 4:0:341:ILE:O    | 1.57                     | 1.01              |
| 1:P:646:PHE:HE2  | 1:P:652:LEU:HD21 | 1.24                     | 1.01              |
| 1:J:529:PRO:C    | 4:W:354:GLN:HB3  | 1.77                     | 1.01              |
| 1:P:795:ARG:HH21 | 3:R:116:GLU:CG   | 1.57                     | 1.01              |
| 1:D:541:MET:HB3  | 4:9:143:TYR:OH   | 1.60                     | 1.01              |
| 1:A:529:PRO:C    | 4:8:354:GLN:HB3  | 1.78                     | 1.01              |
| 1:G:84:MLY:NZ    | 1:G:724:TYR:HE2  | 1.58                     | 1.01              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:HB2  | 1.42                     | 1.01              |
| 4:0:112:PRO:HG3  | 4:1:196:ARG:N    | 1.67                     | 1.01              |
| 4:9:290:ARG:NH2  | 4:W:202:THR:CG2  | 2.23                     | 1.01              |
| 1:G:769:ALA:HB3  | 1:G:770:GLY:CA   | 1.90                     | 1.01              |
| 2:E:150:TYR:O    | 2:E:151:LYS:CB   | 2.06                     | 1.01              |
| 1:J:795:ARG:HB2  | 3:L:35:ARG:NH1   | 1.74                     | 1.01              |
| 1:D:727:LEU:CD1  | 1:D:782:MLY:CE   | 2.32                     | 1.01              |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:HG2  | 1.25                     | 1.01              |
| 1:M:817:GLN:HB3  | 2:N:127:ARG:HH11 | 0.90                     | 1.01              |
| 1:J:642:LYS:HG3  | 4:W:23:GLY:H     | 0.86                     | 1.01              |
| 1:D:553:MLY:HG2  | 4:W:44:MET:O     | 1.59                     | 1.01              |
| 1:A:831:TRP:HH2  | 2:B:50:THR:CB    | 1.69                     | 1.01              |
| 1:P:503:TYR:OH   | 1:P:711:PHE:HD2  | 1.42                     | 1.01              |
| 1:G:599:ASN:CA   | 1:G:649:VAL:HB   | 1.89                     | 1.01              |
| 1:M:98:HIS:HB3   | 1:M:100:PRO:HD2  | 1.42                     | 1.01              |
| 4:9:3:ASP:HA     | 4:9:6:THR:HB     | 1.36                     | 1.01              |
| 1:A:502:GLU:HA   | 1:A:762:HIS:N    | 1.76                     | 1.01              |
| 2:N:121:LEU:HG   | 2:N:128:PHE:CA   | 1.60                     | 1.01              |
| 1:G:529:PRO:C    | 4:V:354:GLN:HB3  | 1.79                     | 1.01              |
| 1:P:642:LYS:HD3  | 4:0:340:TRP:CZ3  | 1.96                     | 1.01              |
| 1:P:642:LYS:HD3  | 4:0:340:TRP:CH2  | 1.95                     | 1.01              |
| 1:P:795:ARG:CG   | 3:R:118:MET:CE   | 2.34                     | 1.01              |
| 1:D:635:GLY:HA3  | 4:9:341:ILE:HD13 | 1.37                     | 1.01              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:HB2  | 1.43                     | 1.01              |
| 1:M:641:LYS:HE3  | 1:M:647:GLN:HB2  | 1.42                     | 1.01              |
| 1:D:712:PRO:HB2  | 1:D:771:LEU:CB   | 1.90                     | 1.01              |
| 1:M:599:ASN:CA   | 1:M:649:VAL:HB   | 1.89                     | 1.01              |
| 1:D:599:ASN:HA   | 1:D:649:VAL:HB   | 1.05                     | 1.01              |
| 1:J:599:ASN:HA   | 1:J:649:VAL:HB   | 1.05                     | 1.01              |
| 1:A:95:THR:HG1   | 1:A:769:ALA:CA   | 1.66                     | 1.01              |
| 4:0:166:TYR:CZ   | 4:2:64:ILE:CG2   | 2.44                     | 1.01              |
| 1:J:756:THR:CG2  | 1:J:776:GLU:CA   | 2.38                     | 1.01              |
| 4:8:290:ARG:NH2  | 4:V:202:THR:CG2  | 2.23                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:48:LYS:O     | 3:C:52:ASN:ND2   | 1.94                     | 1.01              |
| 2:N:150:TYR:O    | 2:N:151:LYS:CB   | 2.07                     | 1.01              |
| 1:A:97:LEU:HD22  | 1:A:712:PRO:HB3  | 1.38                     | 1.00              |
| 1:G:642:LYS:HD3  | 4:V:340:TRP:CH2  | 1.96                     | 1.00              |
| 1:G:820:VAL:HG11 | 2:H:136:MET:HE3  | 1.40                     | 1.00              |
| 1:G:813:ILE:CG2  | 2:H:128:PHE:CZ   | 2.40                     | 1.00              |
| 1:G:206:LYS:HD2  | 1:G:217:THR:HG23 | 1.41                     | 1.00              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:HD21 | 1.24                     | 1.00              |
| 1:J:642:LYS:HD3  | 4:W:340:TRP:CH2  | 1.96                     | 1.00              |
| 1:D:557:GLU:N    | 4:W:48:GLY:CA    | 2.12                     | 1.00              |
| 1:A:797:PHE:CD1  | 3:C:146:ILE:HG23 | 1.95                     | 1.00              |
| 1:A:576:GLU:HG2  | 1:A:577:ALA:H    | 0.85                     | 1.00              |
| 1:P:836:PHE:CE1  | 2:Q:159:HIS:CA   | 2.44                     | 1.00              |
| 1:M:84:MLY:NZ    | 1:M:724:TYR:HE2  | 1.57                     | 1.00              |
| 1:M:84:MLY:CG    | 1:M:723:ARG:CD   | 2.38                     | 1.00              |
| 1:D:831:TRP:NE1  | 2:E:51:PHE:HZ    | 1.47                     | 1.00              |
| 1:M:35:MLY:CH2   | 1:M:778:MET:CG   | 2.38                     | 1.00              |
| 1:J:757:GLN:HA   | 1:J:776:GLU:HG3  | 1.42                     | 1.00              |
| 1:G:834:LEU:HD13 | 2:H:51:PHE:CE1   | 1.95                     | 1.00              |
| 4:9:287:ILE:HB   | 4:W:204:ALA:H    | 1.25                     | 1.00              |
| 3:L:48:LYS:O     | 3:L:52:ASN:ND2   | 1.94                     | 1.00              |
| 1:A:56:GLU:HB2   | 1:A:59:MLY:HB3   | 1.40                     | 1.00              |
| 1:G:752:ASP:O    | 1:G:780:ASP:OD1  | 1.77                     | 1.00              |
| 1:G:541:MET:HB3  | 4:V:143:TYR:OH   | 1.59                     | 1.00              |
| 2:H:121:LEU:HG   | 2:H:128:PHE:CA   | 1.60                     | 1.00              |
| 2:K:121:LEU:C    | 2:K:128:PHE:HB3  | 1.72                     | 1.00              |
| 1:J:84:MLY:CH2   | 1:J:720:PHE:CA   | 2.25                     | 1.00              |
| 1:M:545:ALA:HA   | 4:1:45:VAL:HG12  | 1.00                     | 1.00              |
| 1:M:534:SER:O    | 4:Z:351:THR:HA   | 1.60                     | 1.00              |
| 1:J:635:GLY:HA3  | 4:W:341:ILE:HD13 | 1.36                     | 1.00              |
| 1:D:534:SER:O    | 4:9:351:THR:HA   | 1.59                     | 1.00              |
| 1:A:576:GLU:HG2  | 1:A:577:ALA:N    | 1.66                     | 1.00              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:HB2  | 1.42                     | 1.00              |
| 1:P:641:LYS:HE3  | 1:P:647:GLN:HB2  | 1.43                     | 1.00              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CB   | 1.91                     | 1.00              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CB   | 1.91                     | 1.00              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE3   | 1.40                     | 1.00              |
| 1:G:97:LEU:HD23  | 1:G:712:PRO:CB   | 1.82                     | 1.00              |
| 1:P:506:GLU:HG2  | 1:P:760:PHE:N    | 1.75                     | 1.00              |
| 1:G:202:SER:CA   | 1:G:207:LYS:CE   | 2.36                     | 1.00              |
| 1:M:642:LYS:HD3  | 4:Z:340:TRP:CH2  | 1.95                     | 1.00              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:215:GLN:CA  | 1:G:340:ILE:HG23 | 1.92                     | 1.00              |
| 3:O:48:LYS:O    | 3:O:52:ASN:ND2   | 1.94                     | 1.00              |
| 1:A:800:ARG:HD2 | 3:C:149:VAL:C    | 1.81                     | 1.00              |
| 3:I:24:LYS:CG   | 3:I:63:ILE:O     | 2.08                     | 1.00              |
| 3:L:24:LYS:HG2  | 3:L:63:ILE:O     | 1.59                     | 1.00              |
| 3:O:24:LYS:HG2  | 3:O:63:ILE:O     | 1.59                     | 1.00              |
| 1:M:534:SER:C   | 4:Z:351:THR:HA   | 1.81                     | 1.00              |
| 1:J:642:LYS:HD3 | 4:W:340:TRP:CZ3  | 1.96                     | 1.00              |
| 1:D:206:LYS:HD2 | 1:D:217:THR:HG23 | 1.41                     | 1.00              |
| 1:D:218:LEU:CA  | 1:D:221:GLN:HG3  | 1.90                     | 1.00              |
| 1:A:797:PHE:CG  | 3:C:146:ILE:HG23 | 1.96                     | 1.00              |
| 1:A:534:SER:O   | 4:8:351:THR:HA   | 1.59                     | 1.00              |
| 1:A:641:LYS:HE3 | 1:A:647:GLN:HB2  | 1.42                     | 1.00              |
| 1:M:215:GLN:CA  | 1:M:340:ILE:HG23 | 1.92                     | 1.00              |
| 3:F:48:LYS:O    | 3:F:52:ASN:ND2   | 1.94                     | 1.00              |
| 3:I:24:LYS:HG2  | 3:I:63:ILE:O     | 1.59                     | 1.00              |
| 1:J:174:SER:HB3 | 1:J:667:THR:HG21 | 1.44                     | 1.00              |
| 1:D:174:SER:HB3 | 1:D:667:THR:HG21 | 1.44                     | 1.00              |
| 1:P:174:SER:HB3 | 1:P:667:THR:HG21 | 1.44                     | 1.00              |
| 1:D:795:ARG:CB  | 3:F:35:ARG:NH1   | 2.23                     | 1.00              |
| 1:A:501:GLU:CB  | 1:A:762:HIS:ND1  | 2.24                     | 1.00              |
| 1:P:534:SER:C   | 4:0:351:THR:HA   | 1.81                     | 1.00              |
| 1:J:534:SER:C   | 4:W:351:THR:HA   | 1.81                     | 1.00              |
| 1:G:730:SER:CB  | 3:I:113:THR:HG21 | 1.90                     | 1.00              |
| 1:M:836:PHE:CE1 | 2:N:159:HIS:CA   | 2.45                     | 1.00              |
| 1:M:800:ARG:NH2 | 3:O:40:ASN:OD1   | 1.95                     | 1.00              |
| 4:V:324:THR:CG2 | 4:X:247:VAL:N    | 2.24                     | 1.00              |
| 1:G:98:HIS:HB3  | 1:G:100:PRO:HD2  | 1.42                     | 1.00              |
| 1:G:642:LYS:HD3 | 4:V:340:TRP:CZ3  | 1.96                     | 1.00              |
| 1:G:534:SER:C   | 4:V:351:THR:HA   | 1.82                     | 1.00              |
| 1:G:817:GLN:CG  | 2:H:127:ARG:HB2  | 1.91                     | 1.00              |
| 1:M:506:GLU:CG  | 1:M:760:PHE:O    | 2.09                     | 1.00              |
| 1:D:642:LYS:HD3 | 4:9:340:TRP:CH2  | 1.96                     | 1.00              |
| 1:G:576:GLU:CG  | 1:G:577:ALA:H    | 1.75                     | 1.00              |
| 1:P:98:HIS:HB3  | 1:P:100:PRO:HD2  | 1.42                     | 1.00              |
| 1:D:98:HIS:HB3  | 1:D:100:PRO:HD2  | 1.42                     | 1.00              |
| 1:A:93:MET:HE1  | 1:A:715:VAL:CG1  | 1.92                     | 1.00              |
| 1:G:646:PHE:HE2 | 1:G:652:LEU:HD21 | 1.24                     | 1.00              |
| 1:M:782:MLY:HD2 | 3:O:86:ASP:OD1   | 1.62                     | 1.00              |
| 4:0:288:ASP:OD2 | 4:2:63:GLY:N     | 1.95                     | 1.00              |
| 1:J:95:THR:HA   | 1:J:713:SER:OG   | 1.61                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:48:LYS:O     | 3:R:52:ASN:ND2   | 1.94                     | 1.00              |
| 1:M:56:GLU:HB2   | 1:M:59:MLY:HB3   | 1.40                     | 1.00              |
| 2:N:139:ALA:O    | 2:N:141:PRO:HD3  | 1.62                     | 1.00              |
| 1:M:218:LEU:CA   | 1:M:221:GLN:HG3  | 1.91                     | 1.00              |
| 1:A:576:GLU:CG   | 1:A:577:ALA:H    | 1.75                     | 1.00              |
| 1:P:836:PHE:HE1  | 2:Q:159:HIS:HA   | 1.18                     | 1.00              |
| 1:M:641:LYS:HE3  | 1:M:647:GLN:CB   | 1.91                     | 1.00              |
| 3:O:24:LYS:CG    | 3:O:63:ILE:O     | 2.08                     | 1.00              |
| 1:G:795:ARG:NH2  | 3:I:116:GLU:HG2  | 1.77                     | 0.99              |
| 1:M:817:GLN:HG2  | 2:N:127:ARG:CB   | 1.91                     | 0.99              |
| 1:G:534:SER:O    | 4:V:351:THR:HA   | 1.60                     | 0.99              |
| 4:X:324:THR:HB   | 4:Z:246:GLN:CA   | 1.84                     | 0.99              |
| 4:3:288:ASP:N    | 4:5:203:THR:HG22 | 1.75                     | 0.99              |
| 1:D:642:LYS:HD3  | 4:9:340:TRP:CZ3  | 1.96                     | 0.99              |
| 1:D:831:TRP:CH2  | 2:E:34:ILE:HG23  | 1.96                     | 0.99              |
| 1:A:206:LYS:HD2  | 1:A:217:THR:HG23 | 1.41                     | 0.99              |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:C    | 1.65                     | 0.99              |
| 1:A:795:ARG:CB   | 3:C:35:ARG:CZ    | 2.32                     | 0.99              |
| 1:A:553:MLY:HG2  | 4:V:44:MET:O     | 1.59                     | 0.99              |
| 1:P:218:LEU:CA   | 1:P:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:M:202:SER:CA   | 1:M:207:LYS:CE   | 2.36                     | 0.99              |
| 1:J:829:TRP:CE2  | 2:K:87:LYS:HE2   | 1.97                     | 0.99              |
| 4:8:286:ASP:OD1  | 4:V:203:THR:HG22 | 1.62                     | 0.99              |
| 1:D:795:ARG:NE   | 3:F:116:GLU:OE2  | 1.95                     | 0.99              |
| 2:Q:141:PRO:HB2  | 2:Q:142:PRO:HD2  | 1.44                     | 0.99              |
| 1:P:729:ALA:CA   | 3:R:93:VAL:HG21  | 1.92                     | 0.99              |
| 2:H:121:LEU:C    | 2:H:128:PHE:HB3  | 1.71                     | 0.99              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:A:797:PHE:HZ   | 3:C:146:ILE:HD13 | 1.27                     | 0.99              |
| 1:M:797:PHE:CZ   | 3:O:146:ILE:HD13 | 1.97                     | 0.99              |
| 1:M:834:LEU:CD1  | 2:N:51:PHE:CE1   | 2.40                     | 0.99              |
| 3:R:49:ILE:HA    | 3:R:52:ASN:HD22  | 1.23                     | 0.99              |
| 2:B:149:ASP:OD2  | 2:B:150:TYR:O    | 1.80                     | 0.99              |
| 1:P:730:SER:N    | 3:R:93:VAL:HG22  | 1.72                     | 0.99              |
| 1:D:639:GLY:CA   | 4:9:345:ILE:CA   | 2.41                     | 0.99              |
| 1:A:534:SER:C    | 4:8:351:THR:HA   | 1.81                     | 0.99              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CB   | 1.91                     | 0.99              |
| 1:G:641:LYS:HE3  | 4:V:348:SER:O    | 1.56                     | 0.99              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:HG22 | 1.92                     | 0.99              |
| 4:7:287:ILE:HB   | 4:9:204:ALA:H    | 1.26                     | 0.99              |
| 3:I:48:LYS:O     | 3:I:52:ASN:ND2   | 1.94                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:150:TYR:C    | 2:N:151:LYS:HG3  | 1.83                     | 0.99              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:CA   | 1.75                     | 0.99              |
| 1:G:795:ARG:NH2  | 3:I:116:GLU:CG   | 2.26                     | 0.99              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:J:639:GLY:CA   | 4:W:345:ILE:CA   | 2.40                     | 0.99              |
| 1:P:785:GLU:HG3  | 3:R:81:GLN:CG    | 1.92                     | 0.99              |
| 1:P:795:ARG:CZ   | 3:R:116:GLU:CD   | 2.30                     | 0.99              |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:HB3  | 1.26                     | 0.99              |
| 1:D:641:LYS:CD   | 4:9:348:SER:HB2  | 1.93                     | 0.99              |
| 1:M:831:TRP:CZ2  | 2:N:47:LEU:CD2   | 2.45                     | 0.99              |
| 4:0:243:PRO:CA   | 4:Y:291:LYS:HE3  | 1.93                     | 0.99              |
| 4:1:203:THR:HG22 | 4:Z:288:ASP:N    | 1.75                     | 0.99              |
| 3:C:49:ILE:HA    | 3:C:52:ASN:HD22  | 1.22                     | 0.99              |
| 2:N:149:ASP:OD2  | 2:N:150:TYR:O    | 1.80                     | 0.99              |
| 2:B:150:TYR:C    | 2:B:151:LYS:HG3  | 1.83                     | 0.99              |
| 1:A:501:GLU:HG2  | 1:A:762:HIS:CE1  | 1.98                     | 0.99              |
| 2:N:130:PRO:O    | 2:N:133:ILE:N    | 1.96                     | 0.99              |
| 2:K:141:PRO:HB2  | 2:K:142:PRO:HD2  | 1.44                     | 0.99              |
| 1:D:534:SER:C    | 4:9:351:THR:HA   | 1.81                     | 0.99              |
| 1:D:639:GLY:N    | 4:9:345:ILE:N    | 1.94                     | 0.99              |
| 1:M:642:LYS:HD3  | 4:Z:340:TRP:CZ3  | 1.96                     | 0.99              |
| 4:8:322:PRO:HB3  | 4:V:244:ASP:OD2  | 1.62                     | 0.99              |
| 4:9:286:ASP:OD1  | 4:W:203:THR:HG22 | 1.62                     | 0.99              |
| 4:1:244:ASP:CB   | 4:Z:322:PRO:CB   | 2.40                     | 0.99              |
| 2:K:150:TYR:O    | 2:K:151:LYS:CB   | 2.06                     | 0.99              |
| 1:A:93:MET:HG2   | 1:A:715:VAL:CG2  | 1.92                     | 0.99              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HD3  | 1.43                     | 0.99              |
| 1:M:576:GLU:CG   | 1:M:577:ALA:H    | 1.75                     | 0.99              |
| 1:D:818:TYR:HB3  | 2:E:90:GLY:CA    | 1.87                     | 0.99              |
| 1:P:506:GLU:CG   | 1:P:760:PHE:N    | 2.25                     | 0.99              |
| 1:A:215:GLN:CA   | 1:A:340:ILE:HG23 | 1.92                     | 0.99              |
| 1:D:508:ILE:HD11 | 1:D:766:PHE:HZ   | 1.22                     | 0.99              |
| 1:J:206:LYS:HD2  | 1:J:217:THR:HG23 | 1.41                     | 0.99              |
| 1:J:553:MLY:HE3  | 4:Y:45:VAL:CG1   | 1.92                     | 0.99              |
| 1:A:553:MLY:CB   | 4:V:46:GLY:CA    | 2.32                     | 0.99              |
| 1:J:768:MLY:HH11 | 1:J:772:LEU:CD1  | 1.85                     | 0.99              |
| 1:M:797:PHE:CE1  | 3:O:149:VAL:HG12 | 1.98                     | 0.99              |
| 4:X:291:LYS:HE3  | 4:Z:243:PRO:HB3  | 1.45                     | 0.99              |
| 1:M:803:TYR:O    | 1:M:807:VAL:N    | 1.94                     | 0.99              |
| 1:G:576:GLU:HG2  | 1:G:577:ALA:N    | 1.66                     | 0.99              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CG   | 1.93                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:218:LEU:CA   | 1:A:221:GLN:HG3  | 1.91                     | 0.99              |
| 1:P:639:GLY:CA   | 4:O:345:ILE:CA   | 2.40                     | 0.99              |
| 1:J:530:MET:CE   | 4:W:354:GLN:CG   | 2.40                     | 0.99              |
| 1:D:529:PRO:C    | 4:9:354:GLN:HB3  | 1.78                     | 0.99              |
| 2:Q:149:ASP:OD2  | 2:Q:150:TYR:O    | 1.80                     | 0.99              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:CA   | 1.75                     | 0.99              |
| 1:P:612:GLN:HE22 | 1:P:627:GLY:CA   | 1.75                     | 0.99              |
| 1:D:56:GLU:HB2   | 1:D:59:MLY:HB3   | 1.40                     | 0.99              |
| 1:G:530:MET:CE   | 4:V:354:GLN:CG   | 2.39                     | 0.99              |
| 2:B:141:PRO:HB2  | 2:B:142:PRO:HD2  | 1.44                     | 0.99              |
| 2:B:112:ILE:O    | 2:B:147:ASN:C    | 2.01                     | 0.99              |
| 1:M:783:LEU:HD12 | 1:M:786:ILE:HD11 | 1.45                     | 0.99              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:HG22 | 1.92                     | 0.99              |
| 4:V:325:MET:HE2  | 4:X:244:ASP:OD2  | 1.62                     | 0.99              |
| 1:G:755:HIS:H    | 1:G:779:ARG:CZ   | 1.75                     | 0.98              |
| 1:G:784:ALA:O    | 1:G:788:THR:N    | 1.96                     | 0.98              |
| 2:B:130:PRO:O    | 2:B:133:ILE:N    | 1.96                     | 0.98              |
| 2:B:139:ALA:O    | 2:B:141:PRO:HD3  | 1.62                     | 0.98              |
| 1:J:534:SER:O    | 4:W:351:THR:HA   | 1.60                     | 0.98              |
| 1:J:534:SER:O    | 4:W:351:THR:HG23 | 1.13                     | 0.98              |
| 1:G:84:MLY:CG    | 1:G:723:ARG:HD2  | 1.93                     | 0.98              |
| 4:O:204:ALA:CB   | 4:Y:288:ASP:HB2  | 1.91                     | 0.98              |
| 1:J:215:GLN:CA   | 1:J:340:ILE:HG23 | 1.92                     | 0.98              |
| 1:P:829:TRP:CZ2  | 2:Q:87:LYS:HE2   | 1.97                     | 0.98              |
| 3:O:49:ILE:HA    | 3:O:52:ASN:HD22  | 1.23                     | 0.98              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:O    | 1.80                     | 0.98              |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:CA   | 1.75                     | 0.98              |
| 1:D:727:LEU:CG   | 1:D:782:MLY:HH12 | 1.93                     | 0.98              |
| 1:A:757:GLN:CD   | 1:A:771:LEU:HD12 | 1.77                     | 0.98              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:CB   | 1.93                     | 0.98              |
| 1:P:729:ALA:HB3  | 3:R:93:VAL:CG2   | 1.90                     | 0.98              |
| 1:D:576:GLU:HG2  | 1:D:577:ALA:H    | 0.85                     | 0.98              |
| 1:A:795:ARG:CZ   | 3:C:43:ASN:OD1   | 2.05                     | 0.98              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:HD21 | 1.24                     | 0.98              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:HG22 | 1.92                     | 0.98              |
| 1:P:649:VAL:CG1  | 1:P:649:VAL:HG22 | 1.92                     | 0.98              |
| 4:O:288:ASP:OD2  | 4:2:63:GLY:CA    | 2.11                     | 0.98              |
| 1:J:831:TRP:HZ3  | 2:K:34:ILE:HD13  | 1.28                     | 0.98              |
| 1:M:94:MET:O     | 1:M:713:SER:HB3  | 1.63                     | 0.98              |
| 1:M:95:THR:OG1   | 1:M:770:GLY:CA   | 2.12                     | 0.98              |
| 1:J:639:GLY:N    | 4:W:345:ILE:N    | 1.94                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:641:LYS:CG   | 4:9:348:SER:HB2  | 1.87                     | 0.98              |
| 1:P:641:LYS:HE3  | 1:P:647:GLN:CB   | 1.91                     | 0.98              |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:CG1  | 1.92                     | 0.98              |
| 1:D:215:GLN:CA   | 1:D:340:ILE:HG23 | 1.92                     | 0.98              |
| 4:3:322:PRO:CB   | 4:5:244:ASP:CB   | 2.40                     | 0.98              |
| 1:D:791:GLN:HE22 | 3:F:116:GLU:N    | 1.55                     | 0.98              |
| 1:A:639:GLY:CA   | 4:8:345:ILE:CA   | 2.41                     | 0.98              |
| 1:M:797:PHE:CE1  | 3:O:149:VAL:CG1  | 2.46                     | 0.98              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CE2   | 1.81                     | 0.98              |
| 3:F:52:ASN:HB2   | 3:F:53:PRO:HD3   | 1.46                     | 0.98              |
| 2:K:150:TYR:C    | 2:K:151:LYS:HG3  | 1.83                     | 0.98              |
| 1:P:817:GLN:HG2  | 2:Q:127:ARG:HD2  | 1.27                     | 0.98              |
| 1:G:818:TYR:CE1  | 2:H:127:ARG:CZ   | 2.45                     | 0.98              |
| 2:H:112:ILE:O    | 2:H:147:ASN:C    | 2.01                     | 0.98              |
| 2:H:139:ALA:O    | 2:H:141:PRO:HD3  | 1.62                     | 0.98              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:CG2   | 2.45                     | 0.98              |
| 1:A:792:ALA:CB   | 3:C:42:THR:HG22  | 1.93                     | 0.98              |
| 1:A:28:GLN:NE2   | 1:A:723:ARG:HH21 | 1.62                     | 0.98              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:CA   | 1.75                     | 0.98              |
| 1:A:98:HIS:HB3   | 1:A:100:PRO:HD2  | 1.42                     | 0.98              |
| 1:D:727:LEU:CD1  | 1:D:782:MLY:HD3  | 1.80                     | 0.98              |
| 1:G:757:GLN:CG   | 1:G:776:GLU:CG   | 2.14                     | 0.98              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:CG   | 2.32                     | 0.98              |
| 1:D:530:MET:CE   | 4:9:354:GLN:CG   | 2.40                     | 0.98              |
| 1:A:530:MET:CE   | 4:8:354:GLN:CG   | 2.41                     | 0.98              |
| 1:P:206:LYS:HD2  | 1:P:217:THR:HG23 | 1.41                     | 0.98              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CB   | 1.91                     | 0.98              |
| 4:V:324:THR:HG21 | 4:X:246:GLN:C    | 1.70                     | 0.98              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:O    | 1.80                     | 0.98              |
| 1:A:149:GLN:CD   | 1:A:716:LEU:HD23 | 1.83                     | 0.98              |
| 1:G:639:GLY:CA   | 4:V:345:ILE:CA   | 2.40                     | 0.98              |
| 2:Q:117:LEU:CB   | 2:Q:147:ASN:CG   | 2.32                     | 0.98              |
| 1:P:576:GLU:HG2  | 1:P:577:ALA:H    | 0.85                     | 0.98              |
| 1:M:783:LEU:HA   | 1:M:786:ILE:HG13 | 1.17                     | 0.98              |
| 4:2:287:ILE:HD13 | 4:4:203:THR:HB   | 1.42                     | 0.98              |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:HG2  | 0.98                     | 0.98              |
| 4:7:286:ASP:OD1  | 4:9:203:THR:HG22 | 1.62                     | 0.98              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:CA   | 1.75                     | 0.98              |
| 1:D:797:PHE:HE1  | 3:F:146:ILE:HA   | 0.82                     | 0.98              |
| 1:A:508:ILE:HD13 | 1:A:759:ALA:HB1  | 1.19                     | 0.98              |
| 2:K:112:ILE:O    | 2:K:147:ASN:C    | 2.01                     | 0.98              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:121:LEU:CB   | 2:B:128:PHE:HB3  | 1.69                     | 0.98              |
| 1:P:641:LYS:HG3  | 1:P:647:GLN:NE2  | 1.58                     | 0.98              |
| 1:A:641:LYS:CG   | 4:8:348:SER:HB2  | 1.87                     | 0.98              |
| 1:D:642:LYS:HD2  | 4:9:24:ASP:O     | 1.64                     | 0.98              |
| 1:P:215:GLN:CA   | 1:P:340:ILE:HG23 | 1.92                     | 0.98              |
| 2:Q:150:TYR:O    | 2:Q:151:LYS:CB   | 2.07                     | 0.98              |
| 2:E:163:ALA:HA   | 2:K:21:GLU:HB3   | 1.46                     | 0.98              |
| 2:N:112:ILE:O    | 2:N:147:ASN:C    | 2.01                     | 0.98              |
| 1:P:831:TRP:CH2  | 2:Q:47:LEU:HD21  | 1.78                     | 0.98              |
| 1:P:727:LEU:HG   | 1:P:779:ARG:HH21 | 1.26                     | 0.98              |
| 1:J:831:TRP:CZ2  | 2:K:47:LEU:HD21  | 1.98                     | 0.98              |
| 3:R:52:ASN:HB2   | 3:R:53:PRO:HD3   | 1.46                     | 0.98              |
| 2:Q:130:PRO:O    | 2:Q:133:ILE:N    | 1.96                     | 0.98              |
| 4:O:244:ASP:N    | 4:Y:291:LYS:CE   | 0.85                     | 0.98              |
| 1:A:215:GLN:H    | 1:A:340:ILE:CG1  | 1.73                     | 0.98              |
| 1:A:792:ALA:HB2  | 3:C:42:THR:HG22  | 0.98                     | 0.98              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:CA   | 2.12                     | 0.98              |
| 1:G:788:THR:O    | 3:I:42:THR:CG2   | 2.11                     | 0.97              |
| 1:A:206:LYS:CD   | 1:A:217:THR:CG2  | 2.16                     | 0.97              |
| 1:M:639:GLY:CA   | 4:Z:345:ILE:CA   | 2.40                     | 0.97              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:CG   | 2.42                     | 0.97              |
| 1:M:649:VAL:CG1  | 1:M:649:VAL:HG22 | 1.92                     | 0.97              |
| 1:A:753:VAL:CG1  | 1:A:775:LEU:HG   | 1.92                     | 0.97              |
| 1:G:789:ALA:HB1  | 3:I:81:GLN:NE2   | 1.78                     | 0.97              |
| 2:N:117:LEU:CB   | 2:N:147:ASN:CG   | 2.32                     | 0.97              |
| 2:Q:139:ALA:O    | 2:Q:141:PRO:HD3  | 1.62                     | 0.97              |
| 2:E:139:ALA:O    | 2:E:141:PRO:HD3  | 1.62                     | 0.97              |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:CE1  | 1.93                     | 0.97              |
| 1:D:576:GLU:CG   | 1:D:577:ALA:H    | 1.75                     | 0.97              |
| 1:P:576:GLU:CG   | 1:P:577:ALA:H    | 1.75                     | 0.97              |
| 1:M:795:ARG:CD   | 3:O:43:ASN:OD1   | 2.10                     | 0.97              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:HZ2  | 1.18                     | 0.97              |
| 2:E:121:LEU:HG   | 2:E:128:PHE:CA   | 1.59                     | 0.97              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:CG   | 2.32                     | 0.97              |
| 2:H:121:LEU:HG   | 2:H:128:PHE:HA   | 1.47                     | 0.97              |
| 1:G:820:VAL:HG11 | 2:H:136:MET:CE   | 1.94                     | 0.97              |
| 1:P:542:PHE:CG   | 4:O:143:TYR:CE1  | 2.53                     | 0.97              |
| 1:A:831:TRP:HZ2  | 2:B:47:LEU:HA    | 1.29                     | 0.97              |
| 1:M:797:PHE:HD1  | 3:O:149:VAL:CG1  | 1.75                     | 0.97              |
| 4:3:287:ILE:HD13 | 4:5:203:THR:CB   | 1.92                     | 0.97              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HD13  | 1.98                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:287:ILE:HB   | 4:V:204:ALA:H    | 1.25                     | 0.97              |
| 1:D:727:LEU:HD12 | 1:D:782:MLY:NZ   | 1.77                     | 0.97              |
| 2:H:130:PRO:O    | 2:H:133:ILE:N    | 1.96                     | 0.97              |
| 2:B:117:LEU:HD13 | 2:B:147:ASN:OD1  | 1.64                     | 0.97              |
| 1:J:84:MLY:HH23  | 1:J:720:PHE:HA   | 1.47                     | 0.97              |
| 1:M:215:GLN:H    | 1:M:340:ILE:CG1  | 1.72                     | 0.97              |
| 3:L:46:ILE:O     | 3:L:50:LEU:HG    | 1.64                     | 0.97              |
| 1:A:174:SER:HB3  | 1:A:667:THR:HG21 | 1.44                     | 0.97              |
| 2:Q:144:VAL:HG13 | 2:Q:153:ILE:HG12 | 1.14                     | 0.97              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:CG   | 2.42                     | 0.97              |
| 1:A:642:LYS:HG2  | 4:8:21:PHE:O     | 1.65                     | 0.97              |
| 1:J:829:TRP:CE3  | 2:K:87:LYS:NZ    | 2.31                     | 0.97              |
| 4:2:324:THR:HG21 | 4:4:244:ASP:O    | 1.60                     | 0.97              |
| 2:K:139:ALA:O    | 2:K:141:PRO:HD3  | 1.62                     | 0.97              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:CG   | 2.42                     | 0.97              |
| 1:J:642:LYS:HG2  | 4:W:21:PHE:O     | 1.65                     | 0.97              |
| 1:A:542:PHE:CG   | 4:8:143:TYR:CE1  | 2.52                     | 0.97              |
| 1:J:641:LYS:CG   | 4:W:348:SER:HB2  | 1.86                     | 0.97              |
| 1:G:641:LYS:HG3  | 1:G:647:GLN:NE2  | 1.58                     | 0.97              |
| 1:M:642:LYS:HG2  | 4:Z:21:PHE:O     | 1.65                     | 0.97              |
| 4:7:322:PRO:HB3  | 4:9:244:ASP:OD2  | 1.62                     | 0.97              |
| 1:J:576:GLU:HG2  | 1:J:577:ALA:H    | 0.85                     | 0.97              |
| 1:M:174:SER:HB3  | 1:M:667:THR:HG21 | 1.44                     | 0.97              |
| 1:G:174:SER:HB3  | 1:G:667:THR:HG21 | 1.44                     | 0.97              |
| 1:D:736:GLN:CA   | 1:D:743:ALA:HB2  | 1.95                     | 0.97              |
| 1:G:754:ASP:N    | 1:G:779:ARG:HD3  | 1.79                     | 0.97              |
| 1:D:508:ILE:CG1  | 1:D:766:PHE:CE1  | 2.46                     | 0.97              |
| 2:N:141:PRO:HB2  | 2:N:142:PRO:HD2  | 1.44                     | 0.97              |
| 1:M:545:ALA:HA   | 4:1:45:VAL:HG11  | 1.45                     | 0.97              |
| 1:J:642:LYS:HD2  | 4:W:24:ASP:O     | 1.64                     | 0.97              |
| 1:P:785:GLU:O    | 1:P:786:ILE:N    | 1.97                     | 0.97              |
| 1:M:795:ARG:HD2  | 3:O:43:ASN:OD1   | 1.64                     | 0.97              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:CA   | 2.42                     | 0.97              |
| 1:D:215:GLN:H    | 1:D:340:ILE:CG1  | 1.73                     | 0.97              |
| 1:J:576:GLU:CG   | 1:J:577:ALA:H    | 1.75                     | 0.97              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:O    | 1.80                     | 0.97              |
| 2:B:150:TYR:O    | 2:B:151:LYS:HG3  | 1.65                     | 0.97              |
| 1:M:819:ASN:CG   | 2:N:90:GLY:O     | 2.03                     | 0.97              |
| 2:E:112:ILE:O    | 2:E:147:ASN:C    | 2.01                     | 0.97              |
| 1:P:795:ARG:HB3  | 3:R:35:ARG:HH22  | 1.21                     | 0.97              |
| 4:X:291:LYS:CB   | 4:Z:244:ASP:CB   | 2.25                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:646:PHE:HE2  | 1:M:652:LEU:HD21 | 1.24                     | 0.97              |
| 1:M:649:VAL:CA   | 1:M:649:VAL:CG2  | 2.43                     | 0.97              |
| 1:A:800:ARG:NH2  | 3:C:40:ASN:ND2   | 2.10                     | 0.97              |
| 1:G:553:MLY:CE   | 4:X:45:VAL:HB    | 1.91                     | 0.97              |
| 1:P:534:SER:O    | 4:O:351:THR:HA   | 1.59                     | 0.97              |
| 1:M:206:LYS:CD   | 1:M:217:THR:CG2  | 2.16                     | 0.97              |
| 1:J:768:MLY:CH1  | 1:J:772:LEU:HD12 | 1.95                     | 0.97              |
| 3:O:52:ASN:HB2   | 3:O:53:PRO:HD3   | 1.46                     | 0.97              |
| 4:W:286:ASP:OD2  | 4:Y:203:THR:HG22 | 1.62                     | 0.97              |
| 1:G:754:ASP:HB2  | 1:G:776:GLU:HA   | 1.43                     | 0.97              |
| 1:G:795:ARG:HE   | 3:I:116:GLU:HB3  | 0.80                     | 0.97              |
| 2:Q:112:ILE:O    | 2:Q:147:ASN:C    | 2.01                     | 0.97              |
| 2:E:141:PRO:HB2  | 2:E:142:PRO:HD2  | 1.44                     | 0.97              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:CG   | 2.32                     | 0.97              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:CG   | 2.32                     | 0.97              |
| 1:P:530:MET:CE   | 4:O:354:GLN:CG   | 2.40                     | 0.97              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:HE2   | 1.90                     | 0.97              |
| 1:D:649:VAL:CG2  | 1:D:649:VAL:CA   | 2.42                     | 0.97              |
| 1:G:642:LYS:HG2  | 4:V:21:PHE:O     | 1.65                     | 0.96              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:CG   | 2.42                     | 0.96              |
| 1:P:218:LEU:CA   | 1:P:221:GLN:CG   | 2.42                     | 0.96              |
| 1:P:649:VAL:CG2  | 1:P:649:VAL:CA   | 2.42                     | 0.96              |
| 4:I:287:ILE:CG1  | 4:3:202:THR:HA   | 1.93                     | 0.96              |
| 2:K:130:PRO:O    | 2:K:133:ILE:N    | 1.96                     | 0.96              |
| 1:D:542:PHE:CG   | 4:9:143:TYR:CE1  | 2.52                     | 0.96              |
| 1:M:218:LEU:CA   | 1:M:221:GLN:CG   | 2.42                     | 0.96              |
| 1:M:836:PHE:HE1  | 2:N:159:HIS:HA   | 1.19                     | 0.96              |
| 3:I:46:ILE:O     | 3:I:50:LEU:HG    | 1.64                     | 0.96              |
| 1:D:727:LEU:HG   | 1:D:782:MLY:HG3  | 1.47                     | 0.96              |
| 1:A:93:MET:CE    | 1:A:715:VAL:HG13 | 1.95                     | 0.96              |
| 1:G:637:LYS:NZ   | 4:V:141:SER:O    | 1.99                     | 0.96              |
| 1:P:817:GLN:HG2  | 2:Q:127:ARG:HB2  | 1.47                     | 0.96              |
| 4:I:287:ILE:CG2  | 4:3:204:ALA:H    | 1.78                     | 0.96              |
| 2:B:144:VAL:HG13 | 2:B:153:ILE:HD11 | 1.22                     | 0.96              |
| 1:M:635:GLY:HA3  | 4:Z:334:GLU:HG2  | 1.47                     | 0.96              |
| 1:M:542:PHE:CG   | 4:Z:143:TYR:CE1  | 2.53                     | 0.96              |
| 1:J:553:MLY:HE3  | 4:Y:45:VAL:HG11  | 1.47                     | 0.96              |
| 1:D:553:MLY:HB3  | 4:W:46:GLY:HA2   | 1.47                     | 0.96              |
| 1:J:710:GLY:HA2  | 1:J:772:LEU:HD21 | 1.46                     | 0.96              |
| 1:A:642:LYS:HD2  | 4:8:24:ASP:O     | 1.64                     | 0.96              |
| 3:O:46:ILE:O     | 3:O:50:LEU:HG    | 1.64                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:322:PRO:HB2  | 4:5:244:ASP:CB   | 1.95                     | 0.96              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:O    | 1.83                     | 0.96              |
| 1:G:642:LYS:HD2  | 4:V:24:ASP:O     | 1.64                     | 0.96              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:CD   | 2.34                     | 0.96              |
| 1:A:538:GLU:N    | 4:8:349:LEU:CD1  | 2.28                     | 0.96              |
| 1:G:649:VAL:CA   | 1:G:649:VAL:CG2  | 2.43                     | 0.96              |
| 1:M:642:LYS:HD2  | 4:Z:24:ASP:O     | 1.65                     | 0.96              |
| 3:C:52:ASN:HB2   | 3:C:53:PRO:HD3   | 1.45                     | 0.96              |
| 2:Q:117:LEU:HD13 | 2:Q:147:ASN:OD1  | 1.64                     | 0.96              |
| 2:H:141:PRO:HB2  | 2:H:142:PRO:HD2  | 1.44                     | 0.96              |
| 2:K:121:LEU:HG   | 2:K:128:PHE:HA   | 1.47                     | 0.96              |
| 1:A:534:SER:O    | 4:8:351:THR:HG23 | 1.13                     | 0.96              |
| 3:L:52:ASN:HB2   | 3:L:53:PRO:HD3   | 1.46                     | 0.96              |
| 2:E:150:TYR:C    | 2:E:151:LYS:HG3  | 1.83                     | 0.96              |
| 2:N:150:TYR:O    | 2:N:151:LYS:HG3  | 1.65                     | 0.96              |
| 1:G:791:GLN:HE21 | 3:I:115:GLY:HA3  | 1.26                     | 0.96              |
| 2:N:144:VAL:HG13 | 2:N:153:ILE:HG12 | 1.14                     | 0.96              |
| 2:K:121:LEU:HG   | 2:K:128:PHE:CA   | 1.59                     | 0.96              |
| 1:M:537:GLU:C    | 4:Z:349:LEU:CD1  | 2.20                     | 0.96              |
| 1:J:543:PRO:CG   | 4:W:143:TYR:O    | 2.14                     | 0.96              |
| 1:M:838:ILE:CD1  | 2:N:54:MET:HE3   | 1.89                     | 0.96              |
| 4:3:288:ASP:H    | 4:5:203:THR:HG22 | 1.29                     | 0.96              |
| 1:D:642:LYS:HG2  | 4:9:21:PHE:O     | 1.65                     | 0.96              |
| 1:J:28:GLN:CD    | 1:J:723:ARG:HH11 | 1.67                     | 0.96              |
| 1:J:542:PHE:CG   | 4:W:143:TYR:CE1  | 2.53                     | 0.96              |
| 1:P:552:ASN:ND2  | 4:2:49:GLN:HB3   | 1.73                     | 0.96              |
| 1:A:649:VAL:CG2  | 1:A:649:VAL:CG1  | 2.43                     | 0.96              |
| 3:I:52:ASN:HB2   | 3:I:53:PRO:HD3   | 1.46                     | 0.96              |
| 1:M:576:GLU:HG2  | 1:M:577:ALA:N    | 1.66                     | 0.96              |
| 1:M:530:MET:CE   | 4:Z:354:GLN:CG   | 2.41                     | 0.96              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:HG   | 0.96                     | 0.96              |
| 1:D:725:ARG:CA   | 1:D:782:MLY:CH2  | 2.41                     | 0.96              |
| 1:G:635:GLY:HA3  | 4:V:334:GLU:HG2  | 1.47                     | 0.96              |
| 1:A:797:PHE:CZ   | 3:C:146:ILE:HD12 | 1.91                     | 0.96              |
| 4:0:199:SER:O    | 4:Y:287:ILE:HG21 | 1.65                     | 0.96              |
| 4:8:288:ASP:HA   | 4:V:204:ALA:HB2  | 1.48                     | 0.96              |
| 1:M:95:THR:HG1   | 1:M:770:GLY:N    | 1.62                     | 0.96              |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:CE1  | 2.00                     | 0.96              |
| 2:H:117:LEU:HD13 | 2:H:147:ASN:OD1  | 1.64                     | 0.96              |
| 1:D:538:GLU:N    | 4:9:349:LEU:CD1  | 2.28                     | 0.96              |
| 1:M:782:MLY:O    | 1:M:786:ILE:HG12 | 1.65                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:823:PHE:CD1  | 2:E:160:GLY:CA   | 2.48                     | 0.96              |
| 2:H:150:TYR:C    | 2:H:151:LYS:HG3  | 1.83                     | 0.96              |
| 2:E:130:PRO:O    | 2:E:133:ILE:N    | 1.96                     | 0.95              |
| 1:P:637:LYS:NZ   | 4:0:141:SER:O    | 1.98                     | 0.95              |
| 1:P:543:PRO:CG   | 4:0:143:TYR:O    | 2.14                     | 0.95              |
| 1:G:735:GLY:C    | 1:G:743:ALA:CA   | 2.34                     | 0.95              |
| 4:2:288:ASP:N    | 4:4:203:THR:HG22 | 1.80                     | 0.95              |
| 4:0:112:PRO:HB3  | 4:1:196:ARG:HA   | 0.99                     | 0.95              |
| 1:A:649:VAL:CA   | 1:A:649:VAL:CG2  | 2.43                     | 0.95              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:CG2  | 2.43                     | 0.95              |
| 1:J:557:GLU:HA   | 4:Y:47:MET:HA    | 1.04                     | 0.95              |
| 1:P:769:ALA:C    | 1:P:771:LEU:N    | 2.18                     | 0.95              |
| 2:K:150:TYR:O    | 2:K:151:LYS:HG3  | 1.65                     | 0.95              |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:HB3  | 1.40                     | 0.95              |
| 1:J:735:GLY:C    | 1:J:743:ALA:CA   | 2.34                     | 0.95              |
| 1:P:639:GLY:N    | 4:0:345:ILE:N    | 1.94                     | 0.95              |
| 4:1:203:THR:HG22 | 4:Z:288:ASP:H    | 1.29                     | 0.95              |
| 1:P:506:GLU:OE1  | 1:P:760:PHE:O    | 1.83                     | 0.95              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:CG2  | 2.44                     | 0.95              |
| 4:9:322:PRO:HB3  | 4:W:244:ASP:OD2  | 1.62                     | 0.95              |
| 3:C:46:ILE:O     | 3:C:50:LEU:HG    | 1.65                     | 0.95              |
| 1:M:95:THR:HA    | 1:M:713:SER:HB3  | 1.48                     | 0.95              |
| 2:E:150:TYR:O    | 2:E:151:LYS:HG3  | 1.65                     | 0.95              |
| 2:Q:150:TYR:C    | 2:Q:151:LYS:HG3  | 1.83                     | 0.95              |
| 1:D:795:ARG:HG2  | 3:F:118:MET:HE3  | 0.98                     | 0.95              |
| 2:N:121:LEU:HG   | 2:N:128:PHE:HA   | 1.47                     | 0.95              |
| 1:J:505:MLY:HD2  | 1:J:762:HIS:ND1  | 1.81                     | 0.95              |
| 1:J:649:VAL:CG2  | 1:J:649:VAL:CG1  | 2.43                     | 0.95              |
| 4:7:288:ASP:HA   | 4:9:204:ALA:HB2  | 1.48                     | 0.95              |
| 4:9:288:ASP:HA   | 4:W:204:ALA:HB2  | 1.48                     | 0.95              |
| 1:D:800:ARG:HH22 | 3:F:40:ASN:ND2   | 1.63                     | 0.95              |
| 1:A:93:MET:CE    | 1:A:716:LEU:H    | 1.80                     | 0.95              |
| 1:G:538:GLU:N    | 4:V:349:LEU:CD1  | 2.29                     | 0.95              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:HB3  | 1.45                     | 0.95              |
| 1:M:538:GLU:N    | 4:Z:349:LEU:CD1  | 2.28                     | 0.95              |
| 1:M:637:LYS:NZ   | 4:Z:141:SER:O    | 1.99                     | 0.95              |
| 1:D:206:LYS:CD   | 1:D:217:THR:CG2  | 2.16                     | 0.95              |
| 4:1:203:THR:CB   | 4:Z:287:ILE:HD13 | 1.92                     | 0.95              |
| 3:F:46:ILE:O     | 3:F:50:LEU:HG    | 1.65                     | 0.95              |
| 1:J:795:ARG:CZ   | 3:L:116:GLU:OE1  | 2.11                     | 0.95              |
| 1:D:735:GLY:C    | 1:D:743:ALA:CA   | 2.35                     | 0.95              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:797:PHE:CE1  | 3:I:146:ILE:HG23 | 2.01                     | 0.95              |
| 1:G:542:PHE:CG   | 4:V:143:TYR:CE1  | 2.53                     | 0.95              |
| 1:P:735:GLY:C    | 1:P:743:ALA:CA   | 2.34                     | 0.95              |
| 1:P:642:LYS:HD2  | 4:O:24:ASP:O     | 1.65                     | 0.95              |
| 1:G:206:LYS:CD   | 1:G:217:THR:CG2  | 2.16                     | 0.95              |
| 1:M:538:GLU:HG3  | 4:Z:352:PHE:N    | 1.81                     | 0.95              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:CD   | 2.34                     | 0.95              |
| 1:P:831:TRP:CZ2  | 2:Q:47:LEU:CD2   | 2.49                     | 0.95              |
| 1:G:789:ALA:HB1  | 3:I:81:GLN:CD    | 1.87                     | 0.95              |
| 1:G:530:MET:HA   | 4:V:354:GLN:HG3  | 0.97                     | 0.95              |
| 1:G:538:GLU:HG3  | 4:V:352:PHE:N    | 1.81                     | 0.95              |
| 1:P:819:ASN:CG   | 2:Q:92:ASP:CB    | 2.34                     | 0.95              |
| 2:E:144:VAL:HG13 | 2:E:153:ILE:HD11 | 1.21                     | 0.95              |
| 2:K:117:LEU:HD13 | 2:K:147:ASN:OD1  | 1.64                     | 0.95              |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:CA   | 1.79                     | 0.95              |
| 1:M:641:LYS:HE3  | 4:Z:348:SER:O    | 1.55                     | 0.95              |
| 1:M:649:VAL:CG2  | 1:M:649:VAL:CG1  | 2.43                     | 0.95              |
| 1:A:831:TRP:CH2  | 2:B:50:THR:HG21  | 2.02                     | 0.95              |
| 1:M:795:ARG:HB3  | 3:O:35:ARG:HH22  | 1.14                     | 0.95              |
| 1:P:649:VAL:CG1  | 1:P:649:VAL:CG2  | 2.43                     | 0.95              |
| 4:1:322:PRO:CB   | 4:3:244:ASP:CB   | 2.44                     | 0.95              |
| 1:G:752:ASP:O    | 1:G:780:ASP:CA   | 2.13                     | 0.95              |
| 1:A:505:MLY:CB   | 1:A:762:HIS:CD2  | 2.09                     | 0.95              |
| 2:E:117:LEU:HD13 | 2:E:147:ASN:OD1  | 1.64                     | 0.95              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:CD   | 2.34                     | 0.95              |
| 1:P:642:LYS:HG2  | 4:O:21:PHE:O     | 1.65                     | 0.95              |
| 1:D:635:GLY:HA3  | 4:9:334:GLU:HG2  | 1.47                     | 0.95              |
| 1:A:831:TRP:CZ3  | 2:B:34:ILE:CG1   | 2.49                     | 0.95              |
| 1:A:541:MET:N    | 4:8:349:LEU:HD21 | 1.80                     | 0.95              |
| 1:M:831:TRP:HE1  | 2:N:67:MET:HB3   | 1.31                     | 0.95              |
| 1:G:546:THR:HG22 | 1:G:548:THR:H    | 1.32                     | 0.95              |
| 4:V:286:ASP:CG   | 4:X:203:THR:HG22 | 1.87                     | 0.95              |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:CD   | 1.52                     | 0.95              |
| 1:M:819:ASN:CG   | 2:N:92:ASP:CB    | 2.35                     | 0.95              |
| 2:N:111:SER:CB   | 2:N:148:VAL:C    | 1.93                     | 0.95              |
| 1:M:553:MLY:HE2  | 4:1:43:VAL:HG21  | 1.30                     | 0.95              |
| 1:J:538:GLU:N    | 4:W:349:LEU:CD1  | 2.28                     | 0.95              |
| 1:A:752:ASP:OD2  | 1:A:782:MLY:CD   | 2.14                     | 0.95              |
| 1:A:637:LYS:NZ   | 4:8:141:SER:O    | 1.99                     | 0.95              |
| 4:2:324:THR:HB   | 4:4:243:PRO:O    | 1.14                     | 0.95              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:CD   | 2.34                     | 0.95              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 4:X:324:THR:HG1 | 4:Z:246:GLN:HA   | 1.21                     | 0.95              |
| 2:B:121:LEU:HG  | 2:B:128:PHE:HA   | 1.46                     | 0.95              |
| 1:P:635:GLY:HA3 | 4:0:334:GLU:HG2  | 1.47                     | 0.95              |
| 1:A:635:GLY:HA3 | 4:8:334:GLU:HG2  | 1.47                     | 0.95              |
| 1:A:543:PRO:CG  | 4:8:143:TYR:O    | 2.14                     | 0.95              |
| 1:D:641:LYS:HD2 | 1:D:647:GLN:CD   | 1.70                     | 0.95              |
| 4:1:244:ASP:CB  | 4:Z:322:PRO:HB2  | 1.95                     | 0.95              |
| 2:H:150:TYR:O   | 2:H:151:LYS:HG3  | 1.65                     | 0.95              |
| 2:H:150:TYR:O   | 2:H:151:LYS:CG   | 2.15                     | 0.95              |
| 1:J:783:LEU:O   | 1:J:787:ILE:N    | 1.99                     | 0.94              |
| 1:D:732:ILE:CG2 | 1:D:782:MLY:HH21 | 1.88                     | 0.94              |
| 1:P:642:LYS:CG  | 4:0:23:GLY:H     | 1.77                     | 0.94              |
| 1:P:538:GLU:HG3 | 4:0:352:PHE:N    | 1.81                     | 0.94              |
| 1:M:548:THR:O   | 4:1:47:MET:CG    | 2.13                     | 0.94              |
| 1:J:637:LYS:NZ  | 4:W:141:SER:O    | 1.98                     | 0.94              |
| 1:J:635:GLY:HA3 | 4:W:334:GLU:HG2  | 1.47                     | 0.94              |
| 1:D:637:LYS:NZ  | 4:9:141:SER:O    | 1.99                     | 0.94              |
| 1:D:543:PRO:CG  | 4:9:143:TYR:O    | 2.14                     | 0.94              |
| 1:M:721:LYS:CA  | 1:M:736:GLN:CD   | 2.34                     | 0.94              |
| 1:D:726:VAL:CG1 | 1:D:785:GLU:HG2  | 1.94                     | 0.94              |
| 4:0:112:PRO:CB  | 4:1:196:ARG:HA   | 1.87                     | 0.94              |
| 1:D:215:GLN:HA  | 1:D:340:ILE:HG23 | 0.95                     | 0.94              |
| 3:R:46:ILE:O    | 3:R:50:LEU:HG    | 1.64                     | 0.94              |
| 2:K:150:TYR:O   | 2:K:151:LYS:CG   | 2.15                     | 0.94              |
| 1:G:753:VAL:C   | 1:G:779:ARG:HD3  | 1.87                     | 0.94              |
| 1:G:818:TYR:CZ  | 2:H:127:ARG:CZ   | 2.50                     | 0.94              |
| 1:A:735:GLY:C   | 1:A:743:ALA:CA   | 2.34                     | 0.94              |
| 1:J:538:GLU:HG3 | 4:W:352:PHE:N    | 1.81                     | 0.94              |
| 1:D:537:GLU:C   | 4:9:349:LEU:CD1  | 2.20                     | 0.94              |
| 1:D:818:TYR:HB3 | 2:E:90:GLY:N     | 1.80                     | 0.94              |
| 1:A:530:MET:HA  | 4:8:354:GLN:HG3  | 0.96                     | 0.94              |
| 2:E:150:TYR:O   | 2:E:151:LYS:CG   | 2.15                     | 0.94              |
| 1:J:797:PHE:CE1 | 3:L:146:ILE:CA   | 2.48                     | 0.94              |
| 1:M:735:GLY:C   | 1:M:743:ALA:CA   | 2.35                     | 0.94              |
| 1:J:836:PHE:CZ  | 2:K:160:GLY:N    | 2.35                     | 0.94              |
| 1:M:831:TRP:HH2 | 2:N:47:LEU:HD23  | 1.32                     | 0.94              |
| 4:0:288:ASP:CB  | 4:2:63:GLY:H     | 1.80                     | 0.94              |
| 1:M:95:THR:HA   | 1:M:713:SER:CB   | 1.96                     | 0.94              |
| 2:E:150:TYR:O   | 2:E:151:LYS:HB2  | 1.67                     | 0.94              |
| 2:H:150:TYR:O   | 2:H:151:LYS:HB2  | 1.67                     | 0.94              |
| 1:M:149:GLN:OE1 | 1:M:763:THR:HG21 | 1.68                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:795:ARG:HH21 | 3:I:116:GLU:CG   | 1.80                     | 0.94              |
| 1:G:642:LYS:CG   | 4:V:23:GLY:H     | 1.76                     | 0.94              |
| 1:P:538:GLU:N    | 4:O:349:LEU:CD1  | 2.28                     | 0.94              |
| 1:A:538:GLU:HG3  | 4:8:352:PHE:N    | 1.82                     | 0.94              |
| 4:O:166:TYR:OH   | 4:2:64:ILE:CG2   | 2.15                     | 0.94              |
| 1:D:724:TYR:CB   | 1:D:782:MLY:CD   | 2.42                     | 0.94              |
| 1:P:530:MET:HA   | 4:O:354:GLN:HG3  | 0.96                     | 0.94              |
| 1:A:736:GLN:CA   | 1:A:743:ALA:HB2  | 1.95                     | 0.94              |
| 1:G:218:LEU:CB   | 1:G:221:GLN:CG   | 2.46                     | 0.94              |
| 1:P:546:THR:HG22 | 1:P:548:THR:H    | 1.32                     | 0.94              |
| 1:A:530:MET:CA   | 4:8:354:GLN:CG   | 2.44                     | 0.94              |
| 2:Q:150:TYR:O    | 2:Q:151:LYS:CG   | 2.16                     | 0.94              |
| 1:M:819:ASN:HA   | 2:N:90:GLY:C     | 1.86                     | 0.94              |
| 1:P:831:TRP:HE1  | 2:Q:67:MET:HB3   | 1.30                     | 0.94              |
| 2:N:117:LEU:HD13 | 2:N:147:ASN:OD1  | 1.63                     | 0.94              |
| 1:G:813:ILE:CG2  | 2:H:128:PHE:HE1  | 1.72                     | 0.94              |
| 1:J:84:MLY:CH1   | 1:J:720:PHE:HD1  | 1.76                     | 0.94              |
| 1:M:543:PRO:CG   | 4:Z:143:TYR:O    | 2.14                     | 0.94              |
| 1:M:218:LEU:CB   | 1:M:221:GLN:CG   | 2.46                     | 0.94              |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CB   | 1.79                     | 0.94              |
| 1:A:818:TYR:CB   | 2:B:90:GLY:HA3   | 1.97                     | 0.94              |
| 1:P:612:GLN:NE2  | 1:P:627:GLY:CA   | 2.31                     | 0.94              |
| 1:D:725:ARG:C    | 1:D:782:MLY:HH22 | 1.88                     | 0.94              |
| 1:A:149:GLN:CB   | 1:A:719:ASP:N    | 2.31                     | 0.94              |
| 4:X:324:THR:CB   | 4:Z:245:GLY:C    | 2.30                     | 0.94              |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:HG22 | 0.96                     | 0.94              |
| 1:P:721:LYS:CA   | 1:P:736:GLN:CD   | 2.34                     | 0.94              |
| 1:A:218:LEU:CB   | 1:A:221:GLN:CG   | 2.46                     | 0.94              |
| 1:J:530:MET:HA   | 4:W:354:GLN:HG3  | 0.96                     | 0.94              |
| 1:D:530:MET:HA   | 4:9:354:GLN:HG3  | 0.96                     | 0.94              |
| 1:D:541:MET:N    | 4:9:349:LEU:HD21 | 1.80                     | 0.94              |
| 1:M:795:ARG:CG   | 3:O:118:MET:HE1  | 1.94                     | 0.94              |
| 1:M:797:PHE:CD1  | 3:O:149:VAL:HG12 | 1.96                     | 0.94              |
| 1:P:503:TYR:CE1  | 1:P:711:PHE:CD2  | 2.55                     | 0.94              |
| 1:A:642:LYS:CG   | 4:8:23:GLY:H     | 1.77                     | 0.94              |
| 1:A:818:TYR:HB3  | 2:B:90:GLY:N     | 1.82                     | 0.94              |
| 1:M:215:GLN:HA   | 1:M:340:ILE:HG23 | 0.95                     | 0.94              |
| 4:3:322:PRO:HB2  | 4:5:244:ASP:HB3  | 1.49                     | 0.94              |
| 1:J:567:LYS:HZ3  | 4:Y:92:ASN:HD22  | 1.02                     | 0.94              |
| 2:N:150:TYR:O    | 2:N:151:LYS:CG   | 2.15                     | 0.94              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:HA3  | 1.83                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:612:GLN:NE2  | 1:P:627:GLY:HA3  | 1.83                     | 0.94              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:CA   | 2.31                     | 0.94              |
| 1:G:795:ARG:C    | 3:I:35:ARG:NH2   | 2.20                     | 0.94              |
| 4:1:288:ASP:CG   | 4:3:203:THR:HG23 | 1.86                     | 0.94              |
| 1:P:797:PHE:CE1  | 3:R:149:VAL:HG12 | 2.02                     | 0.94              |
| 1:D:538:GLU:HG3  | 4:9:352:PHE:N    | 1.82                     | 0.94              |
| 1:D:546:THR:HG22 | 1:D:548:THR:H    | 1.32                     | 0.94              |
| 1:J:710:GLY:C    | 1:J:772:LEU:HD22 | 1.88                     | 0.94              |
| 1:M:800:ARG:HB3  | 3:O:149:VAL:CG2  | 1.97                     | 0.94              |
| 2:Q:150:TYR:O    | 2:Q:151:LYS:HG3  | 1.65                     | 0.94              |
| 1:A:739:ASP:HB3  | 1:A:742:LYS:CB   | 1.98                     | 0.94              |
| 2:E:121:LEU:HG   | 2:E:128:PHE:HA   | 1.47                     | 0.94              |
| 1:G:508:ILE:HD11 | 1:G:759:ALA:CB   | 1.96                     | 0.94              |
| 1:M:84:MLY:CD    | 1:M:723:ARG:HD2  | 1.97                     | 0.94              |
| 1:G:567:LYS:HZ1  | 4:X:92:ASN:HD22  | 1.11                     | 0.94              |
| 4:X:325:MET:HE2  | 4:Z:244:ASP:OD2  | 1.67                     | 0.94              |
| 1:G:832:MET:SD   | 2:H:84:PHE:CE2   | 2.61                     | 0.94              |
| 1:A:800:ARG:C    | 3:C:149:VAL:HG21 | 1.88                     | 0.94              |
| 1:M:612:GLN:NE2  | 1:M:627:GLY:HA3  | 1.83                     | 0.94              |
| 1:J:795:ARG:HD3  | 3:L:43:ASN:CG    | 1.88                     | 0.93              |
| 1:A:502:GLU:OE1  | 1:A:763:THR:N    | 2.00                     | 0.93              |
| 1:G:543:PRO:CG   | 4:V:143:TYR:O    | 2.15                     | 0.93              |
| 1:P:530:MET:CA   | 4:O:354:GLN:CG   | 2.44                     | 0.93              |
| 1:M:641:LYS:HG3  | 1:M:647:GLN:NE2  | 1.59                     | 0.93              |
| 1:D:799:MET:HE1  | 3:F:32:ASP:HB3   | 1.48                     | 0.93              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:HA3  | 1.83                     | 0.93              |
| 1:D:727:LEU:CG   | 1:D:782:MLY:HE2  | 1.97                     | 0.93              |
| 2:H:121:LEU:CB   | 2:H:128:PHE:HB3  | 1.69                     | 0.93              |
| 1:A:793:ARG:HH21 | 3:C:147:MET:HE3  | 1.32                     | 0.93              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HA    | 2.03                     | 0.93              |
| 2:Q:150:TYR:O    | 2:Q:151:LYS:HB2  | 1.67                     | 0.93              |
| 1:D:736:GLN:HA   | 1:D:743:ALA:HB2  | 1.51                     | 0.93              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB2  | 1.51                     | 0.93              |
| 1:M:530:MET:HA   | 4:Z:354:GLN:HG3  | 0.96                     | 0.93              |
| 1:J:537:GLU:C    | 4:W:349:LEU:CD1  | 2.20                     | 0.93              |
| 1:M:795:ARG:HG2  | 3:O:118:MET:HE3  | 0.94                     | 0.93              |
| 1:P:641:LYS:HD2  | 1:P:647:GLN:CD   | 1.70                     | 0.93              |
| 1:P:149:GLN:CG   | 1:P:716:LEU:HD11 | 1.98                     | 0.93              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:CB   | 2.14                     | 0.93              |
| 4:1:244:ASP:HB3  | 4:Z:322:PRO:HB2  | 1.49                     | 0.93              |
| 2:Q:121:LEU:HG   | 2:Q:128:PHE:HA   | 1.47                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:736:GLN:CA   | 1:J:743:ALA:HB2  | 1.95                     | 0.93              |
| 1:G:736:GLN:CA   | 1:G:743:ALA:HB2  | 1.95                     | 0.93              |
| 1:A:553:MLY:HB3  | 4:V:46:GLY:HA2   | 1.47                     | 0.93              |
| 1:G:90:ASP:OD2   | 1:G:764:MLY:HH11 | 1.66                     | 0.93              |
| 1:M:629:GLU:CB   | 1:M:643:GLY:O    | 2.17                     | 0.93              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:HA3  | 1.83                     | 0.93              |
| 1:J:797:PHE:CE1  | 3:L:146:ILE:HA   | 2.02                     | 0.93              |
| 1:G:541:MET:N    | 4:V:349:LEU:HD21 | 1.80                     | 0.93              |
| 1:P:215:GLN:H    | 1:P:340:ILE:CG1  | 1.72                     | 0.93              |
| 1:M:34:ALA:HB3   | 1:M:777:GLU:CD   | 1.86                     | 0.93              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:CG   | 2.37                     | 0.93              |
| 1:J:792:ALA:HB2  | 3:L:42:THR:HG23  | 0.96                     | 0.93              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:HH22  | 1.31                     | 0.93              |
| 1:D:813:ILE:HD13 | 2:E:128:PHE:HE1  | 1.12                     | 0.93              |
| 1:P:537:GLU:C    | 4:0:349:LEU:CD1  | 2.20                     | 0.93              |
| 1:J:530:MET:CA   | 4:W:354:GLN:CG   | 2.44                     | 0.93              |
| 4:0:167:GLU:OE1  | 4:2:42:GLY:HA2   | 1.69                     | 0.93              |
| 1:G:503:TYR:CE1  | 1:G:711:PHE:CD2  | 2.56                     | 0.93              |
| 1:M:84:MLY:CB    | 1:M:723:ARG:CD   | 2.38                     | 0.93              |
| 1:M:642:LYS:CB   | 4:Z:21:PHE:O     | 2.17                     | 0.93              |
| 1:D:739:ASP:HB3  | 1:D:742:LYS:CB   | 1.98                     | 0.93              |
| 4:1:288:ASP:N    | 4:3:203:THR:HG22 | 1.82                     | 0.93              |
| 1:G:503:TYR:CE1  | 1:G:711:PHE:HE2  | 1.83                     | 0.93              |
| 4:V:325:MET:CE   | 4:X:244:ASP:CG   | 2.37                     | 0.93              |
| 4:3:324:THR:HG23 | 4:5:244:ASP:C    | 1.86                     | 0.93              |
| 1:A:709:LYS:C    | 1:A:710:GLY:HA3  | 1.89                     | 0.93              |
| 1:J:800:ARG:NH2  | 3:L:40:ASN:CG    | 2.21                     | 0.93              |
| 1:G:797:PHE:CD1  | 3:I:146:ILE:HG23 | 2.04                     | 0.93              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG21  | 1.46                     | 0.93              |
| 1:G:830:PRO:CB   | 2:H:67:MET:CE    | 2.46                     | 0.93              |
| 2:E:149:ASP:CG   | 2:E:150:TYR:H    | 1.73                     | 0.93              |
| 1:J:788:THR:O    | 3:L:42:THR:HG21  | 1.67                     | 0.93              |
| 1:A:707:CYS:SG   | 1:A:714:ARG:NH1  | 2.41                     | 0.93              |
| 1:P:729:ALA:CA   | 3:R:93:VAL:CG2   | 2.44                     | 0.93              |
| 1:P:648:THR:HG21 | 1:P:651:ALA:HB2  | 1.50                     | 0.93              |
| 1:J:538:GLU:N    | 4:W:351:THR:H    | 1.67                     | 0.93              |
| 4:X:291:LYS:HD2  | 4:Z:243:PRO:CB   | 1.98                     | 0.93              |
| 1:A:549:SER:C    | 4:V:46:GLY:HA3   | 1.90                     | 0.93              |
| 1:G:215:GLN:HA   | 1:G:340:ILE:HG23 | 0.95                     | 0.93              |
| 1:G:796:GLY:N    | 3:I:35:ARG:CZ    | 2.33                     | 0.92              |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CZ   | 2.01                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:324:THR:CG2  | 4:Z:247:VAL:N    | 1.92                     | 0.92              |
| 1:P:642:LYS:CB   | 4:O:21:PHE:O     | 2.17                     | 0.92              |
| 1:M:530:MET:CA   | 4:Z:354:GLN:CG   | 2.44                     | 0.92              |
| 1:D:557:GLU:H    | 4:W:48:GLY:HA2   | 1.32                     | 0.92              |
| 1:M:736:GLN:CA   | 1:M:743:ALA:HB2  | 1.95                     | 0.92              |
| 1:A:629:GLU:CB   | 1:A:643:GLY:O    | 2.17                     | 0.92              |
| 1:A:818:TYR:HB2  | 2:B:90:GLY:N     | 1.83                     | 0.92              |
| 2:B:150:TYR:O    | 2:B:151:LYS:HB2  | 1.67                     | 0.92              |
| 1:D:549:SER:C    | 4:W:46:GLY:HA3   | 1.90                     | 0.92              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:CE   | 2.32                     | 0.92              |
| 1:A:648:THR:HG21 | 1:A:651:ALA:HB2  | 1.50                     | 0.92              |
| 1:P:218:LEU:CB   | 1:P:221:GLN:CG   | 2.46                     | 0.92              |
| 1:G:92:ALA:O     | 1:G:714:ARG:HG2  | 1.68                     | 0.92              |
| 2:B:54:MET:CA    | 2:H:21:GLU:OE1   | 2.17                     | 0.92              |
| 1:G:739:ASP:HB3  | 1:G:742:LYS:CB   | 1.99                     | 0.92              |
| 1:J:546:THR:HG22 | 1:J:548:THR:H    | 1.32                     | 0.92              |
| 1:M:612:GLN:NE2  | 1:M:627:GLY:CA   | 2.31                     | 0.92              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:CA   | 2.31                     | 0.92              |
| 4:V:286:ASP:OD2  | 4:X:203:THR:HG22 | 1.69                     | 0.92              |
| 1:D:727:LEU:HB2  | 1:D:782:MLY:HH12 | 1.13                     | 0.92              |
| 2:N:121:LEU:CB   | 2:N:128:PHE:HB3  | 1.68                     | 0.92              |
| 1:G:530:MET:CA   | 4:V:354:GLN:CG   | 2.45                     | 0.92              |
| 4:I:287:ILE:CD1  | 4:3:203:THR:HB   | 1.98                     | 0.92              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:CB   | 2.46                     | 0.92              |
| 1:M:638:GLY:HA3  | 4:Z:341:ILE:O    | 1.70                     | 0.92              |
| 1:J:648:THR:HG21 | 1:J:651:ALA:HB2  | 1.50                     | 0.92              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CG   | 2.33                     | 0.92              |
| 1:A:546:THR:HG22 | 1:A:548:THR:H    | 1.32                     | 0.92              |
| 1:P:838:ILE:CD1  | 2:Q:54:MET:HE3   | 1.93                     | 0.92              |
| 1:G:148:ARG:HH21 | 1:G:764:MLY:HH21 | 1.33                     | 0.92              |
| 1:A:641:LYS:HE3  | 1:A:647:GLN:CG   | 2.00                     | 0.92              |
| 1:A:642:LYS:CB   | 4:8:21:PHE:O     | 2.17                     | 0.92              |
| 1:J:215:GLN:HA   | 1:J:340:ILE:HG23 | 0.95                     | 0.92              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:CA   | 2.31                     | 0.92              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:HA3  | 1.83                     | 0.92              |
| 1:J:792:ALA:HB2  | 3:L:42:THR:HG22  | 1.04                     | 0.92              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:CA   | 2.18                     | 0.92              |
| 1:G:629:GLU:CB   | 1:G:643:GLY:O    | 2.17                     | 0.92              |
| 1:G:642:LYS:CB   | 4:V:21:PHE:O     | 2.17                     | 0.92              |
| 1:P:636:LYS:HD2  | 4:O:332:PRO:HB3  | 1.52                     | 0.92              |
| 1:J:206:LYS:CD   | 1:J:217:THR:CG2  | 2.16                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:213:LYS:HA   | 1:D:220:ASP:CG   | 1.90                     | 0.92              |
| 1:J:739:ASP:HB3  | 1:J:742:LYS:CB   | 1.99                     | 0.92              |
| 1:M:739:ASP:HB3  | 1:M:742:LYS:CB   | 1.98                     | 0.92              |
| 2:B:150:TYR:O    | 2:B:151:LYS:CG   | 2.15                     | 0.92              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:CA   | 2.31                     | 0.92              |
| 1:G:783:LEU:O    | 1:G:787:ILE:HB   | 1.70                     | 0.92              |
| 1:A:768:MLY:HB2  | 1:A:771:LEU:HB2  | 1.48                     | 0.92              |
| 1:P:538:GLU:N    | 4:O:351:THR:H    | 1.68                     | 0.92              |
| 1:M:546:THR:HG22 | 1:M:548:THR:H    | 1.32                     | 0.92              |
| 1:J:642:LYS:CB   | 4:W:21:PHE:O     | 2.17                     | 0.92              |
| 1:P:739:ASP:HB3  | 1:P:742:LYS:CB   | 1.98                     | 0.92              |
| 1:J:792:ALA:N    | 3:L:42:THR:HG22  | 1.84                     | 0.92              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:CB   | 2.46                     | 0.92              |
| 1:M:541:MET:N    | 4:Z:349:LEU:HD21 | 1.80                     | 0.92              |
| 1:P:785:GLU:CG   | 3:R:81:GLN:CG    | 2.47                     | 0.92              |
| 1:P:786:ILE:CA   | 1:P:787:ILE:N    | 2.31                     | 0.92              |
| 1:A:795:ARG:CG   | 3:C:35:ARG:HH12  | 1.83                     | 0.92              |
| 1:D:629:GLU:CB   | 1:D:643:GLY:O    | 2.17                     | 0.92              |
| 1:A:215:GLN:HA   | 1:A:340:ILE:HG23 | 0.96                     | 0.92              |
| 4:W:286:ASP:OD1  | 4:Y:202:THR:HB   | 1.69                     | 0.92              |
| 1:D:278:GLN:HG2  | 1:D:317:GLU:HB2  | 1.52                     | 0.92              |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:HD23 | 1.50                     | 0.92              |
| 1:D:798:LEU:HD12 | 3:F:126:LEU:HD21 | 1.49                     | 0.92              |
| 1:G:648:THR:HG21 | 1:G:651:ALA:HB2  | 1.50                     | 0.92              |
| 1:D:813:ILE:CG2  | 2:E:128:PHE:CZ   | 2.51                     | 0.92              |
| 1:J:636:LYS:HD2  | 4:W:332:PRO:HB3  | 1.52                     | 0.92              |
| 1:P:783:LEU:HA   | 1:P:786:ILE:CG1  | 2.00                     | 0.92              |
| 1:D:530:MET:CA   | 4:9:354:GLN:CG   | 2.45                     | 0.92              |
| 1:M:735:GLY:C    | 1:M:743:ALA:HA   | 1.90                     | 0.92              |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CA   | 2.00                     | 0.92              |
| 1:G:829:TRP:CZ3  | 2:H:87:LYS:NZ    | 2.38                     | 0.92              |
| 1:A:502:GLU:HG3  | 1:A:760:PHE:C    | 1.89                     | 0.92              |
| 1:A:149:GLN:HG3  | 1:A:719:ASP:OD1  | 1.66                     | 0.92              |
| 4:1:287:ILE:CG1  | 4:3:202:THR:HB   | 2.00                     | 0.92              |
| 1:J:629:GLU:CB   | 1:J:643:GLY:O    | 2.17                     | 0.92              |
| 1:P:797:PHE:HZ   | 3:R:146:ILE:HD13 | 1.34                     | 0.92              |
| 1:G:754:ASP:CA   | 1:G:776:GLU:OE1  | 2.12                     | 0.92              |
| 1:G:537:GLU:C    | 4:V:349:LEU:CD1  | 2.21                     | 0.92              |
| 1:P:819:ASN:CG   | 2:Q:90:GLY:O     | 2.07                     | 0.92              |
| 4:1:287:ILE:HG12 | 4:3:202:THR:HA   | 1.48                     | 0.92              |
| 1:J:213:LYS:HA   | 1:J:220:ASP:CG   | 1.90                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:541:MET:N    | 4:W:349:LEU:HD21 | 1.80                     | 0.92              |
| 1:P:797:PHE:CE1  | 3:R:146:ILE:CA   | 2.53                     | 0.92              |
| 1:D:537:GLU:O    | 4:9:349:LEU:HD13 | 0.74                     | 0.92              |
| 1:D:550:PHE:HA   | 4:W:46:GLY:CA    | 2.00                     | 0.92              |
| 1:A:557:GLU:N    | 4:V:48:GLY:CA    | 2.12                     | 0.92              |
| 4:3:288:ASP:OD1  | 4:5:203:THR:HG23 | 1.70                     | 0.92              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:CA   | 2.45                     | 0.92              |
| 1:D:813:ILE:HG21 | 2:E:128:PHE:CE1  | 2.04                     | 0.92              |
| 1:P:629:GLU:CB   | 1:P:643:GLY:O    | 2.17                     | 0.92              |
| 1:P:783:LEU:HA   | 1:P:786:ILE:HG13 | 1.52                     | 0.92              |
| 1:P:213:LYS:HA   | 1:P:220:ASP:CG   | 1.90                     | 0.92              |
| 1:P:649:VAL:CG1  | 1:P:649:VAL:C    | 2.38                     | 0.92              |
| 1:J:537:GLU:O    | 4:W:349:LEU:HD13 | 0.73                     | 0.91              |
| 1:D:648:THR:HG21 | 1:D:651:ALA:HB2  | 1.50                     | 0.91              |
| 1:P:641:LYS:HE3  | 1:P:647:GLN:CG   | 2.00                     | 0.91              |
| 1:G:641:LYS:HE3  | 1:G:647:GLN:CG   | 2.00                     | 0.91              |
| 1:A:818:TYR:CB   | 2:B:90:GLY:CA    | 2.48                     | 0.91              |
| 1:A:149:GLN:HB3  | 1:A:718:ALA:C    | 1.89                     | 0.91              |
| 4:1:287:ILE:HB   | 4:3:203:THR:N    | 1.82                     | 0.91              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:HD2  | 2.00                     | 0.91              |
| 2:H:144:VAL:HG13 | 2:H:153:ILE:HG12 | 1.14                     | 0.91              |
| 1:P:537:GLU:O    | 4:0:349:LEU:HD13 | 0.73                     | 0.91              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HA   | 1.91                     | 0.91              |
| 1:M:545:ALA:CA   | 4:1:45:VAL:HG12  | 1.92                     | 0.91              |
| 1:D:218:LEU:CB   | 1:D:221:GLN:CG   | 2.46                     | 0.91              |
| 1:A:636:LYS:HD2  | 4:8:332:PRO:HB3  | 1.51                     | 0.91              |
| 1:M:28:GLN:HB3   | 1:M:723:ARG:CZ   | 2.00                     | 0.91              |
| 1:D:642:LYS:CB   | 4:9:21:PHE:O     | 2.17                     | 0.91              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:C    | 2.38                     | 0.91              |
| 1:J:278:GLN:HG2  | 1:J:317:GLU:HB2  | 1.52                     | 0.91              |
| 1:P:735:GLY:C    | 1:P:743:ALA:HA   | 1.90                     | 0.91              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:CG   | 2.01                     | 0.91              |
| 1:J:538:GLU:N    | 4:W:349:LEU:HD12 | 1.86                     | 0.91              |
| 1:J:641:LYS:HE3  | 1:J:647:GLN:CG   | 2.00                     | 0.91              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:SD    | 2.09                     | 0.91              |
| 4:W:325:MET:CE   | 4:Y:244:ASP:CG   | 2.37                     | 0.91              |
| 1:A:505:MLY:CG   | 1:A:741:LYS:NZ   | 2.32                     | 0.91              |
| 1:P:818:TYR:CZ   | 2:Q:127:ARG:NH2  | 2.25                     | 0.91              |
| 1:P:541:MET:N    | 4:0:349:LEU:HD21 | 1.80                     | 0.91              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:CG   | 2.01                     | 0.91              |
| 1:D:636:LYS:HD2  | 4:9:332:PRO:HB3  | 1.52                     | 0.91              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:557:GLU:H   | 4:V:48:GLY:HA2   | 1.31                     | 0.91              |
| 1:P:836:PHE:CE2 | 2:Q:160:GLY:N    | 2.39                     | 0.91              |
| 1:P:218:LEU:HA  | 1:P:221:GLN:CG   | 2.00                     | 0.91              |
| 1:J:97:LEU:HD23 | 1:J:712:PRO:HB3  | 1.51                     | 0.91              |
| 1:G:537:GLU:O   | 4:V:349:LEU:HD13 | 0.74                     | 0.91              |
| 2:Q:121:LEU:CB  | 2:Q:128:PHE:HB3  | 1.69                     | 0.91              |
| 4:1:287:ILE:CG1 | 4:3:202:THR:CB   | 2.48                     | 0.91              |
| 1:J:218:LEU:CB  | 1:J:221:GLN:CG   | 2.46                     | 0.91              |
| 1:J:836:PHE:CE2 | 2:K:160:GLY:N    | 2.39                     | 0.91              |
| 3:L:62:ALA:O    | 3:L:63:ILE:CG1   | 2.19                     | 0.91              |
| 1:D:838:ILE:CD1 | 2:E:54:MET:SD    | 2.59                     | 0.91              |
| 4:0:288:ASP:CB  | 4:2:63:GLY:N     | 2.33                     | 0.91              |
| 1:M:630:ALA:O   | 4:Z:25:ASP:CG    | 2.09                     | 0.91              |
| 4:1:244:ASP:C   | 4:Z:324:THR:HG23 | 1.86                     | 0.91              |
| 2:H:149:ASP:CG  | 2:H:150:TYR:H    | 1.73                     | 0.91              |
| 2:N:150:TYR:O   | 2:N:151:LYS:HB2  | 1.67                     | 0.91              |
| 1:D:724:TYR:HB3 | 1:D:782:MLY:HD3  | 1.50                     | 0.91              |
| 1:G:410:ASN:OD1 | 4:V:334:GLU:C    | 2.09                     | 0.91              |
| 1:A:735:GLY:O   | 1:A:743:ALA:CA   | 2.19                     | 0.91              |
| 1:M:544:LYS:HD2 | 4:Z:147:ARG:HB3  | 1.53                     | 0.91              |
| 1:P:795:ARG:HD3 | 3:R:43:ASN:OD1   | 1.71                     | 0.91              |
| 1:D:538:GLU:N   | 4:9:351:THR:H    | 1.68                     | 0.91              |
| 1:J:710:GLY:C   | 1:J:772:LEU:CD2  | 2.37                     | 0.91              |
| 1:M:736:GLN:HA  | 1:M:743:ALA:HB2  | 1.51                     | 0.91              |
| 1:M:829:TRP:CZ2 | 2:N:87:LYS:HE2   | 2.06                     | 0.91              |
| 1:G:544:LYS:HD2 | 4:V:147:ARG:HB3  | 1.53                     | 0.91              |
| 1:M:537:GLU:O   | 4:Z:349:LEU:HD13 | 0.73                     | 0.91              |
| 1:P:795:ARG:CB  | 3:R:35:ARG:HH12  | 1.83                     | 0.91              |
| 1:M:213:LYS:HA  | 1:M:220:ASP:CG   | 1.90                     | 0.91              |
| 1:A:537:GLU:C   | 4:8:349:LEU:CD1  | 2.20                     | 0.91              |
| 1:A:638:GLY:HA3 | 4:8:341:ILE:O    | 1.70                     | 0.91              |
| 1:A:649:VAL:CG1 | 1:A:649:VAL:C    | 2.38                     | 0.91              |
| 4:V:324:THR:CG2 | 4:X:247:VAL:H    | 1.84                     | 0.91              |
| 1:P:278:GLN:HG2 | 1:P:317:GLU:HB2  | 1.52                     | 0.91              |
| 1:A:93:MET:SD   | 1:A:715:VAL:HG22 | 2.11                     | 0.91              |
| 1:D:508:ILE:CD1 | 1:D:766:PHE:CE2  | 2.54                     | 0.91              |
| 1:G:538:GLU:N   | 4:V:351:THR:H    | 1.68                     | 0.91              |
| 1:P:735:GLY:O   | 1:P:743:ALA:CA   | 2.19                     | 0.91              |
| 1:P:736:GLN:CA  | 1:P:743:ALA:HB2  | 1.95                     | 0.91              |
| 1:G:819:ASN:CG  | 2:H:92:ASP:CB    | 2.37                     | 0.91              |
| 1:M:218:LEU:HA  | 1:M:221:GLN:CG   | 2.01                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:537:GLU:O    | 4:8:349:LEU:HD13 | 0.74                     | 0.91              |
| 1:J:836:PHE:HE1  | 2:K:159:HIS:HA   | 1.25                     | 0.91              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE1   | 1.50                     | 0.91              |
| 1:J:826:VAL:HG21 | 2:K:88:LEU:HD23  | 1.49                     | 0.91              |
| 1:P:215:GLN:HA   | 1:P:340:ILE:HG23 | 0.95                     | 0.91              |
| 1:D:735:GLY:O    | 1:D:743:ALA:CA   | 2.19                     | 0.91              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HA   | 1.90                     | 0.91              |
| 1:M:410:ASN:OD1  | 4:Z:334:GLU:C    | 2.10                     | 0.91              |
| 1:A:538:GLU:N    | 4:8:349:LEU:HD12 | 1.86                     | 0.91              |
| 1:A:538:GLU:N    | 4:8:351:THR:H    | 1.67                     | 0.91              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HE2   | 0.94                     | 0.91              |
| 4:1:203:THR:HG23 | 4:Z:288:ASP:OD1  | 1.70                     | 0.91              |
| 1:J:561:LYS:HE3  | 4:Y:48:GLY:HA3   | 1.51                     | 0.91              |
| 1:A:800:ARG:HH22 | 3:C:40:ASN:HD21  | 0.91                     | 0.91              |
| 3:R:62:ALA:O     | 3:R:63:ILE:HG12  | 1.71                     | 0.91              |
| 2:K:150:TYR:O    | 2:K:151:LYS:HB2  | 1.67                     | 0.91              |
| 1:A:544:LYS:HD2  | 4:8:147:ARG:HB3  | 1.53                     | 0.91              |
| 1:D:732:ILE:HG21 | 1:D:782:MLY:HH21 | 0.92                     | 0.90              |
| 1:D:747:LEU:HD21 | 1:D:782:MLY:HH11 | 1.52                     | 0.90              |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:H    | 1.34                     | 0.90              |
| 1:M:505:MLY:HD2  | 1:M:762:HIS:HE1  | 1.36                     | 0.90              |
| 1:A:831:TRP:CE3  | 2:B:34:ILE:HG12  | 2.06                     | 0.90              |
| 1:G:649:VAL:CB   | 1:G:649:VAL:CG2  | 2.49                     | 0.90              |
| 1:D:649:VAL:C    | 1:D:649:VAL:CG1  | 2.38                     | 0.90              |
| 3:C:62:ALA:O     | 3:C:63:ILE:CG1   | 2.19                     | 0.90              |
| 1:J:800:ARG:NH2  | 3:L:40:ASN:ND2   | 2.18                     | 0.90              |
| 1:J:800:ARG:HG2  | 3:L:149:VAL:HG22 | 1.51                     | 0.90              |
| 1:D:798:LEU:CD1  | 3:F:126:LEU:HD21 | 2.01                     | 0.90              |
| 1:J:735:GLY:O    | 1:J:743:ALA:CA   | 2.19                     | 0.90              |
| 1:M:636:LYS:HD2  | 4:Z:332:PRO:HB3  | 1.52                     | 0.90              |
| 1:A:831:TRP:CH2  | 2:B:34:ILE:CG2   | 2.53                     | 0.90              |
| 1:A:550:PHE:HA   | 4:V:46:GLY:CA    | 2.00                     | 0.90              |
| 1:D:641:LYS:HE3  | 1:D:647:GLN:CG   | 2.00                     | 0.90              |
| 1:A:836:PHE:HZ   | 2:B:160:GLY:H    | 1.11                     | 0.90              |
| 1:A:649:VAL:CG2  | 1:A:649:VAL:CB   | 2.50                     | 0.90              |
| 1:M:649:VAL:CB   | 1:M:649:VAL:CG2  | 2.49                     | 0.90              |
| 1:J:756:THR:O    | 1:J:776:GLU:OE1  | 1.88                     | 0.90              |
| 1:G:215:GLN:H    | 1:G:340:ILE:CG1  | 1.72                     | 0.90              |
| 1:G:278:GLN:HG2  | 1:G:317:GLU:HB2  | 1.52                     | 0.90              |
| 1:D:795:ARG:CG   | 3:F:118:MET:CE   | 2.45                     | 0.90              |
| 1:D:553:MLY:HE2  | 4:W:45:VAL:HA    | 1.53                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:218:LEU:HA   | 1:D:221:GLN:CG   | 2.00                     | 0.90              |
| 1:P:838:ILE:CD1  | 2:Q:54:MET:HE1   | 1.95                     | 0.90              |
| 1:M:641:LYS:HE3  | 1:M:647:GLN:CG   | 2.00                     | 0.90              |
| 1:M:753:VAL:HG13 | 1:M:775:LEU:CD2  | 2.01                     | 0.90              |
| 1:J:544:LYS:HD2  | 4:W:147:ARG:HB3  | 1.53                     | 0.90              |
| 1:G:538:GLU:N    | 4:V:349:LEU:HD12 | 1.87                     | 0.90              |
| 1:P:820:VAL:HG11 | 2:Q:136:MET:HE3  | 1.53                     | 0.90              |
| 2:E:137:TRP:HA   | 2:E:145:ALA:HB2  | 1.54                     | 0.90              |
| 1:P:544:LYS:HD2  | 4:O:147:ARG:HB3  | 1.53                     | 0.90              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:CG   | 1.90                     | 0.90              |
| 1:D:538:GLU:O    | 4:9:349:LEU:CG   | 2.20                     | 0.90              |
| 1:A:823:PHE:HE1  | 2:B:160:GLY:CA   | 1.85                     | 0.90              |
| 1:D:649:VAL:HG13 | 1:D:649:VAL:CG2  | 2.02                     | 0.90              |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:CE1   | 2.04                     | 0.90              |
| 1:M:278:GLN:HG2  | 1:M:317:GLU:HB2  | 1.52                     | 0.90              |
| 1:J:797:PHE:CE1  | 3:L:146:ILE:CG2  | 1.95                     | 0.90              |
| 1:G:638:GLY:HA3  | 4:V:341:ILE:O    | 1.70                     | 0.90              |
| 1:G:636:LYS:HD2  | 4:V:332:PRO:HB3  | 1.52                     | 0.90              |
| 1:M:648:THR:HG21 | 1:M:651:ALA:HB2  | 1.50                     | 0.90              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:OE2  | 1.96                     | 0.90              |
| 1:M:735:GLY:O    | 1:M:743:ALA:CA   | 2.19                     | 0.90              |
| 1:M:649:VAL:C    | 1:M:649:VAL:CG1  | 2.38                     | 0.90              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:C    | 2.38                     | 0.90              |
| 1:J:799:MET:SD   | 3:L:32:ASP:HB3   | 2.11                     | 0.90              |
| 1:J:792:ALA:CB   | 3:L:42:THR:HG23  | 1.88                     | 0.90              |
| 1:D:721:LYS:CB   | 1:D:736:GLN:OE1  | 2.20                     | 0.90              |
| 4:1:287:ILE:CD1  | 4:3:203:THR:N    | 2.34                     | 0.90              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:CG   | 2.01                     | 0.90              |
| 1:M:538:GLU:N    | 4:Z:351:THR:H    | 1.67                     | 0.90              |
| 1:D:538:GLU:N    | 4:9:349:LEU:HD12 | 1.86                     | 0.90              |
| 1:G:649:VAL:C    | 1:G:649:VAL:CG1  | 2.38                     | 0.90              |
| 1:P:649:VAL:CG2  | 1:P:649:VAL:HG13 | 2.02                     | 0.90              |
| 1:J:649:VAL:HG13 | 1:J:649:VAL:CG2  | 2.02                     | 0.90              |
| 1:M:817:GLN:HG2  | 2:N:127:ARG:CG   | 2.02                     | 0.90              |
| 2:Q:137:TRP:HA   | 2:Q:145:ALA:HB2  | 1.54                     | 0.90              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:CG   | 1.90                     | 0.90              |
| 1:G:97:LEU:HD23  | 1:G:712:PRO:HB3  | 0.90                     | 0.90              |
| 4:X:325:MET:SD   | 4:Z:244:ASP:HB2  | 2.12                     | 0.90              |
| 1:M:629:GLU:HG2  | 1:M:643:GLY:O    | 1.72                     | 0.90              |
| 3:I:24:LYS:HB3   | 3:I:63:ILE:O     | 1.72                     | 0.90              |
| 2:Q:149:ASP:CG   | 2:Q:150:TYR:H    | 1.73                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:544:LYS:HD2  | 4:9:147:ARG:HB3  | 1.53                     | 0.90              |
| 1:A:278:GLN:HG2  | 1:A:317:GLU:HB2  | 1.52                     | 0.90              |
| 1:G:797:PHE:HE2  | 3:I:126:LEU:HD22 | 1.10                     | 0.90              |
| 2:E:121:LEU:CB   | 2:E:128:PHE:HB3  | 1.69                     | 0.90              |
| 4:1:287:ILE:HG21 | 4:3:202:THR:CB   | 2.02                     | 0.90              |
| 1:P:410:ASN:OD1  | 4:0:334:GLU:C    | 2.10                     | 0.90              |
| 1:J:530:MET:N    | 4:W:354:GLN:HB3  | 1.87                     | 0.90              |
| 1:D:534:SER:O    | 4:9:351:THR:HG23 | 1.13                     | 0.90              |
| 1:D:638:GLY:HA3  | 4:9:341:ILE:O    | 1.70                     | 0.90              |
| 1:G:721:LYS:CB   | 1:G:736:GLN:OE1  | 2.20                     | 0.90              |
| 1:A:410:ASN:OD1  | 4:8:334:GLU:C    | 2.10                     | 0.90              |
| 1:P:630:ALA:O    | 4:0:25:ASP:CG    | 2.09                     | 0.90              |
| 3:C:62:ALA:O     | 3:C:63:ILE:HG12  | 1.71                     | 0.90              |
| 1:G:753:VAL:CA   | 1:G:780:ASP:OD1  | 2.19                     | 0.90              |
| 2:N:121:LEU:CA   | 2:N:128:PHE:CB   | 2.46                     | 0.90              |
| 3:F:62:ALA:O     | 3:F:63:ILE:CG1   | 2.19                     | 0.90              |
| 3:O:62:ALA:O     | 3:O:63:ILE:HG12  | 1.72                     | 0.90              |
| 1:M:97:LEU:CD2   | 1:M:712:PRO:CB   | 2.50                     | 0.90              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HA   | 1.91                     | 0.90              |
| 1:A:501:GLU:CA   | 1:A:762:HIS:CE1  | 2.55                     | 0.90              |
| 1:P:538:GLU:O    | 4:0:349:LEU:CG   | 2.20                     | 0.90              |
| 1:P:635:GLY:CA   | 4:0:341:ILE:HD13 | 2.02                     | 0.90              |
| 1:J:538:GLU:O    | 4:W:349:LEU:CG   | 2.20                     | 0.90              |
| 1:D:550:PHE:CA   | 4:W:46:GLY:HA3   | 2.02                     | 0.90              |
| 1:M:805:ALA:CA   | 1:M:808:GLU:HB2  | 1.99                     | 0.90              |
| 2:B:149:ASP:CG   | 2:B:150:TYR:H    | 1.73                     | 0.90              |
| 1:G:792:ALA:HB1  | 3:I:42:THR:N     | 1.86                     | 0.89              |
| 1:G:629:GLU:HG2  | 1:G:643:GLY:O    | 1.72                     | 0.89              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:HD2  | 1.55                     | 0.89              |
| 1:M:534:SER:HA   | 4:Z:350:SER:O    | 1.71                     | 0.89              |
| 1:J:768:MLY:CH1  | 1:J:772:LEU:CD1  | 2.32                     | 0.89              |
| 1:G:553:MLY:NZ   | 4:X:45:VAL:HG11  | 1.88                     | 0.89              |
| 1:P:821:ARG:HH21 | 2:Q:127:ARG:HG2  | 1.34                     | 0.89              |
| 1:J:721:LYS:CB   | 1:J:736:GLN:OE1  | 2.20                     | 0.89              |
| 1:M:553:MLY:CE   | 4:1:43:VAL:CG2   | 2.43                     | 0.89              |
| 1:J:635:GLY:CA   | 4:W:341:ILE:HD13 | 2.02                     | 0.89              |
| 1:J:410:ASN:OD1  | 4:W:334:GLU:C    | 2.10                     | 0.89              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HA   | 1.90                     | 0.89              |
| 1:A:791:GLN:OE1  | 3:C:116:GLU:CG   | 2.19                     | 0.89              |
| 1:P:206:LYS:CD   | 1:P:217:THR:CG2  | 2.16                     | 0.89              |
| 1:D:649:VAL:CB   | 1:D:649:VAL:CG2  | 2.49                     | 0.89              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:629:GLU:HG2 | 1:A:643:GLY:O    | 1.72                     | 0.89              |
| 1:P:649:VAL:CG2 | 1:P:649:VAL:CB   | 2.49                     | 0.89              |
| 1:J:215:GLN:H   | 1:J:340:ILE:CG1  | 1.73                     | 0.89              |
| 3:R:62:ALA:O    | 3:R:63:ILE:CG1   | 2.19                     | 0.89              |
| 3:C:24:LYS:HB3  | 3:C:63:ILE:O     | 1.72                     | 0.89              |
| 1:G:757:GLN:CG  | 1:G:776:GLU:OE2  | 2.20                     | 0.89              |
| 2:H:137:TRP:HA  | 2:H:145:ALA:HB2  | 1.53                     | 0.89              |
| 1:J:534:SER:HA  | 4:W:350:SER:O    | 1.71                     | 0.89              |
| 1:G:567:LYS:HZ2 | 4:X:92:ASN:HD22  | 1.12                     | 0.89              |
| 1:G:599:ASN:OD1 | 1:G:649:VAL:HB   | 1.72                     | 0.89              |
| 3:I:62:ALA:O    | 3:I:63:ILE:CG1   | 2.19                     | 0.89              |
| 3:L:24:LYS:HB3  | 3:L:63:ILE:O     | 1.72                     | 0.89              |
| 2:E:162:ASP:O   | 2:K:21:GLU:HB2   | 1.72                     | 0.89              |
| 1:D:793:ARG:NH2 | 3:F:147:MET:CE   | 2.36                     | 0.89              |
| 2:K:137:TRP:HA  | 2:K:145:ALA:HB2  | 1.53                     | 0.89              |
| 1:A:721:LYS:CB  | 1:A:736:GLN:OE1  | 2.20                     | 0.89              |
| 1:M:553:MLY:CG  | 4:1:43:VAL:CG2   | 2.50                     | 0.89              |
| 1:D:553:MLY:CG  | 4:W:44:MET:O     | 2.20                     | 0.89              |
| 1:A:530:MET:N   | 4:8:354:GLN:HB3  | 1.87                     | 0.89              |
| 1:A:553:MLY:CG  | 4:V:44:MET:O     | 2.20                     | 0.89              |
| 1:J:710:GLY:N   | 1:J:772:LEU:HD22 | 1.87                     | 0.89              |
| 1:J:649:VAL:CG2 | 1:J:649:VAL:CB   | 2.49                     | 0.89              |
| 4:X:286:ASP:OD2 | 4:Z:203:THR:HG22 | 1.72                     | 0.89              |
| 1:J:630:ALA:O   | 4:W:25:ASP:CG    | 2.09                     | 0.89              |
| 1:A:508:ILE:CG1 | 1:A:759:ALA:HB1  | 2.03                     | 0.89              |
| 2:B:137:TRP:HA  | 2:B:145:ALA:HB2  | 1.54                     | 0.89              |
| 1:M:538:GLU:O   | 4:Z:349:LEU:CG   | 2.20                     | 0.89              |
| 1:M:542:PHE:HA  | 4:Z:143:TYR:HE1  | 1.34                     | 0.89              |
| 1:M:538:GLU:N   | 4:Z:349:LEU:HD12 | 1.86                     | 0.89              |
| 1:G:735:GLY:O   | 1:G:743:ALA:CA   | 2.19                     | 0.89              |
| 1:M:84:MLY:CB   | 1:M:723:ARG:NE   | 2.34                     | 0.89              |
| 1:M:93:MET:HE1  | 1:M:764:MLY:HD2  | 1.55                     | 0.89              |
| 1:D:823:PHE:CE1 | 2:E:160:GLY:HA3  | 2.03                     | 0.89              |
| 3:I:62:ALA:O    | 3:I:63:ILE:HG12  | 1.71                     | 0.89              |
| 1:G:797:PHE:HZ  | 3:I:146:ILE:CD1  | 1.58                     | 0.89              |
| 1:P:530:MET:N   | 4:0:354:GLN:HB3  | 1.87                     | 0.89              |
| 1:D:530:MET:N   | 4:9:354:GLN:HB3  | 1.87                     | 0.89              |
| 1:D:635:GLY:CA  | 4:9:341:ILE:HD13 | 2.03                     | 0.89              |
| 1:G:93:MET:HG2  | 1:G:714:ARG:CA   | 2.01                     | 0.89              |
| 1:D:630:ALA:O   | 4:9:25:ASP:CG    | 2.09                     | 0.89              |
| 1:G:795:ARG:CZ  | 3:I:116:GLU:CD   | 2.41                     | 0.89              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:505:MLY:CH2  | 1:A:762:HIS:O   | 2.20                     | 0.89              |
| 1:G:538:GLU:O    | 4:V:349:LEU:CG  | 2.20                     | 0.89              |
| 1:P:534:SER:HA   | 4:0:350:SER:O   | 1.71                     | 0.89              |
| 1:M:553:MLY:HE2  | 4:1:43:VAL:HG22 | 1.54                     | 0.89              |
| 1:M:641:LYS:CD   | 1:M:647:GLN:OE1 | 2.18                     | 0.89              |
| 1:M:506:GLU:CD   | 1:M:760:PHE:O   | 2.11                     | 0.89              |
| 1:J:831:TRP:CZ2  | 2:K:47:LEU:CD2  | 2.55                     | 0.89              |
| 3:F:62:ALA:O     | 3:F:63:ILE:HG12 | 1.71                     | 0.89              |
| 3:O:62:ALA:O     | 3:O:63:ILE:CG1  | 2.19                     | 0.89              |
| 1:P:721:LYS:CB   | 1:P:736:GLN:OE1 | 2.20                     | 0.89              |
| 1:D:410:ASN:OD1  | 4:9:334:GLU:C   | 2.10                     | 0.89              |
| 1:A:534:SER:HA   | 4:8:350:SER:O   | 1.70                     | 0.89              |
| 1:M:721:LYS:CB   | 1:M:736:GLN:OE1 | 2.20                     | 0.89              |
| 1:D:629:GLU:HG2  | 1:D:643:GLY:O   | 1.72                     | 0.89              |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HE1 | 1.37                     | 0.89              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:HB3 | 1.88                     | 0.89              |
| 1:G:534:SER:HA   | 4:V:350:SER:O   | 1.71                     | 0.89              |
| 1:M:541:MET:CB   | 4:Z:143:TYR:OH  | 2.20                     | 0.89              |
| 1:D:534:SER:HA   | 4:9:350:SER:O   | 1.71                     | 0.89              |
| 1:A:550:PHE:CA   | 4:V:46:GLY:HA3  | 2.02                     | 0.89              |
| 1:D:641:LYS:HD2  | 4:9:348:SER:CB  | 2.03                     | 0.89              |
| 1:M:642:LYS:HG2  | 4:Z:22:ALA:CA   | 2.03                     | 0.89              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:HH12 | 1.38                     | 0.88              |
| 1:M:817:GLN:CD   | 2:N:127:ARG:CD  | 2.35                     | 0.88              |
| 1:A:553:MLY:HE2  | 4:V:45:VAL:HA   | 1.53                     | 0.88              |
| 1:M:838:ILE:CD1  | 2:N:54:MET:HE1  | 1.94                     | 0.88              |
| 1:D:641:LYS:CD   | 1:D:647:GLN:OE1 | 2.17                     | 0.88              |
| 1:J:641:LYS:HD2  | 4:W:348:SER:CB  | 2.02                     | 0.88              |
| 1:M:84:MLY:HH21  | 1:M:720:PHE:CA  | 2.03                     | 0.88              |
| 1:G:792:ALA:CB   | 3:I:42:THR:N    | 2.35                     | 0.88              |
| 2:B:137:TRP:HA   | 2:B:145:ALA:CB  | 2.04                     | 0.88              |
| 1:P:638:GLY:HA3  | 4:0:341:ILE:O   | 1.70                     | 0.88              |
| 1:P:792:ALA:HB2  | 3:R:42:THR:HG22 | 0.90                     | 0.88              |
| 1:D:541:MET:CB   | 4:9:143:TYR:OH  | 2.21                     | 0.88              |
| 1:A:791:GLN:NE2  | 3:C:115:GLY:HA3 | 1.88                     | 0.88              |
| 1:A:538:GLU:O    | 4:8:349:LEU:CG  | 2.20                     | 0.88              |
| 1:A:641:LYS:HG3  | 1:A:647:GLN:NE2 | 1.58                     | 0.88              |
| 1:A:630:ALA:O    | 4:8:25:ASP:CG   | 2.10                     | 0.88              |
| 1:M:817:GLN:HG2  | 2:N:127:ARG:HB2 | 1.55                     | 0.88              |
| 1:G:530:MET:N    | 4:V:354:GLN:HB3 | 1.88                     | 0.88              |
| 1:P:642:LYS:HG2  | 4:0:22:ALA:CA   | 2.03                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:204:ALA:H    | 4:Z:287:ILE:CG2  | 1.87                     | 0.88              |
| 1:M:649:VAL:HG13 | 1:M:649:VAL:CG2  | 2.02                     | 0.88              |
| 3:F:24:LYS:HB3   | 3:F:63:ILE:O     | 1.72                     | 0.88              |
| 4:1:322:PRO:HB3  | 4:3:244:ASP:CG   | 1.93                     | 0.88              |
| 1:A:707:CYS:SG   | 1:A:714:ARG:HD2  | 2.13                     | 0.88              |
| 1:M:544:LYS:O    | 4:1:45:VAL:HG11  | 1.73                     | 0.88              |
| 1:J:638:GLY:HA3  | 4:W:341:ILE:O    | 1.70                     | 0.88              |
| 4:0:205:GLU:OE2  | 4:Y:287:ILE:HG22 | 1.70                     | 0.88              |
| 1:M:836:PHE:CE2  | 2:N:160:GLY:N    | 2.37                     | 0.88              |
| 1:M:797:PHE:CE1  | 3:O:146:ILE:HA   | 2.08                     | 0.88              |
| 1:P:641:LYS:HD2  | 4:0:348:SER:CB   | 2.03                     | 0.88              |
| 1:D:724:TYR:CD1  | 1:D:782:MLY:HD3  | 2.09                     | 0.88              |
| 1:G:552:ASN:O    | 4:X:47:MET:HE1   | 1.72                     | 0.88              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:CB   | 2.46                     | 0.88              |
| 1:M:642:LYS:CG   | 4:Z:21:PHE:O     | 2.22                     | 0.88              |
| 1:G:541:MET:CB   | 4:V:143:TYR:OH   | 2.21                     | 0.88              |
| 1:P:642:LYS:CG   | 4:0:21:PHE:O     | 2.22                     | 0.88              |
| 1:M:546:THR:O    | 4:1:46:GLY:CA    | 2.21                     | 0.88              |
| 1:J:642:LYS:HG2  | 4:W:22:ALA:CA    | 2.03                     | 0.88              |
| 1:D:635:GLY:HA2  | 4:9:334:GLU:CG   | 2.03                     | 0.88              |
| 1:J:505:MLY:HG3  | 1:J:762:HIS:CE1  | 2.07                     | 0.88              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:HB   | 1.73                     | 0.88              |
| 1:A:642:LYS:HG2  | 4:8:22:ALA:CA    | 2.04                     | 0.88              |
| 4:0:288:ASP:CG   | 4:2:63:GLY:CA    | 2.42                     | 0.88              |
| 1:J:541:MET:CB   | 4:W:143:TYR:OH   | 2.20                     | 0.88              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:HD13 | 2.07                     | 0.88              |
| 1:J:710:GLY:O    | 1:J:772:LEU:HB2  | 1.74                     | 0.88              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:OE1  | 2.17                     | 0.88              |
| 1:A:95:THR:OG1   | 1:A:769:ALA:C    | 2.12                     | 0.88              |
| 1:P:215:GLN:H    | 1:P:340:ILE:HG12 | 1.05                     | 0.88              |
| 1:J:215:GLN:H    | 1:J:340:ILE:HG12 | 1.05                     | 0.88              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:HB3   | 0.75                     | 0.88              |
| 3:R:24:LYS:HB3   | 3:R:63:ILE:O     | 1.72                     | 0.88              |
| 3:L:62:ALA:O     | 3:L:63:ILE:HG12  | 1.71                     | 0.88              |
| 3:O:24:LYS:HB3   | 3:O:63:ILE:O     | 1.72                     | 0.88              |
| 1:G:789:ALA:CB   | 3:I:81:GLN:CD    | 2.41                     | 0.88              |
| 1:P:97:LEU:CD2   | 1:P:712:PRO:HB3  | 2.03                     | 0.88              |
| 1:D:727:LEU:HD13 | 1:D:782:MLY:HH12 | 1.55                     | 0.88              |
| 1:A:149:GLN:HG2  | 1:A:719:ASP:H    | 1.37                     | 0.88              |
| 1:A:93:MET:CE    | 1:A:715:VAL:CA   | 2.34                     | 0.88              |
| 1:G:642:LYS:HG2  | 4:V:22:ALA:CA    | 2.03                     | 0.88              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:635:GLY:CA   | 4:Z:341:ILE:HD13 | 2.02                     | 0.88              |
| 1:J:642:LYS:CG   | 4:W:21:PHE:O     | 2.22                     | 0.88              |
| 1:P:798:LEU:HD21 | 3:R:126:LEU:HD11 | 1.10                     | 0.88              |
| 1:G:736:GLN:HA   | 1:G:743:ALA:HB2  | 1.51                     | 0.88              |
| 1:G:93:MET:CA    | 1:G:714:ARG:H    | 1.82                     | 0.88              |
| 1:A:641:LYS:HD2  | 4:8:348:SER:CB   | 2.03                     | 0.88              |
| 4:V:286:ASP:OD1  | 4:X:203:THR:HG22 | 1.74                     | 0.88              |
| 1:D:798:LEU:HD11 | 3:F:126:LEU:CD2  | 2.02                     | 0.88              |
| 1:G:642:LYS:CG   | 4:V:21:PHE:O     | 2.22                     | 0.88              |
| 2:Q:137:TRP:HA   | 2:Q:145:ALA:CB   | 2.04                     | 0.88              |
| 1:G:819:ASN:ND2  | 2:H:92:ASP:CB    | 2.37                     | 0.88              |
| 1:J:84:MLY:HH22  | 1:J:719:ASP:O    | 1.74                     | 0.88              |
| 1:J:629:GLU:HG2  | 1:J:643:GLY:O    | 1.72                     | 0.88              |
| 1:P:795:ARG:HG2  | 3:R:118:MET:HE2  | 1.56                     | 0.88              |
| 1:A:541:MET:CB   | 4:8:143:TYR:OH   | 2.20                     | 0.88              |
| 1:D:215:GLN:H    | 1:D:340:ILE:HG12 | 1.06                     | 0.88              |
| 4:X:286:ASP:OD1  | 4:Z:203:THR:N    | 2.06                     | 0.88              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HB2  | 1.82                     | 0.88              |
| 1:A:502:GLU:OE1  | 1:A:764:MLY:N    | 2.07                     | 0.88              |
| 1:P:817:GLN:HG2  | 2:Q:127:ARG:CG   | 2.03                     | 0.88              |
| 2:E:137:TRP:HA   | 2:E:145:ALA:CB   | 2.04                     | 0.88              |
| 1:P:629:GLU:HG2  | 1:P:643:GLY:O    | 1.72                     | 0.88              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:HE1  | 1.88                     | 0.88              |
| 1:A:795:ARG:HH21 | 3:C:116:GLU:CG   | 1.87                     | 0.88              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:CD1  | 2.57                     | 0.88              |
| 1:D:798:LEU:CD1  | 3:F:126:LEU:CD2  | 2.51                     | 0.87              |
| 1:G:797:PHE:CZ   | 3:I:146:ILE:HD13 | 2.08                     | 0.87              |
| 2:N:137:TRP:HA   | 2:N:145:ALA:HB2  | 1.54                     | 0.87              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CD1  | 2.58                     | 0.87              |
| 1:P:819:ASN:HA   | 2:Q:90:GLY:C     | 1.93                     | 0.87              |
| 1:G:84:MLY:HD3   | 1:G:723:ARG:CD   | 2.03                     | 0.87              |
| 3:R:139:TYR:HA   | 3:R:142:PHE:HB3  | 1.56                     | 0.87              |
| 1:A:736:GLN:HA   | 1:A:743:ALA:HB2  | 1.51                     | 0.87              |
| 1:M:530:MET:N    | 4:Z:354:GLN:HB3  | 1.87                     | 0.87              |
| 4:3:287:ILE:CG2  | 4:5:204:ALA:H    | 1.87                     | 0.87              |
| 1:A:72:VAL:CG1   | 1:A:76:GLN:HB3   | 2.05                     | 0.87              |
| 1:D:797:PHE:CE1  | 3:F:146:ILE:HG23 | 2.08                     | 0.87              |
| 1:G:754:ASP:HA   | 1:G:779:ARG:HD3  | 1.52                     | 0.87              |
| 1:G:635:GLY:CA   | 4:V:341:ILE:HD13 | 2.03                     | 0.87              |
| 2:H:137:TRP:HA   | 2:H:145:ALA:CB   | 2.04                     | 0.87              |
| 1:P:541:MET:CB   | 4:0:143:TYR:OH   | 2.20                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:635:GLY:CA   | 4:8:341:ILE:HD13 | 2.02                     | 0.87              |
| 1:D:642:LYS:CG   | 4:9:21:PHE:O     | 2.22                     | 0.87              |
| 1:A:642:LYS:CG   | 4:8:21:PHE:O     | 2.22                     | 0.87              |
| 1:M:35:MLY:HH23  | 1:M:778:MET:HG2  | 1.55                     | 0.87              |
| 1:A:215:GLN:H    | 1:A:340:ILE:HG12 | 1.06                     | 0.87              |
| 1:G:819:ASN:CB   | 2:H:90:GLY:O     | 2.21                     | 0.87              |
| 1:J:635:GLY:HA2  | 4:W:334:GLU:CG   | 2.03                     | 0.87              |
| 1:P:503:TYR:CE1  | 1:P:711:PHE:CE2  | 2.62                     | 0.87              |
| 1:J:756:THR:HG21 | 1:J:776:GLU:CA   | 2.00                     | 0.87              |
| 1:G:755:HIS:HA   | 1:G:758:TYR:CE1  | 2.10                     | 0.87              |
| 1:D:813:ILE:HG21 | 2:E:128:PHE:HE1  | 1.38                     | 0.87              |
| 1:J:821:ARG:HH21 | 2:K:127:ARG:HG2  | 1.04                     | 0.87              |
| 1:P:636:LYS:H    | 4:0:334:GLU:CD   | 1.78                     | 0.87              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:CD1  | 2.58                     | 0.87              |
| 1:P:785:GLU:C    | 1:P:786:ILE:CA   | 2.42                     | 0.87              |
| 1:M:793:ARG:NH1  | 3:O:40:ASN:HD21  | 1.64                     | 0.87              |
| 1:M:800:ARG:HB3  | 3:O:149:VAL:HG22 | 1.55                     | 0.87              |
| 1:D:85:TYR:HH    | 1:D:772:LEU:CD2  | 1.81                     | 0.87              |
| 1:D:642:LYS:HG2  | 4:9:22:ALA:CA    | 2.04                     | 0.87              |
| 1:M:646:PHE:CD2  | 1:M:652:LEU:HD11 | 2.09                     | 0.87              |
| 1:D:649:VAL:CG1  | 1:D:649:VAL:CA   | 2.53                     | 0.87              |
| 1:J:756:THR:CG2  | 1:J:776:GLU:HA   | 2.02                     | 0.87              |
| 1:A:800:ARG:O    | 3:C:149:VAL:CG2  | 2.23                     | 0.87              |
| 4:1:324:THR:HG23 | 4:3:244:ASP:HA   | 1.55                     | 0.87              |
| 3:L:139:TYR:HA   | 3:L:142:PHE:HB3  | 1.56                     | 0.87              |
| 3:F:139:TYR:HA   | 3:F:142:PHE:HB3  | 1.56                     | 0.87              |
| 1:D:795:ARG:HD2  | 3:F:35:ARG:HH12  | 1.37                     | 0.87              |
| 2:N:137:TRP:HA   | 2:N:145:ALA:CB   | 2.04                     | 0.87              |
| 1:G:503:TYR:CZ   | 1:G:711:PHE:CE2  | 2.62                     | 0.87              |
| 1:M:641:LYS:HD2  | 4:Z:348:SER:CB   | 2.02                     | 0.87              |
| 1:G:649:VAL:CA   | 1:G:649:VAL:CG1  | 2.53                     | 0.87              |
| 1:G:649:VAL:CG2  | 1:G:649:VAL:HG13 | 2.02                     | 0.87              |
| 1:A:649:VAL:CA   | 1:A:649:VAL:CG1  | 2.53                     | 0.87              |
| 4:9:322:PRO:HB2  | 4:W:244:ASP:CG   | 1.94                     | 0.87              |
| 4:8:322:PRO:HB2  | 4:V:244:ASP:CG   | 1.94                     | 0.87              |
| 1:P:72:VAL:CG1   | 1:P:76:GLN:HB3   | 2.05                     | 0.87              |
| 4:1:324:THR:CG2  | 4:3:244:ASP:HA   | 2.05                     | 0.87              |
| 1:J:797:PHE:CD1  | 3:L:146:ILE:HG22 | 2.08                     | 0.87              |
| 1:G:792:ALA:CA   | 3:I:42:THR:HA    | 2.04                     | 0.87              |
| 1:G:534:SER:O    | 4:V:351:THR:HG23 | 1.12                     | 0.87              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:CD   | 2.05                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:817:GLN:CG   | 2:K:127:ARG:CD   | 2.50                     | 0.87              |
| 1:J:818:TYR:HE1  | 2:K:127:ARG:NH2  | 1.65                     | 0.87              |
| 1:P:538:GLU:N    | 4:0:349:LEU:HD12 | 1.86                     | 0.87              |
| 1:P:786:ILE:CB   | 1:P:787:ILE:N    | 2.37                     | 0.87              |
| 1:P:797:PHE:CE1  | 3:R:149:VAL:CG1  | 2.58                     | 0.87              |
| 1:G:641:LYS:HD2  | 4:V:348:SER:CB   | 2.03                     | 0.87              |
| 1:G:567:LYS:HZ3  | 4:X:92:ASN:ND2   | 1.73                     | 0.87              |
| 1:G:72:VAL:CG1   | 1:G:76:GLN:HB3   | 2.05                     | 0.87              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:CB   | 2.46                     | 0.87              |
| 1:M:636:LYS:H    | 4:Z:334:GLU:CD   | 1.78                     | 0.87              |
| 1:J:636:LYS:H    | 4:W:334:GLU:CD   | 1.78                     | 0.87              |
| 4:7:322:PRO:HB2  | 4:9:244:ASP:CG   | 1.94                     | 0.87              |
| 1:P:755:HIS:HA   | 1:P:758:TYR:CE1  | 2.10                     | 0.87              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:C    | 2.12                     | 0.87              |
| 1:P:635:GLY:HA2  | 4:0:334:GLU:CG   | 2.03                     | 0.87              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:HB   | 1.73                     | 0.87              |
| 4:X:286:ASP:CG   | 4:Z:202:THR:HB   | 1.93                     | 0.87              |
| 1:A:28:GLN:HE22  | 1:A:723:ARG:HH21 | 0.89                     | 0.87              |
| 1:J:799:MET:SD   | 3:L:32:ASP:CB    | 2.63                     | 0.87              |
| 1:M:649:VAL:CA   | 1:M:649:VAL:CG1  | 2.53                     | 0.86              |
| 1:P:649:VAL:CG1  | 1:P:649:VAL:CA   | 2.53                     | 0.86              |
| 1:J:649:VAL:CA   | 1:J:649:VAL:CG1  | 2.53                     | 0.86              |
| 1:G:636:LYS:H    | 4:V:334:GLU:CD   | 1.78                     | 0.86              |
| 1:P:534:SER:O    | 4:0:351:THR:HG23 | 1.13                     | 0.86              |
| 1:J:838:ILE:HD11 | 2:K:54:MET:HE1   | 0.89                     | 0.86              |
| 1:D:712:PRO:HB2  | 1:D:771:LEU:HB3  | 1.55                     | 0.86              |
| 1:J:755:HIS:HA   | 1:J:758:TYR:CE1  | 2.10                     | 0.86              |
| 2:N:149:ASP:CG   | 2:N:150:TYR:H    | 1.73                     | 0.86              |
| 4:W:286:ASP:CG   | 4:Y:203:THR:HG22 | 1.96                     | 0.86              |
| 1:D:755:HIS:HA   | 1:D:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:G:752:ASP:C    | 1:G:780:ASP:OD1  | 2.12                     | 0.86              |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:CD2  | 2.04                     | 0.86              |
| 1:A:508:ILE:HD11 | 1:A:759:ALA:CA   | 2.05                     | 0.86              |
| 1:A:757:GLN:CB   | 1:A:771:LEU:CG   | 2.33                     | 0.86              |
| 1:G:646:PHE:CD2  | 1:G:652:LEU:HD11 | 2.09                     | 0.86              |
| 4:1:287:ILE:HB   | 4:3:203:THR:CG2  | 2.04                     | 0.86              |
| 1:P:783:LEU:HG   | 1:P:786:ILE:HD11 | 0.90                     | 0.86              |
| 1:D:636:LYS:H    | 4:9:334:GLU:CD   | 1.77                     | 0.86              |
| 1:G:148:ARG:NH2  | 1:G:764:MLY:HH11 | 1.88                     | 0.86              |
| 1:P:641:LYS:CD   | 1:P:647:GLN:OE1  | 2.18                     | 0.86              |
| 1:G:97:LEU:HD22  | 1:G:712:PRO:HB3  | 1.57                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:646:PHE:CE2  | 1:M:652:LEU:CD1  | 2.58                     | 0.86              |
| 1:A:649:VAL:HG13 | 1:A:649:VAL:CG2  | 2.02                     | 0.86              |
| 1:D:800:ARG:O    | 3:F:149:VAL:CG2  | 2.22                     | 0.86              |
| 4:1:322:PRO:CB   | 4:3:244:ASP:HB3  | 2.04                     | 0.86              |
| 1:M:799:MET:SD   | 3:O:32:ASP:HB3   | 2.15                     | 0.86              |
| 1:G:542:PHE:HA   | 4:V:143:TYR:HE1  | 1.34                     | 0.86              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:CD   | 2.37                     | 0.86              |
| 1:J:641:LYS:CD   | 1:J:647:GLN:OE1  | 2.18                     | 0.86              |
| 1:D:646:PHE:CD2  | 1:D:652:LEU:HD11 | 2.09                     | 0.86              |
| 4:8:287:ILE:CG2  | 4:V:205:GLU:HG2  | 2.05                     | 0.86              |
| 1:J:310:TYR:CZ   | 1:J:320:ILE:HD11 | 2.11                     | 0.86              |
| 1:J:791:GLN:NE2  | 3:L:115:GLY:HA3  | 1.90                     | 0.86              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:NH2   | 1.90                     | 0.86              |
| 1:A:505:MLY:CG   | 1:A:741:LYS:HZ2  | 1.86                     | 0.86              |
| 1:P:730:SER:N    | 3:R:93:VAL:HG23  | 1.86                     | 0.86              |
| 1:G:725:ARG:CZ   | 1:G:733:PRO:HB3  | 2.06                     | 0.86              |
| 1:A:530:MET:HG2  | 4:8:354:GLN:CG   | 2.05                     | 0.86              |
| 1:A:636:LYS:H    | 4:8:334:GLU:CD   | 1.77                     | 0.86              |
| 1:D:769:ALA:N    | 1:D:771:LEU:HD12 | 1.90                     | 0.86              |
| 1:P:831:TRP:HZ3  | 2:Q:34:ILE:HD13  | 1.40                     | 0.86              |
| 1:J:557:GLU:HA   | 4:Y:48:GLY:N     | 1.90                     | 0.86              |
| 4:X:324:THR:HG23 | 4:Z:247:VAL:HG22 | 1.57                     | 0.86              |
| 1:J:756:THR:CA   | 1:J:776:GLU:OE1  | 2.23                     | 0.86              |
| 1:G:215:GLN:H    | 1:G:340:ILE:HG12 | 1.06                     | 0.86              |
| 1:D:72:VAL:CG1   | 1:D:76:GLN:HB3   | 2.05                     | 0.86              |
| 1:D:310:TYR:CZ   | 1:D:320:ILE:HD11 | 2.11                     | 0.86              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:CB   | 2.06                     | 0.86              |
| 1:D:530:MET:HG2  | 4:9:354:GLN:CG   | 2.05                     | 0.86              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:CB   | 2.06                     | 0.86              |
| 1:A:797:PHE:HE1  | 3:C:146:ILE:HA   | 1.04                     | 0.86              |
| 1:J:72:VAL:CG1   | 1:J:76:GLN:HB3   | 2.05                     | 0.86              |
| 2:K:149:ASP:CG   | 2:K:150:TYR:H    | 1.73                     | 0.86              |
| 3:C:139:TYR:HA   | 3:C:142:PHE:HB3  | 1.56                     | 0.86              |
| 1:G:530:MET:HG2  | 4:V:354:GLN:CG   | 2.05                     | 0.86              |
| 1:P:530:MET:HG2  | 4:0:354:GLN:CG   | 2.06                     | 0.86              |
| 1:A:538:GLU:OE2  | 4:8:355:MET:HE3  | 1.73                     | 0.86              |
| 1:D:708:ARG:C    | 1:D:710:GLY:N    | 2.29                     | 0.86              |
| 3:O:139:TYR:HA   | 3:O:142:PHE:HB3  | 1.56                     | 0.86              |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CD1  | 2.10                     | 0.86              |
| 1:G:819:ASN:HA   | 2:H:90:GLY:C     | 1.96                     | 0.86              |
| 2:K:137:TRP:HA   | 2:K:145:ALA:CB   | 2.04                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:117:LEU:CG   | 2:B:147:ASN:CG   | 2.44                     | 0.86              |
| 1:J:530:MET:HG2  | 4:W:354:GLN:CG   | 2.06                     | 0.86              |
| 1:A:795:ARG:HG2  | 3:C:118:MET:CE   | 2.06                     | 0.86              |
| 1:A:542:PHE:HA   | 4:8:143:TYR:HE1  | 1.34                     | 0.86              |
| 1:D:831:TRP:CH2  | 2:E:47:LEU:HA    | 2.11                     | 0.86              |
| 1:M:310:TYR:CZ   | 1:M:320:ILE:HD11 | 2.11                     | 0.86              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:CG   | 2.59                     | 0.86              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:CG   | 2.44                     | 0.86              |
| 1:J:725:ARG:CZ   | 1:J:733:PRO:HB3  | 2.06                     | 0.86              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:HB2  | 1.58                     | 0.86              |
| 1:J:818:TYR:CE1  | 2:K:127:ARG:CZ   | 2.58                     | 0.86              |
| 1:P:538:GLU:OE2  | 4:0:355:MET:HE3  | 1.74                     | 0.86              |
| 1:M:538:GLU:N    | 4:Z:351:THR:N    | 2.24                     | 0.86              |
| 1:M:206:LYS:HD3  | 1:M:217:THR:CB   | 2.06                     | 0.86              |
| 1:M:93:MET:HE1   | 1:M:764:MLY:CD   | 2.05                     | 0.86              |
| 1:M:72:VAL:CG1   | 1:M:76:GLN:HB3   | 2.05                     | 0.86              |
| 1:A:755:HIS:HA   | 1:A:758:TYR:CE1  | 2.10                     | 0.86              |
| 1:M:820:VAL:HG11 | 2:N:136:MET:HE3  | 1.57                     | 0.85              |
| 1:J:410:ASN:OD1  | 4:W:334:GLU:CA   | 2.24                     | 0.85              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:HB2  | 2.11                     | 0.85              |
| 1:J:505:MLY:HD2  | 1:J:762:HIS:HE1  | 1.36                     | 0.85              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:CA   | 2.24                     | 0.85              |
| 1:G:752:ASP:OD2  | 1:G:780:ASP:O    | 1.94                     | 0.85              |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:HB2  | 1.57                     | 0.85              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:CB   | 2.06                     | 0.85              |
| 1:M:530:MET:HG2  | 4:Z:354:GLN:CG   | 2.06                     | 0.85              |
| 1:A:538:GLU:N    | 4:8:351:THR:N    | 2.24                     | 0.85              |
| 1:M:755:HIS:HA   | 1:M:758:TYR:CE1  | 2.10                     | 0.85              |
| 1:P:646:PHE:CD2  | 1:P:652:LEU:HD11 | 2.10                     | 0.85              |
| 1:P:548:THR:HG22 | 4:2:49:GLN:N     | 1.84                     | 0.85              |
| 1:M:84:MLY:HG2   | 1:M:723:ARG:CD   | 2.05                     | 0.85              |
| 1:G:204:GLU:H    | 1:G:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:D:800:ARG:C    | 3:F:149:VAL:HG21 | 1.97                     | 0.85              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HB2  | 1.57                     | 0.85              |
| 4:2:287:ILE:HD13 | 4:4:203:THR:CB   | 1.97                     | 0.85              |
| 1:M:202:SER:HA   | 1:M:207:LYS:HE2  | 0.85                     | 0.85              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:CA   | 2.25                     | 0.85              |
| 4:1:322:PRO:HB2  | 4:3:244:ASP:HB3  | 1.57                     | 0.85              |
| 2:E:163:ALA:CA   | 2:K:21:GLU:HB3   | 2.06                     | 0.85              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:HA2  | 2.06                     | 0.85              |
| 1:D:797:PHE:HE1  | 3:F:146:ILE:CA   | 1.77                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:410:ASN:OD1  | 4:V:334:GLU:CA   | 2.24                     | 0.85              |
| 1:G:553:MLY:HG3  | 4:X:45:VAL:C     | 1.96                     | 0.85              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:HG11  | 1.58                     | 0.85              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:CB   | 2.06                     | 0.85              |
| 1:P:795:ARG:CB   | 3:R:35:ARG:CZ    | 2.54                     | 0.85              |
| 1:D:641:LYS:HG3  | 1:D:647:GLN:NE2  | 1.58                     | 0.85              |
| 1:A:641:LYS:CD   | 1:A:647:GLN:OE1  | 2.17                     | 0.85              |
| 1:P:204:GLU:H    | 1:P:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:J:630:ALA:C    | 4:W:25:ASP:OD2   | 2.15                     | 0.85              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:CG   | 2.45                     | 0.85              |
| 1:P:410:ASN:OD1  | 4:0:334:GLU:CA   | 2.24                     | 0.85              |
| 1:J:646:PHE:CD2  | 1:J:652:LEU:HD11 | 2.10                     | 0.85              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:CD2  | 2.43                     | 0.85              |
| 4:0:167:GLU:HB3  | 4:2:41:GLN:O     | 1.76                     | 0.85              |
| 1:M:785:GLU:C    | 1:M:786:ILE:CA   | 2.44                     | 0.85              |
| 1:G:310:TYR:CZ   | 1:G:320:ILE:HD11 | 2.11                     | 0.85              |
| 1:P:310:TYR:CZ   | 1:P:320:ILE:HD11 | 2.11                     | 0.85              |
| 1:A:502:GLU:HA   | 1:A:761:GLY:C    | 1.95                     | 0.85              |
| 2:Q:117:LEU:CG   | 2:Q:147:ASN:CG   | 2.44                     | 0.85              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:CD   | 2.55                     | 0.85              |
| 1:M:783:LEU:CB   | 1:M:786:ILE:CD1  | 2.55                     | 0.85              |
| 1:G:503:TYR:CZ   | 1:G:711:PHE:CD2  | 2.65                     | 0.85              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:CA   | 2.25                     | 0.85              |
| 1:D:630:ALA:C    | 4:9:25:ASP:OD2   | 2.15                     | 0.85              |
| 1:D:814:PHE:HA   | 2:E:127:ARG:NH1  | 1.89                     | 0.85              |
| 2:N:117:LEU:CG   | 2:N:147:ASN:CG   | 2.44                     | 0.85              |
| 1:G:538:GLU:N    | 4:V:351:THR:N    | 2.24                     | 0.85              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:CB   | 2.44                     | 0.85              |
| 1:J:640:LYS:CB   | 1:J:645:SER:OG   | 2.25                     | 0.85              |
| 1:P:795:ARG:NH2  | 3:R:116:GLU:HG2  | 1.88                     | 0.85              |
| 1:A:635:GLY:HA2  | 4:8:334:GLU:CG   | 2.03                     | 0.85              |
| 1:M:735:GLY:C    | 1:M:743:ALA:HB2  | 1.82                     | 0.85              |
| 1:D:204:GLU:H    | 1:D:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:G:202:SER:HA   | 1:G:207:LYS:HE2  | 0.85                     | 0.85              |
| 1:A:646:PHE:CD2  | 1:A:652:LEU:HD11 | 2.10                     | 0.85              |
| 1:M:107:MLY:HB3  | 1:M:686:MET:HE2  | 1.59                     | 0.85              |
| 1:A:725:ARG:CZ   | 1:A:733:PRO:HB3  | 2.06                     | 0.85              |
| 1:J:410:ASN:ND2  | 4:W:336:LYS:HG2  | 1.92                     | 0.85              |
| 1:P:206:LYS:HD3  | 1:P:217:THR:CB   | 2.06                     | 0.85              |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:HB2  | 1.57                     | 0.85              |
| 1:A:204:GLU:H    | 1:A:207:LYS:HE3  | 1.42                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:204:GLU:H    | 1:M:207:LYS:HE3  | 1.42                     | 0.85              |
| 1:A:630:ALA:C    | 4:8:25:ASP:OD2   | 2.15                     | 0.85              |
| 1:D:410:ASN:OD1  | 4:9:334:GLU:CA   | 2.24                     | 0.85              |
| 1:A:798:LEU:CD1  | 3:C:126:LEU:CD1  | 2.45                     | 0.85              |
| 1:M:831:TRP:HZ3  | 2:N:34:ILE:HD13  | 1.40                     | 0.85              |
| 1:M:28:GLN:HB2   | 1:M:723:ARG:HH12 | 1.40                     | 0.85              |
| 1:J:505:MLY:CG   | 1:J:762:HIS:CE1  | 2.60                     | 0.85              |
| 1:A:640:LYS:C    | 4:8:23:GLY:O     | 2.15                     | 0.85              |
| 1:M:94:MET:C     | 1:M:713:SER:HB3  | 1.96                     | 0.85              |
| 1:J:800:ARG:NH2  | 3:L:40:ASN:HD21  | 1.75                     | 0.84              |
| 1:D:725:ARG:CD   | 1:D:733:PRO:HB3  | 2.07                     | 0.84              |
| 1:D:735:GLY:C    | 1:D:743:ALA:HB1  | 1.84                     | 0.84              |
| 1:G:795:ARG:HA   | 3:I:118:MET:HE1  | 1.57                     | 0.84              |
| 1:M:410:ASN:ND2  | 4:Z:336:LYS:HG2  | 1.92                     | 0.84              |
| 1:J:529:PRO:CB   | 4:W:353:GLN:OE1  | 2.25                     | 0.84              |
| 4:0:243:PRO:CA   | 4:Y:291:LYS:CE   | 2.52                     | 0.84              |
| 1:M:93:MET:CE    | 1:M:764:MLY:HD3  | 2.07                     | 0.84              |
| 1:D:202:SER:HA   | 1:D:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:M:599:ASN:OD1  | 1:M:649:VAL:HB   | 1.73                     | 0.84              |
| 1:D:418:THR:HB   | 1:D:421:GLU:HG3  | 1.59                     | 0.84              |
| 1:J:795:ARG:CG   | 3:L:35:ARG:HH12  | 1.90                     | 0.84              |
| 4:X:324:THR:HB   | 4:Z:245:GLY:O    | 1.77                     | 0.84              |
| 1:P:725:ARG:CD   | 1:P:733:PRO:HB3  | 2.07                     | 0.84              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:HD13 | 1.34                     | 0.84              |
| 4:0:205:GLU:HG3  | 4:Y:287:ILE:CD1  | 2.07                     | 0.84              |
| 1:A:837:MLY:HH21 | 2:H:20:ASP:HA    | 1.57                     | 0.84              |
| 1:J:202:SER:HA   | 1:J:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:P:599:ASN:OD1  | 1:P:649:VAL:CA   | 2.25                     | 0.84              |
| 1:P:630:ALA:C    | 4:0:25:ASP:OD2   | 2.15                     | 0.84              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:NE   | 1.75                     | 0.84              |
| 1:P:543:PRO:HG3  | 4:0:143:TYR:O    | 1.77                     | 0.84              |
| 1:J:543:PRO:HG3  | 4:W:143:TYR:O    | 1.77                     | 0.84              |
| 1:A:202:SER:HA   | 1:A:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:M:599:ASN:OD1  | 1:M:649:VAL:CA   | 2.25                     | 0.84              |
| 3:I:139:TYR:HA   | 3:I:142:PHE:HB3  | 1.56                     | 0.84              |
| 1:D:508:ILE:CD1  | 1:D:766:PHE:CD1  | 2.59                     | 0.84              |
| 1:D:557:GLU:H    | 4:W:48:GLY:HA3   | 1.28                     | 0.84              |
| 1:M:215:GLN:H    | 1:M:340:ILE:HG12 | 1.05                     | 0.84              |
| 4:9:287:ILE:CG2  | 4:W:205:GLU:HG2  | 2.05                     | 0.84              |
| 1:D:795:ARG:HG2  | 3:F:118:MET:HE1  | 1.58                     | 0.84              |
| 1:G:410:ASN:ND2  | 4:V:336:LYS:HG2  | 1.92                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:84:MLY:CH1   | 1:J:724:TYR:CE2  | 2.43                     | 0.84              |
| 1:J:640:LYS:C    | 4:W:23:GLY:O     | 2.15                     | 0.84              |
| 1:G:90:ASP:OD2   | 1:G:764:MLY:CH1  | 2.26                     | 0.84              |
| 4:W:291:LYS:HD2  | 4:Y:243:PRO:CB   | 2.07                     | 0.84              |
| 4:7:287:ILE:CG2  | 4:9:205:GLU:HG2  | 2.05                     | 0.84              |
| 1:P:418:THR:HB   | 1:P:421:GLU:HG3  | 1.60                     | 0.84              |
| 1:J:418:THR:HB   | 1:J:421:GLU:HG3  | 1.60                     | 0.84              |
| 1:D:727:LEU:CD1  | 1:D:782:MLY:CH1  | 2.50                     | 0.84              |
| 1:G:648:THR:CG2  | 1:G:651:ALA:HB2  | 2.08                     | 0.84              |
| 1:D:813:ILE:HG23 | 2:E:128:PHE:HZ   | 1.37                     | 0.84              |
| 1:J:725:ARG:CD   | 1:J:733:PRO:HB3  | 2.07                     | 0.84              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:CG   | 2.44                     | 0.84              |
| 1:A:813:ILE:HG22 | 2:B:127:ARG:HD3  | 1.60                     | 0.84              |
| 1:M:534:SER:O    | 4:Z:351:THR:HG23 | 1.13                     | 0.84              |
| 1:P:796:GLY:CA   | 3:R:35:ARG:HD3   | 2.05                     | 0.84              |
| 1:M:725:ARG:CZ   | 1:M:733:PRO:HB3  | 2.06                     | 0.84              |
| 1:P:202:SER:HA   | 1:P:207:LYS:HE2  | 0.85                     | 0.84              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:HB   | 1.72                     | 0.84              |
| 1:A:310:TYR:CZ   | 1:A:320:ILE:HD11 | 2.11                     | 0.84              |
| 1:A:502:GLU:HA   | 1:A:762:HIS:H    | 1.42                     | 0.84              |
| 1:M:818:TYR:CZ   | 2:N:127:ARG:NH2  | 2.33                     | 0.84              |
| 1:P:821:ARG:NH2  | 2:Q:127:ARG:CG   | 2.39                     | 0.84              |
| 1:P:538:GLU:N    | 4:O:351:THR:N    | 2.24                     | 0.84              |
| 1:J:84:MLY:CH2   | 1:J:719:ASP:O    | 2.26                     | 0.84              |
| 1:D:529:PRO:CB   | 4:9:353:GLN:OE1  | 2.25                     | 0.84              |
| 1:A:410:ASN:OD1  | 4:8:334:GLU:CA   | 2.24                     | 0.84              |
| 1:P:508:ILE:CD1  | 1:P:759:ALA:CB   | 2.37                     | 0.84              |
| 1:M:640:LYS:CB   | 1:M:645:SER:OG   | 2.25                     | 0.84              |
| 1:D:649:VAL:C    | 1:D:649:VAL:HG12 | 1.98                     | 0.84              |
| 1:J:649:VAL:HG12 | 1:J:649:VAL:C    | 1.98                     | 0.84              |
| 2:E:163:ALA:O    | 2:K:22:THR:N     | 2.09                     | 0.84              |
| 4:9:237:GLU:HA   | 4:9:251:GLY:HA2  | 1.60                     | 0.84              |
| 1:G:635:GLY:HA2  | 4:V:334:GLU:CG   | 2.03                     | 0.84              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:CB   | 2.46                     | 0.84              |
| 1:P:640:LYS:CB   | 1:P:645:SER:OG   | 2.25                     | 0.84              |
| 1:M:410:ASN:OD1  | 4:Z:334:GLU:CA   | 2.24                     | 0.84              |
| 1:D:818:TYR:CG   | 2:E:90:GLY:HA3   | 2.11                     | 0.84              |
| 1:M:84:MLY:CH1   | 1:M:724:TYR:HE2  | 1.89                     | 0.84              |
| 1:J:204:GLU:H    | 1:J:207:LYS:HE3  | 1.42                     | 0.84              |
| 1:D:640:LYS:C    | 4:9:23:GLY:O     | 2.15                     | 0.84              |
| 1:P:599:ASN:OD1  | 1:P:649:VAL:HB   | 1.73                     | 0.84              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:P:769:ALA:O    | 1:P:771:LEU:HB2 | 1.78                     | 0.84              |
| 1:P:829:TRP:CH2  | 2:Q:87:LYS:HE2  | 2.12                     | 0.84              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:HA  | 1.76                     | 0.84              |
| 4:W:237:GLU:HA   | 4:W:251:GLY:HA2 | 1.60                     | 0.84              |
| 4:7:237:GLU:HA   | 4:7:251:GLY:HA2 | 1.60                     | 0.84              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HB2 | 1.57                     | 0.84              |
| 1:P:640:LYS:C    | 4:0:23:GLY:O    | 2.15                     | 0.84              |
| 1:P:629:GLU:CG   | 1:P:643:GLY:O   | 2.26                     | 0.84              |
| 1:M:543:PRO:HG3  | 4:Z:143:TYR:O   | 1.77                     | 0.84              |
| 1:P:791:GLN:OE1  | 3:R:116:GLU:HG3 | 1.76                     | 0.84              |
| 1:D:538:GLU:N    | 4:9:351:THR:N   | 2.24                     | 0.84              |
| 1:A:542:PHE:CA   | 4:8:143:TYR:CE1 | 2.61                     | 0.84              |
| 1:A:543:PRO:HG3  | 4:8:143:TYR:O   | 1.77                     | 0.84              |
| 1:J:641:LYS:HG3  | 1:J:647:GLN:NE2 | 1.58                     | 0.84              |
| 1:M:640:LYS:C    | 4:Z:23:GLY:O    | 2.15                     | 0.84              |
| 1:M:95:THR:OG1   | 1:M:770:GLY:HA2 | 1.77                     | 0.84              |
| 1:J:629:GLU:CG   | 1:J:643:GLY:O   | 2.26                     | 0.84              |
| 1:J:542:PHE:CA   | 4:W:143:TYR:CE1 | 2.61                     | 0.84              |
| 1:P:793:ARG:CD   | 3:R:40:ASN:ND2  | 2.40                     | 0.84              |
| 1:D:410:ASN:ND2  | 4:9:336:LYS:HG2 | 1.92                     | 0.84              |
| 1:A:410:ASN:ND2  | 4:8:336:LYS:HG2 | 1.93                     | 0.84              |
| 1:P:831:TRP:HH2  | 2:Q:47:LEU:HD23 | 1.41                     | 0.84              |
| 4:7:286:ASP:OD1  | 4:9:203:THR:CG2 | 2.26                     | 0.84              |
| 4:0:237:GLU:HA   | 4:0:251:GLY:HA2 | 1.60                     | 0.84              |
| 1:M:821:ARG:HH21 | 2:N:127:ARG:HG2 | 1.38                     | 0.83              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:CD  | 2.56                     | 0.83              |
| 2:K:141:PRO:CB   | 2:K:142:PRO:CD  | 2.56                     | 0.83              |
| 1:P:529:PRO:CB   | 4:0:353:GLN:OE1 | 2.25                     | 0.83              |
| 1:A:648:THR:CG2  | 1:A:651:ALA:HB2 | 2.08                     | 0.83              |
| 1:M:795:ARG:CB   | 3:O:35:ARG:NH2  | 2.37                     | 0.83              |
| 1:G:503:TYR:HE1  | 1:G:711:PHE:CE2 | 1.90                     | 0.83              |
| 1:D:629:GLU:CG   | 1:D:643:GLY:O   | 2.26                     | 0.83              |
| 4:Y:237:GLU:HA   | 4:Y:251:GLY:HA2 | 1.60                     | 0.83              |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:CH1 | 2.05                     | 0.83              |
| 1:A:508:ILE:CD1  | 1:A:759:ALA:HB3 | 2.07                     | 0.83              |
| 1:P:410:ASN:ND2  | 4:0:336:LYS:HG2 | 1.92                     | 0.83              |
| 1:A:725:ARG:CD   | 1:A:733:PRO:HB3 | 2.07                     | 0.83              |
| 1:M:529:PRO:CB   | 4:Z:353:GLN:OE1 | 2.25                     | 0.83              |
| 1:D:640:LYS:CB   | 1:D:645:SER:OG  | 2.25                     | 0.83              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:CA  | 2.25                     | 0.83              |
| 1:J:561:LYS:CE   | 4:Y:48:GLY:HA3  | 2.07                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:727:LEU:N    | 1:D:782:MLY:HE2  | 1.93                     | 0.83              |
| 1:D:730:SER:O    | 1:D:734:GLU:HG3  | 1.78                     | 0.83              |
| 1:D:791:GLN:CD   | 3:F:116:GLU:N    | 2.20                     | 0.83              |
| 2:B:111:SER:OG   | 2:B:148:VAL:C    | 2.15                     | 0.83              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HB2  | 1.58                     | 0.83              |
| 1:P:795:ARG:HH21 | 3:R:116:GLU:HB3  | 0.69                     | 0.83              |
| 1:D:648:THR:CG2  | 1:D:651:ALA:HB2  | 2.08                     | 0.83              |
| 1:G:725:ARG:CD   | 1:G:733:PRO:HB3  | 2.07                     | 0.83              |
| 1:A:798:LEU:HD12 | 3:C:126:LEU:HD21 | 1.60                     | 0.83              |
| 4:O:202:THR:OG1  | 4:Y:287:ILE:N    | 2.11                     | 0.83              |
| 1:J:797:PHE:HD1  | 3:L:146:ILE:HG23 | 1.31                     | 0.83              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:CE1  | 2.12                     | 0.83              |
| 1:G:529:PRO:CB   | 4:V:353:GLN:OE1  | 2.25                     | 0.83              |
| 2:Q:121:LEU:CA   | 2:Q:128:PHE:CB   | 2.46                     | 0.83              |
| 1:P:729:ALA:HB3  | 3:R:93:VAL:HG23  | 1.60                     | 0.83              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HB2  | 1.82                     | 0.83              |
| 1:P:648:THR:CG2  | 1:P:651:ALA:HB2  | 2.08                     | 0.83              |
| 1:M:635:GLY:HA2  | 4:Z:334:GLU:CG   | 2.03                     | 0.83              |
| 1:A:549:SER:O    | 4:V:46:GLY:HA3   | 1.77                     | 0.83              |
| 1:A:557:GLU:H    | 4:V:48:GLY:HA3   | 1.28                     | 0.83              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CD1  | 2.58                     | 0.83              |
| 4:1:244:ASP:OD2  | 4:Z:322:PRO:HB3  | 1.78                     | 0.83              |
| 1:G:94:MET:C     | 1:G:713:SER:HB3  | 1.99                     | 0.83              |
| 4:W:286:ASP:OD1  | 4:Y:203:THR:N    | 2.11                     | 0.83              |
| 4:2:237:GLU:HA   | 4:2:251:GLY:HA2  | 1.60                     | 0.83              |
| 1:G:640:LYS:C    | 4:V:23:GLY:O     | 2.16                     | 0.83              |
| 1:A:553:MLY:HG2  | 4:V:47:MET:H     | 1.44                     | 0.83              |
| 4:O:287:ILE:HG22 | 4:2:203:THR:HG22 | 1.60                     | 0.83              |
| 1:P:805:ALA:CA   | 1:P:808:GLU:HB2  | 2.03                     | 0.83              |
| 1:J:829:TRP:CH2  | 2:K:87:LYS:NZ    | 2.46                     | 0.83              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:CB   | 2.55                     | 0.83              |
| 1:D:279:LEU:HB2  | 1:D:282:GLU:HG3  | 1.60                     | 0.83              |
| 1:M:418:THR:HB   | 1:M:421:GLU:HG3  | 1.59                     | 0.83              |
| 1:M:798:LEU:CG   | 3:O:126:LEU:HD11 | 1.88                     | 0.83              |
| 1:M:797:PHE:CE2  | 3:O:146:ILE:CD1  | 2.60                     | 0.83              |
| 1:G:97:LEU:HD22  | 1:G:712:PRO:CB   | 2.06                     | 0.83              |
| 1:G:640:LYS:CB   | 1:G:645:SER:OG   | 2.25                     | 0.83              |
| 1:J:730:SER:O    | 1:J:734:GLU:HG3  | 1.79                     | 0.83              |
| 2:H:141:PRO:CB   | 2:H:142:PRO:CD   | 2.56                     | 0.83              |
| 1:J:84:MLY:CH1   | 1:J:720:PHE:CE1  | 2.55                     | 0.83              |
| 1:M:553:MLY:HG3  | 4:1:43:VAL:HG21  | 1.60                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:792:ALA:HB2  | 3:R:42:THR:CB    | 2.08                     | 0.83              |
| 1:P:797:PHE:CE1  | 3:R:146:ILE:C    | 2.52                     | 0.83              |
| 1:D:549:SER:O    | 4:W:46:GLY:HA3   | 1.77                     | 0.83              |
| 1:A:529:PRO:CB   | 4:8:353:GLN:OE1  | 2.25                     | 0.83              |
| 1:M:783:LEU:HG   | 1:M:786:ILE:HD12 | 0.83                     | 0.83              |
| 1:G:84:MLY:HB3   | 1:G:723:ARG:NE   | 1.93                     | 0.83              |
| 4:X:291:LYS:HE3  | 4:Z:243:PRO:CB   | 2.09                     | 0.83              |
| 1:A:629:GLU:CG   | 1:A:643:GLY:O    | 2.26                     | 0.83              |
| 1:M:630:ALA:C    | 4:Z:25:ASP:OD2   | 2.15                     | 0.83              |
| 1:J:279:LEU:HB2  | 1:J:282:GLU:HG3  | 1.60                     | 0.83              |
| 4:3:237:GLU:HA   | 4:3:251:GLY:HA2  | 1.60                     | 0.83              |
| 4:5:237:GLU:HA   | 4:5:251:GLY:HA2  | 1.60                     | 0.83              |
| 2:Q:141:PRO:CB   | 2:Q:142:PRO:CD   | 2.56                     | 0.83              |
| 1:J:218:LEU:HB3  | 1:J:221:GLN:HG3  | 1.61                     | 0.83              |
| 1:M:542:PHE:CA   | 4:Z:143:TYR:CE1  | 2.61                     | 0.83              |
| 1:J:538:GLU:N    | 4:W:351:THR:N    | 2.24                     | 0.83              |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:HD13 | 1.60                     | 0.83              |
| 4:3:287:ILE:CD1  | 4:5:203:THR:HB   | 2.06                     | 0.83              |
| 1:J:756:THR:CG2  | 1:J:776:GLU:OE1  | 2.27                     | 0.83              |
| 4:9:286:ASP:OD1  | 4:W:203:THR:CG2  | 2.26                     | 0.83              |
| 4:3:322:PRO:HB3  | 4:5:244:ASP:OD2  | 1.78                     | 0.83              |
| 1:G:542:PHE:CA   | 4:V:143:TYR:CE1  | 2.61                     | 0.83              |
| 1:P:646:PHE:CE2  | 1:P:652:LEU:CD1  | 2.58                     | 0.83              |
| 1:J:641:LYS:HG2  | 1:J:647:GLN:HG3  | 1.61                     | 0.83              |
| 1:P:641:LYS:HG2  | 1:P:647:GLN:HG3  | 1.61                     | 0.83              |
| 1:D:726:VAL:O    | 1:D:785:GLU:HG2  | 1.78                     | 0.83              |
| 1:M:34:ALA:HB3   | 1:M:777:GLU:CG   | 2.08                     | 0.83              |
| 1:G:769:ALA:CB   | 1:G:770:GLY:N    | 2.42                     | 0.83              |
| 1:M:556:ASP:H    | 4:1:49:GLN:N     | 1.72                     | 0.83              |
| 1:G:418:THR:HB   | 1:G:421:GLU:HG3  | 1.59                     | 0.83              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD13 | 0.91                     | 0.83              |
| 1:G:792:ALA:CB   | 3:I:42:THR:HG23  | 2.09                     | 0.83              |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:CD1  | 2.09                     | 0.83              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:CD   | 2.09                     | 0.83              |
| 1:P:542:PHE:CA   | 4:0:143:TYR:HE1  | 1.92                     | 0.83              |
| 1:D:542:PHE:CA   | 4:9:143:TYR:CE1  | 2.61                     | 0.83              |
| 1:D:553:MLY:HG2  | 4:W:47:MET:H     | 1.44                     | 0.83              |
| 1:P:218:LEU:HA   | 1:P:221:GLN:HG2  | 1.61                     | 0.83              |
| 1:D:747:LEU:CD1  | 1:D:782:MLY:CH2  | 2.42                     | 0.82              |
| 2:N:141:PRO:CB   | 2:N:142:PRO:CD   | 2.56                     | 0.82              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:HD13 | 1.34                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:542:PHE:CA   | 4:W:143:TYR:HE1  | 1.92                     | 0.82              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:HB2  | 1.57                     | 0.82              |
| 1:D:819:ASN:N    | 2:E:90:GLY:O     | 2.11                     | 0.82              |
| 1:M:836:PHE:CE2  | 2:N:160:GLY:HA3  | 2.14                     | 0.82              |
| 1:D:641:LYS:HG2  | 1:D:647:GLN:HG3  | 1.60                     | 0.82              |
| 1:M:730:SER:O    | 1:M:734:GLU:HG3  | 1.79                     | 0.82              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:HE1   | 1.90                     | 0.82              |
| 4:4:237:GLU:HA   | 4:4:251:GLY:HA2  | 1.60                     | 0.82              |
| 1:P:279:LEU:HB2  | 1:P:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:J:783:LEU:O    | 1:J:787:ILE:HB   | 1.78                     | 0.82              |
| 1:A:501:GLU:CG   | 1:A:762:HIS:CE1  | 2.59                     | 0.82              |
| 1:G:538:GLU:OE2  | 4:V:355:MET:HE3  | 1.78                     | 0.82              |
| 1:M:732:ILE:CG2  | 1:M:747:LEU:HD13 | 1.34                     | 0.82              |
| 1:D:799:MET:SD   | 3:F:32:ASP:CA    | 2.66                     | 0.82              |
| 1:A:809:ARG:NH1  | 2:B:124:GLY:HA2  | 1.94                     | 0.82              |
| 1:P:730:SER:O    | 1:P:734:GLU:HG3  | 1.79                     | 0.82              |
| 2:K:121:LEU:CG   | 2:K:128:PHE:CA   | 2.48                     | 0.82              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:HG2  | 1.62                     | 0.82              |
| 1:J:648:THR:CG2  | 1:J:651:ALA:HB2  | 2.08                     | 0.82              |
| 1:M:786:ILE:O    | 1:M:790:THR:N    | 2.12                     | 0.82              |
| 1:M:641:LYS:HD2  | 4:Z:348:SER:CA   | 2.09                     | 0.82              |
| 4:8:290:ARG:NH1  | 4:V:202:THR:HG21 | 1.94                     | 0.82              |
| 1:D:800:ARG:CD   | 3:F:149:VAL:C    | 2.48                     | 0.82              |
| 1:A:418:THR:HB   | 1:A:421:GLU:HG3  | 1.59                     | 0.82              |
| 1:G:279:LEU:HB2  | 1:G:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:A:279:LEU:HB2  | 1:A:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:D:725:ARG:CZ   | 1:D:733:PRO:HB3  | 2.06                     | 0.82              |
| 1:D:795:ARG:NE   | 3:F:43:ASN:OD1   | 2.11                     | 0.82              |
| 1:G:754:ASP:N    | 1:G:779:ARG:CD   | 2.36                     | 0.82              |
| 1:G:643:GLY:N    | 4:V:24:ASP:HA    | 1.94                     | 0.82              |
| 1:J:817:GLN:CB   | 2:K:127:ARG:HD2  | 2.08                     | 0.82              |
| 1:M:795:ARG:HG3  | 3:O:118:MET:HE3  | 1.61                     | 0.82              |
| 1:M:725:ARG:CD   | 1:M:733:PRO:HB3  | 2.08                     | 0.82              |
| 4:W:325:MET:HE1  | 4:Y:244:ASP:CG   | 1.99                     | 0.82              |
| 1:P:127:ASN:HD22 | 1:P:128:PRO:HD2  | 1.44                     | 0.82              |
| 2:N:121:LEU:CG   | 2:N:128:PHE:CA   | 2.49                     | 0.82              |
| 1:G:629:GLU:CG   | 1:G:643:GLY:O    | 2.26                     | 0.82              |
| 1:P:819:ASN:OD1  | 2:Q:91:ALA:C     | 2.18                     | 0.82              |
| 2:B:121:LEU:CG   | 2:B:128:PHE:CA   | 2.48                     | 0.82              |
| 1:M:639:GLY:CA   | 4:Z:344:SER:C    | 2.48                     | 0.82              |
| 1:M:648:THR:CG2  | 1:M:651:ALA:HB2  | 2.08                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:543:PRO:HG3  | 4:9:143:TYR:O    | 1.78                     | 0.82              |
| 1:A:830:PRO:CB   | 2:B:51:PHE:CE1   | 2.61                     | 0.82              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:G:530:MET:HE1  | 4:V:355:MET:SD   | 2.19                     | 0.82              |
| 4:1:287:ILE:HG21 | 4:3:204:ALA:H    | 1.42                     | 0.82              |
| 1:P:639:GLY:CA   | 4:0:344:SER:C    | 2.48                     | 0.82              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:P:798:LEU:HD11 | 3:R:126:LEU:HD22 | 1.61                     | 0.82              |
| 1:A:578:HIS:HB3  | 1:A:592:ILE:HD12 | 1.62                     | 0.82              |
| 1:D:713:SER:CB   | 1:D:775:LEU:HD22 | 2.08                     | 0.82              |
| 1:D:800:ARG:NH2  | 3:F:40:ASN:CG    | 2.32                     | 0.82              |
| 1:A:709:LYS:O    | 1:A:710:GLY:HA3  | 1.80                     | 0.82              |
| 1:A:149:GLN:HE21 | 1:A:718:ALA:HB3  | 1.27                     | 0.82              |
| 1:A:757:GLN:CA   | 1:A:771:LEU:HD11 | 2.10                     | 0.82              |
| 1:G:543:PRO:HG3  | 4:V:143:TYR:O    | 1.78                     | 0.82              |
| 1:P:725:ARG:CZ   | 1:P:733:PRO:HB3  | 2.06                     | 0.82              |
| 1:P:734:GLU:O    | 1:P:738:MET:CG   | 2.28                     | 0.82              |
| 1:G:813:ILE:HG21 | 2:H:128:PHE:CE1  | 2.12                     | 0.82              |
| 2:B:141:PRO:CB   | 2:B:142:PRO:CD   | 2.56                     | 0.82              |
| 1:A:730:SER:O    | 1:A:734:GLU:HG3  | 1.78                     | 0.82              |
| 1:P:218:LEU:CA   | 1:P:221:GLN:HG2  | 2.10                     | 0.82              |
| 1:G:84:MLY:HH21  | 1:G:720:PHE:HA   | 1.58                     | 0.82              |
| 1:A:641:LYS:HG2  | 1:A:647:GLN:HG3  | 1.60                     | 0.82              |
| 1:M:629:GLU:CG   | 1:M:643:GLY:O    | 2.26                     | 0.82              |
| 1:J:754:ASP:C    | 1:J:780:ASP:OD2  | 2.17                     | 0.82              |
| 1:J:754:ASP:CG   | 1:J:780:ASP:OD2  | 2.03                     | 0.82              |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:HD2  | 1.44                     | 0.82              |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:HD2  | 1.45                     | 0.82              |
| 1:M:279:LEU:HB2  | 1:M:282:GLU:HG3  | 1.60                     | 0.82              |
| 1:D:727:LEU:CB   | 1:D:782:MLY:HE2  | 2.10                     | 0.82              |
| 1:P:736:GLN:HA   | 1:P:743:ALA:HB2  | 1.51                     | 0.82              |
| 1:G:817:GLN:CD   | 2:H:127:ARG:CG   | 2.48                     | 0.82              |
| 1:G:813:ILE:HG23 | 2:H:128:PHE:HZ   | 1.36                     | 0.82              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:M:795:ARG:CD   | 3:O:118:MET:HE1  | 2.09                     | 0.82              |
| 1:M:734:GLU:O    | 1:M:738:MET:CG   | 2.28                     | 0.82              |
| 4:8:286:ASP:OD1  | 4:V:203:THR:CG2  | 2.26                     | 0.82              |
| 4:7:290:ARG:NH1  | 4:9:202:THR:HG21 | 1.95                     | 0.82              |
| 1:G:578:HIS:HB3  | 1:G:592:ILE:HD12 | 1.62                     | 0.82              |
| 1:J:769:ALA:CB   | 1:J:770:GLY:CA   | 2.57                     | 0.82              |
| 1:J:792:ALA:H    | 3:L:42:THR:HG22  | 1.44                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:817:GLN:CD   | 2:Q:127:ARG:CD   | 2.39                     | 0.82              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:CG1  | 2.10                     | 0.82              |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:CD1  | 2.10                     | 0.82              |
| 1:J:643:GLY:N    | 4:W:24:ASP:HA    | 1.93                     | 0.82              |
| 1:D:218:LEU:HB3  | 1:D:221:GLN:HG3  | 1.61                     | 0.82              |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:CG1  | 2.10                     | 0.82              |
| 1:G:93:MET:HE2   | 1:G:764:MLY:CD   | 1.87                     | 0.82              |
| 2:Q:144:VAL:HG12 | 2:Q:153:ILE:CD1  | 2.10                     | 0.82              |
| 1:A:795:ARG:CZ   | 3:C:116:GLU:CD   | 2.38                     | 0.82              |
| 1:P:578:HIS:HB3  | 1:P:592:ILE:HD12 | 1.62                     | 0.82              |
| 1:P:218:LEU:HB3  | 1:P:221:GLN:HG3  | 1.61                     | 0.82              |
| 1:P:806:MET:CA   | 1:P:807:VAL:N    | 2.43                     | 0.82              |
| 1:J:829:TRP:CH2  | 2:K:84:PHE:CD1   | 2.67                     | 0.82              |
| 1:P:829:TRP:HZ3  | 2:Q:84:PHE:CZ    | 1.98                     | 0.82              |
| 4:8:237:GLU:HA   | 4:8:251:GLY:HA2  | 1.60                     | 0.82              |
| 1:G:557:GLU:HB2  | 4:X:46:GLY:C     | 2.00                     | 0.81              |
| 1:P:826:VAL:HG21 | 2:Q:88:LEU:CD2   | 2.10                     | 0.81              |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:CD1  | 2.10                     | 0.81              |
| 1:P:735:GLY:C    | 1:P:743:ALA:HB2  | 1.82                     | 0.81              |
| 1:M:553:MLY:CG   | 4:1:43:VAL:HG11  | 2.09                     | 0.81              |
| 1:M:551:MLY:O    | 4:1:48:GLY:HA3   | 1.80                     | 0.81              |
| 1:D:549:SER:O    | 4:W:46:GLY:C     | 2.18                     | 0.81              |
| 1:G:730:SER:O    | 1:G:734:GLU:HG3  | 1.79                     | 0.81              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CB   | 1.85                     | 0.81              |
| 1:P:548:THR:HG21 | 4:2:48:GLY:C     | 1.99                     | 0.81              |
| 1:P:218:LEU:HD22 | 1:P:222:ILE:CG1  | 2.10                     | 0.81              |
| 1:J:599:ASN:CA   | 1:J:649:VAL:CB   | 2.53                     | 0.81              |
| 1:G:769:ALA:O    | 1:G:773:GLY:CA   | 2.28                     | 0.81              |
| 1:A:800:ARG:C    | 3:C:149:VAL:CG2  | 2.47                     | 0.81              |
| 1:M:571:ALA:O    | 1:M:572:LYS:CG   | 2.28                     | 0.81              |
| 4:V:237:GLU:HA   | 4:V:251:GLY:HA2  | 1.60                     | 0.81              |
| 4:1:237:GLU:HA   | 4:1:251:GLY:HA2  | 1.60                     | 0.81              |
| 1:P:542:PHE:CA   | 4:0:143:TYR:CE1  | 2.61                     | 0.81              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:HG2  | 1.61                     | 0.81              |
| 1:A:549:SER:O    | 4:V:46:GLY:CA    | 2.28                     | 0.81              |
| 1:M:641:LYS:HG2  | 1:M:647:GLN:HG3  | 1.61                     | 0.81              |
| 4:1:203:THR:HB   | 4:Z:287:ILE:CD1  | 2.06                     | 0.81              |
| 1:D:643:GLY:N    | 4:9:24:ASP:HA    | 1.93                     | 0.81              |
| 1:P:820:VAL:HG11 | 2:Q:136:MET:CE   | 2.10                     | 0.81              |
| 1:P:795:ARG:HG2  | 3:R:118:MET:HE1  | 0.82                     | 0.81              |
| 1:D:542:PHE:CA   | 4:9:143:TYR:HE1  | 1.92                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:549:SER:O    | 4:W:46:GLY:CA    | 2.27                     | 0.81              |
| 1:A:830:PRO:HB2  | 2:B:51:PHE:CZ    | 2.14                     | 0.81              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD13 | 0.91                     | 0.81              |
| 1:A:639:GLY:CA   | 4:8:344:SER:C    | 2.48                     | 0.81              |
| 1:M:795:ARG:HG3  | 3:O:118:MET:CE   | 2.10                     | 0.81              |
| 1:M:782:MLY:HE3  | 3:O:86:ASP:OD2   | 1.79                     | 0.81              |
| 1:P:641:LYS:HD2  | 4:0:348:SER:CA   | 2.09                     | 0.81              |
| 1:D:726:VAL:HG11 | 1:D:785:GLU:CB   | 1.97                     | 0.81              |
| 1:D:712:PRO:HD2  | 1:D:771:LEU:HD13 | 1.62                     | 0.81              |
| 1:M:93:MET:CE    | 1:M:764:MLY:CD   | 2.58                     | 0.81              |
| 1:M:643:GLY:N    | 4:Z:24:ASP:HA    | 1.93                     | 0.81              |
| 1:A:643:GLY:N    | 4:8:24:ASP:HA    | 1.93                     | 0.81              |
| 1:A:640:LYS:CB   | 1:A:645:SER:OG   | 2.25                     | 0.81              |
| 1:D:571:ALA:O    | 1:D:572:LYS:CG   | 2.28                     | 0.81              |
| 1:M:829:TRP:HZ3  | 2:N:84:PHE:CZ    | 1.98                     | 0.81              |
| 1:J:578:HIS:HB3  | 1:J:592:ILE:HD12 | 1.61                     | 0.81              |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:HD2  | 1.45                     | 0.81              |
| 1:A:549:SER:O    | 4:V:46:GLY:C     | 2.19                     | 0.81              |
| 4:2:290:ARG:HH21 | 4:4:202:THR:HG23 | 1.41                     | 0.81              |
| 1:G:84:MLY:NZ    | 1:G:724:TYR:CE2  | 2.47                     | 0.81              |
| 1:P:215:GLN:N    | 1:P:340:ILE:CD1  | 2.44                     | 0.81              |
| 1:M:232:PHE:CZ   | 1:M:287:ILE:HD13 | 2.16                     | 0.81              |
| 1:G:232:PHE:CZ   | 1:G:287:ILE:HD13 | 2.16                     | 0.81              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:HD22 | 1.45                     | 0.81              |
| 4:Z:237:GLU:HA   | 4:Z:251:GLY:HA2  | 1.60                     | 0.81              |
| 1:D:727:LEU:CG   | 1:D:782:MLY:CG   | 2.58                     | 0.81              |
| 1:P:795:ARG:HB3  | 3:R:35:ARG:NH1   | 1.88                     | 0.81              |
| 1:D:639:GLY:CA   | 4:9:344:SER:C    | 2.48                     | 0.81              |
| 1:G:641:LYS:HD2  | 4:V:348:SER:CA   | 2.10                     | 0.81              |
| 1:M:831:TRP:HE1  | 2:N:67:MET:CB    | 1.94                     | 0.81              |
| 1:J:826:VAL:CG2  | 2:K:88:LEU:HD21  | 2.08                     | 0.81              |
| 1:G:829:TRP:CH2  | 2:H:87:LYS:HE2   | 2.16                     | 0.81              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:HD22 | 1.45                     | 0.81              |
| 4:X:237:GLU:HA   | 4:X:251:GLY:HA2  | 1.60                     | 0.81              |
| 1:A:107:MLY:HB3  | 1:A:686:MET:HE2  | 1.61                     | 0.81              |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:HD2  | 1.45                     | 0.81              |
| 1:D:734:GLU:O    | 1:D:738:MET:CG   | 2.28                     | 0.81              |
| 1:G:639:GLY:CA   | 4:V:344:SER:C    | 2.48                     | 0.81              |
| 1:J:734:GLU:O    | 1:J:738:MET:CG   | 2.28                     | 0.81              |
| 1:P:643:GLY:N    | 4:0:24:ASP:HA    | 1.93                     | 0.81              |
| 1:P:538:GLU:CA   | 4:0:351:THR:H    | 1.93                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:538:GLU:CA   | 4:9:351:THR:H    | 1.93                     | 0.81              |
| 1:D:550:PHE:CA   | 4:W:46:GLY:CA    | 2.59                     | 0.81              |
| 1:D:641:LYS:HD2  | 4:9:348:SER:CA   | 2.09                     | 0.81              |
| 1:M:506:GLU:OE2  | 1:M:761:GLY:HA2  | 1.80                     | 0.81              |
| 1:A:505:MLY:HE2  | 1:A:762:HIS:CG   | 1.99                     | 0.81              |
| 1:P:735:GLY:C    | 1:P:743:ALA:HB1  | 1.84                     | 0.81              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:CB   | 2.10                     | 0.81              |
| 1:J:639:GLY:CA   | 4:W:344:SER:C    | 2.48                     | 0.81              |
| 1:P:788:THR:O    | 3:R:42:THR:HG21  | 1.81                     | 0.81              |
| 1:A:831:TRP:CZ2  | 2:B:47:LEU:HA    | 2.15                     | 0.81              |
| 4:0:201:VAL:N    | 4:Y:287:ILE:CG1  | 2.07                     | 0.81              |
| 1:J:641:LYS:HD2  | 4:W:348:SER:CA   | 2.09                     | 0.81              |
| 1:G:641:LYS:HG2  | 1:G:647:GLN:HG3  | 1.61                     | 0.81              |
| 1:J:754:ASP:HA   | 1:J:780:ASP:OD2  | 1.80                     | 0.81              |
| 1:P:724:TYR:HE1  | 1:P:776:GLU:CD   | 1.84                     | 0.81              |
| 1:J:831:TRP:HZ3  | 2:K:34:ILE:CD1   | 1.94                     | 0.81              |
| 4:9:223:PHE:HE1  | 4:9:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:P:374:GLN:HG3  | 1:P:375:ALA:N    | 1.96                     | 0.81              |
| 4:W:223:PHE:HE1  | 4:W:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:CB   | 1.84                     | 0.81              |
| 2:B:144:VAL:CA   | 2:B:153:ILE:HD11 | 2.11                     | 0.81              |
| 1:M:538:GLU:CA   | 4:Z:351:THR:H    | 1.93                     | 0.81              |
| 1:D:578:HIS:HD2  | 1:D:591:ASN:HA   | 1.45                     | 0.81              |
| 1:D:557:GLU:N    | 4:W:48:GLY:HA2   | 1.90                     | 0.81              |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:HD12 | 0.81                     | 0.81              |
| 1:A:538:GLU:CA   | 4:8:351:THR:H    | 1.93                     | 0.81              |
| 1:D:838:ILE:CD1  | 2:E:54:MET:CE    | 2.59                     | 0.81              |
| 4:8:223:PHE:HE1  | 4:8:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:A:505:MLY:NZ   | 1:A:762:HIS:C    | 2.22                     | 0.81              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:HD21 | 2.14                     | 0.81              |
| 1:P:732:ILE:CG2  | 1:P:747:LEU:HD13 | 1.34                     | 0.81              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:HG2  | 1.62                     | 0.81              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD13 | 0.91                     | 0.81              |
| 1:G:817:GLN:HE21 | 2:H:127:ARG:HB2  | 1.45                     | 0.81              |
| 2:H:111:SER:OG   | 2:H:148:VAL:C    | 2.15                     | 0.81              |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:CD1  | 2.09                     | 0.81              |
| 1:M:578:HIS:HD2  | 1:M:591:ASN:HA   | 1.45                     | 0.81              |
| 1:M:84:MLY:NZ    | 1:M:724:TYR:CE2  | 2.46                     | 0.81              |
| 1:A:799:MET:SD   | 3:C:32:ASP:HA    | 2.18                     | 0.81              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:HD21 | 2.14                     | 0.81              |
| 4:9:290:ARG:NH1  | 4:W:202:THR:HG21 | 1.95                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:799:MET:SD   | 3:L:32:ASP:CG    | 2.60                     | 0.81              |
| 1:M:127:ASN:HD22 | 1:M:128:PRO:HD2  | 1.45                     | 0.81              |
| 4:7:223:PHE:HE1  | 4:7:255:PHE:HB2  | 1.46                     | 0.81              |
| 1:G:796:GLY:HA2  | 3:I:35:ARG:HD3   | 0.83                     | 0.81              |
| 1:M:409:GLY:N    | 1:M:636:LYS:CG   | 2.44                     | 0.81              |
| 1:A:831:TRP:CZ2  | 2:B:34:ILE:HG23  | 2.15                     | 0.81              |
| 1:D:218:LEU:CA   | 1:D:221:GLN:HG2  | 2.10                     | 0.81              |
| 1:P:836:PHE:CE2  | 2:Q:160:GLY:HA3  | 2.15                     | 0.81              |
| 1:D:712:PRO:HG2  | 1:D:771:LEU:CB   | 2.07                     | 0.81              |
| 1:A:95:THR:HG1   | 1:A:769:ALA:HA   | 0.74                     | 0.81              |
| 1:M:374:GLN:HG3  | 1:M:375:ALA:N    | 1.96                     | 0.81              |
| 1:G:538:GLU:CA   | 4:V:351:THR:H    | 1.92                     | 0.80              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD13 | 0.91                     | 0.80              |
| 1:M:542:PHE:CA   | 4:Z:143:TYR:HE1  | 1.92                     | 0.80              |
| 1:J:538:GLU:CA   | 4:W:351:THR:H    | 1.93                     | 0.80              |
| 1:M:721:LYS:CA   | 1:M:736:GLN:NE2  | 2.43                     | 0.80              |
| 1:A:641:LYS:HD2  | 4:8:348:SER:CA   | 2.10                     | 0.80              |
| 4:V:325:MET:SD   | 4:X:244:ASP:HB3  | 2.19                     | 0.80              |
| 1:M:215:GLN:N    | 1:M:340:ILE:CD1  | 2.44                     | 0.80              |
| 4:3:324:THR:HG21 | 4:5:244:ASP:N    | 1.80                     | 0.80              |
| 1:D:107:MLY:HB3  | 1:D:686:MET:HE2  | 1.63                     | 0.80              |
| 2:N:144:VAL:CA   | 2:N:153:ILE:HD11 | 2.11                     | 0.80              |
| 2:H:121:LEU:CG   | 2:H:128:PHE:CA   | 2.49                     | 0.80              |
| 1:M:578:HIS:HB3  | 1:M:592:ILE:HD12 | 1.62                     | 0.80              |
| 1:A:550:PHE:CA   | 4:V:46:GLY:CA    | 2.59                     | 0.80              |
| 1:M:797:PHE:HE2  | 3:O:126:LEU:HD22 | 1.46                     | 0.80              |
| 1:D:823:PHE:HE1  | 2:E:160:GLY:C    | 1.84                     | 0.80              |
| 1:M:646:PHE:CE2  | 1:M:652:LEU:HD21 | 2.15                     | 0.80              |
| 1:M:599:ASN:CA   | 1:M:649:VAL:CB   | 2.53                     | 0.80              |
| 3:O:49:ILE:N     | 3:O:52:ASN:ND2   | 2.29                     | 0.80              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:CG2  | 2.09                     | 0.80              |
| 1:M:829:TRP:CH2  | 2:N:87:LYS:HE2   | 2.16                     | 0.80              |
| 1:J:578:HIS:HD2  | 1:J:591:ASN:HA   | 1.45                     | 0.80              |
| 1:D:374:GLN:HG3  | 1:D:375:ALA:N    | 1.96                     | 0.80              |
| 1:D:724:TYR:CG   | 1:D:782:MLY:HD3  | 2.17                     | 0.80              |
| 1:A:94:MET:O     | 1:A:713:SER:CB   | 2.29                     | 0.80              |
| 2:K:141:PRO:CB   | 2:K:142:PRO:HD2  | 2.11                     | 0.80              |
| 2:K:144:VAL:CA   | 2:K:153:ILE:HD11 | 2.11                     | 0.80              |
| 1:J:218:LEU:CA   | 1:J:221:GLN:HG2  | 2.10                     | 0.80              |
| 1:M:798:LEU:HD23 | 3:O:122:GLU:HB3  | 1.62                     | 0.80              |
| 1:D:215:GLN:N    | 1:D:340:ILE:CD1  | 2.44                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:215:GLN:N    | 1:J:340:ILE:CD1  | 2.44                     | 0.80              |
| 1:G:571:ALA:O    | 1:G:572:LYS:CG   | 2.28                     | 0.80              |
| 1:D:814:PHE:HA   | 2:E:127:ARG:HH11 | 1.44                     | 0.80              |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:HD22 | 1.45                     | 0.80              |
| 1:A:232:PHE:CZ   | 1:A:287:ILE:HD13 | 2.16                     | 0.80              |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:HD12 | 0.81                     | 0.80              |
| 1:P:571:ALA:O    | 1:P:572:LYS:CG   | 2.28                     | 0.80              |
| 1:J:374:GLN:HG3  | 1:J:375:ALA:N    | 1.96                     | 0.80              |
| 1:P:799:MET:SD   | 3:R:32:ASP:CG    | 2.60                     | 0.80              |
| 1:J:795:ARG:HH21 | 3:L:116:GLU:HG2  | 1.45                     | 0.80              |
| 1:D:747:LEU:CD2  | 1:D:782:MLY:HH11 | 2.10                     | 0.80              |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:HD23 | 1.61                     | 0.80              |
| 1:G:796:GLY:N    | 3:I:35:ARG:NH2   | 2.30                     | 0.80              |
| 1:G:734:GLU:O    | 1:G:738:MET:CG   | 2.28                     | 0.80              |
| 1:P:552:ASN:ND2  | 4:2:49:GLN:CD    | 2.34                     | 0.80              |
| 1:M:93:MET:HE2   | 1:M:764:MLY:HD3  | 1.62                     | 0.80              |
| 4:0:288:ASP:HB2  | 4:2:63:GLY:HA3   | 0.84                     | 0.80              |
| 1:J:756:THR:HG22 | 1:J:776:GLU:CG   | 2.10                     | 0.80              |
| 3:L:49:ILE:N     | 3:L:52:ASN:ND2   | 2.30                     | 0.80              |
| 4:X:223:PHE:HE1  | 4:X:255:PHE:HB2  | 1.46                     | 0.80              |
| 4:2:223:PHE:HE1  | 4:2:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:J:784:ALA:O    | 1:J:788:THR:N    | 2.14                     | 0.80              |
| 1:G:553:MLY:CH1  | 4:X:45:VAL:CG1   | 2.49                     | 0.80              |
| 1:G:538:GLU:HG3  | 4:V:351:THR:C    | 2.02                     | 0.80              |
| 1:G:817:GLN:NE2  | 2:H:127:ARG:CB   | 2.43                     | 0.80              |
| 2:K:141:PRO:HB2  | 2:K:142:PRO:CD   | 2.12                     | 0.80              |
| 1:D:578:HIS:HB3  | 1:D:592:ILE:HD12 | 1.62                     | 0.80              |
| 1:P:232:PHE:CZ   | 1:P:287:ILE:HD13 | 2.16                     | 0.80              |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:CD1  | 2.09                     | 0.80              |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:HD12 | 0.81                     | 0.80              |
| 1:P:641:LYS:HD2  | 1:P:647:GLN:OE1  | 1.81                     | 0.80              |
| 1:A:823:PHE:CE1  | 2:B:160:GLY:CA   | 2.65                     | 0.80              |
| 1:A:215:GLN:N    | 1:A:340:ILE:CD1  | 2.44                     | 0.80              |
| 3:C:49:ILE:N     | 3:C:52:ASN:ND2   | 2.29                     | 0.80              |
| 2:E:163:ALA:O    | 2:K:21:GLU:N     | 2.14                     | 0.80              |
| 1:P:480:ILE:HG22 | 1:P:481:ASN:HD22 | 1.45                     | 0.80              |
| 1:A:506:GLU:CG   | 1:A:760:PHE:O    | 2.25                     | 0.80              |
| 1:A:505:MLY:CG   | 1:A:762:HIS:CD2  | 2.65                     | 0.80              |
| 1:G:542:PHE:CA   | 4:V:143:TYR:HE1  | 1.93                     | 0.80              |
| 1:P:795:ARG:HH22 | 3:R:116:GLU:CG   | 1.95                     | 0.80              |
| 1:G:215:GLN:N    | 1:G:340:ILE:CD1  | 2.44                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:94:MET:O     | 1:G:713:SER:CB   | 2.29                     | 0.80              |
| 1:G:578:HIS:HD2  | 1:G:591:ASN:HA   | 1.44                     | 0.80              |
| 4:5:223:PHE:HE1  | 4:5:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:A:374:GLN:HG3  | 1:A:375:ALA:N    | 1.96                     | 0.80              |
| 1:A:768:MLY:HG2  | 1:A:771:LEU:CD1  | 2.02                     | 0.80              |
| 2:Q:144:VAL:CA   | 2:Q:153:ILE:HD11 | 2.11                     | 0.80              |
| 1:A:734:GLU:O    | 1:A:738:MET:CG   | 2.28                     | 0.80              |
| 1:A:831:TRP:HZ3  | 2:B:34:ILE:HG12  | 1.39                     | 0.80              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:HD13 | 1.34                     | 0.80              |
| 1:A:791:GLN:HE22 | 3:C:115:GLY:HA3  | 1.42                     | 0.80              |
| 1:P:578:HIS:HD2  | 1:P:591:ASN:HA   | 1.45                     | 0.80              |
| 1:D:713:SER:HB2  | 1:D:775:LEU:CD2  | 2.11                     | 0.80              |
| 1:A:823:PHE:CE1  | 2:B:160:GLY:HA2  | 2.16                     | 0.80              |
| 1:J:232:PHE:CZ   | 1:J:287:ILE:HD13 | 2.16                     | 0.80              |
| 1:D:95:THR:O     | 1:D:770:GLY:N    | 2.14                     | 0.80              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:HD22 | 1.45                     | 0.80              |
| 4:0:173:HIS:CD2  | 4:1:268:GLY:HA3  | 2.17                     | 0.80              |
| 4:4:223:PHE:HE1  | 4:4:255:PHE:HB2  | 1.46                     | 0.80              |
| 1:D:724:TYR:HB3  | 1:D:782:MLY:NZ   | 1.97                     | 0.79              |
| 1:G:817:GLN:HG2  | 2:H:127:ARG:HB2  | 1.52                     | 0.79              |
| 2:B:141:PRO:CB   | 2:B:142:PRO:HD2  | 2.12                     | 0.79              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:HG2  | 1.62                     | 0.79              |
| 1:A:578:HIS:HD2  | 1:A:591:ASN:HA   | 1.45                     | 0.79              |
| 1:G:599:ASN:CA   | 1:G:649:VAL:CB   | 2.53                     | 0.79              |
| 1:J:831:TRP:HH2  | 2:K:47:LEU:HD21  | 1.47                     | 0.79              |
| 4:V:223:PHE:HE1  | 4:V:255:PHE:HB2  | 1.46                     | 0.79              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:HD22 | 1.45                     | 0.79              |
| 1:G:374:GLN:HG3  | 1:G:375:ALA:N    | 1.96                     | 0.79              |
| 1:D:232:PHE:CZ   | 1:D:287:ILE:HD13 | 2.16                     | 0.79              |
| 1:A:501:GLU:HA   | 1:A:762:HIS:CE1  | 2.16                     | 0.79              |
| 1:A:93:MET:CE    | 1:A:716:LEU:N    | 2.45                     | 0.79              |
| 2:N:141:PRO:CB   | 2:N:142:PRO:HD2  | 2.12                     | 0.79              |
| 4:1:287:ILE:HG13 | 4:3:202:THR:HA   | 1.64                     | 0.79              |
| 4:1:288:ASP:N    | 4:3:203:THR:CG2  | 2.45                     | 0.79              |
| 1:P:732:ILE:HG22 | 1:P:747:LEU:HD12 | 0.81                     | 0.79              |
| 2:B:141:PRO:HB2  | 2:B:142:PRO:CD   | 2.12                     | 0.79              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CG   | 2.60                     | 0.79              |
| 1:J:756:THR:HG22 | 1:J:776:GLU:OE1  | 1.81                     | 0.79              |
| 3:I:50:LEU:C     | 3:I:53:PRO:HD2   | 2.03                     | 0.79              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:NH1   | 2.33                     | 0.79              |
| 2:Q:141:PRO:CB   | 2:Q:142:PRO:HD2  | 2.11                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:144:VAL:CA   | 2:E:153:ILE:HD11 | 2.11                     | 0.79              |
| 2:H:141:PRO:CB   | 2:H:142:PRO:HD2  | 2.12                     | 0.79              |
| 1:P:797:PHE:HE1  | 3:R:146:ILE:O    | 1.62                     | 0.79              |
| 1:A:795:ARG:NE   | 3:C:116:GLU:OE2  | 2.16                     | 0.79              |
| 1:M:791:GLN:NE2  | 3:O:114:LEU:O    | 2.15                     | 0.79              |
| 1:G:84:MLY:HH11  | 1:G:724:TYR:CE2  | 2.16                     | 0.79              |
| 1:J:756:THR:CG2  | 1:J:776:GLU:CB   | 2.61                     | 0.79              |
| 1:J:571:ALA:O    | 1:J:572:LYS:CG   | 2.28                     | 0.79              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:NE2  | 2.43                     | 0.79              |
| 2:N:141:PRO:HB2  | 2:N:142:PRO:CD   | 2.12                     | 0.79              |
| 2:Q:141:PRO:HB2  | 2:Q:142:PRO:CD   | 2.11                     | 0.79              |
| 2:H:141:PRO:HB2  | 2:H:142:PRO:CD   | 2.11                     | 0.79              |
| 2:K:111:SER:OG   | 2:K:148:VAL:C    | 2.15                     | 0.79              |
| 1:M:553:MLY:HG2  | 4:1:43:VAL:HG21  | 1.61                     | 0.79              |
| 1:M:553:MLY:HG3  | 4:1:43:VAL:HG11  | 1.64                     | 0.79              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:NE2  | 2.43                     | 0.79              |
| 1:A:797:PHE:CD1  | 3:C:146:ILE:CG2  | 2.66                     | 0.79              |
| 3:F:49:ILE:N     | 3:F:52:ASN:ND2   | 2.29                     | 0.79              |
| 3:F:50:LEU:C     | 3:F:53:PRO:HD2   | 2.03                     | 0.79              |
| 1:M:95:THR:CA    | 1:M:713:SER:HB3  | 2.13                     | 0.79              |
| 1:A:571:ALA:O    | 1:A:572:LYS:CG   | 2.28                     | 0.79              |
| 2:E:141:PRO:HB2  | 2:E:142:PRO:CD   | 2.12                     | 0.79              |
| 4:8:287:ILE:HB   | 4:V:204:ALA:N    | 1.97                     | 0.79              |
| 1:G:769:ALA:HB1  | 1:G:770:GLY:HA2  | 1.62                     | 0.79              |
| 3:O:50:LEU:C     | 3:O:53:PRO:HD2   | 2.03                     | 0.79              |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:HD12 | 0.81                     | 0.79              |
| 1:G:796:GLY:HA2  | 3:I:35:ARG:NE    | 1.96                     | 0.79              |
| 2:E:141:PRO:CB   | 2:E:142:PRO:HD2  | 2.12                     | 0.79              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:NE2  | 2.43                     | 0.79              |
| 2:H:144:VAL:CA   | 2:H:153:ILE:HD11 | 2.11                     | 0.79              |
| 1:M:537:GLU:O    | 4:Z:350:SER:N    | 2.16                     | 0.79              |
| 1:J:410:ASN:CG   | 4:W:334:GLU:CA   | 2.47                     | 0.79              |
| 1:A:798:LEU:CD2  | 3:C:126:LEU:HD11 | 2.12                     | 0.79              |
| 1:P:503:TYR:HE1  | 1:P:711:PHE:CD2  | 2.01                     | 0.79              |
| 1:A:800:ARG:NH2  | 3:C:40:ASN:OD1   | 2.16                     | 0.79              |
| 1:G:789:ALA:CB   | 3:I:81:GLN:NE2   | 2.46                     | 0.79              |
| 1:A:174:SER:CB   | 1:A:667:THR:HG21 | 2.13                     | 0.79              |
| 1:A:556:ASP:HA   | 4:V:49:GLN:O     | 1.70                     | 0.79              |
| 4:Y:223:PHE:HE1  | 4:Y:255:PHE:HB2  | 1.46                     | 0.79              |
| 4:0:223:PHE:HE1  | 4:0:255:PHE:HB2  | 1.46                     | 0.79              |
| 1:M:819:ASN:CB   | 2:N:90:GLY:O     | 2.30                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:530:MET:HE1  | 4:W:355:MET:SD   | 2.23                     | 0.79              |
| 1:P:785:GLU:HG3  | 3:R:81:GLN:HG3   | 1.49                     | 0.79              |
| 1:D:550:PHE:HA   | 4:W:46:GLY:HA2   | 1.64                     | 0.79              |
| 1:A:409:GLY:N    | 1:A:636:LYS:CG   | 2.44                     | 0.79              |
| 1:A:550:PHE:N    | 4:V:46:GLY:HA3   | 1.97                     | 0.79              |
| 1:M:641:LYS:HD2  | 4:Z:348:SER:HB2  | 1.54                     | 0.79              |
| 1:A:599:ASN:CA   | 1:A:649:VAL:CB   | 2.53                     | 0.79              |
| 3:I:49:ILE:N     | 3:I:52:ASN:ND2   | 2.29                     | 0.79              |
| 3:L:50:LEU:C     | 3:L:53:PRO:HD2   | 2.03                     | 0.79              |
| 4:3:223:PHE:HE1  | 4:3:255:PHE:HB2  | 1.46                     | 0.79              |
| 1:D:798:LEU:CD1  | 3:F:126:LEU:HD13 | 2.11                     | 0.79              |
| 1:G:795:ARG:CB   | 3:I:118:MET:HE1  | 2.13                     | 0.79              |
| 1:A:502:GLU:HG2  | 1:A:764:MLY:O    | 1.83                     | 0.79              |
| 2:N:111:SER:OG   | 2:N:148:VAL:C    | 2.15                     | 0.79              |
| 1:G:537:GLU:O    | 4:V:350:SER:N    | 2.16                     | 0.79              |
| 1:M:538:GLU:HG3  | 4:Z:351:THR:C    | 2.03                     | 0.79              |
| 1:D:409:GLY:N    | 1:D:636:LYS:CG   | 2.44                     | 0.79              |
| 1:D:537:GLU:O    | 4:9:350:SER:N    | 2.16                     | 0.79              |
| 1:M:218:LEU:CA   | 1:M:221:GLN:HG2  | 2.10                     | 0.79              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:HB2  | 2.13                     | 0.79              |
| 1:M:732:ILE:HG22 | 1:M:747:LEU:HD12 | 0.81                     | 0.79              |
| 1:G:92:ALA:O     | 1:G:714:ARG:CG   | 2.30                     | 0.79              |
| 1:M:642:LYS:HG2  | 4:Z:22:ALA:HA    | 1.65                     | 0.79              |
| 2:Q:121:LEU:CG   | 2:Q:128:PHE:CA   | 2.48                     | 0.79              |
| 1:P:538:GLU:HG3  | 4:0:351:THR:C    | 2.03                     | 0.79              |
| 1:J:538:GLU:HG3  | 4:W:351:THR:C    | 2.03                     | 0.79              |
| 1:D:407:GLY:HA2  | 1:D:412:ALA:HA   | 1.65                     | 0.79              |
| 1:A:537:GLU:O    | 4:8:350:SER:N    | 2.16                     | 0.79              |
| 1:A:538:GLU:HG3  | 4:8:351:THR:C    | 2.03                     | 0.79              |
| 1:G:506:GLU:OE2  | 1:G:760:PHE:O    | 1.99                     | 0.79              |
| 1:J:829:TRP:CZ2  | 2:K:87:LYS:CE    | 2.64                     | 0.79              |
| 3:R:49:ILE:N     | 3:R:52:ASN:ND2   | 2.29                     | 0.79              |
| 2:E:162:ASP:O    | 2:K:21:GLU:CB    | 2.31                     | 0.79              |
| 1:G:174:SER:CB   | 1:G:667:THR:HG21 | 2.13                     | 0.79              |
| 1:D:291:ILE:HA   | 1:D:331:LEU:HD11 | 1.64                     | 0.79              |
| 1:J:291:ILE:HA   | 1:J:331:LEU:HD11 | 1.64                     | 0.79              |
| 1:J:83:PRO:O     | 1:J:723:ARG:NH2  | 2.14                     | 0.79              |
| 1:M:792:ALA:HB2  | 3:O:42:THR:CG2   | 2.13                     | 0.79              |
| 1:A:800:ARG:HD2  | 3:C:149:VAL:O    | 1.83                     | 0.79              |
| 1:D:800:ARG:NH2  | 3:F:40:ASN:OD1   | 2.16                     | 0.79              |
| 1:P:826:VAL:HG21 | 2:Q:88:LEU:HD21  | 1.66                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:117:LEU:HB2  | 2:K:147:ASN:HD21 | 1.47                     | 0.78              |
| 1:P:409:GLY:N    | 1:P:636:LYS:CG   | 2.44                     | 0.78              |
| 1:J:639:GLY:CA   | 4:W:345:ILE:N    | 2.47                     | 0.78              |
| 4:X:325:MET:SD   | 4:Z:244:ASP:CB   | 2.71                     | 0.78              |
| 1:A:642:LYS:HG2  | 4:8:22:ALA:HA    | 1.65                     | 0.78              |
| 1:J:829:TRP:HZ2  | 2:K:83:MET:CE    | 1.96                     | 0.78              |
| 1:J:407:GLY:HA2  | 1:J:412:ALA:HA   | 1.65                     | 0.78              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:HD13 | 1.34                     | 0.78              |
| 1:G:796:GLY:CA   | 3:I:35:ARG:CD    | 2.43                     | 0.78              |
| 1:J:818:TYR:CD1  | 2:K:127:ARG:NH1  | 2.51                     | 0.78              |
| 1:J:642:LYS:CG   | 4:W:23:GLY:H     | 1.77                     | 0.78              |
| 1:P:798:LEU:HD12 | 3:R:126:LEU:HD21 | 1.64                     | 0.78              |
| 1:A:542:PHE:CA   | 4:8:143:TYR:HE1  | 1.92                     | 0.78              |
| 1:M:838:ILE:HD11 | 2:N:54:MET:SD    | 2.23                     | 0.78              |
| 1:M:641:LYS:HD2  | 1:M:647:GLN:OE1  | 1.81                     | 0.78              |
| 1:P:84:MLY:HH11  | 1:P:724:TYR:CE2  | 2.17                     | 0.78              |
| 1:P:174:SER:CB   | 1:P:667:THR:HG21 | 2.13                     | 0.78              |
| 1:G:799:MET:SD   | 3:I:32:ASP:CG    | 2.61                     | 0.78              |
| 1:G:537:GLU:HG3  | 4:V:350:SER:O    | 1.79                     | 0.78              |
| 1:J:537:GLU:O    | 4:W:350:SER:N    | 2.16                     | 0.78              |
| 1:P:797:PHE:CD1  | 3:R:149:VAL:CG1  | 2.66                     | 0.78              |
| 1:D:550:PHE:N    | 4:W:46:GLY:HA3   | 1.97                     | 0.78              |
| 1:A:795:ARG:HG2  | 3:C:118:MET:HE3  | 1.63                     | 0.78              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:CG   | 2.60                     | 0.78              |
| 1:P:506:GLU:CD   | 1:P:760:PHE:C    | 2.38                     | 0.78              |
| 3:R:50:LEU:C     | 3:R:53:PRO:HD2   | 2.03                     | 0.78              |
| 1:G:798:LEU:HG   | 3:I:122:GLU:HB3  | 1.64                     | 0.78              |
| 1:G:407:GLY:HA2  | 1:G:412:ALA:HA   | 1.65                     | 0.78              |
| 1:A:218:LEU:CA   | 1:A:221:GLN:HG2  | 2.10                     | 0.78              |
| 1:P:646:PHE:HE2  | 1:P:652:LEU:CD2  | 1.97                     | 0.78              |
| 1:G:218:LEU:CA   | 1:G:221:GLN:HG2  | 2.10                     | 0.78              |
| 1:M:529:PRO:C    | 4:Z:354:GLN:CB   | 2.48                     | 0.78              |
| 1:M:538:GLU:OE2  | 4:Z:355:MET:HE3  | 1.79                     | 0.78              |
| 1:J:409:GLY:N    | 1:J:636:LYS:CG   | 2.44                     | 0.78              |
| 1:J:530:MET:CG   | 4:W:354:GLN:CB   | 2.30                     | 0.78              |
| 1:A:553:MLY:NZ   | 4:V:45:VAL:HA    | 1.84                     | 0.78              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:N    | 2.46                     | 0.78              |
| 1:D:646:PHE:CE2  | 1:D:652:LEU:HD21 | 2.14                     | 0.78              |
| 1:A:815:CYS:O    | 2:B:90:GLY:O     | 2.01                     | 0.78              |
| 1:P:829:TRP:CH2  | 2:Q:87:LYS:NZ    | 2.49                     | 0.78              |
| 1:D:481:ASN:N    | 1:D:481:ASN:HD22 | 1.82                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:107:MLY:HB3  | 1:G:686:MET:HE2  | 1.64                     | 0.78              |
| 1:M:291:ILE:HA   | 1:M:331:LEU:HD11 | 1.64                     | 0.78              |
| 1:G:754:ASP:CA   | 1:G:779:ARG:HD3  | 2.04                     | 0.78              |
| 1:P:537:GLU:O    | 4:0:350:SER:N    | 2.16                     | 0.78              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:CD2  | 1.97                     | 0.78              |
| 1:M:34:ALA:HB1   | 1:M:777:GLU:OE2  | 1.83                     | 0.78              |
| 4:7:287:ILE:HB   | 4:9:204:ALA:N    | 1.98                     | 0.78              |
| 4:9:287:ILE:HB   | 4:W:204:ALA:N    | 1.97                     | 0.78              |
| 1:J:174:SER:CB   | 1:J:667:THR:HG21 | 2.13                     | 0.78              |
| 1:M:174:SER:CB   | 1:M:667:THR:HG21 | 2.13                     | 0.78              |
| 1:A:51:THR:O     | 1:A:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:G:836:PHE:CE1  | 2:H:159:HIS:HA   | 2.18                     | 0.78              |
| 4:1:223:PHE:HE1  | 4:1:255:PHE:HB2  | 1.46                     | 0.78              |
| 1:G:752:ASP:OD1  | 1:G:783:LEU:HB2  | 1.84                     | 0.78              |
| 1:G:646:PHE:HE2  | 1:G:652:LEU:CD2  | 1.97                     | 0.78              |
| 1:M:635:GLY:HA3  | 4:Z:341:ILE:CD1  | 2.14                     | 0.78              |
| 1:A:550:PHE:HA   | 4:V:46:GLY:HA2   | 1.65                     | 0.78              |
| 1:A:557:GLU:N    | 4:V:48:GLY:HA2   | 1.90                     | 0.78              |
| 1:M:797:PHE:CD1  | 3:O:146:ILE:O    | 2.37                     | 0.78              |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:HD13 | 0.90                     | 0.78              |
| 1:G:641:LYS:HD2  | 4:V:348:SER:HB2  | 1.54                     | 0.78              |
| 1:M:646:PHE:HE2  | 1:M:652:LEU:CD2  | 1.97                     | 0.78              |
| 1:M:804:ARG:O    | 1:M:808:GLU:HG3  | 1.84                     | 0.78              |
| 1:M:806:MET:CA   | 1:M:807:VAL:N    | 2.46                     | 0.78              |
| 1:J:756:THR:CG2  | 1:J:776:GLU:CD   | 2.52                     | 0.78              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:HB2  | 1.66                     | 0.78              |
| 1:P:291:ILE:HA   | 1:P:331:LEU:HD11 | 1.64                     | 0.78              |
| 1:D:798:LEU:HD13 | 3:F:126:LEU:CD1  | 1.94                     | 0.78              |
| 1:G:642:LYS:HG2  | 4:V:22:ALA:HA    | 1.65                     | 0.78              |
| 4:0:205:GLU:OE2  | 4:Y:287:ILE:CG2  | 2.08                     | 0.78              |
| 1:J:641:LYS:CE   | 1:J:647:GLN:HB2  | 2.13                     | 0.78              |
| 1:M:641:LYS:CE   | 1:M:647:GLN:HB2  | 2.13                     | 0.78              |
| 1:D:712:PRO:CB   | 1:D:771:LEU:CB   | 2.61                     | 0.78              |
| 1:J:51:THR:O     | 1:J:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:A:502:GLU:O    | 1:A:761:GLY:HA2  | 1.84                     | 0.78              |
| 1:M:545:ALA:HA   | 4:1:45:VAL:HG13  | 1.62                     | 0.78              |
| 4:3:288:ASP:N    | 4:5:203:THR:CG2  | 2.46                     | 0.78              |
| 3:C:50:LEU:C     | 3:C:53:PRO:HD2   | 2.03                     | 0.78              |
| 1:M:95:THR:HA    | 1:M:713:SER:OG   | 1.84                     | 0.78              |
| 1:A:496:PHE:CD2  | 1:A:514:ASP:HA   | 2.19                     | 0.78              |
| 1:G:219:GLU:O    | 1:G:223:ILE:HG13 | 1.84                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:817:GLN:HB3  | 2:N:127:ARG:HD3  | 1.66                     | 0.78              |
| 1:G:409:GLY:N    | 1:G:636:LYS:CG   | 2.44                     | 0.78              |
| 1:P:407:GLY:HA2  | 1:P:412:ALA:HA   | 1.65                     | 0.78              |
| 1:J:149:GLN:OE1  | 1:J:763:THR:HG21 | 1.84                     | 0.78              |
| 1:M:530:MET:CG   | 4:Z:354:GLN:CB   | 2.30                     | 0.78              |
| 1:M:218:LEU:HA   | 1:M:221:GLN:HG2  | 1.62                     | 0.78              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:HG21 | 1.60                     | 0.78              |
| 1:G:28:GLN:HB3   | 1:G:723:ARG:HH12 | 1.46                     | 0.78              |
| 4:4:223:PHE:HD2  | 4:4:312:ARG:HH21 | 1.32                     | 0.78              |
| 1:J:107:MLY:HB3  | 1:J:686:MET:HE2  | 1.66                     | 0.78              |
| 1:M:219:GLU:O    | 1:M:223:ILE:HG13 | 1.84                     | 0.78              |
| 4:Z:223:PHE:HE1  | 4:Z:255:PHE:HB2  | 1.46                     | 0.78              |
| 1:P:107:MLY:HB3  | 1:P:686:MET:HE2  | 1.66                     | 0.78              |
| 1:P:496:PHE:CD2  | 1:P:514:ASP:HA   | 2.19                     | 0.78              |
| 1:G:51:THR:O     | 1:G:62:VAL:HG13  | 1.84                     | 0.78              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:HG2  | 1.95                     | 0.78              |
| 1:M:553:MLY:HA   | 4:1:43:VAL:HG11  | 1.64                     | 0.78              |
| 1:D:538:GLU:HG3  | 4:9:351:THR:C    | 2.03                     | 0.78              |
| 1:A:641:LYS:HD2  | 4:8:348:SER:HB2  | 1.54                     | 0.78              |
| 1:P:599:ASN:CA   | 1:P:649:VAL:CB   | 2.53                     | 0.78              |
| 4:1:324:THR:HG23 | 4:3:244:ASP:CA   | 2.14                     | 0.78              |
| 4:1:324:THR:CG2  | 4:3:244:ASP:CA   | 2.59                     | 0.78              |
| 1:A:407:GLY:HA2  | 1:A:412:ALA:HA   | 1.65                     | 0.78              |
| 3:C:3:SER:O      | 3:C:4:LYS:HB2    | 1.84                     | 0.78              |
| 1:A:219:GLU:O    | 1:A:223:ILE:HG13 | 1.84                     | 0.78              |
| 1:M:407:GLY:HA2  | 1:M:412:ALA:HA   | 1.65                     | 0.77              |
| 1:M:530:MET:HE1  | 4:Z:355:MET:SD   | 2.24                     | 0.77              |
| 1:M:785:GLU:C    | 1:M:786:ILE:N    | 2.38                     | 0.77              |
| 1:P:641:LYS:CE   | 1:P:647:GLN:HB2  | 2.13                     | 0.77              |
| 4:2:322:PRO:CB   | 4:4:244:ASP:OD2  | 2.26                     | 0.77              |
| 4:3:322:PRO:HB3  | 4:5:244:ASP:CB   | 2.10                     | 0.77              |
| 1:M:496:PHE:CD2  | 1:M:514:ASP:HA   | 2.19                     | 0.77              |
| 1:M:767:PHE:CE1  | 1:M:772:LEU:HD22 | 2.19                     | 0.77              |
| 1:G:496:PHE:CD2  | 1:G:514:ASP:HA   | 2.19                     | 0.77              |
| 1:G:291:ILE:HA   | 1:G:331:LEU:HD11 | 1.64                     | 0.77              |
| 1:J:496:PHE:CD2  | 1:J:514:ASP:HA   | 2.19                     | 0.77              |
| 1:G:530:MET:HE3  | 4:V:354:GLN:HG2  | 1.65                     | 0.77              |
| 1:G:733:PRO:C    | 1:G:737:PHE:HD1  | 1.88                     | 0.77              |
| 1:P:552:ASN:ND2  | 4:2:49:GLN:HG3   | 1.82                     | 0.77              |
| 1:A:639:GLY:CA   | 4:8:345:ILE:N    | 2.47                     | 0.77              |
| 1:D:641:LYS:CE   | 1:D:647:GLN:CG   | 2.60                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:834:LEU:CD2  | 2:E:54:MET:HE3   | 2.13                     | 0.77              |
| 1:P:707:CYS:SG   | 1:P:714:ARG:NH1  | 2.57                     | 0.77              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:HB3  | 2.14                     | 0.77              |
| 3:C:49:ILE:N     | 3:C:52:ASN:HD22  | 1.82                     | 0.77              |
| 1:G:639:GLY:CA   | 4:V:345:ILE:N    | 2.47                     | 0.77              |
| 1:P:721:LYS:CA   | 1:P:736:GLN:NE2  | 2.43                     | 0.77              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:HD21 | 2.14                     | 0.77              |
| 1:D:530:MET:HE1  | 4:9:355:MET:SD   | 2.24                     | 0.77              |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:HG12 | 1.67                     | 0.77              |
| 1:M:796:GLY:HA2  | 3:O:35:ARG:CD    | 2.13                     | 0.77              |
| 1:G:148:ARG:NH2  | 1:G:764:MLY:HH21 | 1.99                     | 0.77              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:HB2  | 2.13                     | 0.77              |
| 4:0:243:PRO:HG2  | 4:Y:288:ASP:HB3  | 1.65                     | 0.77              |
| 1:M:84:MLY:CH1   | 1:M:724:TYR:CE2  | 2.67                     | 0.77              |
| 4:0:223:PHE:HD2  | 4:0:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:P:116:TYR:O    | 1:P:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:D:795:ARG:CB   | 3:F:35:ARG:HH12  | 1.89                     | 0.77              |
| 1:M:821:ARG:NH2  | 2:N:127:ARG:CG   | 2.46                     | 0.77              |
| 1:P:817:GLN:HB3  | 2:Q:127:ARG:HD3  | 1.63                     | 0.77              |
| 1:G:503:TYR:HE1  | 1:G:711:PHE:CD2  | 2.00                     | 0.77              |
| 4:X:325:MET:SD   | 4:Z:244:ASP:CG   | 2.63                     | 0.77              |
| 1:D:174:SER:CB   | 1:D:667:THR:HG21 | 2.13                     | 0.77              |
| 1:M:51:THR:O     | 1:M:62:VAL:HG13  | 1.84                     | 0.77              |
| 1:P:51:THR:O     | 1:P:62:VAL:HG13  | 1.84                     | 0.77              |
| 1:P:219:GLU:O    | 1:P:223:ILE:HG13 | 1.84                     | 0.77              |
| 1:J:820:VAL:HG11 | 2:K:136:MET:HE3  | 1.66                     | 0.77              |
| 1:P:639:GLY:CA   | 4:0:345:ILE:N    | 2.47                     | 0.77              |
| 1:A:725:ARG:HG3  | 1:A:733:PRO:HA   | 1.67                     | 0.77              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG12 | 1.66                     | 0.77              |
| 1:D:818:TYR:CB   | 2:E:90:GLY:N     | 2.44                     | 0.77              |
| 4:0:205:GLU:CG   | 4:Y:287:ILE:CB   | 2.03                     | 0.77              |
| 4:0:243:PRO:C    | 4:Y:291:LYS:NZ   | 2.34                     | 0.77              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:CD2  | 1.97                     | 0.77              |
| 2:H:150:TYR:C    | 2:H:151:LYS:CG   | 2.48                     | 0.77              |
| 1:J:799:MET:SD   | 3:L:32:ASP:OD2   | 2.42                     | 0.77              |
| 1:J:769:ALA:HB2  | 1:J:770:GLY:CA   | 2.14                     | 0.77              |
| 4:Y:223:PHE:HD2  | 4:Y:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:J:116:TYR:O    | 1:J:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:D:723:ARG:NH2  | 1:D:779:ARG:NH2  | 2.32                     | 0.77              |
| 1:D:727:LEU:CA   | 1:D:782:MLY:HH13 | 2.14                     | 0.77              |
| 1:A:502:GLU:C    | 1:A:761:GLY:HA3  | 2.04                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:639:GLY:CA   | 4:9:345:ILE:N    | 2.47                     | 0.77              |
| 1:M:721:LYS:CA   | 1:M:736:GLN:OE1  | 2.33                     | 0.77              |
| 4:0:245:GLY:H    | 4:Y:291:LYS:HB2  | 1.49                     | 0.77              |
| 1:P:831:TRP:HE1  | 2:Q:67:MET:CB    | 1.98                     | 0.77              |
| 1:D:629:GLU:HA   | 1:D:643:GLY:C    | 2.05                     | 0.77              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:CD2  | 1.97                     | 0.77              |
| 1:M:35:MLY:HH21  | 1:M:778:MET:CG   | 2.09                     | 0.77              |
| 4:V:325:MET:HE1  | 4:X:244:ASP:CG   | 2.03                     | 0.77              |
| 4:1:324:THR:CB   | 4:3:244:ASP:HA   | 2.14                     | 0.77              |
| 4:9:223:PHE:HD2  | 4:9:312:ARG:HH21 | 1.33                     | 0.77              |
| 4:5:223:PHE:HD2  | 4:5:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:D:51:THR:O     | 1:D:62:VAL:HG13  | 1.84                     | 0.77              |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:CD2   | 2.14                     | 0.77              |
| 1:J:795:ARG:HB3  | 3:L:35:ARG:NH2   | 2.00                     | 0.77              |
| 1:D:724:TYR:HE1  | 1:D:778:MET:C    | 1.87                     | 0.77              |
| 1:G:754:ASP:CB   | 1:G:776:GLU:HA   | 2.15                     | 0.77              |
| 1:A:732:ILE:N    | 1:A:733:PRO:HD2  | 2.00                     | 0.77              |
| 1:G:725:ARG:HG3  | 1:G:733:PRO:HA   | 1.67                     | 0.77              |
| 1:D:116:TYR:O    | 1:D:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:D:496:PHE:CD2  | 1:D:514:ASP:HA   | 2.19                     | 0.77              |
| 1:D:94:MET:CE    | 1:D:101:ALA:HB1  | 2.15                     | 0.77              |
| 1:G:116:TYR:O    | 1:G:153:PRO:HB2  | 1.85                     | 0.77              |
| 1:A:291:ILE:HA   | 1:A:331:LEU:HD11 | 1.64                     | 0.77              |
| 4:1:287:ILE:HG21 | 4:3:202:THR:C    | 2.05                     | 0.77              |
| 2:K:121:LEU:CG   | 2:K:128:PHE:HA   | 2.14                     | 0.77              |
| 1:D:836:PHE:CZ   | 2:E:160:GLY:N    | 2.53                     | 0.77              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:H    | 1.98                     | 0.77              |
| 4:3:288:ASP:H    | 4:5:203:THR:CG2  | 1.98                     | 0.77              |
| 1:A:815:CYS:SG   | 2:B:92:ASP:HB2   | 2.25                     | 0.77              |
| 4:W:223:PHE:HD2  | 4:W:312:ARG:HH21 | 1.33                     | 0.77              |
| 1:J:219:GLU:O    | 1:J:223:ILE:HG13 | 1.84                     | 0.77              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:CD1  | 2.15                     | 0.77              |
| 1:G:529:PRO:C    | 4:V:354:GLN:CB   | 2.50                     | 0.77              |
| 1:P:721:LYS:CA   | 1:P:736:GLN:OE1  | 2.33                     | 0.77              |
| 1:G:818:TYR:HB3  | 2:H:90:GLY:HA3   | 1.66                     | 0.77              |
| 2:B:121:LEU:CG   | 2:B:128:PHE:HA   | 2.14                     | 0.77              |
| 1:J:635:GLY:HA3  | 4:W:341:ILE:CD1  | 2.14                     | 0.77              |
| 1:D:635:GLY:HA3  | 4:9:341:ILE:CD1  | 2.14                     | 0.77              |
| 1:M:786:ILE:CA   | 1:M:787:ILE:N    | 2.48                     | 0.77              |
| 1:M:795:ARG:CZ   | 3:O:116:GLU:OE2  | 2.33                     | 0.77              |
| 1:M:797:PHE:CE2  | 3:O:126:LEU:HD22 | 2.19                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:0:166:TYR:OH   | 4:2:64:ILE:HD13  | 1.85                     | 0.77              |
| 1:G:830:PRO:CG   | 2:H:67:MET:HE2   | 2.15                     | 0.77              |
| 4:X:223:PHE:HD2  | 4:X:312:ARG:HH21 | 1.32                     | 0.77              |
| 1:J:834:LEU:CD1  | 2:K:51:PHE:CE1   | 2.68                     | 0.77              |
| 1:A:707:CYS:HA   | 1:A:714:ARG:HH12 | 0.96                     | 0.77              |
| 1:A:149:GLN:CG   | 1:A:719:ASP:H    | 1.97                     | 0.77              |
| 1:G:530:MET:CG   | 4:V:354:GLN:CB   | 2.30                     | 0.77              |
| 2:E:121:LEU:CG   | 2:E:128:PHE:CA   | 2.48                     | 0.77              |
| 1:P:729:ALA:CB   | 3:R:93:VAL:HG23  | 2.11                     | 0.77              |
| 1:P:725:ARG:HG3  | 1:P:733:PRO:HA   | 1.67                     | 0.77              |
| 1:P:836:PHE:CE1  | 2:Q:160:GLY:N    | 2.51                     | 0.77              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:HB2  | 2.13                     | 0.77              |
| 1:M:506:GLU:HG2  | 1:M:760:PHE:O    | 1.85                     | 0.77              |
| 1:P:829:TRP:CH2  | 2:Q:87:LYS:CE    | 2.67                     | 0.77              |
| 4:7:223:PHE:HD2  | 4:7:312:ARG:HH21 | 1.32                     | 0.77              |
| 4:2:223:PHE:HD2  | 4:2:312:ARG:HH21 | 1.33                     | 0.77              |
| 4:3:223:PHE:HD2  | 4:3:312:ARG:HH21 | 1.33                     | 0.77              |
| 3:F:3:SER:O      | 3:F:4:LYS:HB2    | 1.84                     | 0.77              |
| 1:J:800:ARG:HH22 | 3:L:40:ASN:CG    | 1.86                     | 0.76              |
| 1:P:530:MET:CG   | 4:0:354:GLN:CB   | 2.30                     | 0.76              |
| 1:P:786:ILE:C    | 1:P:787:ILE:CA   | 2.53                     | 0.76              |
| 1:J:710:GLY:O    | 1:J:772:LEU:CB   | 2.32                     | 0.76              |
| 1:M:84:MLY:HA    | 1:M:723:ARG:CZ   | 2.15                     | 0.76              |
| 1:D:642:LYS:HG2  | 4:9:22:ALA:HA    | 1.65                     | 0.76              |
| 4:8:223:PHE:HD2  | 4:8:312:ARG:HH21 | 1.33                     | 0.76              |
| 1:P:94:MET:CE    | 1:P:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:D:727:LEU:H    | 1:D:782:MLY:CE   | 1.97                     | 0.76              |
| 1:A:94:MET:CE    | 1:A:101:ALA:HB1  | 2.15                     | 0.76              |
| 2:E:121:LEU:CG   | 2:E:128:PHE:HA   | 2.14                     | 0.76              |
| 1:J:725:ARG:HG3  | 1:J:733:PRO:HA   | 1.67                     | 0.76              |
| 1:P:635:GLY:HA3  | 4:0:341:ILE:CD1  | 2.14                     | 0.76              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG12 | 1.67                     | 0.76              |
| 1:M:639:GLY:CA   | 4:Z:345:ILE:N    | 2.46                     | 0.76              |
| 1:M:725:ARG:HG3  | 1:M:733:PRO:HA   | 1.67                     | 0.76              |
| 1:M:93:MET:HA    | 1:M:714:ARG:H    | 1.48                     | 0.76              |
| 1:A:629:GLU:HA   | 1:A:643:GLY:C    | 2.05                     | 0.76              |
| 1:J:94:MET:CE    | 1:J:101:ALA:HB1  | 2.15                     | 0.76              |
| 4:1:244:ASP:HB2  | 4:Z:322:PRO:CB   | 2.14                     | 0.76              |
| 1:M:820:VAL:HG11 | 2:N:136:MET:CE   | 2.14                     | 0.76              |
| 1:P:642:LYS:HG2  | 4:0:22:ALA:HA    | 1.65                     | 0.76              |
| 1:P:783:LEU:CA   | 1:P:786:ILE:HG13 | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:534:SER:O    | 4:9:351:THR:N    | 2.19                     | 0.76              |
| 1:M:786:ILE:O    | 1:M:789:ALA:HB3  | 1.85                     | 0.76              |
| 1:P:506:GLU:HG3  | 1:P:760:PHE:H    | 1.47                     | 0.76              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:CB   | 2.63                     | 0.76              |
| 1:P:799:MET:SD   | 3:R:32:ASP:HB3   | 2.25                     | 0.76              |
| 1:P:481:ASN:HD22 | 1:P:481:ASN:N    | 1.82                     | 0.76              |
| 4:1:223:PHE:HD2  | 4:1:312:ARG:HH21 | 1.33                     | 0.76              |
| 1:D:219:GLU:O    | 1:D:223:ILE:HG13 | 1.84                     | 0.76              |
| 1:D:727:LEU:CG   | 1:D:782:MLY:CH1  | 2.60                     | 0.76              |
| 1:J:721:LYS:CA   | 1:J:736:GLN:OE1  | 2.33                     | 0.76              |
| 1:G:218:LEU:HB2  | 1:G:221:GLN:CG   | 2.09                     | 0.76              |
| 1:M:785:GLU:O    | 1:M:789:ALA:HB2  | 1.86                     | 0.76              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:CA   | 2.68                     | 0.76              |
| 1:M:94:MET:CE    | 1:M:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:A:505:MLY:HD3  | 1:A:762:HIS:HA   | 0.76                     | 0.76              |
| 2:N:121:LEU:CG   | 2:N:128:PHE:HA   | 2.14                     | 0.76              |
| 1:G:629:GLU:HA   | 1:G:643:GLY:C    | 2.05                     | 0.76              |
| 1:P:733:PRO:C    | 1:P:737:PHE:HD1  | 1.88                     | 0.76              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG12 | 1.67                     | 0.76              |
| 2:H:121:LEU:CG   | 2:H:128:PHE:HA   | 2.14                     | 0.76              |
| 1:P:646:PHE:CE2  | 1:P:652:LEU:HD21 | 2.14                     | 0.76              |
| 1:P:782:MLY:HH22 | 3:R:80:ASP:O     | 1.86                     | 0.76              |
| 1:D:537:GLU:HG3  | 4:9:350:SER:O    | 1.79                     | 0.76              |
| 1:M:732:ILE:N    | 1:M:733:PRO:HD2  | 2.00                     | 0.76              |
| 1:M:629:GLU:HA   | 1:M:643:GLY:C    | 2.05                     | 0.76              |
| 1:D:800:ARG:HD3  | 3:F:149:VAL:C    | 2.06                     | 0.76              |
| 1:D:800:ARG:HH21 | 3:F:40:ASN:CG    | 1.88                     | 0.76              |
| 4:V:223:PHE:HD2  | 4:V:312:ARG:HH21 | 1.33                     | 0.76              |
| 1:J:834:LEU:CD1  | 2:K:51:PHE:HE1   | 1.98                     | 0.76              |
| 3:O:3:SER:O      | 3:O:4:LYS:HB2    | 1.85                     | 0.76              |
| 3:R:3:SER:O      | 3:R:4:LYS:HB2    | 1.85                     | 0.76              |
| 1:D:793:ARG:NH2  | 3:F:147:MET:HE1  | 1.98                     | 0.76              |
| 1:G:792:ALA:HA   | 3:I:42:THR:HA    | 1.67                     | 0.76              |
| 1:G:795:ARG:HA   | 3:I:118:MET:CE   | 2.15                     | 0.76              |
| 4:1:288:ASP:OD1  | 4:3:203:THR:HG23 | 1.84                     | 0.76              |
| 1:J:818:TYR:CZ   | 2:K:127:ARG:NH2  | 2.40                     | 0.76              |
| 1:A:733:PRO:C    | 1:A:737:PHE:HD1  | 1.88                     | 0.76              |
| 1:M:546:THR:O    | 4:1:46:GLY:HA2   | 1.84                     | 0.76              |
| 4:9:290:ARG:NH1  | 4:W:202:THR:CG2  | 2.49                     | 0.76              |
| 1:D:623:PHE:CA   | 1:D:623:PHE:CG   | 2.68                     | 0.76              |
| 1:P:623:PHE:CG   | 1:P:623:PHE:CA   | 2.68                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:623:PHE:CG   | 1:A:623:PHE:CA   | 2.68                     | 0.76              |
| 3:L:49:ILE:N     | 3:L:52:ASN:HD22  | 1.83                     | 0.76              |
| 4:1:244:ASP:CB   | 4:Z:322:PRO:HB3  | 2.10                     | 0.76              |
| 1:J:567:LYS:HZ3  | 4:Y:92:ASN:ND2   | 1.80                     | 0.76              |
| 1:M:664:LEU:O    | 1:M:667:THR:HB   | 1.86                     | 0.76              |
| 4:Z:223:PHE:HD2  | 4:Z:312:ARG:HH21 | 1.33                     | 0.76              |
| 1:M:116:TYR:O    | 1:M:153:PRO:HB2  | 1.85                     | 0.76              |
| 1:A:116:TYR:O    | 1:A:153:PRO:HB2  | 1.85                     | 0.76              |
| 1:D:795:ARG:CD   | 3:F:35:ARG:HH12  | 1.98                     | 0.76              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:NE2  | 2.43                     | 0.76              |
| 1:M:795:ARG:HB3  | 3:O:35:ARG:CZ    | 2.13                     | 0.76              |
| 1:M:797:PHE:CE2  | 3:O:146:ILE:HD12 | 2.20                     | 0.76              |
| 1:P:218:LEU:HD22 | 1:P:222:ILE:HG12 | 1.67                     | 0.76              |
| 4:W:291:LYS:HB3  | 4:Y:244:ASP:HB3  | 1.66                     | 0.76              |
| 1:J:756:THR:HG22 | 1:J:776:GLU:HB3  | 1.67                     | 0.76              |
| 2:K:150:TYR:C    | 2:K:151:LYS:CG   | 2.48                     | 0.76              |
| 1:G:754:ASP:HA   | 1:G:779:ARG:HD2  | 0.93                     | 0.76              |
| 1:A:505:MLY:CD   | 1:A:762:HIS:CA   | 2.22                     | 0.76              |
| 1:A:218:LEU:HB3  | 1:A:221:GLN:HG3  | 1.61                     | 0.76              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:CD   | 2.63                     | 0.76              |
| 1:D:529:PRO:C    | 4:9:354:GLN:CB   | 2.49                     | 0.76              |
| 1:A:831:TRP:HZ3  | 2:B:50:THR:HG21  | 0.83                     | 0.76              |
| 1:G:28:GLN:O     | 1:G:723:ARG:NH2  | 2.19                     | 0.76              |
| 1:G:641:LYS:HD2  | 1:G:647:GLN:OE1  | 1.81                     | 0.76              |
| 1:D:721:LYS:CA   | 1:D:736:GLN:OE1  | 2.33                     | 0.76              |
| 1:D:732:ILE:N    | 1:D:733:PRO:HD2  | 2.00                     | 0.76              |
| 1:A:218:LEU:HB2  | 1:A:221:GLN:CG   | 2.09                     | 0.76              |
| 1:D:538:GLU:OE2  | 4:9:355:MET:HE3  | 1.86                     | 0.76              |
| 1:D:553:MLY:NZ   | 4:W:45:VAL:HA    | 1.84                     | 0.76              |
| 1:P:641:LYS:CE   | 1:P:647:GLN:CG   | 2.61                     | 0.76              |
| 4:0:166:TYR:CE1  | 4:2:64:ILE:HG21  | 2.21                     | 0.76              |
| 4:8:290:ARG:NH1  | 4:V:202:THR:CG2  | 2.49                     | 0.76              |
| 1:G:94:MET:CE    | 1:G:101:ALA:HB1  | 2.15                     | 0.76              |
| 1:D:664:LEU:O    | 1:D:667:THR:HB   | 1.86                     | 0.76              |
| 1:J:817:GLN:HB3  | 2:K:127:ARG:NH1  | 1.98                     | 0.76              |
| 1:A:530:MET:HE1  | 4:8:355:MET:SD   | 2.26                     | 0.76              |
| 1:G:649:VAL:CB   | 1:G:649:VAL:CG1  | 2.64                     | 0.76              |
| 1:D:649:VAL:CB   | 1:D:649:VAL:CG1  | 2.64                     | 0.76              |
| 1:D:831:TRP:CZ3  | 2:E:34:ILE:CG2   | 2.67                     | 0.76              |
| 1:M:623:PHE:CG   | 1:M:623:PHE:CA   | 2.68                     | 0.76              |
| 1:J:481:ASN:N    | 1:J:481:ASN:HD22 | 1.82                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:795:ARG:CD   | 3:L:35:ARG:HH12  | 1.99                     | 0.75              |
| 1:P:732:ILE:HG21 | 1:P:747:LEU:HD13 | 0.91                     | 0.75              |
| 1:P:732:ILE:N    | 1:P:733:PRO:HD2  | 2.00                     | 0.75              |
| 1:P:786:ILE:HB   | 1:P:787:ILE:N    | 2.01                     | 0.75              |
| 1:G:732:ILE:N    | 1:G:733:PRO:HD2  | 2.00                     | 0.75              |
| 4:W:324:THR:CG2  | 4:Y:247:VAL:HG22 | 2.17                     | 0.75              |
| 1:P:149:GLN:HB3  | 1:P:716:LEU:CD2  | 2.06                     | 0.75              |
| 1:M:649:VAL:CB   | 1:M:649:VAL:CG1  | 2.64                     | 0.75              |
| 1:D:599:ASN:CA   | 1:D:649:VAL:CB   | 2.53                     | 0.75              |
| 1:P:769:ALA:CB   | 1:P:770:GLY:N    | 2.47                     | 0.75              |
| 1:J:797:PHE:HE1  | 3:L:146:ILE:CA   | 1.65                     | 0.75              |
| 1:J:800:ARG:HD2  | 3:L:149:VAL:HG13 | 1.66                     | 0.75              |
| 1:G:534:SER:O    | 4:V:351:THR:N    | 2.20                     | 0.75              |
| 4:1:287:ILE:HG13 | 4:3:202:THR:CA   | 2.16                     | 0.75              |
| 2:B:117:LEU:HB2  | 2:B:147:ASN:HD21 | 1.47                     | 0.75              |
| 1:A:831:TRP:CZ3  | 2:B:34:ILE:HG23  | 2.18                     | 0.75              |
| 1:G:721:LYS:CA   | 1:G:736:GLN:OE1  | 2.33                     | 0.75              |
| 1:A:530:MET:CG   | 4:8:354:GLN:CB   | 2.30                     | 0.75              |
| 1:M:836:PHE:CE2  | 2:N:160:GLY:CA   | 2.68                     | 0.75              |
| 1:M:84:MLY:HH21  | 1:M:719:ASP:O    | 1.81                     | 0.75              |
| 3:R:49:ILE:N     | 3:R:52:ASN:HD22  | 1.82                     | 0.75              |
| 4:3:322:PRO:CB   | 4:5:244:ASP:HB2  | 2.14                     | 0.75              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:HG22 | 1.68                     | 0.75              |
| 1:G:481:ASN:HD22 | 1:G:481:ASN:N    | 1.82                     | 0.75              |
| 1:D:797:PHE:CE1  | 3:F:146:ILE:CB   | 2.65                     | 0.75              |
| 1:A:502:GLU:CD   | 1:A:764:MLY:O    | 2.24                     | 0.75              |
| 1:G:813:ILE:HG21 | 2:H:128:PHE:HE1  | 1.49                     | 0.75              |
| 1:G:506:GLU:CD   | 1:G:760:PHE:O    | 2.25                     | 0.75              |
| 1:A:649:VAL:CB   | 1:A:649:VAL:CG1  | 2.64                     | 0.75              |
| 1:G:829:TRP:HH2  | 2:H:83:MET:HE3   | 1.52                     | 0.75              |
| 3:I:49:ILE:N     | 3:I:52:ASN:HD22  | 1.82                     | 0.75              |
| 1:J:798:LEU:CD1  | 3:L:126:LEU:HD13 | 1.79                     | 0.75              |
| 1:D:725:ARG:HG3  | 1:D:733:PRO:HA   | 1.68                     | 0.75              |
| 2:Q:111:SER:OG   | 2:Q:148:VAL:C    | 2.15                     | 0.75              |
| 1:P:534:SER:O    | 4:0:351:THR:N    | 2.19                     | 0.75              |
| 1:P:538:GLU:O    | 4:0:349:LEU:HG   | 1.86                     | 0.75              |
| 1:P:541:MET:O    | 4:0:143:TYR:CZ   | 2.40                     | 0.75              |
| 1:J:642:LYS:HG2  | 4:W:22:ALA:HA    | 1.65                     | 0.75              |
| 1:M:797:PHE:CE1  | 3:O:149:VAL:HG11 | 2.15                     | 0.75              |
| 3:O:49:ILE:N     | 3:O:52:ASN:HD22  | 1.82                     | 0.75              |
| 1:D:166:MET:HE1  | 1:D:254:PHE:HB2  | 1.68                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:3:SER:O      | 3:I:4:LYS:HB2    | 1.84                     | 0.75              |
| 1:M:505:MLY:CE   | 1:M:762:HIS:HE1  | 1.99                     | 0.75              |
| 1:M:534:SER:O    | 4:Z:351:THR:N    | 2.19                     | 0.75              |
| 1:P:797:PHE:CD2  | 3:R:146:ILE:HG23 | 2.22                     | 0.75              |
| 1:A:795:ARG:HB2  | 3:C:35:ARG:NH1   | 1.99                     | 0.75              |
| 4:2:290:ARG:NH2  | 4:4:202:THR:HG22 | 1.97                     | 0.75              |
| 1:M:642:LYS:CG   | 4:Z:23:GLY:H     | 1.77                     | 0.75              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:CB   | 2.64                     | 0.75              |
| 1:D:800:ARG:CB   | 3:F:149:VAL:HG22 | 2.15                     | 0.75              |
| 1:D:727:LEU:CG   | 1:D:782:MLY:CE   | 2.63                     | 0.75              |
| 1:G:783:LEU:O    | 1:G:787:ILE:CB   | 2.35                     | 0.75              |
| 1:A:97:LEU:HD23  | 1:A:712:PRO:HB3  | 1.67                     | 0.75              |
| 1:J:736:GLN:HA   | 1:J:743:ALA:HB1  | 1.26                     | 0.75              |
| 1:P:410:ASN:CG   | 4:0:334:GLU:CA   | 2.47                     | 0.75              |
| 1:P:530:MET:HE2  | 4:0:354:GLN:HG3  | 1.69                     | 0.75              |
| 1:M:541:MET:O    | 4:Z:143:TYR:CZ   | 2.40                     | 0.75              |
| 1:J:541:MET:O    | 4:W:143:TYR:CZ   | 2.40                     | 0.75              |
| 1:D:550:PHE:HA   | 4:W:46:GLY:HA3   | 1.66                     | 0.75              |
| 1:D:713:SER:HB2  | 1:D:775:LEU:HD22 | 1.65                     | 0.75              |
| 1:D:642:LYS:CG   | 4:9:23:GLY:H     | 1.77                     | 0.75              |
| 1:P:649:VAL:CG1  | 1:P:649:VAL:CB   | 2.64                     | 0.75              |
| 3:F:49:ILE:N     | 3:F:52:ASN:HD22  | 1.82                     | 0.75              |
| 1:A:481:ASN:N    | 1:A:481:ASN:HD22 | 1.82                     | 0.75              |
| 3:R:4:LYS:N      | 3:R:5:ALA:O      | 2.16                     | 0.75              |
| 1:J:800:ARG:HD3  | 3:L:149:VAL:C    | 2.07                     | 0.75              |
| 2:N:117:LEU:HB2  | 2:N:147:ASN:HD21 | 1.47                     | 0.75              |
| 2:N:117:LEU:CB   | 2:N:147:ASN:ND2  | 2.35                     | 0.75              |
| 2:E:111:SER:OG   | 2:E:148:VAL:C    | 2.15                     | 0.75              |
| 1:P:800:ARG:HB3  | 3:R:149:VAL:HG22 | 1.68                     | 0.75              |
| 1:M:218:LEU:HB3  | 1:M:221:GLN:HG3  | 1.61                     | 0.75              |
| 1:G:641:LYS:CE   | 1:G:647:GLN:CG   | 2.61                     | 0.75              |
| 1:J:97:LEU:HD23  | 1:J:712:PRO:CB   | 2.17                     | 0.75              |
| 1:P:664:LEU:O    | 1:P:667:THR:HB   | 1.86                     | 0.75              |
| 1:A:664:LEU:O    | 1:A:667:THR:HB   | 1.86                     | 0.75              |
| 1:G:664:LEU:O    | 1:G:667:THR:HB   | 1.86                     | 0.75              |
| 1:J:350:ALA:O    | 1:J:354:LEU:HB2  | 1.87                     | 0.75              |
| 1:J:820:VAL:HG11 | 2:K:136:MET:CE   | 2.17                     | 0.75              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG12 | 1.67                     | 0.75              |
| 1:A:534:SER:O    | 4:8:351:THR:N    | 2.18                     | 0.75              |
| 1:J:97:LEU:CD2   | 1:J:712:PRO:CB   | 2.65                     | 0.75              |
| 1:G:623:PHE:CA   | 1:G:623:PHE:CG   | 2.68                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:664:LEU:O    | 1:J:667:THR:HB   | 1.86                     | 0.75              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:HA2  | 1.69                     | 0.75              |
| 1:J:800:ARG:O    | 3:L:149:VAL:HG21 | 1.87                     | 0.75              |
| 4:X:324:THR:HG21 | 4:Z:246:GLN:C    | 2.07                     | 0.75              |
| 4:1:287:ILE:CB   | 4:3:203:THR:HG22 | 2.14                     | 0.75              |
| 1:J:733:PRO:C    | 1:J:737:PHE:HD1  | 1.88                     | 0.75              |
| 1:P:529:PRO:C    | 4:0:354:GLN:CB   | 2.49                     | 0.75              |
| 1:P:792:ALA:HB2  | 3:R:42:THR:HG23  | 1.60                     | 0.75              |
| 1:P:795:ARG:NE   | 3:R:116:GLU:HB3  | 2.01                     | 0.75              |
| 1:J:829:TRP:HH2  | 2:K:84:PHE:CD1   | 2.05                     | 0.75              |
| 1:P:829:TRP:CZ3  | 2:Q:84:PHE:CZ    | 2.75                     | 0.75              |
| 1:A:28:GLN:NE2   | 1:A:723:ARG:NH2  | 2.29                     | 0.75              |
| 1:M:310:TYR:CE2  | 1:M:320:ILE:HD11 | 2.22                     | 0.75              |
| 1:P:310:TYR:CE2  | 1:P:320:ILE:HD11 | 2.22                     | 0.75              |
| 1:M:481:ASN:N    | 1:M:481:ASN:HD22 | 1.82                     | 0.75              |
| 1:J:798:LEU:HD12 | 3:L:126:LEU:CD1  | 2.04                     | 0.74              |
| 1:D:727:LEU:HG   | 1:D:782:MLY:CG   | 2.17                     | 0.74              |
| 1:A:754:ASP:OD2  | 1:A:778:MET:HE1  | 1.87                     | 0.74              |
| 1:G:541:MET:O    | 4:V:143:TYR:CZ   | 2.40                     | 0.74              |
| 1:J:538:GLU:OE2  | 4:W:355:MET:HE3  | 1.87                     | 0.74              |
| 1:A:795:ARG:HH22 | 3:C:116:GLU:CD   | 1.90                     | 0.74              |
| 1:A:541:MET:O    | 4:8:143:TYR:CZ   | 2.40                     | 0.74              |
| 1:M:84:MLY:HH11  | 1:M:720:PHE:CD1  | 2.21                     | 0.74              |
| 1:M:805:ALA:O    | 1:M:809:ARG:CB   | 2.35                     | 0.74              |
| 4:V:325:MET:CE   | 4:X:244:ASP:OD2  | 2.34                     | 0.74              |
| 1:J:310:TYR:CE2  | 1:J:320:ILE:HD11 | 2.22                     | 0.74              |
| 1:A:350:ALA:O    | 1:A:354:LEU:HB2  | 1.87                     | 0.74              |
| 4:5:253:GLU:HA   | 4:5:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:M:538:GLU:HA   | 4:Z:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:D:538:GLU:O    | 4:9:349:LEU:HG   | 1.86                     | 0.74              |
| 1:A:635:GLY:HA3  | 4:8:341:ILE:CD1  | 2.14                     | 0.74              |
| 1:M:786:ILE:C    | 1:M:790:THR:H    | 1.89                     | 0.74              |
| 4:8:288:ASP:H    | 4:V:203:THR:HG22 | 1.52                     | 0.74              |
| 4:9:288:ASP:H    | 4:W:203:THR:HG22 | 1.52                     | 0.74              |
| 4:1:253:GLU:HA   | 4:1:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:9:253:GLU:HA   | 4:9:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:W:253:GLU:HA   | 4:W:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:3:253:GLU:HA   | 4:3:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:P:636:LYS:O    | 1:P:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:J:84:MLY:HH21  | 1:J:720:PHE:HA   | 0.74                     | 0.74              |
| 1:M:733:PRO:C    | 1:M:737:PHE:HD1  | 1.88                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:707:CYS:SG   | 1:G:714:ARG:CZ   | 2.74                     | 0.74              |
| 1:M:641:LYS:CE   | 1:M:647:GLN:CG   | 2.60                     | 0.74              |
| 1:A:839:MLY:CH1  | 2:B:159:HIS:CD2  | 2.71                     | 0.74              |
| 1:M:215:GLN:NE2  | 1:M:336:SER:O    | 2.20                     | 0.74              |
| 1:A:215:GLN:NE2  | 1:A:336:SER:O    | 2.20                     | 0.74              |
| 1:D:272:MLY:HH13 | 1:D:435:GLU:OE1  | 1.87                     | 0.74              |
| 1:A:436:MLY:HE3  | 1:A:626:TYR:CE1  | 2.22                     | 0.74              |
| 4:Z:253:GLU:HA   | 4:Z:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:G:754:ASP:HB2  | 1:G:776:GLU:CA   | 2.17                     | 0.74              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:NH2   | 2.01                     | 0.74              |
| 2:E:117:LEU:HB2  | 2:E:147:ASN:HD21 | 1.47                     | 0.74              |
| 1:J:732:ILE:N    | 1:J:733:PRO:HD2  | 2.01                     | 0.74              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HB2  | 1.82                     | 0.74              |
| 1:M:636:LYS:O    | 1:M:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:J:640:LYS:O    | 4:W:23:GLY:O     | 2.06                     | 0.74              |
| 1:A:538:GLU:O    | 4:8:349:LEU:HG   | 1.86                     | 0.74              |
| 1:A:636:LYS:O    | 1:A:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:D:215:GLN:NE2  | 1:D:336:SER:O    | 2.20                     | 0.74              |
| 4:7:288:ASP:H    | 4:9:203:THR:HG22 | 1.52                     | 0.74              |
| 1:D:350:ALA:O    | 1:D:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:D:732:ILE:HD12 | 1:D:782:MLY:HH13 | 1.68                     | 0.74              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:P:538:GLU:HA   | 4:0:349:LEU:HD12 | 0.75                     | 0.74              |
| 1:M:546:THR:O    | 4:1:46:GLY:HA3   | 1.86                     | 0.74              |
| 1:J:636:LYS:O    | 1:J:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:D:541:MET:O    | 4:9:143:TYR:CZ   | 2.40                     | 0.74              |
| 1:G:732:ILE:N    | 1:G:733:PRO:CD   | 2.51                     | 0.74              |
| 1:A:793:ARG:NH2  | 3:C:147:MET:HE3  | 2.00                     | 0.74              |
| 4:7:290:ARG:HH22 | 4:9:202:THR:HG23 | 1.50                     | 0.74              |
| 1:D:310:TYR:CE2  | 1:D:320:ILE:HD11 | 2.22                     | 0.74              |
| 1:J:272:MLY:HH13 | 1:J:435:GLU:OE1  | 1.87                     | 0.74              |
| 1:G:791:GLN:CD   | 3:I:116:GLU:HG3  | 2.08                     | 0.74              |
| 1:P:732:ILE:N    | 1:P:733:PRO:CD   | 2.51                     | 0.74              |
| 1:A:721:LYS:CB   | 1:A:736:GLN:CD   | 2.56                     | 0.74              |
| 1:M:537:GLU:HG3  | 4:Z:350:SER:O    | 1.78                     | 0.74              |
| 1:G:721:LYS:CB   | 1:G:736:GLN:CD   | 2.56                     | 0.74              |
| 1:P:836:PHE:CE2  | 2:Q:160:GLY:CA   | 2.70                     | 0.74              |
| 1:P:215:GLN:NE2  | 1:P:336:SER:O    | 2.21                     | 0.74              |
| 1:J:757:GLN:HA   | 1:J:776:GLU:CG   | 2.15                     | 0.74              |
| 4:0:253:GLU:HA   | 4:0:256:ARG:HG3  | 1.69                     | 0.74              |
| 4:X:253:GLU:HA   | 4:X:256:ARG:HG3  | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:486:MLY:HH13 | 1:P:527:GLU:OE1  | 1.87                     | 0.74              |
| 4:7:253:GLU:HA   | 4:7:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:P:640:LYS:O    | 4:0:23:GLY:O     | 2.06                     | 0.74              |
| 1:G:218:LEU:HB3  | 1:G:221:GLN:HG3  | 1.60                     | 0.74              |
| 1:M:538:GLU:O    | 4:Z:349:LEU:HG   | 1.86                     | 0.74              |
| 1:J:534:SER:O    | 4:W:351:THR:N    | 2.19                     | 0.74              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:D:530:MET:CG   | 4:9:354:GLN:CB   | 2.30                     | 0.74              |
| 1:D:636:LYS:O    | 1:D:637:LYS:HB2  | 1.86                     | 0.74              |
| 1:M:735:GLY:CA   | 1:M:743:ALA:HA   | 2.18                     | 0.74              |
| 1:A:823:PHE:HE1  | 2:B:160:GLY:HA2  | 1.52                     | 0.74              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:CB   | 2.66                     | 0.74              |
| 1:D:799:MET:SD   | 3:F:32:ASP:HA    | 2.28                     | 0.74              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HD23  | 2.22                     | 0.74              |
| 1:P:84:MLY:HH11  | 1:P:724:TYR:HE2  | 1.51                     | 0.74              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CE1   | 1.88                     | 0.74              |
| 1:P:350:ALA:O    | 1:P:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:G:350:ALA:O    | 1:G:354:LEU:HB2  | 1.87                     | 0.74              |
| 4:Y:253:GLU:HA   | 4:Y:256:ARG:HG3  | 1.69                     | 0.74              |
| 1:D:727:LEU:HG   | 1:D:782:MLY:HE2  | 1.69                     | 0.74              |
| 1:D:721:LYS:CB   | 1:D:736:GLN:CD   | 2.56                     | 0.74              |
| 1:G:797:PHE:HE2  | 3:I:126:LEU:CD2  | 1.71                     | 0.74              |
| 1:G:792:ALA:HB3  | 3:I:42:THR:CG2   | 1.91                     | 0.74              |
| 1:A:505:MLY:HD2  | 1:A:741:LYS:HZ3  | 1.51                     | 0.74              |
| 2:Q:121:LEU:CG   | 2:Q:128:PHE:HA   | 2.14                     | 0.74              |
| 2:Q:117:LEU:CB   | 2:Q:147:ASN:ND2  | 2.35                     | 0.74              |
| 2:E:114:LYS:HA   | 2:E:146:GLY:C    | 2.03                     | 0.74              |
| 1:A:732:ILE:N    | 1:A:733:PRO:CD   | 2.51                     | 0.74              |
| 1:J:84:MLY:NZ    | 1:J:724:TYR:HD2  | 1.81                     | 0.74              |
| 1:J:538:GLU:O    | 4:W:349:LEU:HG   | 1.86                     | 0.74              |
| 1:A:538:GLU:CD   | 4:8:355:MET:HE3  | 2.08                     | 0.74              |
| 1:M:735:GLY:C    | 1:M:743:ALA:HB1  | 1.84                     | 0.74              |
| 1:A:640:LYS:O    | 4:8:23:GLY:O     | 2.06                     | 0.74              |
| 1:G:829:TRP:HZ3  | 2:H:84:PHE:CZ    | 2.06                     | 0.74              |
| 1:M:94:MET:O     | 1:M:713:SER:CB   | 2.34                     | 0.74              |
| 1:D:436:MLY:HE3  | 1:D:626:TYR:CE1  | 2.23                     | 0.74              |
| 1:A:498:LEU:CD2  | 1:A:764:MLY:HH22 | 2.17                     | 0.74              |
| 1:J:732:ILE:N    | 1:J:733:PRO:CD   | 2.51                     | 0.74              |
| 1:J:410:ASN:OD1  | 4:W:335:ARG:N    | 2.21                     | 0.74              |
| 1:G:735:GLY:CA   | 1:G:743:ALA:HA   | 2.17                     | 0.74              |
| 4:0:205:GLU:CG   | 4:Y:287:ILE:CD1  | 2.66                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:409:GLY:HA3  | 4:8:333:PRO:N    | 2.02                     | 0.74              |
| 1:M:782:MLY:O    | 1:M:786:ILE:CG1  | 2.34                     | 0.74              |
| 1:D:640:LYS:O    | 4:9:23:GLY:O     | 2.06                     | 0.74              |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:HD21  | 1.67                     | 0.74              |
| 1:P:436:MLY:HE3  | 1:P:626:TYR:CE1  | 2.23                     | 0.74              |
| 1:M:436:MLY:HE3  | 1:M:626:TYR:CE1  | 2.23                     | 0.74              |
| 3:L:3:SER:O      | 3:L:4:LYS:HB2    | 1.84                     | 0.74              |
| 1:G:757:GLN:CG   | 1:G:776:GLU:CD   | 2.56                     | 0.74              |
| 1:A:97:LEU:HD22  | 1:A:712:PRO:HB2  | 1.68                     | 0.74              |
| 2:N:130:PRO:O    | 2:N:132:GLU:N    | 2.21                     | 0.74              |
| 1:G:636:LYS:O    | 1:G:637:LYS:HB2  | 1.86                     | 0.74              |
| 2:E:130:PRO:O    | 2:E:132:GLU:N    | 2.21                     | 0.74              |
| 1:P:735:GLY:CA   | 1:P:743:ALA:HA   | 2.18                     | 0.74              |
| 2:K:130:PRO:O    | 2:K:132:GLU:N    | 2.21                     | 0.74              |
| 2:B:130:PRO:O    | 2:B:132:GLU:N    | 2.21                     | 0.74              |
| 1:A:721:LYS:CA   | 1:A:736:GLN:OE1  | 2.33                     | 0.74              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:HD12 | 0.74                     | 0.74              |
| 1:J:641:LYS:HD2  | 1:J:647:GLN:OE1  | 1.81                     | 0.74              |
| 1:M:732:ILE:N    | 1:M:733:PRO:CD   | 2.51                     | 0.74              |
| 1:D:712:PRO:CB   | 1:D:771:LEU:HB2  | 2.17                     | 0.74              |
| 1:M:84:MLY:CH2   | 1:M:719:ASP:C    | 2.55                     | 0.74              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CD2   | 2.70                     | 0.74              |
| 1:G:829:TRP:CZ2  | 2:H:87:LYS:HE2   | 2.23                     | 0.74              |
| 1:D:800:ARG:HB3  | 3:F:149:VAL:CG1  | 2.18                     | 0.74              |
| 1:P:166:MET:HE1  | 1:P:254:PHE:HB2  | 1.69                     | 0.74              |
| 1:M:350:ALA:O    | 1:M:354:LEU:HB2  | 1.87                     | 0.74              |
| 1:A:486:MLY:HH13 | 1:A:527:GLU:OE1  | 1.88                     | 0.74              |
| 1:G:754:ASP:OD2  | 1:G:776:GLU:HA   | 1.88                     | 0.73              |
| 2:H:117:LEU:HB2  | 2:H:147:ASN:HD21 | 1.47                     | 0.73              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:CG   | 2.01                     | 0.73              |
| 1:P:629:GLU:HA   | 1:P:643:GLY:C    | 2.05                     | 0.73              |
| 1:P:791:GLN:NE2  | 3:R:115:GLY:HA3  | 1.99                     | 0.73              |
| 1:P:795:ARG:CB   | 3:R:35:ARG:NH2   | 2.46                     | 0.73              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HB2  | 1.82                     | 0.73              |
| 1:A:530:MET:CE   | 4:8:355:MET:SD   | 2.76                     | 0.73              |
| 1:J:710:GLY:C    | 1:J:772:LEU:HD23 | 2.08                     | 0.73              |
| 1:J:505:MLY:CG   | 1:J:762:HIS:HE1  | 1.98                     | 0.73              |
| 1:G:567:LYS:HZ1  | 4:X:92:ASN:ND2   | 1.69                     | 0.73              |
| 1:P:149:GLN:HG2  | 1:P:716:LEU:CD1  | 2.07                     | 0.73              |
| 1:P:503:TYR:CZ   | 1:P:711:PHE:CD2  | 2.75                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:800:ARG:NH2  | 3:C:40:ASN:CG    | 2.41                     | 0.73              |
| 1:G:310:TYR:CE2  | 1:G:320:ILE:HD11 | 2.22                     | 0.73              |
| 1:P:272:MLY:HH13 | 1:P:435:GLU:OE1  | 1.87                     | 0.73              |
| 1:G:635:GLY:HA3  | 4:V:341:ILE:CD1  | 2.14                     | 0.73              |
| 2:Q:114:LYS:HA   | 2:Q:146:GLY:C    | 2.03                     | 0.73              |
| 1:P:729:ALA:O    | 3:R:93:VAL:HG22  | 1.88                     | 0.73              |
| 1:P:410:ASN:OD1  | 4:O:335:ARG:N    | 2.21                     | 0.73              |
| 1:J:510:TRP:CH2  | 1:J:772:LEU:HD11 | 2.23                     | 0.73              |
| 1:D:726:VAL:HG12 | 1:D:785:GLU:HG3  | 1.62                     | 0.73              |
| 3:F:24:LYS:CA    | 3:F:63:ILE:O     | 2.36                     | 0.73              |
| 1:M:149:GLN:CD   | 1:M:763:THR:HG21 | 2.07                     | 0.73              |
| 1:D:487:LEU:O    | 1:D:490:PHE:HB3  | 1.88                     | 0.73              |
| 1:D:721:LYS:HG2  | 1:D:736:GLN:CD   | 1.86                     | 0.73              |
| 1:P:441:MET:O    | 1:P:445:ILE:HG13 | 1.88                     | 0.73              |
| 1:J:836:PHE:CZ   | 2:K:159:HIS:HA   | 2.16                     | 0.73              |
| 4:1:203:THR:HG22 | 4:Z:287:ILE:HB   | 1.69                     | 0.73              |
| 1:G:486:MLY:HH13 | 1:G:527:GLU:OE1  | 1.87                     | 0.73              |
| 1:G:410:ASN:CG   | 4:V:334:GLU:CA   | 2.47                     | 0.73              |
| 1:P:819:ASN:ND2  | 2:Q:92:ASP:CB    | 2.46                     | 0.73              |
| 1:M:505:MLY:CD   | 1:M:762:HIS:HE1  | 1.92                     | 0.73              |
| 1:M:534:SER:CA   | 4:Z:351:THR:HA   | 2.19                     | 0.73              |
| 1:D:534:SER:CA   | 4:9:351:THR:HA   | 2.19                     | 0.73              |
| 1:A:542:PHE:CD2  | 4:8:143:TYR:CE1  | 2.76                     | 0.73              |
| 4:8:253:GLU:HA   | 4:8:256:ARG:HG3  | 1.69                     | 0.73              |
| 4:V:253:GLU:HA   | 4:V:256:ARG:HG3  | 1.69                     | 0.73              |
| 1:A:502:GLU:CG   | 1:A:764:MLY:O    | 2.36                     | 0.73              |
| 1:G:410:ASN:OD1  | 4:V:335:ARG:N    | 2.21                     | 0.73              |
| 1:J:821:ARG:HH12 | 2:K:127:ARG:CZ   | 2.00                     | 0.73              |
| 1:P:530:MET:CE   | 4:O:355:MET:SD   | 2.77                     | 0.73              |
| 1:P:640:LYS:O    | 1:P:645:SER:OG   | 2.06                     | 0.73              |
| 1:J:441:MET:O    | 1:J:445:ILE:HG13 | 1.88                     | 0.73              |
| 1:M:409:GLY:HA3  | 4:Z:333:PRO:N    | 2.03                     | 0.73              |
| 1:J:629:GLU:HA   | 1:J:643:GLY:C    | 2.05                     | 0.73              |
| 1:J:534:SER:CA   | 4:W:351:THR:HA   | 2.19                     | 0.73              |
| 1:P:536:LEU:HD13 | 1:P:550:PHE:CZ   | 2.24                     | 0.73              |
| 1:M:721:LYS:CB   | 1:M:736:GLN:CD   | 2.56                     | 0.73              |
| 4:3:288:ASP:CB   | 4:5:203:THR:CG2  | 2.66                     | 0.73              |
| 1:A:310:TYR:CE2  | 1:A:320:ILE:HD11 | 2.22                     | 0.73              |
| 1:M:21:GLU:O     | 1:M:25:ILE:HG13  | 1.88                     | 0.73              |
| 1:J:795:ARG:HD2  | 3:L:43:ASN:CG    | 2.08                     | 0.73              |
| 1:D:732:ILE:N    | 1:D:733:PRO:CD   | 2.51                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:796:GLY:CA   | 3:I:35:ARG:NE    | 2.52                     | 0.73              |
| 1:G:556:ASP:CG   | 4:X:47:MET:HE2   | 1.50                     | 0.73              |
| 2:Q:117:LEU:HB2  | 2:Q:147:ASN:HD21 | 1.47                     | 0.73              |
| 1:G:733:PRO:C    | 1:G:737:PHE:CD1  | 2.62                     | 0.73              |
| 4:0:243:PRO:N    | 4:Y:291:LYS:HE3  | 2.03                     | 0.73              |
| 1:D:768:MLY:N    | 1:D:771:LEU:HD11 | 2.02                     | 0.73              |
| 1:G:838:ILE:HD11 | 2:H:54:MET:HE2   | 1.67                     | 0.73              |
| 1:P:503:TYR:CZ   | 1:P:711:PHE:HD2  | 2.06                     | 0.73              |
| 1:M:806:MET:HA   | 1:M:809:ARG:HD2  | 1.69                     | 0.73              |
| 1:P:767:PHE:CE1  | 1:P:772:LEU:HD21 | 2.23                     | 0.73              |
| 1:G:215:GLN:NE2  | 1:G:336:SER:O    | 2.20                     | 0.73              |
| 4:8:290:ARG:HH22 | 4:V:202:THR:HG23 | 1.51                     | 0.73              |
| 3:R:24:LYS:CA    | 3:R:63:ILE:O     | 2.36                     | 0.73              |
| 3:I:24:LYS:CA    | 3:I:63:ILE:O     | 2.37                     | 0.73              |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CZ   | 2.24                     | 0.73              |
| 1:G:487:LEU:O    | 1:G:490:PHE:HB3  | 1.89                     | 0.73              |
| 4:2:253:GLU:HA   | 4:2:256:ARG:HG3  | 1.69                     | 0.73              |
| 1:D:292:MET:HE3  | 1:D:309:PRO:HA   | 1.70                     | 0.73              |
| 1:D:486:MLY:HH13 | 1:D:527:GLU:OE1  | 1.88                     | 0.73              |
| 1:P:487:LEU:O    | 1:P:490:PHE:HB3  | 1.88                     | 0.73              |
| 1:J:487:LEU:O    | 1:J:490:PHE:HB3  | 1.89                     | 0.73              |
| 1:P:190:MLY:HE3  | 1:P:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:D:727:LEU:HD11 | 1:D:782:MLY:CD   | 2.09                     | 0.73              |
| 1:G:409:GLY:HA3  | 4:V:333:PRO:N    | 2.03                     | 0.73              |
| 2:H:130:PRO:O    | 2:H:132:GLU:N    | 2.21                     | 0.73              |
| 1:P:537:GLU:HG3  | 4:0:350:SER:O    | 1.78                     | 0.73              |
| 1:M:410:ASN:OD1  | 4:Z:335:ARG:N    | 2.21                     | 0.73              |
| 1:J:530:MET:CE   | 4:W:355:MET:SD   | 2.77                     | 0.73              |
| 1:D:530:MET:CE   | 4:9:355:MET:SD   | 2.77                     | 0.73              |
| 1:D:409:GLY:HA3  | 4:9:333:PRO:N    | 2.03                     | 0.73              |
| 1:D:542:PHE:CD2  | 4:9:143:TYR:CE1  | 2.77                     | 0.73              |
| 1:A:410:ASN:OD1  | 4:8:335:ARG:N    | 2.22                     | 0.73              |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CZ   | 2.24                     | 0.73              |
| 1:A:834:LEU:HD21 | 2:B:54:MET:HE3   | 0.74                     | 0.73              |
| 1:M:804:ARG:O    | 1:M:808:GLU:CG   | 2.35                     | 0.73              |
| 1:M:753:VAL:CG1  | 1:M:775:LEU:CD2  | 2.67                     | 0.73              |
| 1:A:131:TRP:C    | 1:A:132:LEU:HD12 | 2.09                     | 0.73              |
| 1:A:237:THR:HG22 | 1:A:239:ARG:H    | 1.53                     | 0.73              |
| 2:N:117:LEU:HD12 | 2:N:147:ASN:CA   | 2.19                     | 0.73              |
| 1:G:640:LYS:O    | 4:V:23:GLY:O     | 2.06                     | 0.73              |
| 1:P:534:SER:CA   | 4:0:351:THR:HA   | 2.19                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:505:MLY:CE   | 1:M:762:HIS:CE1  | 2.71                     | 0.73              |
| 1:J:529:PRO:C    | 4:W:354:GLN:CB   | 2.48                     | 0.73              |
| 1:G:730:SER:HG   | 3:I:113:THR:HG21 | 1.46                     | 0.73              |
| 4:2:288:ASP:H    | 4:4:203:THR:CG2  | 1.98                     | 0.73              |
| 1:D:640:LYS:O    | 1:D:645:SER:OG   | 2.06                     | 0.73              |
| 1:M:640:LYS:O    | 4:Z:23:GLY:O     | 2.06                     | 0.73              |
| 1:D:214:MET:HA   | 1:D:340:ILE:HD11 | 1.70                     | 0.73              |
| 1:J:215:GLN:NE2  | 1:J:336:SER:O    | 2.20                     | 0.73              |
| 1:J:802:GLU:O    | 1:J:806:MET:HG3  | 1.88                     | 0.73              |
| 1:M:131:TRP:C    | 1:M:132:LEU:HD12 | 2.09                     | 0.73              |
| 1:G:190:MLY:HE3  | 1:G:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:J:486:MLY:HH13 | 1:J:527:GLU:OE1  | 1.88                     | 0.73              |
| 1:J:735:GLY:CA   | 1:J:743:ALA:HA   | 2.18                     | 0.73              |
| 2:B:144:VAL:CB   | 2:B:153:ILE:HD11 | 2.19                     | 0.73              |
| 1:P:530:MET:HE1  | 4:0:355:MET:SD   | 2.29                     | 0.73              |
| 4:0:110:LEU:O    | 4:1:195:GLU:CA   | 2.34                     | 0.73              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:CA   | 2.18                     | 0.73              |
| 1:P:290:GLN:C    | 1:P:331:LEU:HD12 | 2.09                     | 0.73              |
| 1:D:237:THR:HG22 | 1:D:239:ARG:H    | 1.54                     | 0.73              |
| 4:4:253:GLU:HA   | 4:4:256:ARG:HG3  | 1.69                     | 0.73              |
| 1:G:802:GLU:O    | 1:G:806:MET:HG3  | 1.89                     | 0.73              |
| 1:D:508:ILE:HG12 | 1:D:766:PHE:CE1  | 2.24                     | 0.73              |
| 2:Q:130:PRO:O    | 2:Q:132:GLU:N    | 2.21                     | 0.73              |
| 1:P:733:PRO:C    | 1:P:737:PHE:CD1  | 2.62                     | 0.73              |
| 2:H:144:VAL:CB   | 2:H:153:ILE:HD11 | 2.19                     | 0.73              |
| 1:A:735:GLY:CA   | 1:A:743:ALA:HA   | 2.18                     | 0.73              |
| 1:D:441:MET:O    | 1:D:445:ILE:HG13 | 1.88                     | 0.73              |
| 1:M:733:PRO:C    | 1:M:737:PHE:CD1  | 2.62                     | 0.73              |
| 1:M:214:MET:HA   | 1:M:340:ILE:HD11 | 1.70                     | 0.73              |
| 4:9:290:ARG:HH22 | 4:W:202:THR:HG23 | 1.50                     | 0.73              |
| 1:M:739:ASP:CB   | 1:M:742:LYS:HB3  | 2.12                     | 0.73              |
| 1:M:519:LEU:N    | 1:M:519:LEU:HD12 | 2.04                     | 0.73              |
| 1:D:36:SER:O     | 1:D:52:ILE:HG12  | 1.89                     | 0.73              |
| 1:M:190:MLY:HE3  | 1:M:230:GLU:OE2  | 1.89                     | 0.73              |
| 1:M:618:THR:O    | 1:M:622:LEU:HD13 | 1.89                     | 0.73              |
| 1:M:486:MLY:HH13 | 1:M:527:GLU:OE1  | 1.88                     | 0.73              |
| 1:D:735:GLY:CA   | 1:D:743:ALA:HA   | 2.18                     | 0.72              |
| 1:D:793:ARG:NH2  | 3:F:147:MET:HE3  | 2.04                     | 0.72              |
| 1:G:797:PHE:CE2  | 3:I:146:ILE:HD12 | 2.16                     | 0.72              |
| 1:A:441:MET:O    | 1:A:445:ILE:HG13 | 1.88                     | 0.72              |
| 1:P:542:PHE:CD2  | 4:0:143:TYR:CE1  | 2.77                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:640:LYS:O    | 1:J:645:SER:OG   | 2.06                     | 0.72              |
| 1:J:409:GLY:HA3  | 4:W:333:PRO:N    | 2.03                     | 0.72              |
| 1:D:410:ASN:OD1  | 4:9:335:ARG:N    | 2.22                     | 0.72              |
| 1:A:839:MLY:CH1  | 2:B:159:HIS:HD2  | 2.02                     | 0.72              |
| 1:M:829:TRP:CZ3  | 2:N:84:PHE:CZ    | 2.76                     | 0.72              |
| 4:V:287:ILE:HD11 | 4:X:201:VAL:O    | 1.75                     | 0.72              |
| 1:J:436:MLY:HE3  | 1:J:626:TYR:CE1  | 2.23                     | 0.72              |
| 1:D:618:THR:O    | 1:D:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:M:272:MLY:HH13 | 1:M:435:GLU:OE1  | 1.88                     | 0.72              |
| 1:G:21:GLU:O     | 1:G:25:ILE:HG13  | 1.89                     | 0.72              |
| 1:M:36:SER:O     | 1:M:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:J:237:THR:HG22 | 1:J:239:ARG:H    | 1.54                     | 0.72              |
| 1:D:725:ARG:HA   | 1:D:782:MLY:CH2  | 2.19                     | 0.72              |
| 1:G:538:GLU:O    | 4:V:349:LEU:HG   | 1.87                     | 0.72              |
| 2:Q:144:VAL:CB   | 2:Q:153:ILE:HD11 | 2.19                     | 0.72              |
| 2:E:144:VAL:CB   | 2:E:153:ILE:HD11 | 2.19                     | 0.72              |
| 1:M:530:MET:CE   | 4:Z:355:MET:SD   | 2.77                     | 0.72              |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CZ   | 2.24                     | 0.72              |
| 1:M:802:GLU:O    | 1:M:806:MET:HG3  | 1.89                     | 0.72              |
| 1:G:214:MET:HA   | 1:G:340:ILE:HD11 | 1.70                     | 0.72              |
| 3:L:24:LYS:CA    | 3:L:63:ILE:O     | 2.37                     | 0.72              |
| 3:O:24:LYS:CA    | 3:O:63:ILE:O     | 2.37                     | 0.72              |
| 1:J:618:THR:O    | 1:J:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:M:487:LEU:O    | 1:M:490:PHE:HB3  | 1.88                     | 0.72              |
| 1:J:36:SER:O     | 1:J:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:J:21:GLU:O     | 1:J:25:ILE:HG13  | 1.89                     | 0.72              |
| 1:G:272:MLY:HH13 | 1:G:435:GLU:OE1  | 1.88                     | 0.72              |
| 1:J:190:MLY:HE3  | 1:J:230:GLU:OE2  | 1.89                     | 0.72              |
| 1:D:798:LEU:CD2  | 3:F:126:LEU:HD11 | 2.19                     | 0.72              |
| 1:A:707:CYS:CA   | 1:A:714:ARG:HH12 | 1.83                     | 0.72              |
| 1:P:721:LYS:CB   | 1:P:736:GLN:CD   | 2.56                     | 0.72              |
| 2:H:117:LEU:HD12 | 2:H:147:ASN:CA   | 2.19                     | 0.72              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:HE   | 1.35                     | 0.72              |
| 1:M:536:LEU:HD13 | 1:M:550:PHE:CZ   | 2.24                     | 0.72              |
| 1:G:838:ILE:CG1  | 2:H:54:MET:CE    | 2.68                     | 0.72              |
| 1:P:295:MLY:HG3  | 1:P:332:MET:CE   | 2.19                     | 0.72              |
| 3:C:24:LYS:CA    | 3:C:63:ILE:O     | 2.36                     | 0.72              |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CZ   | 2.24                     | 0.72              |
| 4:2:3:ASP:HA     | 4:2:6:THR:CB     | 2.18                     | 0.72              |
| 1:M:237:THR:HG22 | 1:M:239:ARG:H    | 1.54                     | 0.72              |
| 1:P:36:SER:O     | 1:P:52:ILE:HG12  | 1.89                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:618:THR:O    | 1:G:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:G:166:MET:HE1  | 1:G:254:PHE:HB2  | 1.71                     | 0.72              |
| 1:D:190:MLY:HE3  | 1:D:230:GLU:OE2  | 1.89                     | 0.72              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:HB2  | 0.75                     | 0.72              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:HD2  | 2.18                     | 0.72              |
| 1:G:441:MET:O    | 1:G:445:ILE:HG13 | 1.88                     | 0.72              |
| 1:J:542:PHE:CD2  | 4:W:143:TYR:CE1  | 2.77                     | 0.72              |
| 1:P:785:GLU:CG   | 3:R:81:GLN:OE1   | 2.35                     | 0.72              |
| 1:J:505:MLY:HG3  | 1:J:762:HIS:HE1  | 1.53                     | 0.72              |
| 4:3:287:ILE:HB   | 4:5:203:THR:HG22 | 1.69                     | 0.72              |
| 4:0:288:ASP:OD2  | 4:2:63:GLY:HA2   | 1.88                     | 0.72              |
| 1:J:214:MET:HA   | 1:J:340:ILE:HD11 | 1.70                     | 0.72              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:HB3  | 1.70                     | 0.72              |
| 1:A:21:GLU:O     | 1:A:25:ILE:HG13  | 1.88                     | 0.72              |
| 1:P:131:TRP:C    | 1:P:132:LEU:HD12 | 2.09                     | 0.72              |
| 1:A:505:MLY:N    | 1:A:762:HIS:NE2  | 2.38                     | 0.72              |
| 1:D:557:GLU:N    | 4:W:48:GLY:HA3   | 1.90                     | 0.72              |
| 1:A:534:SER:CA   | 4:8:351:THR:HA   | 2.18                     | 0.72              |
| 1:D:836:PHE:CE1  | 2:E:159:HIS:HB2  | 2.23                     | 0.72              |
| 1:G:830:PRO:HB3  | 2:H:67:MET:CE    | 2.10                     | 0.72              |
| 1:A:802:GLU:O    | 1:A:806:MET:HG3  | 1.89                     | 0.72              |
| 1:P:618:THR:O    | 1:P:622:LEU:HD13 | 1.89                     | 0.72              |
| 1:G:436:MLY:HE3  | 1:G:626:TYR:CE1  | 2.23                     | 0.72              |
| 1:A:272:MLY:HH13 | 1:A:435:GLU:OE1  | 1.88                     | 0.72              |
| 1:A:36:SER:O     | 1:A:52:ILE:HG12  | 1.89                     | 0.72              |
| 1:G:530:MET:CE   | 4:V:355:MET:SD   | 2.78                     | 0.72              |
| 4:1:288:ASP:H    | 4:3:203:THR:HG22 | 1.54                     | 0.72              |
| 4:1:287:ILE:HG23 | 4:3:202:THR:HB   | 0.88                     | 0.72              |
| 1:J:84:MLY:HH13  | 1:J:724:TYR:CE2  | 2.24                     | 0.72              |
| 1:P:797:PHE:HE2  | 3:R:146:ILE:HD12 | 1.49                     | 0.72              |
| 1:G:84:MLY:HH21  | 1:G:719:ASP:O    | 1.88                     | 0.72              |
| 1:D:769:ALA:C    | 1:D:774:LEU:HB2  | 2.08                     | 0.72              |
| 1:D:85:TYR:HH    | 1:D:772:LEU:HD23 | 1.45                     | 0.72              |
| 1:G:829:TRP:HZ3  | 2:H:84:PHE:CE1   | 2.06                     | 0.72              |
| 1:D:739:ASP:CB   | 1:D:742:LYS:HB3  | 2.12                     | 0.72              |
| 4:1:3:ASP:HA     | 4:1:6:THR:CB     | 2.17                     | 0.72              |
| 4:8:3:ASP:HA     | 4:8:6:THR:CB     | 2.18                     | 0.72              |
| 1:M:290:GLN:C    | 1:M:331:LEU:HD12 | 2.09                     | 0.72              |
| 1:M:486:MLY:HH22 | 1:M:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:G:237:THR:HG22 | 1:G:239:ARG:H    | 1.54                     | 0.72              |
| 1:J:131:TRP:C    | 1:J:132:LEU:HD12 | 2.09                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:144:VAL:CB   | 2:N:153:ILE:HD11 | 2.19                     | 0.72              |
| 1:P:409:GLY:HA3  | 4:0:333:PRO:N    | 2.03                     | 0.72              |
| 1:J:28:GLN:OE1   | 1:J:723:ARG:HG2  | 1.89                     | 0.72              |
| 1:M:552:ASN:CB   | 4:1:47:MET:C     | 2.12                     | 0.72              |
| 1:P:546:THR:HG21 | 4:2:48:GLY:HA2   | 1.71                     | 0.72              |
| 1:P:214:MET:HA   | 1:P:340:ILE:HD11 | 1.70                     | 0.72              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:CE   | 2.20                     | 0.72              |
| 4:7:290:ARG:NH1  | 4:9:202:THR:CG2  | 2.49                     | 0.72              |
| 4:3:3:ASP:HA     | 4:3:6:THR:CB     | 2.18                     | 0.72              |
| 1:G:176:LEU:N    | 1:G:176:LEU:HD12 | 2.05                     | 0.72              |
| 1:P:754:ASP:HB3  | 1:P:757:GLN:HG2  | 1.72                     | 0.72              |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:OE2  | 1.90                     | 0.72              |
| 1:P:762:HIS:CD2  | 1:P:762:HIS:H    | 2.07                     | 0.72              |
| 1:D:732:ILE:HD12 | 1:D:782:MLY:CH1  | 2.19                     | 0.72              |
| 1:G:797:PHE:CE1  | 3:I:146:ILE:HD13 | 2.21                     | 0.72              |
| 2:N:114:LYS:HA   | 2:N:146:GLY:C    | 2.03                     | 0.72              |
| 1:P:819:ASN:CB   | 2:Q:90:GLY:O     | 2.37                     | 0.72              |
| 1:M:800:ARG:HB3  | 3:O:149:VAL:HG21 | 1.70                     | 0.72              |
| 4:2:287:ILE:CD1  | 4:4:203:THR:HB   | 2.19                     | 0.72              |
| 1:A:641:LYS:HD2  | 1:A:647:GLN:OE1  | 1.81                     | 0.72              |
| 1:J:295:MLY:HG3  | 1:J:332:MET:CE   | 2.20                     | 0.72              |
| 1:D:290:GLN:C    | 1:D:331:LEU:HD12 | 2.09                     | 0.72              |
| 1:A:290:GLN:C    | 1:A:331:LEU:HD12 | 2.09                     | 0.72              |
| 1:D:802:GLU:O    | 1:D:806:MET:HG3  | 1.89                     | 0.72              |
| 1:P:21:GLU:O     | 1:P:25:ILE:HG13  | 1.89                     | 0.72              |
| 1:D:519:LEU:N    | 1:D:519:LEU:HD12 | 2.04                     | 0.72              |
| 1:D:733:PRO:C    | 1:D:737:PHE:HD1  | 1.88                     | 0.72              |
| 1:A:93:MET:CE    | 1:A:715:VAL:CG1  | 2.62                     | 0.72              |
| 1:J:721:LYS:CB   | 1:J:736:GLN:CD   | 2.56                     | 0.72              |
| 2:K:144:VAL:CB   | 2:K:153:ILE:HD11 | 2.19                     | 0.72              |
| 2:B:117:LEU:HD12 | 2:B:147:ASN:CA   | 2.20                     | 0.72              |
| 1:M:217:THR:C    | 1:M:221:GLN:HE21 | 1.92                     | 0.72              |
| 1:M:836:PHE:CE1  | 2:N:160:GLY:N    | 2.51                     | 0.72              |
| 1:M:730:SER:CB   | 3:O:96:LYS:HB3   | 2.19                     | 0.72              |
| 1:M:640:LYS:O    | 1:M:645:SER:OG   | 2.06                     | 0.72              |
| 4:V:286:ASP:OD1  | 4:X:203:THR:N    | 2.23                     | 0.72              |
| 3:C:4:LYS:N      | 3:C:5:ALA:O      | 2.16                     | 0.72              |
| 1:A:14:ALA:HB3   | 1:A:15:PRO:HD3   | 1.72                     | 0.72              |
| 1:A:519:LEU:HD12 | 1:A:519:LEU:N    | 2.04                     | 0.72              |
| 1:G:131:TRP:C    | 1:G:132:LEU:HD12 | 2.09                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:21:GLU:O     | 1:D:25:ILE:HG13  | 1.89                     | 0.72              |
| 1:J:791:GLN:HE21 | 3:L:115:GLY:HA3  | 1.52                     | 0.72              |
| 1:G:791:GLN:NE2  | 3:I:116:GLU:H    | 1.87                     | 0.72              |
| 1:M:553:MLY:HG2  | 4:1:43:VAL:CB    | 2.20                     | 0.72              |
| 1:P:792:ALA:HB2  | 3:R:42:THR:CA    | 2.18                     | 0.72              |
| 1:D:217:THR:C    | 1:D:221:GLN:HE21 | 1.92                     | 0.72              |
| 1:M:508:ILE:HD11 | 1:M:759:ALA:CB   | 2.20                     | 0.72              |
| 1:P:739:ASP:CB   | 1:P:742:LYS:HB3  | 2.12                     | 0.72              |
| 2:N:150:TYR:C    | 2:N:151:LYS:CG   | 2.48                     | 0.72              |
| 4:9:3:ASP:HA     | 4:9:6:THR:CB     | 2.18                     | 0.72              |
| 1:G:290:GLN:C    | 1:G:331:LEU:HD12 | 2.09                     | 0.72              |
| 1:G:534:SER:CA   | 4:V:351:THR:HA   | 2.19                     | 0.71              |
| 1:G:640:LYS:O    | 1:G:645:SER:OG   | 2.06                     | 0.71              |
| 4:1:287:ILE:HG21 | 4:3:202:THR:OG1  | 1.89                     | 0.71              |
| 2:K:136:MET:O    | 2:K:140:PHE:HB2  | 1.90                     | 0.71              |
| 1:J:84:MLY:HH21  | 1:J:720:PHE:C    | 2.10                     | 0.71              |
| 1:M:542:PHE:CD2  | 4:Z:143:TYR:CE1  | 2.77                     | 0.71              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CD1   | 2.77                     | 0.71              |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:OE2  | 1.90                     | 0.71              |
| 1:G:36:SER:O     | 1:G:52:ILE:HG12  | 1.90                     | 0.71              |
| 1:A:762:HIS:H    | 1:A:762:HIS:CD2  | 2.08                     | 0.71              |
| 1:G:542:PHE:CD2  | 4:V:143:TYR:CE1  | 2.78                     | 0.71              |
| 1:A:217:THR:O    | 1:A:220:ASP:HB2  | 1.91                     | 0.71              |
| 1:A:217:THR:C    | 1:A:221:GLN:HE21 | 1.93                     | 0.71              |
| 1:M:547:ASP:O    | 4:1:46:GLY:O     | 2.07                     | 0.71              |
| 4:Z:3:ASP:HA     | 4:Z:6:THR:CB     | 2.17                     | 0.71              |
| 1:J:176:LEU:N    | 1:J:176:LEU:HD12 | 2.05                     | 0.71              |
| 1:P:176:LEU:N    | 1:P:176:LEU:HD12 | 2.05                     | 0.71              |
| 1:J:290:GLN:C    | 1:J:331:LEU:HD12 | 2.09                     | 0.71              |
| 1:P:486:MLY:HH22 | 1:P:527:GLU:OE2  | 1.90                     | 0.71              |
| 1:D:131:TRP:C    | 1:D:132:LEU:HD12 | 2.09                     | 0.71              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CB   | 1.84                     | 0.71              |
| 1:G:795:ARG:CA   | 3:I:118:MET:CE   | 2.65                     | 0.71              |
| 1:J:817:GLN:HB3  | 2:K:127:ARG:CD   | 2.20                     | 0.71              |
| 1:A:733:PRO:C    | 1:A:737:PHE:CD1  | 2.62                     | 0.71              |
| 1:D:217:THR:O    | 1:D:220:ASP:HB2  | 1.90                     | 0.71              |
| 1:D:641:LYS:HD2  | 1:D:647:GLN:OE1  | 1.81                     | 0.71              |
| 4:0:204:ALA:CB   | 4:Y:288:ASP:CB   | 2.67                     | 0.71              |
| 1:D:769:ALA:HA   | 1:D:771:LEU:HA   | 0.75                     | 0.71              |
| 1:P:802:GLU:O    | 1:P:806:MET:HG3  | 1.89                     | 0.71              |
| 1:P:806:MET:O    | 1:P:810:ARG:N    | 2.23                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:806:MET:HA   | 1:P:809:ARG:HD2  | 1.72                     | 0.71              |
| 1:M:295:MLY:HG3  | 1:M:332:MET:CE   | 2.20                     | 0.71              |
| 1:M:754:ASP:HB3  | 1:M:757:GLN:HG2  | 1.71                     | 0.71              |
| 1:G:519:LEU:N    | 1:G:519:LEU:HD12 | 2.05                     | 0.71              |
| 1:A:190:MLY:HE3  | 1:A:230:GLU:OE2  | 1.89                     | 0.71              |
| 1:A:166:MET:HE1  | 1:A:254:PHE:HB2  | 1.72                     | 0.71              |
| 1:A:618:THR:O    | 1:A:622:LEU:HD13 | 1.89                     | 0.71              |
| 1:P:86:ASP:OD2   | 1:P:87:MLY:HH13  | 1.91                     | 0.71              |
| 2:Q:136:MET:O    | 2:Q:140:PHE:HB2  | 1.90                     | 0.71              |
| 2:B:136:MET:O    | 2:B:140:PHE:HB2  | 1.90                     | 0.71              |
| 1:G:217:THR:C    | 1:G:221:GLN:HE21 | 1.92                     | 0.71              |
| 1:M:783:LEU:CB   | 1:M:786:ILE:HD11 | 2.17                     | 0.71              |
| 1:P:217:THR:O    | 1:P:220:ASP:HB2  | 1.91                     | 0.71              |
| 1:D:823:PHE:HE1  | 2:E:161:GLU:N    | 1.88                     | 0.71              |
| 1:A:640:LYS:O    | 1:A:645:SER:OG   | 2.06                     | 0.71              |
| 1:A:214:MET:HA   | 1:A:340:ILE:HD11 | 1.71                     | 0.71              |
| 4:5:3:ASP:HA     | 4:5:6:THR:CB     | 2.18                     | 0.71              |
| 1:D:176:LEU:HD12 | 1:D:176:LEU:N    | 2.05                     | 0.71              |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:OE2  | 1.90                     | 0.71              |
| 1:A:487:LEU:O    | 1:A:490:PHE:HB3  | 1.88                     | 0.71              |
| 1:P:14:ALA:HB3   | 1:P:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:M:14:ALA:HB3   | 1:M:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:G:14:ALA:HB3   | 1:G:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:J:217:THR:C    | 1:J:221:GLN:HE21 | 1.92                     | 0.71              |
| 4:2:287:ILE:CG2  | 4:4:204:ALA:H    | 2.04                     | 0.71              |
| 4:2:287:ILE:HB   | 4:4:204:ALA:H    | 1.55                     | 0.71              |
| 1:P:217:THR:C    | 1:P:221:GLN:HE21 | 1.92                     | 0.71              |
| 1:D:831:TRP:NE1  | 2:E:51:PHE:CE2   | 2.57                     | 0.71              |
| 4:X:3:ASP:HA     | 4:X:6:THR:CB     | 2.17                     | 0.71              |
| 1:J:72:VAL:HG13  | 1:J:76:GLN:CB    | 2.19                     | 0.71              |
| 1:P:519:LEU:N    | 1:P:519:LEU:HD12 | 2.04                     | 0.71              |
| 1:D:86:ASP:OD2   | 1:D:87:MLY:HH13  | 1.91                     | 0.71              |
| 1:D:727:LEU:HB2  | 1:D:782:MLY:NZ   | 2.01                     | 0.71              |
| 1:D:793:ARG:HH21 | 3:F:147:MET:HE3  | 1.53                     | 0.71              |
| 1:A:505:MLY:CA   | 1:A:762:HIS:CD2  | 2.74                     | 0.71              |
| 1:D:762:HIS:H    | 1:D:762:HIS:CD2  | 2.08                     | 0.71              |
| 1:P:818:TYR:CE1  | 2:Q:127:ARG:CZ   | 2.72                     | 0.71              |
| 1:A:735:GLY:C    | 1:A:743:ALA:HB1  | 1.84                     | 0.71              |
| 1:M:441:MET:O    | 1:M:445:ILE:HG13 | 1.88                     | 0.71              |
| 1:A:530:MET:HE2  | 4:8:354:GLN:HG3  | 1.71                     | 0.71              |
| 1:A:839:MLY:HH13 | 2:B:159:HIS:CD2  | 2.25                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:X:291:LYS:CD   | 4:Z:243:PRO:CB   | 2.64                     | 0.71              |
| 1:J:295:MLY:HG3  | 1:J:332:MET:HE1  | 1.72                     | 0.71              |
| 1:G:829:TRP:CZ3  | 2:H:84:PHE:CE1   | 2.79                     | 0.71              |
| 1:D:245:ARG:HD3  | 1:D:271:GLU:OE1  | 1.90                     | 0.71              |
| 1:J:797:PHE:HD1  | 3:L:146:ILE:CG2  | 1.86                     | 0.71              |
| 1:G:755:HIS:N    | 1:G:779:ARG:CZ   | 2.52                     | 0.71              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:CE   | 2.19                     | 0.71              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:N    | 2.17                     | 0.71              |
| 1:D:56:GLU:CB    | 1:D:59:MLY:HB3   | 2.20                     | 0.71              |
| 1:G:274:ARG:NH2  | 1:G:282:GLU:OE1  | 2.24                     | 0.71              |
| 1:M:274:ARG:NH2  | 1:M:282:GLU:OE1  | 2.24                     | 0.71              |
| 1:A:499:GLU:CD   | 1:A:766:PHE:CZ   | 2.64                     | 0.71              |
| 1:J:721:LYS:HG2  | 1:J:736:GLN:CD   | 1.86                     | 0.71              |
| 1:J:818:TYR:CE1  | 2:K:127:ARG:NH1  | 2.59                     | 0.71              |
| 1:M:762:HIS:CD2  | 1:M:762:HIS:H    | 2.07                     | 0.71              |
| 1:D:767:PHE:C    | 1:D:771:LEU:CD1  | 2.43                     | 0.71              |
| 1:G:834:LEU:CD1  | 2:H:51:PHE:CD1   | 2.74                     | 0.71              |
| 1:J:56:GLU:CB    | 1:J:59:MLY:HB3   | 2.19                     | 0.71              |
| 4:7:3:ASP:HA     | 4:7:6:THR:CB     | 2.18                     | 0.71              |
| 1:J:274:ARG:NH2  | 1:J:282:GLU:OE1  | 2.24                     | 0.71              |
| 1:J:14:ALA:HB3   | 1:J:15:PRO:HD3   | 1.72                     | 0.71              |
| 1:J:519:LEU:HD12 | 1:J:519:LEU:N    | 2.04                     | 0.71              |
| 1:M:166:MET:HE3  | 1:M:254:PHE:CD2  | 2.26                     | 0.71              |
| 1:P:237:THR:HG22 | 1:P:239:ARG:H    | 1.54                     | 0.71              |
| 1:J:791:GLN:OE1  | 3:L:116:GLU:HG3  | 1.91                     | 0.71              |
| 1:G:753:VAL:N    | 1:G:780:ASP:OD1  | 2.24                     | 0.71              |
| 1:A:754:ASP:HB3  | 1:A:757:GLN:HG2  | 1.72                     | 0.71              |
| 2:E:136:MET:O    | 2:E:140:PHE:HB2  | 1.90                     | 0.71              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:HG23 | 0.71                     | 0.71              |
| 1:J:821:ARG:NH2  | 2:K:127:ARG:NE   | 2.38                     | 0.71              |
| 1:P:795:ARG:CG   | 3:R:118:MET:HE2  | 2.15                     | 0.71              |
| 4:1:244:ASP:N    | 4:Z:324:THR:HG21 | 1.80                     | 0.71              |
| 1:P:97:LEU:HD22  | 1:P:712:PRO:HB3  | 1.72                     | 0.71              |
| 1:P:245:ARG:HD3  | 1:P:271:GLU:OE1  | 1.90                     | 0.71              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:HG23 | 0.71                     | 0.71              |
| 1:G:728:ASN:HD21 | 3:I:114:LEU:HA   | 1.56                     | 0.71              |
| 1:J:754:ASP:HB3  | 1:J:757:GLN:HG2  | 1.72                     | 0.71              |
| 1:J:831:TRP:HH2  | 2:K:47:LEU:CD2   | 2.02                     | 0.71              |
| 1:M:829:TRP:CH2  | 2:N:87:LYS:CE    | 2.74                     | 0.71              |
| 1:A:176:LEU:HD12 | 1:A:176:LEU:N    | 2.05                     | 0.71              |
| 1:J:245:ARG:HD3  | 1:J:271:GLU:OE1  | 1.90                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:834:LEU:HD13 | 2:K:51:PHE:CE1   | 2.26                     | 0.71              |
| 1:D:723:ARG:HE   | 1:D:779:ARG:HG3  | 1.57                     | 0.70              |
| 1:A:149:GLN:HA   | 1:A:719:ASP:OD1  | 1.91                     | 0.70              |
| 1:A:787:ILE:HG22 | 1:A:788:THR:N    | 2.06                     | 0.70              |
| 1:D:834:LEU:HD21 | 2:E:54:MET:HE3   | 1.65                     | 0.70              |
| 1:D:643:GLY:N    | 4:9:24:ASP:CA    | 2.46                     | 0.70              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:CE   | 2.20                     | 0.70              |
| 4:V:3:ASP:HA     | 4:V:6:THR:CB     | 2.18                     | 0.70              |
| 1:M:56:GLU:CB    | 1:M:59:MLY:HB3   | 2.19                     | 0.70              |
| 3:L:4:LYS:N      | 3:L:5:ALA:O      | 2.16                     | 0.70              |
| 1:D:14:ALA:HB3   | 1:D:15:PRO:HD3   | 1.72                     | 0.70              |
| 1:G:557:GLU:HA   | 4:X:48:GLY:CA    | 2.18                     | 0.70              |
| 1:P:819:ASN:OD1  | 2:Q:92:ASP:CB    | 2.37                     | 0.70              |
| 1:G:217:THR:O    | 1:G:220:ASP:HB2  | 1.91                     | 0.70              |
| 1:J:217:THR:O    | 1:J:220:ASP:HB2  | 1.91                     | 0.70              |
| 1:A:831:TRP:CE3  | 2:B:34:ILE:CD1   | 2.74                     | 0.70              |
| 1:M:206:LYS:HD3  | 1:M:217:THR:HG23 | 0.71                     | 0.70              |
| 1:D:641:LYS:HD2  | 4:9:348:SER:HA   | 1.73                     | 0.70              |
| 1:D:836:PHE:HZ   | 2:E:160:GLY:H    | 1.39                     | 0.70              |
| 1:J:97:LEU:CD2   | 1:J:712:PRO:HB3  | 2.21                     | 0.70              |
| 1:A:72:VAL:HG13  | 1:A:76:GLN:CB    | 2.19                     | 0.70              |
| 1:M:176:LEU:HD12 | 1:M:176:LEU:N    | 2.05                     | 0.70              |
| 1:G:86:ASP:OD2   | 1:G:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:J:166:MET:HE1  | 1:J:254:PHE:HB2  | 1.73                     | 0.70              |
| 1:G:245:ARG:HD3  | 1:G:271:GLU:OE1  | 1.90                     | 0.70              |
| 1:D:754:ASP:HB3  | 1:D:757:GLN:HG2  | 1.72                     | 0.70              |
| 1:M:245:ARG:HD3  | 1:M:271:GLU:OE1  | 1.90                     | 0.70              |
| 1:J:86:ASP:OD2   | 1:J:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:J:800:ARG:CG   | 3:L:149:VAL:HG22 | 2.20                     | 0.70              |
| 1:D:791:GLN:OE1  | 3:F:116:GLU:N    | 2.24                     | 0.70              |
| 1:D:813:ILE:CD1  | 2:E:128:PHE:CE1  | 2.66                     | 0.70              |
| 1:D:530:MET:HE2  | 4:9:354:GLN:HG3  | 1.73                     | 0.70              |
| 1:D:577:ALA:O    | 1:D:578:HIS:CG   | 2.45                     | 0.70              |
| 1:M:217:THR:O    | 1:M:220:ASP:HB2  | 1.91                     | 0.70              |
| 1:M:796:GLY:CA   | 3:O:35:ARG:HD3   | 2.18                     | 0.70              |
| 1:P:206:LYS:HD3  | 1:P:217:THR:HG23 | 0.71                     | 0.70              |
| 1:J:641:LYS:HD2  | 4:W:348:SER:HA   | 1.73                     | 0.70              |
| 4:0:287:ILE:HG21 | 4:2:203:THR:HG22 | 0.72                     | 0.70              |
| 1:J:762:HIS:CD2  | 1:J:762:HIS:H    | 2.08                     | 0.70              |
| 1:P:630:ALA:O    | 4:0:25:ASP:HB2   | 1.91                     | 0.70              |
| 1:A:274:ARG:NH2  | 1:A:282:GLU:OE1  | 2.24                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:86:ASP:OD2   | 1:A:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:M:579:PHE:HD2  | 1:M:592:ILE:HD11 | 1.56                     | 0.70              |
| 1:P:577:ALA:O    | 1:P:578:HIS:CG   | 2.45                     | 0.70              |
| 4:2:324:THR:HG21 | 4:4:243:PRO:C    | 2.11                     | 0.70              |
| 3:I:25:ILE:O     | 3:I:63:ILE:HB    | 1.92                     | 0.70              |
| 4:1:244:ASP:C    | 4:Z:324:THR:CG2  | 2.55                     | 0.70              |
| 1:G:579:PHE:HD2  | 1:G:592:ILE:HD11 | 1.57                     | 0.70              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:HD11 | 1.73                     | 0.70              |
| 4:3:1:ASP:HA     | 4:3:4:GLU:HB3    | 1.74                     | 0.70              |
| 2:N:136:MET:O    | 2:N:140:PHE:HB2  | 1.90                     | 0.70              |
| 1:D:579:PHE:HD2  | 1:D:592:ILE:HD11 | 1.56                     | 0.70              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:CD1  | 2.69                     | 0.70              |
| 1:M:798:LEU:HD22 | 3:O:126:LEU:CD1  | 2.05                     | 0.70              |
| 4:W:324:THR:HG23 | 4:Y:247:VAL:HG22 | 1.70                     | 0.70              |
| 1:G:56:GLU:CB    | 1:G:59:MLY:HB3   | 2.19                     | 0.70              |
| 1:D:274:ARG:NH2  | 1:D:282:GLU:OE1  | 2.24                     | 0.70              |
| 1:P:274:ARG:NH2  | 1:P:282:GLU:OE1  | 2.24                     | 0.70              |
| 1:M:86:ASP:OD2   | 1:M:87:MLY:HH13  | 1.91                     | 0.70              |
| 1:D:725:ARG:CA   | 1:D:782:MLY:HH22 | 2.16                     | 0.70              |
| 1:G:792:ALA:CA   | 3:I:42:THR:HG22  | 2.21                     | 0.70              |
| 1:A:92:ALA:O     | 1:A:713:SER:HA   | 1.92                     | 0.70              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CB   | 1.85                     | 0.70              |
| 1:M:530:MET:HE3  | 4:Z:354:GLN:HG2  | 1.73                     | 0.70              |
| 1:A:546:THR:HG22 | 1:A:548:THR:N    | 2.05                     | 0.70              |
| 1:P:213:LYS:HA   | 1:P:220:ASP:OD1  | 1.92                     | 0.70              |
| 1:M:831:TRP:CZ3  | 2:N:34:ILE:HD13  | 2.27                     | 0.70              |
| 1:D:831:TRP:CD2  | 2:E:51:PHE:CZ    | 2.79                     | 0.70              |
| 1:J:630:ALA:O    | 4:W:25:ASP:HB2   | 1.91                     | 0.70              |
| 4:1:244:ASP:CG   | 4:Z:322:PRO:CB   | 2.54                     | 0.70              |
| 4:Y:3:ASP:HA     | 4:Y:6:THR:CB     | 2.18                     | 0.70              |
| 1:P:123:CYS:HB2  | 1:P:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:J:213:LYS:HA   | 1:J:220:ASP:OD1  | 1.92                     | 0.70              |
| 1:P:793:ARG:CZ   | 3:R:40:ASN:ND2   | 2.54                     | 0.70              |
| 1:M:797:PHE:HE2  | 3:O:126:LEU:CD2  | 2.04                     | 0.70              |
| 1:P:641:LYS:HD2  | 4:0:348:SER:HA   | 1.73                     | 0.70              |
| 3:C:48:LYS:HB3   | 3:C:52:ASN:HD21  | 1.57                     | 0.70              |
| 1:G:739:ASP:CB   | 1:G:742:LYS:HB3  | 2.12                     | 0.70              |
| 1:D:72:VAL:HG13  | 1:D:76:GLN:CB    | 2.20                     | 0.70              |
| 4:0:3:ASP:HA     | 4:0:6:THR:CB     | 2.18                     | 0.70              |
| 1:D:556:ASP:HA   | 4:W:49:GLN:O     | 1.70                     | 0.70              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:HD11 | 1.73                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:123:CYS:HB2  | 1:J:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:HD13 | 2.20                     | 0.70              |
| 1:P:820:VAL:CG1  | 2:Q:136:MET:HE1  | 2.22                     | 0.70              |
| 4:1:287:ILE:CG2  | 4:3:203:THR:N    | 2.55                     | 0.70              |
| 2:H:136:MET:O    | 2:H:140:PHE:HB2  | 1.90                     | 0.70              |
| 2:K:111:SER:OG   | 2:K:148:VAL:HG12 | 1.92                     | 0.70              |
| 1:P:538:GLU:CD   | 4:0:355:MET:HE3  | 2.11                     | 0.70              |
| 1:M:553:MLY:HG2  | 4:1:43:VAL:CG2   | 2.20                     | 0.70              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:OD1  | 1.92                     | 0.70              |
| 1:A:579:PHE:HD2  | 1:A:592:ILE:HD11 | 1.57                     | 0.70              |
| 1:G:97:LEU:HD21  | 1:G:712:PRO:CB   | 2.22                     | 0.70              |
| 1:P:93:MET:HA    | 1:P:714:ARG:H    | 1.56                     | 0.70              |
| 1:D:831:TRP:HZ3  | 2:E:50:THR:HG21  | 1.55                     | 0.70              |
| 4:X:1:ASP:HA     | 4:X:4:GLU:HB3    | 1.74                     | 0.70              |
| 1:D:725:ARG:O    | 1:D:782:MLY:HH22 | 1.90                     | 0.70              |
| 1:G:791:GLN:NE2  | 3:I:116:GLU:N    | 2.39                     | 0.70              |
| 1:G:797:PHE:HE2  | 3:I:126:LEU:CG   | 2.05                     | 0.70              |
| 1:M:530:MET:HE2  | 4:Z:354:GLN:HG3  | 1.73                     | 0.70              |
| 1:A:537:GLU:HG3  | 4:8:350:SER:O    | 1.79                     | 0.70              |
| 1:P:838:ILE:HD11 | 2:Q:54:MET:SD    | 2.31                     | 0.70              |
| 1:M:810:ARG:HH11 | 1:M:810:ARG:HG2  | 1.57                     | 0.70              |
| 1:P:806:MET:O    | 1:P:809:ARG:HB2  | 1.92                     | 0.70              |
| 1:J:757:GLN:NE2  | 1:J:777:GLU:H    | 1.88                     | 0.70              |
| 1:D:630:ALA:O    | 4:9:25:ASP:HB2   | 1.92                     | 0.70              |
| 1:J:829:TRP:CZ2  | 2:K:83:MET:CE    | 2.74                     | 0.70              |
| 1:J:577:ALA:O    | 1:J:578:HIS:CG   | 2.45                     | 0.70              |
| 1:G:546:THR:HG22 | 1:G:548:THR:N    | 2.05                     | 0.70              |
| 3:O:4:LYS:N      | 3:O:5:ALA:O      | 2.16                     | 0.70              |
| 4:1:1:ASP:HA     | 4:1:4:GLU:HB3    | 1.74                     | 0.70              |
| 1:A:245:ARG:HD3  | 1:A:271:GLU:OE1  | 1.90                     | 0.70              |
| 2:Q:117:LEU:CB   | 2:Q:147:ASN:OD1  | 2.39                     | 0.70              |
| 1:A:802:GLU:OE1  | 1:A:802:GLU:HA   | 1.92                     | 0.70              |
| 1:D:810:ARG:HH11 | 1:D:810:ARG:HG2  | 1.57                     | 0.70              |
| 1:M:123:CYS:HB2  | 1:M:158:ILE:HD11 | 1.73                     | 0.70              |
| 1:G:810:ARG:HH11 | 1:G:810:ARG:HG2  | 1.56                     | 0.70              |
| 1:D:732:ILE:HG21 | 1:D:747:LEU:HD11 | 0.72                     | 0.69              |
| 2:N:117:LEU:CB   | 2:N:147:ASN:OD1  | 2.39                     | 0.69              |
| 1:G:643:GLY:N    | 4:V:24:ASP:CA    | 2.47                     | 0.69              |
| 2:Q:111:SER:OG   | 2:Q:148:VAL:HG12 | 1.92                     | 0.69              |
| 1:P:541:MET:CG   | 4:0:345:ILE:O    | 2.40                     | 0.69              |
| 1:M:218:LEU:HB2  | 1:M:221:GLN:CG   | 2.09                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:823:PHE:CD1  | 2:E:160:GLY:HA3  | 2.24                     | 0.69              |
| 4:0:287:ILE:HG21 | 4:2:203:THR:CB   | 2.22                     | 0.69              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:CA    | 2.75                     | 0.69              |
| 1:G:769:ALA:O    | 1:G:773:GLY:HA3  | 1.91                     | 0.69              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:HA   | 1.90                     | 0.69              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:HD11 | 1.26                     | 0.69              |
| 1:D:218:LEU:HB2  | 1:D:221:GLN:CG   | 2.09                     | 0.69              |
| 1:A:782:MLY:C    | 1:A:783:LEU:HD12 | 2.22                     | 0.69              |
| 4:0:201:VAL:H    | 4:Y:287:ILE:HG12 | 0.89                     | 0.69              |
| 1:P:579:PHE:HD2  | 1:P:592:ILE:HD11 | 1.56                     | 0.69              |
| 1:A:577:ALA:O    | 1:A:578:HIS:CG   | 2.45                     | 0.69              |
| 1:J:630:ALA:O    | 4:W:25:ASP:CB    | 2.41                     | 0.69              |
| 1:J:579:PHE:HD2  | 1:J:592:ILE:HD11 | 1.57                     | 0.69              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:HD11 | 1.73                     | 0.69              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:OD1  | 2.39                     | 0.69              |
| 1:J:817:GLN:HG3  | 2:K:128:PHE:CE1  | 2.26                     | 0.69              |
| 1:J:819:ASN:HD21 | 2:K:92:ASP:HB2   | 1.49                     | 0.69              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:HG23 | 0.71                     | 0.69              |
| 1:M:641:LYS:HD2  | 4:Z:348:SER:HA   | 1.72                     | 0.69              |
| 4:W:324:THR:HG23 | 4:Y:247:VAL:H    | 1.45                     | 0.69              |
| 1:P:630:ALA:O    | 4:0:25:ASP:CB    | 2.41                     | 0.69              |
| 1:G:72:VAL:HG13  | 1:G:76:GLN:CB    | 2.19                     | 0.69              |
| 4:Z:1:ASP:HA     | 4:Z:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:P:732:ILE:HG21 | 1:P:747:LEU:HD11 | 0.73                     | 0.69              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CB   | 1.84                     | 0.69              |
| 1:M:505:MLY:HH23 | 1:M:762:HIS:ND1  | 2.07                     | 0.69              |
| 1:M:577:ALA:O    | 1:M:578:HIS:CG   | 2.45                     | 0.69              |
| 1:P:797:PHE:CE2  | 3:R:146:ILE:HG23 | 2.27                     | 0.69              |
| 1:P:546:THR:HG22 | 1:P:548:THR:N    | 2.05                     | 0.69              |
| 1:G:28:GLN:HB3   | 1:G:723:ARG:NH1  | 2.06                     | 0.69              |
| 1:A:641:LYS:HD2  | 4:8:348:SER:HA   | 1.73                     | 0.69              |
| 1:M:802:GLU:HA   | 1:M:802:GLU:OE1  | 1.93                     | 0.69              |
| 1:P:810:ARG:HH11 | 1:P:810:ARG:HG2  | 1.57                     | 0.69              |
| 1:J:215:GLN:CA   | 1:J:340:ILE:CG2  | 2.62                     | 0.69              |
| 3:O:25:ILE:O     | 3:O:63:ILE:HB    | 1.92                     | 0.69              |
| 1:P:72:VAL:HG13  | 1:P:76:GLN:CB    | 2.19                     | 0.69              |
| 1:G:762:HIS:H    | 1:G:762:HIS:CD2  | 2.08                     | 0.69              |
| 1:J:810:ARG:HH11 | 1:J:810:ARG:HG2  | 1.57                     | 0.69              |
| 1:J:782:MLY:C    | 1:J:783:LEU:HD12 | 2.22                     | 0.69              |
| 2:N:111:SER:OG   | 2:N:148:VAL:HG12 | 1.92                     | 0.69              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:ND2  | 2.35                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:546:THR:HG22 | 1:M:548:THR:N    | 2.05                     | 0.69              |
| 1:J:530:MET:HE2  | 4:W:354:GLN:HG3  | 1.74                     | 0.69              |
| 1:M:787:ILE:HG22 | 1:M:788:THR:N    | 2.07                     | 0.69              |
| 1:G:641:LYS:HD2  | 4:V:348:SER:HA   | 1.73                     | 0.69              |
| 3:F:25:ILE:O     | 3:F:63:ILE:HB    | 1.92                     | 0.69              |
| 1:M:97:LEU:HD22  | 1:M:712:PRO:CB   | 2.21                     | 0.69              |
| 1:P:56:GLU:CB    | 1:P:59:MLY:HB3   | 2.19                     | 0.69              |
| 1:J:218:LEU:HB2  | 1:J:221:GLN:CG   | 2.09                     | 0.69              |
| 1:D:541:MET:CG   | 4:9:345:ILE:O    | 2.41                     | 0.69              |
| 1:D:553:MLY:HG2  | 4:W:47:MET:N     | 2.07                     | 0.69              |
| 1:P:218:LEU:HB2  | 1:P:221:GLN:CG   | 2.09                     | 0.69              |
| 4:0:243:PRO:CB   | 4:Y:291:LYS:HE3  | 2.23                     | 0.69              |
| 1:M:642:LYS:HB3  | 4:Z:21:PHE:O     | 1.92                     | 0.69              |
| 1:D:831:TRP:HZ2  | 2:E:47:LEU:CA    | 2.04                     | 0.69              |
| 3:F:4:LYS:N      | 3:F:5:ALA:O      | 2.16                     | 0.69              |
| 1:J:791:GLN:CD   | 3:L:116:GLU:HG3  | 2.13                     | 0.69              |
| 1:J:801:VAL:CG2  | 3:L:126:LEU:CD2  | 2.69                     | 0.69              |
| 1:A:813:ILE:HG21 | 2:B:127:ARG:CD   | 1.98                     | 0.69              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:HG23 | 0.70                     | 0.69              |
| 1:J:537:GLU:HG3  | 4:W:350:SER:O    | 1.78                     | 0.69              |
| 1:P:782:MLY:C    | 1:P:783:LEU:HD12 | 2.22                     | 0.69              |
| 1:M:506:GLU:OE2  | 1:M:760:PHE:C    | 2.30                     | 0.69              |
| 1:P:831:TRP:CZ2  | 2:Q:47:LEU:HD21  | 2.24                     | 0.69              |
| 1:P:807:VAL:O    | 1:P:810:ARG:HB2  | 1.93                     | 0.69              |
| 1:J:739:ASP:CB   | 1:J:742:LYS:HB3  | 2.12                     | 0.69              |
| 3:R:48:LYS:HB3   | 3:R:52:ASN:HD21  | 1.57                     | 0.69              |
| 3:R:25:ILE:O     | 3:R:63:ILE:HB    | 1.92                     | 0.69              |
| 1:J:546:THR:HG22 | 1:J:548:THR:N    | 2.05                     | 0.69              |
| 1:M:97:LEU:HD22  | 1:M:712:PRO:HB3  | 1.73                     | 0.69              |
| 4:W:3:ASP:HA     | 4:W:6:THR:CB     | 2.18                     | 0.69              |
| 1:G:577:ALA:O    | 1:G:578:HIS:CG   | 2.45                     | 0.69              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:CD1  | 2.23                     | 0.69              |
| 4:V:1:ASP:HA     | 4:V:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:D:733:PRO:C    | 1:D:737:PHE:CD1  | 2.62                     | 0.69              |
| 1:G:796:GLY:CA   | 3:I:35:ARG:CZ    | 2.71                     | 0.69              |
| 1:G:795:ARG:NH2  | 3:I:116:GLU:CD   | 2.44                     | 0.69              |
| 1:M:817:GLN:CB   | 2:N:127:ARG:HD3  | 2.21                     | 0.69              |
| 1:P:815:CYS:O    | 1:P:819:ASN:HB2  | 1.93                     | 0.69              |
| 1:P:817:GLN:CG   | 2:Q:127:ARG:HB2  | 2.22                     | 0.69              |
| 1:P:820:VAL:CG1  | 2:Q:136:MET:CE   | 2.71                     | 0.69              |
| 2:B:117:LEU:CB   | 2:B:147:ASN:OD1  | 2.39                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:813:ILE:HG22 | 2:B:127:ARG:HD2  | 0.69                     | 0.69              |
| 1:M:410:ASN:CG   | 4:Z:334:GLU:CA   | 2.47                     | 0.69              |
| 1:M:533:PHE:O    | 1:M:537:GLU:HG2  | 1.93                     | 0.69              |
| 1:P:793:ARG:HA   | 3:R:40:ASN:HB3   | 1.73                     | 0.69              |
| 1:A:553:MLY:HG2  | 4:V:47:MET:N     | 2.07                     | 0.69              |
| 1:G:506:GLU:OE2  | 1:G:760:PHE:HB2  | 1.91                     | 0.69              |
| 1:M:831:TRP:NE1  | 2:N:67:MET:HB3   | 2.08                     | 0.69              |
| 1:D:642:LYS:HB3  | 4:9:21:PHE:O     | 1.93                     | 0.69              |
| 1:A:642:LYS:HB3  | 4:8:21:PHE:O     | 1.92                     | 0.69              |
| 1:P:727:LEU:HG   | 1:P:779:ARG:NH2  | 2.04                     | 0.69              |
| 1:A:630:ALA:O    | 4:8:25:ASP:HB2   | 1.92                     | 0.69              |
| 1:J:829:TRP:HZ2  | 2:K:83:MET:HE3   | 1.56                     | 0.69              |
| 3:I:48:LYS:HB3   | 3:I:52:ASN:HD21  | 1.56                     | 0.69              |
| 3:L:25:ILE:O     | 3:L:63:ILE:HB    | 1.92                     | 0.69              |
| 4:4:3:ASP:HA     | 4:4:6:THR:CB     | 2.18                     | 0.69              |
| 1:J:166:MET:HE3  | 1:J:254:PHE:CD2  | 2.28                     | 0.69              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:CD1  | 2.23                     | 0.69              |
| 1:P:123:CYS:HB2  | 1:P:158:ILE:CD1  | 2.23                     | 0.69              |
| 1:D:807:VAL:O    | 1:D:810:ARG:HB2  | 1.93                     | 0.69              |
| 1:A:810:ARG:HG2  | 1:A:810:ARG:HH11 | 1.57                     | 0.69              |
| 4:4:1:ASP:HA     | 4:4:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:J:795:ARG:HG2  | 3:L:118:MET:CE   | 2.19                     | 0.69              |
| 1:D:782:MLY:C    | 1:D:783:LEU:HD12 | 2.22                     | 0.69              |
| 2:H:111:SER:OG   | 2:H:148:VAL:HG12 | 1.92                     | 0.69              |
| 1:J:538:GLU:CD   | 4:W:355:MET:HE1  | 2.12                     | 0.69              |
| 1:D:713:SER:O    | 1:D:771:LEU:HD21 | 1.91                     | 0.69              |
| 1:M:652:LEU:O    | 1:M:655:GLU:N    | 2.26                     | 0.69              |
| 1:M:806:MET:O    | 1:M:809:ARG:HB2  | 1.93                     | 0.69              |
| 1:M:215:GLN:CA   | 1:M:340:ILE:CG2  | 2.62                     | 0.69              |
| 1:M:630:ALA:O    | 4:Z:25:ASP:HB2   | 1.92                     | 0.69              |
| 1:M:630:ALA:O    | 4:Z:25:ASP:CB    | 2.41                     | 0.69              |
| 3:I:3:SER:O      | 3:I:4:LYS:CB     | 2.41                     | 0.69              |
| 4:5:1:ASP:HA     | 4:5:4:GLU:HB3    | 1.74                     | 0.69              |
| 4:7:1:ASP:HA     | 4:7:4:GLU:HB3    | 1.74                     | 0.69              |
| 1:D:787:ILE:HG22 | 1:D:788:THR:N    | 2.07                     | 0.69              |
| 1:G:556:ASP:OD2  | 4:X:47:MET:CE    | 2.39                     | 0.69              |
| 1:D:815:CYS:O    | 1:D:819:ASN:HB2  | 1.93                     | 0.69              |
| 1:A:815:CYS:O    | 1:A:819:ASN:HB2  | 1.93                     | 0.69              |
| 4:Y:1:ASP:HA     | 4:Y:4:GLU:HB3    | 1.74                     | 0.69              |
| 2:E:117:LEU:HD12 | 2:E:147:ASN:CA   | 2.19                     | 0.68              |
| 1:P:538:GLU:CD   | 4:0:355:MET:CE   | 2.62                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:834:LEU:CD2  | 2:B:54:MET:HE2   | 1.92                     | 0.68              |
| 3:L:48:LYS:C     | 3:L:52:ASN:HD21  | 1.96                     | 0.68              |
| 1:M:72:VAL:HG13  | 1:M:76:GLN:CB    | 2.19                     | 0.68              |
| 1:P:62:VAL:HG12  | 1:P:63:MLY:O     | 1.93                     | 0.68              |
| 3:O:3:SER:O      | 3:O:4:LYS:CB     | 2.41                     | 0.68              |
| 4:9:1:ASP:HA     | 4:9:4:GLU:HB3    | 1.74                     | 0.68              |
| 4:0:1:ASP:HA     | 4:0:4:GLU:HB3    | 1.74                     | 0.68              |
| 1:A:498:LEU:HD23 | 1:A:764:MLY:HH22 | 1.75                     | 0.68              |
| 1:M:817:GLN:CB   | 2:N:127:ARG:NH1  | 2.38                     | 0.68              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG2   | 2.21                     | 0.68              |
| 2:Q:117:LEU:HD12 | 2:Q:147:ASN:CA   | 2.19                     | 0.68              |
| 1:G:815:CYS:O    | 1:G:819:ASN:HB2  | 1.93                     | 0.68              |
| 2:B:111:SER:OG   | 2:B:148:VAL:HG12 | 1.92                     | 0.68              |
| 1:J:541:MET:CG   | 4:W:345:ILE:O    | 2.40                     | 0.68              |
| 1:J:538:GLU:CD   | 4:W:355:MET:CE   | 2.62                     | 0.68              |
| 1:P:788:THR:O    | 3:R:42:THR:CG2   | 2.41                     | 0.68              |
| 1:M:213:LYS:HA   | 1:M:220:ASP:OD1  | 1.92                     | 0.68              |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:CB   | 1.84                     | 0.68              |
| 1:M:807:VAL:O    | 1:M:810:ARG:HB2  | 1.93                     | 0.68              |
| 3:O:48:LYS:HB3   | 3:O:52:ASN:HD21  | 1.57                     | 0.68              |
| 1:D:62:VAL:HG12  | 1:D:63:MLY:O     | 1.93                     | 0.68              |
| 3:F:3:SER:O      | 3:F:4:LYS:CB     | 2.41                     | 0.68              |
| 4:8:1:ASP:HA     | 4:8:4:GLU:HB3    | 1.74                     | 0.68              |
| 1:M:815:CYS:O    | 1:M:819:ASN:HB2  | 1.93                     | 0.68              |
| 1:G:533:PHE:O    | 1:G:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:G:652:LEU:O    | 1:G:655:GLU:N    | 2.27                     | 0.68              |
| 1:J:530:MET:HE3  | 4:W:354:GLN:HG2  | 1.72                     | 0.68              |
| 1:A:795:ARG:CB   | 3:C:35:ARG:NH2   | 2.51                     | 0.68              |
| 1:P:831:TRP:CH2  | 2:Q:47:LEU:HD23  | 2.22                     | 0.68              |
| 1:P:802:GLU:OE1  | 1:P:802:GLU:HA   | 1.93                     | 0.68              |
| 1:D:630:ALA:O    | 4:9:25:ASP:CB    | 2.41                     | 0.68              |
| 3:C:3:SER:O      | 3:C:4:LYS:CB     | 2.41                     | 0.68              |
| 4:3:160:THR:HG21 | 4:3:274:ILE:HD11 | 1.76                     | 0.68              |
| 1:J:797:PHE:CG   | 3:L:146:ILE:CG2  | 2.61                     | 0.68              |
| 1:G:755:HIS:CE1  | 1:G:779:ARG:HH12 | 2.06                     | 0.68              |
| 1:G:782:MLY:C    | 1:G:783:LEU:HD12 | 2.22                     | 0.68              |
| 1:G:784:ALA:O    | 1:G:788:THR:HB   | 1.94                     | 0.68              |
| 1:G:798:LEU:CD2  | 3:I:118:MET:HB3  | 2.22                     | 0.68              |
| 2:E:111:SER:OG   | 2:E:148:VAL:HG12 | 1.92                     | 0.68              |
| 4:X:324:THR:CG2  | 4:Z:246:GLN:HA   | 2.23                     | 0.68              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:OD1  | 1.92                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:213:LYS:HA   | 1:G:220:ASP:OD1  | 1.92                     | 0.68              |
| 1:M:408:VAL:HG12 | 4:Z:332:PRO:HB3  | 1.76                     | 0.68              |
| 1:M:548:THR:O    | 4:1:47:MET:CB    | 2.42                     | 0.68              |
| 1:P:787:ILE:HG22 | 1:P:788:THR:N    | 2.07                     | 0.68              |
| 1:M:52:ILE:N     | 1:M:52:ILE:HD13  | 2.09                     | 0.68              |
| 4:W:1:ASP:HA     | 4:W:4:GLU:HB3    | 1.74                     | 0.68              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:OE1  | 2.27                     | 0.68              |
| 1:G:757:GLN:HG2  | 1:G:776:GLU:CD   | 2.14                     | 0.68              |
| 1:G:787:ILE:HG22 | 1:G:788:THR:N    | 2.07                     | 0.68              |
| 1:J:815:CYS:O    | 1:J:819:ASN:HB2  | 1.93                     | 0.68              |
| 1:J:533:PHE:O    | 1:J:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:M:806:MET:C    | 1:M:809:ARG:HB2  | 2.13                     | 0.68              |
| 1:A:652:LEU:O    | 1:A:655:GLU:N    | 2.27                     | 0.68              |
| 3:L:48:LYS:HB3   | 3:L:52:ASN:HD21  | 1.57                     | 0.68              |
| 1:A:52:ILE:HD13  | 1:A:52:ILE:N     | 2.08                     | 0.68              |
| 1:D:802:GLU:HA   | 1:D:802:GLU:OE1  | 1.93                     | 0.68              |
| 4:W:160:THR:HG21 | 4:W:274:ILE:HD11 | 1.76                     | 0.68              |
| 4:9:160:THR:HG21 | 4:9:274:ILE:HD11 | 1.76                     | 0.68              |
| 4:2:1:ASP:HA     | 4:2:4:GLU:HB3    | 1.74                     | 0.68              |
| 4:Y:160:THR:HG21 | 4:Y:274:ILE:HD11 | 1.76                     | 0.68              |
| 1:J:787:ILE:HG22 | 1:J:788:THR:N    | 2.07                     | 0.68              |
| 1:D:538:GLU:CD   | 4:9:355:MET:CE   | 2.62                     | 0.68              |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:CD1   | 2.27                     | 0.68              |
| 1:D:800:ARG:CG   | 3:F:149:VAL:HG22 | 2.23                     | 0.68              |
| 4:0:160:THR:HG21 | 4:0:274:ILE:HD11 | 1.76                     | 0.68              |
| 1:G:292:MET:HE3  | 1:G:309:PRO:HA   | 1.75                     | 0.68              |
| 1:J:292:MET:HE3  | 1:J:309:PRO:HA   | 1.74                     | 0.68              |
| 4:7:160:THR:HG21 | 4:7:274:ILE:HD11 | 1.76                     | 0.68              |
| 1:A:93:MET:C     | 1:A:713:SER:HB3  | 2.14                     | 0.68              |
| 1:P:642:LYS:HB3  | 4:0:21:PHE:O     | 1.92                     | 0.68              |
| 1:M:541:MET:CG   | 4:Z:345:ILE:O    | 2.40                     | 0.68              |
| 1:J:642:LYS:HB3  | 4:W:21:PHE:O     | 1.92                     | 0.68              |
| 1:D:533:PHE:O    | 1:D:537:GLU:HG2  | 1.93                     | 0.68              |
| 1:M:782:MLY:C    | 1:M:783:LEU:HD12 | 2.22                     | 0.68              |
| 1:D:712:PRO:CD   | 1:D:771:LEU:HD13 | 2.23                     | 0.68              |
| 1:A:630:ALA:O    | 4:8:25:ASP:CB    | 2.41                     | 0.68              |
| 1:G:52:ILE:HD13  | 1:G:52:ILE:N     | 2.09                     | 0.68              |
| 1:M:123:CYS:HB2  | 1:M:158:ILE:CD1  | 2.23                     | 0.68              |
| 4:2:153:LEU:HD11 | 4:2:274:ILE:HG13 | 1.76                     | 0.68              |
| 1:A:499:GLU:OE2  | 1:A:766:PHE:CE2  | 2.47                     | 0.68              |
| 1:G:408:VAL:HG12 | 4:V:332:PRO:HB3  | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:556:ASP:OD2  | 4:X:47:MET:HE2   | 1.91                     | 0.68              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:OD1  | 2.39                     | 0.68              |
| 1:M:550:PHE:HE2  | 1:M:592:ILE:HG23 | 1.59                     | 0.68              |
| 1:P:550:PHE:HE2  | 1:P:592:ILE:HG23 | 1.59                     | 0.68              |
| 1:P:806:MET:CA   | 1:P:809:ARG:HB2  | 2.23                     | 0.68              |
| 1:J:829:TRP:CE2  | 2:K:87:LYS:CE    | 2.76                     | 0.68              |
| 3:C:25:ILE:O     | 3:C:63:ILE:HB    | 1.92                     | 0.68              |
| 3:R:3:SER:O      | 3:R:4:LYS:CB     | 2.41                     | 0.68              |
| 1:J:802:GLU:OE1  | 1:J:802:GLU:HA   | 1.93                     | 0.68              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:CD1  | 2.23                     | 0.68              |
| 1:A:807:VAL:O    | 1:A:810:ARG:HB2  | 1.93                     | 0.68              |
| 1:P:292:MET:HE3  | 1:P:309:PRO:HA   | 1.74                     | 0.68              |
| 1:D:795:ARG:HH22 | 3:F:116:GLU:CD   | 1.93                     | 0.68              |
| 1:G:541:MET:CG   | 4:V:345:ILE:O    | 2.41                     | 0.68              |
| 1:D:550:PHE:HE2  | 1:D:592:ILE:HG23 | 1.59                     | 0.68              |
| 4:0:202:THR:OG1  | 4:Y:286:ASP:C    | 2.29                     | 0.68              |
| 1:D:713:SER:HB3  | 1:D:775:LEU:HD22 | 1.75                     | 0.68              |
| 1:M:806:MET:CA   | 1:M:809:ARG:HB2  | 2.23                     | 0.68              |
| 1:J:826:VAL:CG2  | 2:K:88:LEU:CD2   | 2.55                     | 0.68              |
| 1:P:806:MET:C    | 1:P:809:ARG:HB2  | 2.14                     | 0.68              |
| 3:F:48:LYS:HB3   | 3:F:52:ASN:HD21  | 1.57                     | 0.68              |
| 2:Q:150:TYR:C    | 2:Q:151:LYS:CG   | 2.48                     | 0.68              |
| 1:G:550:PHE:HE2  | 1:G:592:ILE:HG23 | 1.59                     | 0.68              |
| 4:1:322:PRO:CB   | 4:3:244:ASP:HB2  | 2.23                     | 0.68              |
| 1:A:56:GLU:CB    | 1:A:59:MLY:HB3   | 2.19                     | 0.68              |
| 1:J:62:VAL:HG12  | 1:J:63:MLY:O     | 1.94                     | 0.68              |
| 1:A:166:MET:HE3  | 1:A:254:PHE:CD2  | 2.29                     | 0.68              |
| 1:G:807:VAL:O    | 1:G:810:ARG:HB2  | 1.93                     | 0.68              |
| 1:J:807:VAL:O    | 1:J:810:ARG:HB2  | 1.93                     | 0.68              |
| 1:G:538:GLU:CD   | 4:V:355:MET:CE   | 2.62                     | 0.68              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:HB3  | 2.24                     | 0.68              |
| 2:K:117:LEU:HD12 | 2:K:147:ASN:CA   | 2.19                     | 0.68              |
| 1:M:505:MLY:HH23 | 1:M:762:HIS:CE1  | 2.29                     | 0.68              |
| 1:M:538:GLU:CD   | 4:Z:355:MET:CE   | 2.62                     | 0.68              |
| 1:P:795:ARG:NE   | 3:R:116:GLU:OE2  | 2.27                     | 0.68              |
| 1:P:798:LEU:CG   | 3:R:126:LEU:CD1  | 2.44                     | 0.68              |
| 1:D:538:GLU:CD   | 4:9:355:MET:HE1  | 2.13                     | 0.68              |
| 1:A:799:MET:HE1  | 3:C:32:ASP:HB3   | 1.73                     | 0.68              |
| 4:1:203:THR:CB   | 4:Z:288:ASP:OD2  | 2.42                     | 0.68              |
| 3:O:102:VAL:HG23 | 3:O:139:TYR:HD1  | 1.59                     | 0.68              |
| 1:G:802:GLU:OE1  | 1:G:802:GLU:HA   | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:166:MET:HE3  | 1:M:254:PHE:HD2  | 1.59                     | 0.68              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:CD1  | 2.23                     | 0.68              |
| 4:4:153:LEU:HD11 | 4:4:274:ILE:HG13 | 1.76                     | 0.68              |
| 1:A:502:GLU:C    | 1:A:761:GLY:CA   | 2.60                     | 0.67              |
| 1:G:642:LYS:HB3  | 4:V:21:PHE:O     | 1.92                     | 0.67              |
| 1:D:819:ASN:ND2  | 2:E:90:GLY:O     | 2.26                     | 0.67              |
| 1:A:408:VAL:HG12 | 4:8:332:PRO:HB3  | 1.76                     | 0.67              |
| 4:1:203:THR:HG21 | 4:Z:288:ASP:CB   | 2.25                     | 0.67              |
| 4:3:288:ASP:CB   | 4:5:203:THR:HG21 | 2.25                     | 0.67              |
| 1:D:652:LEU:O    | 1:D:655:GLU:N    | 2.26                     | 0.67              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:N    | 2.43                     | 0.67              |
| 4:X:160:THR:HG21 | 4:X:274:ILE:HD11 | 1.76                     | 0.67              |
| 1:A:58:GLY:HA2   | 1:A:74:GLU:OE1   | 1.95                     | 0.67              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:HH22  | 2.06                     | 0.67              |
| 2:B:141:PRO:O    | 2:B:145:ALA:CB   | 2.43                     | 0.67              |
| 1:J:643:GLY:N    | 4:W:24:ASP:CA    | 2.46                     | 0.67              |
| 1:D:546:THR:HG22 | 1:D:548:THR:N    | 2.05                     | 0.67              |
| 1:A:541:MET:CG   | 4:8:345:ILE:O    | 2.40                     | 0.67              |
| 1:A:546:THR:H    | 1:A:549:SER:HB3  | 1.59                     | 0.67              |
| 1:G:838:ILE:CD1  | 2:H:54:MET:HE1   | 2.13                     | 0.67              |
| 1:P:148:ARG:NH2  | 1:P:764:MLY:HH21 | 2.09                     | 0.67              |
| 4:V:325:MET:CE   | 4:X:244:ASP:CB   | 2.70                     | 0.67              |
| 2:B:150:TYR:C    | 2:B:151:LYS:CG   | 2.48                     | 0.67              |
| 1:P:799:MET:SD   | 3:R:32:ASP:CB    | 2.83                     | 0.67              |
| 1:M:290:GLN:O    | 1:M:331:LEU:HD12 | 1.95                     | 0.67              |
| 3:L:3:SER:O      | 3:L:4:LYS:CB     | 2.41                     | 0.67              |
| 4:Y:153:LEU:HD11 | 4:Y:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:0:153:LEU:HD11 | 4:0:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:1:160:THR:HG21 | 4:1:274:ILE:HD11 | 1.76                     | 0.67              |
| 1:G:788:THR:C    | 3:I:42:THR:HG21  | 2.13                     | 0.67              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:HB3  | 2.24                     | 0.67              |
| 1:P:546:THR:H    | 1:P:549:SER:HB3  | 1.59                     | 0.67              |
| 1:A:530:MET:HE3  | 4:8:354:GLN:HG2  | 1.76                     | 0.67              |
| 1:P:806:MET:C    | 1:P:807:VAL:CA   | 2.63                     | 0.67              |
| 1:J:374:GLN:HG3  | 1:J:375:ALA:H    | 1.59                     | 0.67              |
| 1:M:166:MET:HE1  | 1:M:254:PHE:HB2  | 1.76                     | 0.67              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:CA   | 2.72                     | 0.67              |
| 2:K:117:LEU:HD11 | 2:K:147:ASN:HB3  | 1.76                     | 0.67              |
| 1:M:505:MLY:HH23 | 1:M:762:HIS:HD1  | 1.60                     | 0.67              |
| 1:D:530:MET:HE3  | 4:9:354:GLN:HG2  | 1.73                     | 0.67              |
| 1:D:546:THR:H    | 1:D:549:SER:HB3  | 1.59                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:215:GLN:HA   | 1:D:340:ILE:CB   | 2.23                     | 0.67              |
| 1:J:546:THR:H    | 1:J:549:SER:HB3  | 1.59                     | 0.67              |
| 4:W:153:LEU:HD11 | 4:W:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:2:160:THR:HG21 | 4:2:274:ILE:HD11 | 1.76                     | 0.67              |
| 4:Z:160:THR:HG21 | 4:Z:274:ILE:HD11 | 1.76                     | 0.67              |
| 4:V:153:LEU:HD11 | 4:V:274:ILE:HG13 | 1.76                     | 0.67              |
| 1:P:730:SER:CB   | 3:R:92:ARG:C     | 2.53                     | 0.67              |
| 1:J:733:PRO:C    | 1:J:737:PHE:CD1  | 2.62                     | 0.67              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:HB3  | 2.24                     | 0.67              |
| 2:K:114:LYS:HA   | 2:K:146:GLY:C    | 2.03                     | 0.67              |
| 1:P:652:LEU:O    | 1:P:655:GLU:N    | 2.27                     | 0.67              |
| 1:A:732:ILE:HG22 | 1:A:747:LEU:CD1  | 1.55                     | 0.67              |
| 1:M:217:THR:O    | 1:M:221:GLN:HG2  | 1.95                     | 0.67              |
| 1:M:218:LEU:HA   | 1:M:221:GLN:HG3  | 1.71                     | 0.67              |
| 1:D:768:MLY:HA   | 1:D:771:LEU:CD1  | 2.23                     | 0.67              |
| 3:F:49:ILE:HA    | 3:F:52:ASN:ND2   | 2.05                     | 0.67              |
| 1:M:374:GLN:HG3  | 1:M:375:ALA:H    | 1.59                     | 0.67              |
| 1:P:131:TRP:O    | 1:P:132:LEU:HD12 | 1.95                     | 0.67              |
| 1:D:131:TRP:O    | 1:D:132:LEU:HD12 | 1.94                     | 0.67              |
| 4:8:153:LEU:HD11 | 4:8:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:5:160:THR:HG21 | 4:5:274:ILE:HD11 | 1.76                     | 0.67              |
| 1:G:797:PHE:CZ   | 3:I:126:LEU:CD2  | 2.60                     | 0.67              |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:HD21  | 1.77                     | 0.67              |
| 1:G:217:THR:O    | 1:G:221:GLN:HG2  | 1.95                     | 0.67              |
| 1:A:550:PHE:HA   | 4:V:46:GLY:HA3   | 1.66                     | 0.67              |
| 1:M:721:LYS:HG2  | 1:M:736:GLN:CD   | 1.85                     | 0.67              |
| 1:G:28:GLN:CB    | 1:G:723:ARG:HH12 | 2.05                     | 0.67              |
| 1:J:838:ILE:CD1  | 2:K:54:MET:HE3   | 2.06                     | 0.67              |
| 1:M:62:VAL:HG12  | 1:M:63:MLY:O     | 1.94                     | 0.67              |
| 1:G:58:GLY:HA2   | 1:G:74:GLU:OE1   | 1.95                     | 0.67              |
| 3:R:102:VAL:HG23 | 3:R:139:TYR:HD1  | 1.59                     | 0.67              |
| 2:H:114:LYS:HA   | 2:H:146:GLY:C    | 2.02                     | 0.67              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:OD1  | 2.39                     | 0.67              |
| 1:A:817:GLN:HG3  | 2:B:127:ARG:CD   | 2.13                     | 0.67              |
| 1:M:537:GLU:C    | 4:Z:351:THR:H    | 1.98                     | 0.67              |
| 1:J:652:LEU:O    | 1:J:655:GLU:N    | 2.27                     | 0.67              |
| 1:A:831:TRP:CE3  | 2:B:34:ILE:CG1   | 2.75                     | 0.67              |
| 1:A:533:PHE:O    | 1:A:537:GLU:HG2  | 1.93                     | 0.67              |
| 1:G:838:ILE:CG1  | 2:H:54:MET:HE1   | 2.25                     | 0.67              |
| 1:P:806:MET:N    | 1:P:807:VAL:N    | 2.43                     | 0.67              |
| 4:2:324:THR:CG2  | 4:4:243:PRO:C    | 2.57                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:567:LYS:HZ1  | 4:Y:92:ASN:HA    | 1.59                     | 0.67              |
| 1:M:78:PHE:HB3   | 1:M:98:HIS:CD2   | 2.30                     | 0.67              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:ND2  | 2.10                     | 0.67              |
| 1:P:374:GLN:HG3  | 1:P:375:ALA:H    | 1.59                     | 0.67              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:ND2  | 2.09                     | 0.67              |
| 1:D:52:ILE:N     | 1:D:52:ILE:HD13  | 2.09                     | 0.67              |
| 1:A:768:MLY:C    | 1:A:771:LEU:CB   | 2.72                     | 0.67              |
| 2:N:117:LEU:CG   | 2:N:147:ASN:HB3  | 2.25                     | 0.67              |
| 1:G:553:MLY:CD   | 4:X:45:VAL:HG12  | 2.23                     | 0.67              |
| 1:A:217:THR:O    | 1:A:221:GLN:HG2  | 1.95                     | 0.67              |
| 2:K:141:PRO:O    | 2:K:145:ALA:CB   | 2.43                     | 0.67              |
| 1:M:648:THR:CB   | 4:Z:350:SER:OG   | 2.43                     | 0.67              |
| 1:J:831:TRP:HE1  | 2:K:67:MET:HB3   | 1.59                     | 0.67              |
| 3:O:48:LYS:C     | 3:O:52:ASN:HD21  | 1.96                     | 0.67              |
| 1:P:612:GLN:NE2  | 1:P:627:GLY:N    | 2.43                     | 0.67              |
| 1:G:752:ASP:OD1  | 1:G:783:LEU:N    | 2.28                     | 0.67              |
| 1:G:537:GLU:C    | 4:V:351:THR:H    | 1.99                     | 0.67              |
| 2:Q:141:PRO:O    | 2:Q:145:ALA:CB   | 2.43                     | 0.67              |
| 2:H:141:PRO:O    | 2:H:145:ALA:CB   | 2.43                     | 0.67              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:HB3  | 2.24                     | 0.67              |
| 1:P:635:GLY:O    | 4:O:341:ILE:HG21 | 1.95                     | 0.67              |
| 1:P:717:TYR:HD1  | 1:P:744:SER:HG   | 1.43                     | 0.67              |
| 1:J:826:VAL:CG2  | 2:K:88:LEU:HD23  | 2.24                     | 0.67              |
| 1:P:767:PHE:CG   | 1:P:772:LEU:CD2  | 2.78                     | 0.67              |
| 1:J:756:THR:CG2  | 1:J:776:GLU:C    | 2.50                     | 0.67              |
| 1:G:831:TRP:HZ3  | 2:H:34:ILE:HG21  | 1.60                     | 0.67              |
| 3:R:24:LYS:HA    | 3:R:63:ILE:O     | 1.95                     | 0.67              |
| 1:G:546:THR:H    | 1:G:549:SER:HB3  | 1.59                     | 0.67              |
| 1:J:290:GLN:O    | 1:J:331:LEU:HD12 | 1.95                     | 0.67              |
| 1:P:290:GLN:O    | 1:P:331:LEU:HD12 | 1.95                     | 0.67              |
| 1:G:166:MET:HE3  | 1:G:254:PHE:CD2  | 2.30                     | 0.67              |
| 1:J:131:TRP:O    | 1:J:132:LEU:HD12 | 1.95                     | 0.67              |
| 1:J:58:GLY:HA2   | 1:J:74:GLU:OE1   | 1.95                     | 0.67              |
| 1:A:505:MLY:HD2  | 1:A:741:LYS:NZ   | 2.09                     | 0.67              |
| 2:N:141:PRO:O    | 2:N:145:ALA:CB   | 2.43                     | 0.67              |
| 1:J:408:VAL:HG12 | 4:W:332:PRO:HB3  | 1.76                     | 0.67              |
| 1:D:648:THR:CB   | 4:9:350:SER:OG   | 2.43                     | 0.67              |
| 1:G:202:SER:HA   | 1:G:207:LYS:HE3  | 1.72                     | 0.67              |
| 1:J:757:GLN:CA   | 1:J:776:GLU:HG3  | 2.23                     | 0.67              |
| 1:J:550:PHE:HE2  | 1:J:592:ILE:HG23 | 1.59                     | 0.67              |
| 1:G:78:PHE:HB3   | 1:G:98:HIS:CD2   | 2.30                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:62:VAL:HG12  | 1:A:63:MLY:O     | 1.93                     | 0.67              |
| 1:A:290:GLN:O    | 1:A:331:LEU:HD12 | 1.95                     | 0.67              |
| 4:X:153:LEU:HD11 | 4:X:274:ILE:HG13 | 1.76                     | 0.67              |
| 4:V:160:THR:HG21 | 4:V:274:ILE:HD11 | 1.76                     | 0.67              |
| 1:D:58:GLY:HA2   | 1:D:74:GLU:OE1   | 1.95                     | 0.67              |
| 1:D:795:ARG:NH2  | 3:F:116:GLU:CB   | 2.30                     | 0.66              |
| 1:A:149:GLN:HG2  | 1:A:719:ASP:OD1  | 1.94                     | 0.66              |
| 1:A:97:LEU:HD23  | 1:A:712:PRO:CB   | 2.21                     | 0.66              |
| 1:P:408:VAL:HG12 | 4:O:332:PRO:HB3  | 1.76                     | 0.66              |
| 1:P:533:PHE:O    | 1:P:537:GLU:HG2  | 1.93                     | 0.66              |
| 1:P:648:THR:CB   | 4:O:350:SER:OG   | 2.43                     | 0.66              |
| 1:J:541:MET:O    | 4:W:143:TYR:OH   | 2.13                     | 0.66              |
| 1:P:804:ARG:O    | 1:P:808:GLU:HG3  | 1.94                     | 0.66              |
| 1:A:800:ARG:CD   | 3:C:149:VAL:O    | 2.43                     | 0.66              |
| 3:I:24:LYS:HA    | 3:I:63:ILE:O     | 1.95                     | 0.66              |
| 1:A:61:THR:HG23  | 1:A:71:THR:OG1   | 1.94                     | 0.66              |
| 1:M:174:SER:O    | 1:M:670:HIS:HB2  | 1.95                     | 0.66              |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:HD1  | 1.60                     | 0.66              |
| 1:P:418:THR:HG22 | 1:P:419:VAL:N    | 2.11                     | 0.66              |
| 1:G:62:VAL:HG12  | 1:G:63:MLY:O     | 1.94                     | 0.66              |
| 1:G:290:GLN:O    | 1:G:331:LEU:HD12 | 1.95                     | 0.66              |
| 4:4:160:THR:HG21 | 4:4:274:ILE:HD11 | 1.76                     | 0.66              |
| 1:A:739:ASP:CB   | 1:A:742:LYS:HB3  | 2.12                     | 0.66              |
| 1:A:550:PHE:HE2  | 1:A:592:ILE:HG23 | 1.59                     | 0.66              |
| 1:P:508:ILE:HD11 | 1:P:759:ALA:HB2  | 0.70                     | 0.66              |
| 1:D:642:LYS:CD   | 4:9:24:ASP:O     | 2.42                     | 0.66              |
| 3:F:48:LYS:C     | 3:F:52:ASN:HD21  | 1.96                     | 0.66              |
| 1:A:78:PHE:HB3   | 1:A:98:HIS:CD2   | 2.30                     | 0.66              |
| 1:D:709:LYS:C    | 1:D:710:GLY:HA2  | 2.15                     | 0.66              |
| 1:D:418:THR:HG22 | 1:D:419:VAL:N    | 2.11                     | 0.66              |
| 1:A:418:THR:HG22 | 1:A:419:VAL:N    | 2.11                     | 0.66              |
| 1:D:374:GLN:HG3  | 1:D:375:ALA:H    | 1.60                     | 0.66              |
| 4:Z:153:LEU:HD11 | 4:Z:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:P:58:GLY:HA2   | 1:P:74:GLU:OE1   | 1.95                     | 0.66              |
| 1:A:757:GLN:HB3  | 1:A:771:LEU:HD13 | 1.63                     | 0.66              |
| 2:E:141:PRO:O    | 2:E:145:ALA:CB   | 2.43                     | 0.66              |
| 1:P:795:ARG:HD2  | 3:R:43:ASN:CG    | 2.16                     | 0.66              |
| 1:A:795:ARG:CD   | 3:C:43:ASN:CG    | 2.63                     | 0.66              |
| 1:A:537:GLU:C    | 4:8:351:THR:H    | 1.99                     | 0.66              |
| 1:M:785:GLU:O    | 1:M:786:ILE:N    | 2.27                     | 0.66              |
| 4:W:324:THR:HG22 | 4:Y:247:VAL:HG13 | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:61:THR:HG23  | 1:G:71:THR:OG1   | 1.94                     | 0.66              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:N    | 2.43                     | 0.66              |
| 1:G:174:SER:O    | 1:G:670:HIS:HB2  | 1.96                     | 0.66              |
| 3:L:102:VAL:HG23 | 3:L:139:TYR:HD1  | 1.59                     | 0.66              |
| 1:M:131:TRP:O    | 1:M:132:LEU:HD12 | 1.95                     | 0.66              |
| 4:8:160:THR:HG21 | 4:8:274:ILE:HD11 | 1.76                     | 0.66              |
| 1:G:557:GLU:HB2  | 4:X:47:MET:C     | 2.16                     | 0.66              |
| 1:P:541:MET:O    | 4:0:143:TYR:OH   | 2.14                     | 0.66              |
| 1:P:544:LYS:NZ   | 4:2:45:VAL:CG2   | 2.59                     | 0.66              |
| 1:D:226:ASN:HB2  | 1:D:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:P:217:THR:O    | 1:P:221:GLN:HG2  | 1.95                     | 0.66              |
| 1:G:599:ASN:OD1  | 1:G:649:VAL:N    | 2.29                     | 0.66              |
| 1:P:599:ASN:OD1  | 1:P:649:VAL:N    | 2.29                     | 0.66              |
| 1:A:174:SER:O    | 1:A:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:J:52:ILE:N     | 1:J:52:ILE:HD13  | 2.09                     | 0.66              |
| 1:G:131:TRP:O    | 1:G:132:LEU:HD12 | 1.95                     | 0.66              |
| 4:9:153:LEU:HD11 | 4:9:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:D:732:ILE:CD1  | 1:D:782:MLY:HH13 | 2.21                     | 0.66              |
| 1:G:648:THR:CB   | 4:V:350:SER:OG   | 2.44                     | 0.66              |
| 2:H:146:GLY:O    | 2:H:147:ASN:HB2  | 1.96                     | 0.66              |
| 2:K:117:LEU:CB   | 2:K:147:ASN:ND2  | 2.35                     | 0.66              |
| 1:P:541:MET:HG2  | 4:0:345:ILE:C    | 2.16                     | 0.66              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:C    | 2.16                     | 0.66              |
| 1:A:648:THR:CB   | 4:8:350:SER:OG   | 2.43                     | 0.66              |
| 1:M:84:MLY:HD3   | 1:M:723:ARG:CD   | 2.25                     | 0.66              |
| 4:X:291:LYS:HB2  | 4:Z:244:ASP:CB   | 2.20                     | 0.66              |
| 1:D:599:ASN:OD1  | 1:D:649:VAL:N    | 2.29                     | 0.66              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:C    | 2.16                     | 0.66              |
| 3:F:102:VAL:HG23 | 3:F:139:TYR:HD1  | 1.59                     | 0.66              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:ND2  | 2.10                     | 0.66              |
| 1:P:339:ASP:OD1  | 1:P:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:A:97:LEU:HD23  | 1:A:712:PRO:CA   | 2.26                     | 0.66              |
| 2:Q:117:LEU:CG   | 2:Q:147:ASN:HB3  | 2.24                     | 0.66              |
| 2:H:117:LEU:CB   | 2:H:147:ASN:ND2  | 2.35                     | 0.66              |
| 2:K:141:PRO:O    | 2:K:145:ALA:HB2  | 1.96                     | 0.66              |
| 2:K:146:GLY:O    | 2:K:147:ASN:HB2  | 1.96                     | 0.66              |
| 1:P:537:GLU:C    | 4:0:351:THR:H    | 1.98                     | 0.66              |
| 1:J:635:GLY:O    | 4:W:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:D:408:VAL:HG12 | 4:9:332:PRO:HB3  | 1.76                     | 0.66              |
| 1:D:726:VAL:CG1  | 1:D:785:GLU:HG3  | 2.23                     | 0.66              |
| 1:P:93:MET:CE    | 1:P:764:MLY:HD3  | 2.25                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:642:LYS:CD   | 4:8:24:ASP:O     | 2.42                     | 0.66              |
| 1:A:643:GLY:N    | 4:8:24:ASP:CA    | 2.46                     | 0.66              |
| 1:J:829:TRP:CZ3  | 2:K:84:PHE:CE2   | 2.69                     | 0.66              |
| 1:J:832:MET:SD   | 2:K:84:PHE:HE2   | 2.17                     | 0.66              |
| 1:J:78:PHE:HB3   | 1:J:98:HIS:CD2   | 2.30                     | 0.66              |
| 1:J:418:THR:HG22 | 1:J:419:VAL:N    | 2.10                     | 0.66              |
| 1:P:480:ILE:HG22 | 1:P:481:ASN:ND2  | 2.09                     | 0.66              |
| 1:D:339:ASP:OD1  | 1:D:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:CD1  | 2.26                     | 0.66              |
| 1:J:795:ARG:NE   | 3:L:43:ASN:OD1   | 2.27                     | 0.66              |
| 2:E:141:PRO:O    | 2:E:145:ALA:HB2  | 1.96                     | 0.66              |
| 1:G:226:ASN:HB2  | 1:G:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:M:530:MET:CA   | 4:Z:354:GLN:CB   | 2.74                     | 0.66              |
| 1:M:635:GLY:O    | 4:Z:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:J:537:GLU:C    | 4:W:351:THR:H    | 1.98                     | 0.66              |
| 1:P:797:PHE:HE1  | 3:R:149:VAL:HG12 | 1.55                     | 0.66              |
| 1:D:635:GLY:O    | 4:9:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:M:795:ARG:HG2  | 3:O:118:MET:SD   | 2.34                     | 0.66              |
| 1:D:831:TRP:CH2  | 2:E:50:THR:HB    | 2.31                     | 0.66              |
| 3:L:24:LYS:HA    | 3:L:63:ILE:O     | 1.95                     | 0.66              |
| 1:D:174:SER:O    | 1:D:670:HIS:HB2  | 1.96                     | 0.66              |
| 1:P:174:SER:O    | 1:P:670:HIS:HB2  | 1.95                     | 0.66              |
| 1:A:131:TRP:O    | 1:A:132:LEU:HD12 | 1.94                     | 0.66              |
| 4:7:153:LEU:HD11 | 4:7:274:ILE:HG13 | 1.76                     | 0.66              |
| 4:1:153:LEU:HD11 | 4:1:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:J:91:MET:HE3   | 1:J:119:SER:HB2  | 1.77                     | 0.66              |
| 1:P:322:VAL:HB   | 1:P:325:ILE:CD1  | 2.26                     | 0.66              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:CD1  | 2.26                     | 0.66              |
| 1:G:783:LEU:O    | 1:G:787:ILE:CA   | 2.43                     | 0.66              |
| 4:X:324:THR:CB   | 4:Z:247:VAL:H    | 2.04                     | 0.66              |
| 1:J:648:THR:CB   | 4:W:350:SER:OG   | 2.43                     | 0.66              |
| 1:P:797:PHE:CZ   | 3:R:146:ILE:CA   | 2.70                     | 0.66              |
| 1:P:789:ALA:HB1  | 3:R:81:GLN:CD    | 2.16                     | 0.66              |
| 1:D:537:GLU:C    | 4:9:351:THR:H    | 1.98                     | 0.66              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:HB3  | 1.78                     | 0.66              |
| 4:2:287:ILE:HG22 | 4:4:204:ALA:HB3  | 1.76                     | 0.66              |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:HD11 | 0.73                     | 0.66              |
| 1:A:839:MLY:HH11 | 2:B:159:HIS:HD2  | 1.59                     | 0.66              |
| 1:P:831:TRP:CZ3  | 2:Q:34:ILE:HD13  | 2.27                     | 0.66              |
| 3:F:24:LYS:HA    | 3:F:63:ILE:O     | 1.95                     | 0.66              |
| 1:M:61:THR:HG23  | 1:M:71:THR:OG1   | 1.95                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:174:SER:O    | 1:J:670:HIS:HB2  | 1.95                     | 0.66              |
| 1:A:612:GLN:NE2  | 1:A:627:GLY:N    | 2.43                     | 0.66              |
| 1:M:418:THR:HG22 | 1:M:419:VAL:N    | 2.11                     | 0.66              |
| 1:D:290:GLN:O    | 1:D:331:LEU:HD12 | 1.95                     | 0.66              |
| 4:V:288:ASP:H    | 4:X:204:ALA:H    | 1.43                     | 0.66              |
| 1:J:339:ASP:OD1  | 1:J:348:MLY:HH13 | 1.95                     | 0.66              |
| 1:G:635:GLY:O    | 4:V:341:ILE:HG21 | 1.95                     | 0.66              |
| 1:P:642:LYS:HA   | 4:O:21:PHE:O     | 1.96                     | 0.66              |
| 1:J:83:PRO:C     | 1:J:723:ARG:NH2  | 2.49                     | 0.66              |
| 1:P:789:ALA:CB   | 3:R:81:GLN:CD    | 2.64                     | 0.66              |
| 1:A:795:ARG:CD   | 3:C:35:ARG:NH1   | 2.29                     | 0.66              |
| 1:A:530:MET:CA   | 4:8:354:GLN:CB   | 2.74                     | 0.66              |
| 1:A:538:GLU:CD   | 4:8:355:MET:CE   | 2.62                     | 0.66              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:C    | 2.16                     | 0.66              |
| 1:P:839:MLY:HH21 | 2:Q:158:THR:HG22 | 1.77                     | 0.66              |
| 4:O:244:ASP:HB2  | 4:Y:291:LYS:C    | 2.13                     | 0.66              |
| 1:D:823:PHE:CE1  | 2:E:161:GLU:N    | 2.64                     | 0.66              |
| 1:P:61:THR:HG23  | 1:P:71:THR:OG1   | 1.95                     | 0.66              |
| 1:M:612:GLN:NE2  | 1:M:627:GLY:N    | 2.43                     | 0.66              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:N    | 2.43                     | 0.66              |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:HD1  | 1.59                     | 0.66              |
| 1:G:374:GLN:HG3  | 1:G:375:ALA:H    | 1.60                     | 0.66              |
| 1:P:52:ILE:N     | 1:P:52:ILE:HD13  | 2.09                     | 0.66              |
| 1:A:296:MLY:HH11 | 1:A:348:MLY:HH21 | 1.78                     | 0.66              |
| 1:A:144:ARG:NH1  | 1:A:160:ASP:OD1  | 2.29                     | 0.66              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:C    | 2.17                     | 0.66              |
| 2:E:146:GLY:O    | 2:E:147:ASN:HB2  | 1.96                     | 0.66              |
| 4:1:288:ASP:H    | 4:3:203:THR:CG2  | 2.08                     | 0.66              |
| 1:J:226:ASN:HB2  | 1:J:227:PRO:HD3  | 1.78                     | 0.66              |
| 1:M:546:THR:H    | 1:M:549:SER:HB3  | 1.59                     | 0.66              |
| 1:D:541:MET:O    | 4:9:143:TYR:OH   | 2.14                     | 0.66              |
| 1:D:217:THR:O    | 1:D:221:GLN:HG2  | 1.95                     | 0.66              |
| 4:O:205:GLU:CG   | 4:Y:287:ILE:HD13 | 2.26                     | 0.66              |
| 1:G:508:ILE:CD1  | 1:G:759:ALA:HB2  | 2.08                     | 0.66              |
| 3:C:45:GLU:O     | 3:C:49:ILE:HG13  | 1.96                     | 0.66              |
| 3:O:24:LYS:HA    | 3:O:63:ILE:O     | 1.95                     | 0.66              |
| 1:D:61:THR:HG23  | 1:D:71:THR:OG1   | 1.95                     | 0.66              |
| 1:A:709:LYS:O    | 1:A:710:GLY:CA   | 2.44                     | 0.66              |
| 1:M:691:VAL:O    | 1:M:695:LEU:HD13 | 1.96                     | 0.66              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:N    | 2.11                     | 0.66              |
| 1:G:480:ILE:HG22 | 1:G:481:ASN:ND2  | 2.10                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:5:153:LEU:HD11 | 4:5:274:ILE:HG13 | 1.76                     | 0.66              |
| 1:D:466:GLY:HA2  | 1:D:484:ASN:HD21 | 1.61                     | 0.66              |
| 1:J:144:ARG:NH1  | 1:J:160:ASP:OD1  | 2.29                     | 0.66              |
| 1:M:538:GLU:HA   | 4:Z:349:LEU:HB3  | 1.78                     | 0.65              |
| 1:P:793:ARG:HD3  | 3:R:40:ASN:HD22  | 1.43                     | 0.65              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:C    | 2.16                     | 0.65              |
| 1:J:599:ASN:OD1  | 1:J:649:VAL:N    | 2.29                     | 0.65              |
| 1:P:78:PHE:HB3   | 1:P:98:HIS:CD2   | 2.30                     | 0.65              |
| 1:D:691:VAL:O    | 1:D:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:N    | 2.11                     | 0.65              |
| 1:M:58:GLY:HA2   | 1:M:74:GLU:OE1   | 1.95                     | 0.65              |
| 1:G:144:ARG:NH1  | 1:G:160:ASP:OD1  | 2.29                     | 0.65              |
| 1:G:339:ASP:OD1  | 1:G:348:MLY:HH13 | 1.95                     | 0.65              |
| 1:G:161:ASN:O    | 1:G:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:D:727:LEU:H    | 1:D:782:MLY:HE2  | 1.58                     | 0.65              |
| 1:G:538:GLU:CD   | 4:V:355:MET:HE3  | 2.17                     | 0.65              |
| 1:M:541:MET:HG2  | 4:Z:345:ILE:C    | 2.16                     | 0.65              |
| 1:G:721:LYS:HG2  | 1:G:736:GLN:CD   | 1.86                     | 0.65              |
| 1:A:795:ARG:HG2  | 3:C:118:MET:HE1  | 1.78                     | 0.65              |
| 1:M:795:ARG:CB   | 3:O:35:ARG:CZ    | 2.73                     | 0.65              |
| 1:M:642:LYS:CD   | 4:Z:24:ASP:O     | 2.43                     | 0.65              |
| 1:M:599:ASN:OD1  | 1:M:649:VAL:N    | 2.29                     | 0.65              |
| 1:J:829:TRP:CH2  | 2:K:87:LYS:CE    | 2.79                     | 0.65              |
| 3:R:48:LYS:O     | 3:R:52:ASN:CG    | 2.34                     | 0.65              |
| 1:J:61:THR:HG23  | 1:J:71:THR:OG1   | 1.95                     | 0.65              |
| 1:D:78:PHE:HB3   | 1:D:98:HIS:CD2   | 2.30                     | 0.65              |
| 1:P:691:VAL:O    | 1:P:695:LEU:HD13 | 1.96                     | 0.65              |
| 4:3:153:LEU:HD11 | 4:3:274:ILE:HG13 | 1.76                     | 0.65              |
| 1:G:466:GLY:HA2  | 1:G:484:ASN:HD21 | 1.61                     | 0.65              |
| 1:P:161:ASN:O    | 1:P:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:M:144:ARG:NH1  | 1:M:160:ASP:OD1  | 2.29                     | 0.65              |
| 1:A:161:ASN:O    | 1:A:165:PHE:HB2  | 1.96                     | 0.65              |
| 2:N:144:VAL:CG1  | 2:N:153:ILE:HD13 | 2.19                     | 0.65              |
| 1:G:541:MET:O    | 4:V:143:TYR:OH   | 2.13                     | 0.65              |
| 1:P:721:LYS:HG2  | 1:P:736:GLN:CD   | 1.86                     | 0.65              |
| 1:A:107:MLY:HB3  | 1:A:686:MET:CE   | 2.26                     | 0.65              |
| 3:F:3:SER:HG     | 3:F:5:ALA:N      | 1.95                     | 0.65              |
| 1:A:339:ASP:OD1  | 1:A:348:MLY:HH13 | 1.96                     | 0.65              |
| 1:M:296:MLY:HH11 | 1:M:348:MLY:HH21 | 1.78                     | 0.65              |
| 1:M:466:GLY:HA2  | 1:M:484:ASN:ND2  | 2.11                     | 0.65              |
| 1:A:149:GLN:CB   | 1:A:719:ASP:OD1  | 2.43                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:217:THR:O    | 1:J:221:GLN:HG2  | 1.95                     | 0.65              |
| 1:A:635:GLY:O    | 4:8:341:ILE:HG21 | 1.95                     | 0.65              |
| 1:M:792:ALA:CB   | 3:O:42:THR:HG22  | 2.19                     | 0.65              |
| 1:P:805:ALA:O    | 1:P:809:ARG:CB   | 2.45                     | 0.65              |
| 1:J:567:LYS:NZ   | 4:Y:92:ASN:HA    | 2.10                     | 0.65              |
| 1:J:691:VAL:O    | 1:J:695:LEU:HD13 | 1.96                     | 0.65              |
| 1:G:296:MLY:HH11 | 1:G:348:MLY:HH21 | 1.79                     | 0.65              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:CG1  | 2.27                     | 0.65              |
| 1:P:530:MET:CA   | 4:0:354:GLN:CB   | 2.74                     | 0.65              |
| 1:J:642:LYS:HA   | 4:W:21:PHE:O     | 1.96                     | 0.65              |
| 1:D:530:MET:CA   | 4:9:354:GLN:CB   | 2.74                     | 0.65              |
| 1:M:831:TRP:HE1  | 2:N:67:MET:CG    | 2.10                     | 0.65              |
| 1:A:599:ASN:OD1  | 1:A:649:VAL:N    | 2.29                     | 0.65              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:CG   | 2.75                     | 0.65              |
| 3:F:45:GLU:O     | 3:F:49:ILE:HG13  | 1.97                     | 0.65              |
| 1:M:480:ILE:HG22 | 1:M:481:ASN:ND2  | 2.10                     | 0.65              |
| 1:G:691:VAL:O    | 1:G:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:J:161:ASN:O    | 1:J:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:D:822:SER:O    | 1:D:825:ASN:HB2  | 1.97                     | 0.65              |
| 2:N:146:GLY:O    | 2:N:147:ASN:HB2  | 1.96                     | 0.65              |
| 1:G:530:MET:CG   | 4:V:354:GLN:CG   | 2.72                     | 0.65              |
| 2:H:141:PRO:O    | 2:H:145:ALA:HB2  | 1.96                     | 0.65              |
| 1:P:534:SER:C    | 4:0:351:THR:CA   | 2.47                     | 0.65              |
| 1:M:226:ASN:HB2  | 1:M:227:PRO:HD3  | 1.77                     | 0.65              |
| 3:I:48:LYS:O     | 3:I:52:ASN:CG    | 2.34                     | 0.65              |
| 3:L:48:LYS:O     | 3:L:52:ASN:CG    | 2.34                     | 0.65              |
| 3:C:24:LYS:HA    | 3:C:63:ILE:O     | 1.95                     | 0.65              |
| 1:G:789:ALA:HB2  | 3:I:81:GLN:CD    | 2.17                     | 0.65              |
| 1:A:691:VAL:O    | 1:A:695:LEU:HD13 | 1.97                     | 0.65              |
| 1:J:791:GLN:NE2  | 3:L:115:GLY:CA   | 2.60                     | 0.65              |
| 1:D:797:PHE:HD1  | 3:F:146:ILE:O    | 1.80                     | 0.65              |
| 1:G:754:ASP:CG   | 1:G:779:ARG:CD   | 2.62                     | 0.65              |
| 4:1:287:ILE:HG21 | 4:3:204:ALA:N    | 2.11                     | 0.65              |
| 2:B:146:GLY:O    | 2:B:147:ASN:HB2  | 1.96                     | 0.65              |
| 1:G:725:ARG:NE   | 1:G:737:PHE:HE1  | 1.95                     | 0.65              |
| 1:M:725:ARG:NE   | 1:M:737:PHE:HE1  | 1.95                     | 0.65              |
| 1:G:84:MLY:HG2   | 1:G:723:ARG:HD2  | 1.75                     | 0.65              |
| 1:M:202:SER:HA   | 1:M:207:LYS:HE3  | 1.72                     | 0.65              |
| 1:J:822:SER:O    | 1:J:825:ASN:HB2  | 1.97                     | 0.65              |
| 4:X:285:CYS:O    | 4:Z:202:THR:CG2  | 2.44                     | 0.65              |
| 3:O:45:GLU:O     | 3:O:49:ILE:HG13  | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:800:ARG:HB3  | 3:F:149:VAL:HG13 | 1.78                     | 0.65              |
| 1:M:829:TRP:CH2  | 2:N:87:LYS:NZ    | 2.57                     | 0.65              |
| 1:P:466:GLY:HA2  | 1:P:484:ASN:HD21 | 1.61                     | 0.65              |
| 1:A:822:SER:O    | 1:A:825:ASN:HB2  | 1.97                     | 0.65              |
| 1:A:466:GLY:HA2  | 1:A:484:ASN:ND2  | 2.11                     | 0.65              |
| 1:A:93:MET:HE1   | 1:A:716:LEU:N    | 2.12                     | 0.65              |
| 2:N:117:LEU:HD11 | 2:N:147:ASN:HB3  | 1.76                     | 0.65              |
| 2:Q:146:GLY:O    | 2:Q:147:ASN:HB2  | 1.96                     | 0.65              |
| 1:P:795:ARG:HH21 | 3:R:116:GLU:CA   | 2.01                     | 0.65              |
| 1:P:795:ARG:NE   | 3:R:43:ASN:OD1   | 2.28                     | 0.65              |
| 1:P:226:ASN:HB2  | 1:P:227:PRO:HD3  | 1.78                     | 0.65              |
| 1:A:642:LYS:HA   | 4:8:21:PHE:O     | 1.96                     | 0.65              |
| 3:L:45:GLU:O     | 3:L:49:ILE:HG13  | 1.96                     | 0.65              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:N    | 1.94                     | 0.65              |
| 1:A:809:ARG:NH1  | 2:B:124:GLY:CA   | 2.59                     | 0.65              |
| 1:A:374:GLN:HG3  | 1:A:375:ALA:H    | 1.60                     | 0.65              |
| 1:A:322:VAL:HB   | 1:A:325:ILE:CD1  | 2.26                     | 0.65              |
| 1:D:724:TYR:HB3  | 1:D:782:MLY:CD   | 2.21                     | 0.65              |
| 2:Q:141:PRO:O    | 2:Q:145:ALA:HB2  | 1.96                     | 0.65              |
| 2:B:117:LEU:HD11 | 2:B:147:ASN:HB3  | 1.75                     | 0.65              |
| 1:J:530:MET:CA   | 4:W:354:GLN:CB   | 2.74                     | 0.65              |
| 1:D:530:MET:CG   | 4:9:354:GLN:CG   | 2.71                     | 0.65              |
| 4:0:205:GLU:HG3  | 4:Y:287:ILE:HB   | 0.70                     | 0.65              |
| 1:A:636:LYS:HG3  | 4:8:334:GLU:CD   | 2.17                     | 0.65              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:CB   | 2.78                     | 0.65              |
| 1:D:838:ILE:HD12 | 2:E:54:MET:CE    | 2.23                     | 0.65              |
| 4:V:324:THR:HG23 | 4:X:247:VAL:H    | 1.61                     | 0.65              |
| 3:C:48:LYS:C     | 3:C:52:ASN:HD21  | 1.97                     | 0.65              |
| 1:P:612:GLN:HE22 | 1:P:627:GLY:N    | 1.95                     | 0.65              |
| 1:G:418:THR:HG22 | 1:G:419:VAL:N    | 2.11                     | 0.65              |
| 1:J:466:GLY:HA2  | 1:J:484:ASN:ND2  | 2.12                     | 0.65              |
| 1:D:479:CYS:HB3  | 1:D:653:PHE:CE2  | 2.32                     | 0.65              |
| 1:J:800:ARG:HH22 | 3:L:40:ASN:HD21  | 1.28                     | 0.65              |
| 1:D:795:ARG:HE   | 3:F:116:GLU:HB3  | 1.62                     | 0.65              |
| 1:D:797:PHE:CD1  | 3:F:146:ILE:CA   | 2.80                     | 0.65              |
| 1:G:797:PHE:HE2  | 3:I:126:LEU:CD1  | 2.10                     | 0.65              |
| 1:A:93:MET:SD    | 1:A:715:VAL:HG13 | 2.36                     | 0.65              |
| 1:A:768:MLY:C    | 1:A:771:LEU:HB3  | 2.28                     | 0.65              |
| 1:M:819:ASN:ND2  | 2:N:92:ASP:CB    | 2.49                     | 0.65              |
| 1:D:813:ILE:CD1  | 2:E:128:PHE:HE1  | 2.00                     | 0.65              |
| 1:A:217:THR:HB   | 1:A:220:ASP:OD2  | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:226:ASN:HB2  | 1:A:227:PRO:HD3  | 1.78                     | 0.65              |
| 1:P:538:GLU:HA   | 4:0:349:LEU:HB3  | 1.78                     | 0.65              |
| 1:P:636:LYS:O    | 1:P:637:LYS:CB   | 2.45                     | 0.65              |
| 1:M:636:LYS:O    | 1:M:637:LYS:CB   | 2.45                     | 0.65              |
| 1:P:797:PHE:HE2  | 3:R:126:LEU:HD22 | 1.62                     | 0.65              |
| 1:D:636:LYS:HG3  | 4:9:334:GLU:CD   | 2.17                     | 0.65              |
| 1:A:553:MLY:CE   | 4:V:45:VAL:CA    | 2.49                     | 0.65              |
| 1:M:642:LYS:HA   | 4:Z:21:PHE:O     | 1.96                     | 0.65              |
| 3:C:48:LYS:O     | 3:C:52:ASN:CG    | 2.34                     | 0.65              |
| 1:P:466:GLY:HA2  | 1:P:484:ASN:ND2  | 2.12                     | 0.65              |
| 1:M:210:GLN:O    | 1:M:211:SER:OG   | 2.15                     | 0.65              |
| 1:M:161:ASN:O    | 1:M:165:PHE:HB2  | 1.96                     | 0.65              |
| 1:D:144:ARG:NH1  | 1:D:160:ASP:OD1  | 2.30                     | 0.65              |
| 2:N:141:PRO:O    | 2:N:145:ALA:HB2  | 1.96                     | 0.64              |
| 1:G:642:LYS:HA   | 4:V:21:PHE:O     | 1.97                     | 0.64              |
| 1:P:819:ASN:OD1  | 2:Q:92:ASP:CA    | 2.45                     | 0.64              |
| 1:P:725:ARG:NE   | 1:P:737:PHE:HE1  | 1.95                     | 0.64              |
| 1:A:218:LEU:CD2  | 1:A:222:ILE:HG12 | 2.28                     | 0.64              |
| 1:G:822:SER:O    | 1:G:825:ASN:HB2  | 1.97                     | 0.64              |
| 1:J:636:LYS:HG3  | 4:W:334:GLU:CD   | 2.17                     | 0.64              |
| 1:M:793:ARG:HD3  | 3:O:40:ASN:ND2   | 2.11                     | 0.64              |
| 1:G:97:LEU:HD22  | 1:G:712:PRO:HB2  | 1.79                     | 0.64              |
| 4:0:112:PRO:HG3  | 4:1:195:GLU:CA   | 2.23                     | 0.64              |
| 1:D:642:LYS:HA   | 4:9:21:PHE:O     | 1.96                     | 0.64              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:N    | 1.94                     | 0.64              |
| 1:A:480:ILE:HG22 | 1:A:481:ASN:N    | 2.11                     | 0.64              |
| 1:G:107:MLY:HB3  | 1:G:686:MET:CE   | 2.26                     | 0.64              |
| 1:D:94:MET:HE1   | 1:D:101:ALA:HB1  | 1.79                     | 0.64              |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:HH21 | 1.78                     | 0.64              |
| 1:D:466:GLY:HA2  | 1:D:484:ASN:ND2  | 2.12                     | 0.64              |
| 1:A:91:MET:HE3   | 1:A:119:SER:HB2  | 1.79                     | 0.64              |
| 1:P:144:ARG:NH1  | 1:P:160:ASP:OD1  | 2.29                     | 0.64              |
| 1:M:817:GLN:HB3  | 2:N:127:ARG:CZ   | 2.27                     | 0.64              |
| 2:Q:140:PHE:HB3  | 2:Q:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:J:725:ARG:NE   | 1:J:737:PHE:HE1  | 1.95                     | 0.64              |
| 2:B:144:VAL:CG1  | 2:B:153:ILE:HD13 | 2.19                     | 0.64              |
| 1:D:636:LYS:O    | 1:D:637:LYS:CB   | 2.45                     | 0.64              |
| 1:P:548:THR:HG22 | 4:2:49:GLN:CG    | 2.27                     | 0.64              |
| 1:P:217:THR:HB   | 1:P:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:D:642:LYS:CD   | 4:9:340:TRP:CZ3  | 2.79                     | 0.64              |
| 1:P:829:TRP:CE3  | 2:Q:87:LYS:NZ    | 2.65                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:48:LYS:O     | 3:F:52:ASN:CG    | 2.34                     | 0.64              |
| 4:3:324:THR:CG2  | 4:5:244:ASP:C    | 2.55                     | 0.64              |
| 1:D:480:ILE:HG22 | 1:D:481:ASN:N    | 2.11                     | 0.64              |
| 1:G:466:GLY:HA2  | 1:G:484:ASN:ND2  | 2.12                     | 0.64              |
| 1:M:339:ASP:OD1  | 1:M:348:MLY:HH13 | 1.95                     | 0.64              |
| 1:A:466:GLY:HA2  | 1:A:484:ASN:HD21 | 1.61                     | 0.64              |
| 1:M:133:PRO:O    | 1:M:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:P:210:GLN:O    | 1:P:211:SER:OG   | 2.15                     | 0.64              |
| 1:D:725:ARG:NE   | 1:D:737:PHE:HE1  | 1.95                     | 0.64              |
| 1:A:768:MLY:HB3  | 1:A:771:LEU:HD13 | 1.79                     | 0.64              |
| 1:P:729:ALA:HB1  | 3:R:93:VAL:HG21  | 0.65                     | 0.64              |
| 2:H:140:PHE:O    | 2:H:141:PRO:C    | 2.33                     | 0.64              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:CB   | 2.76                     | 0.64              |
| 1:J:217:THR:HB   | 1:J:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:J:84:MLY:HH12  | 1:J:720:PHE:HD1  | 1.60                     | 0.64              |
| 1:G:732:ILE:HG21 | 1:G:747:LEU:HD11 | 0.72                     | 0.64              |
| 4:0:245:GLY:N    | 4:Y:291:LYS:CB   | 2.60                     | 0.64              |
| 1:J:505:MLY:CD   | 1:J:762:HIS:HE1  | 1.90                     | 0.64              |
| 1:P:831:TRP:NE1  | 2:Q:67:MET:HB3   | 2.08                     | 0.64              |
| 1:D:202:SER:CA   | 1:D:207:LYS:HE3  | 2.27                     | 0.64              |
| 1:M:806:MET:C    | 1:M:807:VAL:CA   | 2.65                     | 0.64              |
| 3:R:45:GLU:O     | 3:R:49:ILE:HG13  | 1.97                     | 0.64              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:N    | 1.94                     | 0.64              |
| 1:P:296:MLY:HH11 | 1:P:348:MLY:HH21 | 1.78                     | 0.64              |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:HH21 | 1.78                     | 0.64              |
| 4:2:148:THR:HG21 | 4:4:45:VAL:CG2   | 2.27                     | 0.64              |
| 1:M:322:VAL:HB   | 1:M:325:ILE:CD1  | 2.26                     | 0.64              |
| 1:G:322:VAL:HB   | 1:G:325:ILE:CD1  | 2.26                     | 0.64              |
| 1:J:133:PRO:O    | 1:J:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:D:795:ARG:HD2  | 3:F:43:ASN:OD1   | 1.91                     | 0.64              |
| 1:G:783:LEU:HD12 | 1:G:783:LEU:N    | 2.13                     | 0.64              |
| 1:M:820:VAL:CG1  | 2:N:136:MET:HE1  | 2.28                     | 0.64              |
| 1:G:819:ASN:N    | 2:H:90:GLY:O     | 2.30                     | 0.64              |
| 1:J:93:MET:SD    | 1:J:716:LEU:HB2  | 2.37                     | 0.64              |
| 1:D:217:THR:HB   | 1:D:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:A:202:SER:CA   | 1:A:207:LYS:HE3  | 2.27                     | 0.64              |
| 4:3:288:ASP:OD2  | 4:5:203:THR:CB   | 2.42                     | 0.64              |
| 1:M:806:MET:O    | 1:M:810:ARG:N    | 2.29                     | 0.64              |
| 1:A:642:LYS:CD   | 4:8:340:TRP:CZ3  | 2.79                     | 0.64              |
| 1:J:95:THR:HA    | 1:J:713:SER:HB3  | 1.64                     | 0.64              |
| 1:D:800:ARG:HG2  | 3:F:149:VAL:HG22 | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:107:MLY:HB3  | 1:J:686:MET:CE   | 2.27                     | 0.64              |
| 1:J:166:MET:HE3  | 1:J:254:PHE:HD2  | 1.60                     | 0.64              |
| 1:A:133:PRO:O    | 1:A:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:G:801:VAL:HG21 | 3:I:126:LEU:HD21 | 1.78                     | 0.64              |
| 1:G:530:MET:CA   | 4:V:354:GLN:CB   | 2.75                     | 0.64              |
| 1:G:553:MLY:O    | 4:X:46:GLY:CA    | 2.45                     | 0.64              |
| 1:G:642:LYS:CA   | 4:V:21:PHE:O     | 2.46                     | 0.64              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:HB3  | 1.79                     | 0.64              |
| 4:1:287:ILE:HG13 | 4:3:202:THR:CB   | 2.26                     | 0.64              |
| 1:P:530:MET:CG   | 4:0:354:GLN:CG   | 2.72                     | 0.64              |
| 1:G:218:LEU:CD2  | 1:G:222:ILE:HG12 | 2.28                     | 0.64              |
| 1:M:538:GLU:CD   | 4:Z:355:MET:HE3  | 2.18                     | 0.64              |
| 1:A:752:ASP:OD2  | 1:A:782:MLY:CG   | 2.46                     | 0.64              |
| 4:2:288:ASP:N    | 4:4:203:THR:CG2  | 2.56                     | 0.64              |
| 1:J:754:ASP:HB3  | 1:J:780:ASP:OD2  | 1.94                     | 0.64              |
| 1:D:107:MLY:HB3  | 1:D:686:MET:CE   | 2.27                     | 0.64              |
| 1:M:466:GLY:HA2  | 1:M:484:ASN:HD21 | 1.61                     | 0.64              |
| 4:1:167:GLU:OE1  | 4:3:44:MET:HA    | 1.98                     | 0.64              |
| 1:G:133:PRO:O    | 1:G:136:ASN:HB2  | 1.98                     | 0.64              |
| 1:J:479:CYS:HB3  | 1:J:653:PHE:CE2  | 2.33                     | 0.64              |
| 1:D:727:LEU:CG   | 1:D:782:MLY:HG3  | 2.19                     | 0.64              |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:N    | 2.13                     | 0.64              |
| 1:G:636:LYS:HG3  | 4:V:334:GLU:CD   | 2.18                     | 0.64              |
| 1:G:642:LYS:CD   | 4:V:24:ASP:O     | 2.43                     | 0.64              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:CG1  | 2.28                     | 0.64              |
| 2:B:144:VAL:HA   | 2:B:153:ILE:HD11 | 1.80                     | 0.64              |
| 1:A:725:ARG:NE   | 1:A:737:PHE:HE1  | 1.95                     | 0.64              |
| 1:G:217:THR:HB   | 1:G:220:ASP:OD2  | 1.97                     | 0.64              |
| 1:J:537:GLU:C    | 4:W:351:THR:N    | 2.51                     | 0.64              |
| 1:J:710:GLY:HA2  | 1:J:772:LEU:HD22 | 0.88                     | 0.64              |
| 1:A:823:PHE:CE1  | 2:B:160:GLY:HA3  | 2.31                     | 0.64              |
| 1:A:823:PHE:HE1  | 2:B:160:GLY:HA3  | 1.59                     | 0.64              |
| 1:M:94:MET:HE1   | 1:M:101:ALA:HB1  | 1.79                     | 0.64              |
| 1:M:753:VAL:CG1  | 1:M:775:LEU:HD22 | 2.27                     | 0.64              |
| 1:G:806:MET:O    | 1:G:809:ARG:HB2  | 1.98                     | 0.64              |
| 1:D:161:ASN:O    | 1:D:165:PHE:HB2  | 1.96                     | 0.64              |
| 1:J:793:ARG:HH21 | 3:L:147:MET:CE   | 2.11                     | 0.64              |
| 1:G:795:ARG:HH21 | 3:I:116:GLU:CB   | 2.10                     | 0.64              |
| 1:A:94:MET:HE1   | 1:A:101:ALA:HB1  | 1.80                     | 0.64              |
| 1:M:820:VAL:CG1  | 2:N:136:MET:CE   | 2.76                     | 0.64              |
| 2:H:117:LEU:HD11 | 2:H:147:ASN:HB3  | 1.76                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:117:LEU:CG   | 2:K:147:ASN:CB   | 2.76                     | 0.64              |
| 2:B:141:PRO:O    | 2:B:145:ALA:HB2  | 1.96                     | 0.64              |
| 1:J:636:LYS:O    | 1:J:637:LYS:CB   | 2.45                     | 0.64              |
| 1:J:642:LYS:CA   | 4:W:21:PHE:O     | 2.45                     | 0.64              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:HB3  | 1.78                     | 0.64              |
| 1:A:636:LYS:O    | 1:A:637:LYS:CB   | 2.45                     | 0.64              |
| 1:P:218:LEU:CD2  | 1:P:222:ILE:HG12 | 2.28                     | 0.64              |
| 1:G:84:MLY:HB3   | 1:G:723:ARG:CZ   | 2.27                     | 0.64              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:CD1   | 2.74                     | 0.64              |
| 3:C:49:ILE:HA    | 3:C:52:ASN:ND2   | 2.05                     | 0.64              |
| 2:E:149:ASP:OD2  | 2:E:150:TYR:C    | 2.36                     | 0.64              |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:N    | 1.95                     | 0.64              |
| 3:R:3:SER:HG     | 3:R:5:ALA:N      | 1.96                     | 0.64              |
| 1:G:210:GLN:O    | 1:G:211:SER:OG   | 2.15                     | 0.64              |
| 1:M:822:SER:O    | 1:M:825:ASN:HB2  | 1.97                     | 0.64              |
| 1:D:506:GLU:HG3  | 1:D:764:MLY:HE3  | 1.78                     | 0.64              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:O    | 1.98                     | 0.64              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:HD11 | 0.73                     | 0.64              |
| 2:H:140:PHE:HB3  | 2:H:144:VAL:CG1  | 2.28                     | 0.64              |
| 1:P:642:LYS:CA   | 4:0:21:PHE:O     | 2.45                     | 0.64              |
| 1:M:537:GLU:C    | 4:Z:351:THR:N    | 2.51                     | 0.64              |
| 1:M:217:THR:HB   | 1:M:220:ASP:OD2  | 1.97                     | 0.64              |
| 4:0:202:THR:HG23 | 4:Y:287:ILE:N    | 1.96                     | 0.64              |
| 1:A:541:MET:O    | 4:8:143:TYR:OH   | 2.14                     | 0.64              |
| 1:M:84:MLY:HH11  | 1:M:720:PHE:HD1  | 1.61                     | 0.64              |
| 1:A:642:LYS:CA   | 4:8:21:PHE:O     | 2.46                     | 0.64              |
| 1:J:556:ASP:O    | 4:Y:48:GLY:N     | 2.29                     | 0.64              |
| 4:X:287:ILE:HG12 | 4:Z:201:VAL:N    | 2.11                     | 0.64              |
| 3:O:48:LYS:O     | 3:O:52:ASN:CG    | 2.34                     | 0.64              |
| 2:N:149:ASP:OD2  | 2:N:150:TYR:C    | 2.36                     | 0.64              |
| 1:J:127:ASN:HD22 | 1:J:128:PRO:CD   | 2.11                     | 0.64              |
| 1:D:127:ASN:HD22 | 1:D:128:PRO:CD   | 2.11                     | 0.64              |
| 1:J:806:MET:O    | 1:J:809:ARG:HB2  | 1.98                     | 0.64              |
| 4:0:190:MET:SD   | 4:0:209:VAL:HG11 | 2.38                     | 0.64              |
| 4:8:190:MET:SD   | 4:8:209:VAL:HG11 | 2.38                     | 0.64              |
| 1:M:292:MET:HE3  | 1:M:309:PRO:HA   | 1.79                     | 0.64              |
| 1:D:795:ARG:CZ   | 3:F:43:ASN:OD1   | 2.42                     | 0.64              |
| 1:G:784:ALA:O    | 1:G:788:THR:CB   | 2.45                     | 0.64              |
| 1:G:795:ARG:NE   | 3:I:116:GLU:CB   | 2.45                     | 0.64              |
| 1:A:149:GLN:CB   | 1:A:718:ALA:C    | 2.64                     | 0.64              |
| 2:N:146:GLY:O    | 2:N:147:ASN:CB   | 2.46                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:140:PHE:HB3  | 2:K:144:VAL:CG1  | 2.27                     | 0.64              |
| 2:K:144:VAL:HA   | 2:K:153:ILE:HD11 | 1.80                     | 0.64              |
| 1:M:530:MET:CG   | 4:Z:354:GLN:CG   | 2.72                     | 0.64              |
| 1:J:636:LYS:N    | 4:W:334:GLU:OE1  | 2.31                     | 0.64              |
| 1:P:796:GLY:HA2  | 3:R:35:ARG:CG    | 2.28                     | 0.64              |
| 1:D:537:GLU:HB3  | 1:D:648:THR:HB   | 1.80                     | 0.64              |
| 3:I:45:GLU:O     | 3:I:49:ILE:HG13  | 1.97                     | 0.64              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:N    | 1.94                     | 0.64              |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:N    | 2.13                     | 0.64              |
| 1:P:107:MLY:HB3  | 1:P:686:MET:CE   | 2.27                     | 0.64              |
| 1:J:466:GLY:HA2  | 1:J:484:ASN:HD21 | 1.61                     | 0.64              |
| 4:Y:190:MET:SD   | 4:Y:209:VAL:HG11 | 2.38                     | 0.64              |
| 1:G:479:CYS:HB3  | 1:G:653:PHE:CE2  | 2.33                     | 0.64              |
| 1:A:505:MLY:N    | 1:A:762:HIS:CD2  | 2.66                     | 0.64              |
| 2:N:132:GLU:O    | 2:N:136:MET:HG2  | 1.98                     | 0.64              |
| 1:G:537:GLU:HB3  | 1:G:648:THR:HB   | 1.80                     | 0.64              |
| 1:J:725:ARG:NE   | 1:J:737:PHE:CE1  | 2.67                     | 0.64              |
| 1:P:642:LYS:CD   | 4:O:340:TRP:CZ3  | 2.79                     | 0.64              |
| 1:P:406:VAL:HG12 | 1:P:407:GLY:N    | 2.13                     | 0.64              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:HD11 | 0.73                     | 0.64              |
| 1:M:541:MET:HG2  | 4:Z:345:ILE:O    | 1.98                     | 0.64              |
| 1:M:577:ALA:O    | 1:M:578:HIS:CD2  | 2.51                     | 0.64              |
| 1:M:541:MET:CA   | 4:Z:143:TYR:OH   | 2.46                     | 0.64              |
| 1:P:798:LEU:CD1  | 3:R:126:LEU:HD13 | 2.19                     | 0.64              |
| 1:G:735:GLY:O    | 1:G:743:ALA:HA   | 1.94                     | 0.64              |
| 1:P:576:GLU:CG   | 1:P:577:ALA:N    | 2.44                     | 0.64              |
| 1:G:148:ARG:HE   | 1:G:764:MLY:HH21 | 1.63                     | 0.64              |
| 1:G:84:MLY:HH13  | 1:G:724:TYR:CE2  | 2.31                     | 0.64              |
| 1:M:724:TYR:HB3  | 1:M:727:LEU:HD12 | 1.80                     | 0.64              |
| 1:G:829:TRP:CH2  | 2:H:83:MET:CE    | 2.81                     | 0.64              |
| 1:J:577:ALA:O    | 1:J:578:HIS:CD2  | 2.51                     | 0.64              |
| 1:P:166:MET:HE3  | 1:P:254:PHE:CD2  | 2.33                     | 0.64              |
| 4:9:190:MET:SD   | 4:9:209:VAL:HG11 | 2.38                     | 0.64              |
| 1:A:505:MLY:CD   | 1:A:741:LYS:HZ3  | 2.11                     | 0.63              |
| 2:N:144:VAL:HA   | 2:N:153:ILE:HD11 | 1.80                     | 0.63              |
| 1:G:530:MET:HE2  | 4:V:354:GLN:HG3  | 1.78                     | 0.63              |
| 1:P:725:ARG:NE   | 1:P:737:PHE:CE1  | 2.66                     | 0.63              |
| 1:J:642:LYS:CG   | 4:W:22:ALA:C     | 2.67                     | 0.63              |
| 1:J:642:LYS:CD   | 4:W:340:TRP:CZ3  | 2.79                     | 0.63              |
| 1:D:537:GLU:C    | 4:9:351:THR:N    | 2.51                     | 0.63              |
| 1:D:218:LEU:CD2  | 1:D:222:ILE:HG12 | 2.28                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:636:LYS:N    | 4:8:334:GLU:OE1  | 2.31                     | 0.63              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:CG   | 2.27                     | 0.63              |
| 4:2:287:ILE:CB   | 4:4:204:ALA:H    | 2.11                     | 0.63              |
| 1:M:34:ALA:C     | 1:M:777:GLU:OE2  | 2.36                     | 0.63              |
| 1:D:792:ALA:HB2  | 3:F:42:THR:HG22  | 0.78                     | 0.63              |
| 1:G:215:GLN:CA   | 1:G:340:ILE:CG2  | 2.62                     | 0.63              |
| 1:G:577:ALA:O    | 1:G:578:HIS:CD2  | 2.52                     | 0.63              |
| 2:E:163:ALA:C    | 2:K:22:THR:N     | 2.51                     | 0.63              |
| 1:A:806:MET:O    | 1:A:809:ARG:HB2  | 1.98                     | 0.63              |
| 1:P:127:ASN:HD22 | 1:P:128:PRO:CD   | 2.11                     | 0.63              |
| 1:A:479:CYS:HB3  | 1:A:653:PHE:CE2  | 2.32                     | 0.63              |
| 1:D:783:LEU:HD12 | 1:D:783:LEU:N    | 2.13                     | 0.63              |
| 1:A:149:GLN:CA   | 1:A:719:ASP:OD1  | 2.46                     | 0.63              |
| 1:D:506:GLU:OE2  | 1:D:764:MLY:HE3  | 1.97                     | 0.63              |
| 1:G:643:GLY:H    | 4:V:23:GLY:C     | 2.02                     | 0.63              |
| 2:Q:132:GLU:O    | 2:Q:136:MET:HG2  | 1.99                     | 0.63              |
| 2:E:117:LEU:CG   | 2:E:147:ASN:CB   | 2.76                     | 0.63              |
| 1:J:817:GLN:CB   | 2:K:127:ARG:HH11 | 2.02                     | 0.63              |
| 1:G:728:ASN:ND2  | 3:I:113:THR:O    | 2.31                     | 0.63              |
| 1:M:218:LEU:CD2  | 1:M:222:ILE:HG12 | 2.28                     | 0.63              |
| 1:A:534:SER:C    | 4:8:351:THR:CA   | 2.47                     | 0.63              |
| 1:M:783:LEU:N    | 1:M:783:LEU:HD12 | 2.13                     | 0.63              |
| 1:M:28:GLN:CB    | 1:M:723:ARG:NH1  | 2.02                     | 0.63              |
| 1:M:642:LYS:CA   | 4:Z:21:PHE:O     | 2.45                     | 0.63              |
| 1:M:642:LYS:CG   | 4:Z:22:ALA:C     | 2.67                     | 0.63              |
| 3:I:48:LYS:C     | 3:I:52:ASN:HD21  | 1.96                     | 0.63              |
| 1:M:94:MET:O     | 1:M:713:SER:HA   | 1.97                     | 0.63              |
| 1:P:480:ILE:HG22 | 1:P:481:ASN:N    | 2.12                     | 0.63              |
| 1:P:94:MET:HE1   | 1:P:101:ALA:HB1  | 1.79                     | 0.63              |
| 1:A:166:MET:HE3  | 1:A:254:PHE:HD2  | 1.62                     | 0.63              |
| 4:Y:257:CYS:HB3  | 4:Y:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:2:190:MET:SD   | 4:2:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:P:133:PRO:O    | 1:P:136:ASN:HB2  | 1.98                     | 0.63              |
| 4:4:190:MET:SD   | 4:4:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:D:133:PRO:O    | 1:D:136:ASN:HB2  | 1.98                     | 0.63              |
| 2:N:140:PHE:HB3  | 2:N:144:VAL:CG1  | 2.28                     | 0.63              |
| 1:G:642:LYS:CG   | 4:V:22:ALA:C     | 2.66                     | 0.63              |
| 2:E:132:GLU:O    | 2:E:136:MET:HG2  | 1.99                     | 0.63              |
| 2:E:140:PHE:O    | 2:E:141:PRO:C    | 2.33                     | 0.63              |
| 1:G:813:ILE:HG22 | 2:H:128:PHE:CE1  | 2.28                     | 0.63              |
| 2:K:144:VAL:CG1  | 2:K:153:ILE:HD13 | 2.20                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:114:LYS:HA   | 2:B:146:GLY:C    | 2.03                     | 0.63              |
| 2:B:146:GLY:O    | 2:B:147:ASN:CB   | 2.46                     | 0.63              |
| 1:P:636:LYS:HG3  | 4:0:334:GLU:CD   | 2.17                     | 0.63              |
| 1:P:636:LYS:N    | 4:0:334:GLU:OE1  | 2.31                     | 0.63              |
| 1:M:636:LYS:HG3  | 4:Z:334:GLU:CD   | 2.17                     | 0.63              |
| 1:D:577:ALA:O    | 1:D:578:HIS:CD2  | 2.51                     | 0.63              |
| 1:D:806:MET:O    | 1:D:809:ARG:HB2  | 1.98                     | 0.63              |
| 1:A:724:TYR:HB3  | 1:A:727:LEU:HD12 | 1.80                     | 0.63              |
| 1:D:797:PHE:CG   | 3:F:146:ILE:CG2  | 2.67                     | 0.63              |
| 2:E:140:PHE:HB3  | 2:E:144:VAL:CG1  | 2.28                     | 0.63              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:HD11 | 1.26                     | 0.63              |
| 1:A:725:ARG:NE   | 1:A:737:PHE:CE1  | 2.67                     | 0.63              |
| 1:A:530:MET:HA   | 4:8:354:GLN:CB   | 2.28                     | 0.63              |
| 1:A:577:ALA:O    | 1:A:578:HIS:CD2  | 2.51                     | 0.63              |
| 1:M:34:ALA:CA    | 1:M:777:GLU:OE2  | 2.45                     | 0.63              |
| 1:J:480:ILE:HG22 | 1:J:481:ASN:N    | 2.11                     | 0.63              |
| 1:M:127:ASN:HD22 | 1:M:128:PRO:CD   | 2.11                     | 0.63              |
| 3:L:3:SER:HG     | 3:L:5:ALA:N      | 1.96                     | 0.63              |
| 1:P:822:SER:O    | 1:P:825:ASN:HB2  | 1.97                     | 0.63              |
| 4:0:257:CYS:HB3  | 4:0:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:D:724:TYR:HD1  | 1:D:727:LEU:HD11 | 1.64                     | 0.63              |
| 1:G:537:GLU:C    | 4:V:351:THR:N    | 2.51                     | 0.63              |
| 1:G:636:LYS:O    | 1:G:637:LYS:CB   | 2.45                     | 0.63              |
| 2:E:146:GLY:O    | 2:E:147:ASN:CB   | 2.46                     | 0.63              |
| 1:J:735:GLY:C    | 1:J:743:ALA:HB1  | 1.84                     | 0.63              |
| 1:G:821:ARG:NH2  | 2:H:127:ARG:CG   | 2.57                     | 0.63              |
| 1:P:642:LYS:CD   | 4:0:24:ASP:O     | 2.43                     | 0.63              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:HB3  | 1.78                     | 0.63              |
| 1:P:724:TYR:HB3  | 1:P:727:LEU:HD12 | 1.80                     | 0.63              |
| 1:P:278:GLN:CG   | 1:P:317:GLU:HB2  | 2.27                     | 0.63              |
| 1:M:107:MLY:HB3  | 1:M:686:MET:CE   | 2.27                     | 0.63              |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:N    | 2.13                     | 0.63              |
| 3:I:4:LYS:N      | 3:I:5:ALA:O      | 2.16                     | 0.63              |
| 4:W:257:CYS:HB3  | 4:W:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:M:771:LEU:O    | 1:M:774:LEU:N    | 2.32                     | 0.63              |
| 1:D:791:GLN:NE2  | 3:F:114:LEU:O    | 2.28                     | 0.63              |
| 1:G:792:ALA:HB1  | 3:I:42:THR:CA    | 2.12                     | 0.63              |
| 1:A:505:MLY:CD   | 1:A:741:LYS:NZ   | 2.61                     | 0.63              |
| 2:N:117:LEU:CG   | 2:N:147:ASN:CB   | 2.76                     | 0.63              |
| 1:P:817:GLN:CB   | 2:Q:127:ARG:HD3  | 2.22                     | 0.63              |
| 2:K:132:GLU:O    | 2:K:136:MET:HG2  | 1.99                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:121:LEU:HA   | 2:B:128:PHE:CG   | 2.34                     | 0.63              |
| 1:J:218:LEU:CD2  | 1:J:222:ILE:HG12 | 2.28                     | 0.63              |
| 1:J:93:MET:SD    | 1:J:716:LEU:N    | 2.71                     | 0.63              |
| 1:J:541:MET:CA   | 4:W:143:TYR:OH   | 2.46                     | 0.63              |
| 1:P:783:LEU:N    | 1:P:783:LEU:HD12 | 2.13                     | 0.63              |
| 1:P:783:LEU:HA   | 1:P:786:ILE:HG12 | 1.81                     | 0.63              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:O    | 1.98                     | 0.63              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:CG   | 2.28                     | 0.63              |
| 1:P:577:ALA:O    | 1:P:578:HIS:CD2  | 2.51                     | 0.63              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:O    | 1.98                     | 0.63              |
| 1:A:557:GLU:N    | 4:V:48:GLY:HA3   | 1.90                     | 0.63              |
| 1:M:725:ARG:NE   | 1:M:737:PHE:CE1  | 2.66                     | 0.63              |
| 1:D:642:LYS:CG   | 4:9:22:ALA:C     | 2.67                     | 0.63              |
| 1:D:831:TRP:CH2  | 2:E:34:ILE:CG2   | 2.77                     | 0.63              |
| 1:J:756:THR:CG2  | 1:J:776:GLU:HB3  | 2.28                     | 0.63              |
| 1:J:831:TRP:CZ2  | 2:K:47:LEU:HD22  | 2.34                     | 0.63              |
| 1:J:829:TRP:CZ2  | 2:K:83:MET:HE2   | 2.33                     | 0.63              |
| 1:J:94:MET:HE1   | 1:J:101:ALA:HB1  | 1.80                     | 0.63              |
| 1:J:141:LEU:HD12 | 1:J:141:LEU:H    | 1.64                     | 0.63              |
| 1:A:724:TYR:HD1  | 1:A:727:LEU:HD11 | 1.64                     | 0.63              |
| 1:P:479:CYS:HB3  | 1:P:653:PHE:CE2  | 2.33                     | 0.63              |
| 4:W:190:MET:SD   | 4:W:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:M:479:CYS:HB3  | 1:M:653:PHE:CE2  | 2.33                     | 0.63              |
| 1:D:724:TYR:HB3  | 1:D:727:LEU:HD12 | 1.80                     | 0.63              |
| 1:P:537:GLU:C    | 4:0:351:THR:N    | 2.51                     | 0.63              |
| 1:P:541:MET:HG2  | 4:0:345:ILE:O    | 1.98                     | 0.63              |
| 1:M:505:MLY:HE3  | 1:M:762:HIS:HE1  | 1.63                     | 0.63              |
| 1:M:505:MLY:CD   | 1:M:762:HIS:NE2  | 2.48                     | 0.63              |
| 1:M:541:MET:C    | 4:Z:143:TYR:CZ   | 2.72                     | 0.63              |
| 1:M:541:MET:O    | 4:Z:143:TYR:OH   | 2.13                     | 0.63              |
| 1:M:544:LYS:HB2  | 4:Z:147:ARG:HA   | 1.80                     | 0.63              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:O    | 1.98                     | 0.63              |
| 1:D:411:GLU:N    | 4:9:333:PRO:HB2  | 2.11                     | 0.63              |
| 1:A:783:LEU:N    | 1:A:783:LEU:HD12 | 2.13                     | 0.63              |
| 1:A:542:PHE:CZ   | 1:A:553:MLY:HH11 | 2.34                     | 0.63              |
| 1:P:141:LEU:HD12 | 1:P:141:LEU:H    | 1.64                     | 0.63              |
| 4:7:257:CYS:HB3  | 4:7:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:X:190:MET:SD   | 4:X:209:VAL:HG11 | 2.38                     | 0.63              |
| 1:A:506:GLU:CB   | 1:A:760:PHE:C    | 2.59                     | 0.63              |
| 2:N:121:LEU:HA   | 2:N:128:PHE:CG   | 2.34                     | 0.63              |
| 2:E:117:LEU:HD11 | 2:E:147:ASN:HB3  | 1.75                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:636:LYS:N    | 4:Z:334:GLU:OE1  | 2.31                     | 0.63              |
| 1:A:831:TRP:HH2  | 2:B:50:THR:OG1   | 1.82                     | 0.63              |
| 1:A:541:MET:CA   | 4:8:143:TYR:OH   | 2.47                     | 0.63              |
| 1:A:537:GLU:C    | 4:8:351:THR:N    | 2.52                     | 0.63              |
| 1:P:839:MLY:HH13 | 2:Q:159:HIS:HD2  | 1.63                     | 0.63              |
| 3:R:48:LYS:C     | 3:R:52:ASN:HD21  | 1.96                     | 0.63              |
| 1:D:166:MET:HE3  | 1:D:254:PHE:CD2  | 2.34                     | 0.63              |
| 4:9:257:CYS:HB3  | 4:9:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:4:257:CYS:HB3  | 4:4:258:PRO:HD3  | 1.81                     | 0.63              |
| 4:2:257:CYS:HB3  | 4:2:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:D:210:GLN:O    | 1:D:211:SER:OG   | 2.15                     | 0.63              |
| 1:J:795:ARG:HB3  | 3:L:35:ARG:HH12  | 0.82                     | 0.63              |
| 2:E:144:VAL:HA   | 2:E:153:ILE:HD11 | 1.80                     | 0.63              |
| 2:H:121:LEU:HA   | 2:H:128:PHE:CG   | 2.34                     | 0.63              |
| 1:J:817:GLN:CB   | 2:K:127:ARG:CD   | 2.77                     | 0.63              |
| 1:P:541:MET:CA   | 4:0:143:TYR:OH   | 2.46                     | 0.63              |
| 1:J:537:GLU:HB3  | 1:J:648:THR:HB   | 1.80                     | 0.63              |
| 1:P:548:THR:HG22 | 4:2:49:GLN:CA    | 2.15                     | 0.63              |
| 1:G:202:SER:CA   | 1:G:207:LYS:HE3  | 2.28                     | 0.63              |
| 1:D:831:TRP:CE2  | 2:E:51:PHE:CE2   | 2.86                     | 0.63              |
| 1:J:95:THR:CA    | 1:J:713:SER:HB3  | 2.28                     | 0.63              |
| 3:L:49:ILE:HA    | 3:L:52:ASN:ND2   | 2.06                     | 0.63              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:C    | 2.36                     | 0.63              |
| 2:H:149:ASP:OD2  | 2:H:150:TYR:C    | 2.36                     | 0.63              |
| 2:Q:149:ASP:OD2  | 2:Q:150:TYR:C    | 2.36                     | 0.63              |
| 1:A:127:ASN:HD22 | 1:A:128:PRO:CD   | 2.11                     | 0.63              |
| 1:M:141:LEU:HD12 | 1:M:141:LEU:H    | 1.64                     | 0.63              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:CB   | 2.29                     | 0.63              |
| 4:5:257:CYS:HB3  | 4:5:258:PRO:HD3  | 1.81                     | 0.63              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:CB   | 2.29                     | 0.63              |
| 1:G:755:HIS:HA   | 1:G:758:TYR:HE1  | 1.64                     | 0.62              |
| 1:G:541:MET:CA   | 4:V:143:TYR:OH   | 2.47                     | 0.62              |
| 2:Q:146:GLY:O    | 2:Q:147:ASN:CB   | 2.46                     | 0.62              |
| 2:K:146:GLY:O    | 2:K:147:ASN:CB   | 2.46                     | 0.62              |
| 1:J:819:ASN:HD21 | 2:K:92:ASP:CB    | 2.06                     | 0.62              |
| 2:B:132:GLU:O    | 2:B:136:MET:HG2  | 1.99                     | 0.62              |
| 1:P:544:LYS:HB2  | 4:0:147:ARG:HA   | 1.80                     | 0.62              |
| 1:J:717:TYR:HD1  | 1:J:744:SER:HG   | 1.45                     | 0.62              |
| 1:M:542:PHE:N    | 4:Z:143:TYR:OH   | 2.32                     | 0.62              |
| 1:J:534:SER:C    | 4:W:351:THR:CA   | 2.47                     | 0.62              |
| 1:D:551:MLY:C    | 4:W:46:GLY:O     | 2.47                     | 0.62              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:G:725:ARG:NE  | 1:G:737:PHE:CE1  | 2.67                     | 0.62              |
| 3:R:24:LYS:HB3  | 3:R:63:ILE:H     | 1.64                     | 0.62              |
| 1:J:278:GLN:CG  | 1:J:317:GLU:HB2  | 2.27                     | 0.62              |
| 1:M:799:MET:SD  | 3:O:32:ASP:CB    | 2.85                     | 0.62              |
| 1:A:274:ARG:HB2 | 1:A:285:TYR:CE2  | 2.34                     | 0.62              |
| 3:C:3:SER:HG    | 3:C:5:ALA:N      | 1.97                     | 0.62              |
| 1:G:166:MET:HE3 | 1:G:254:PHE:HD2  | 1.62                     | 0.62              |
| 1:G:141:LEU:H   | 1:G:141:LEU:HD12 | 1.64                     | 0.62              |
| 1:J:251:ARG:HB2 | 1:J:264:ASP:CB   | 2.29                     | 0.62              |
| 1:D:725:ARG:NE  | 1:D:737:PHE:CE1  | 2.67                     | 0.62              |
| 1:G:636:LYS:N   | 4:V:334:GLU:OE1  | 2.31                     | 0.62              |
| 1:D:813:ILE:CG2 | 2:E:128:PHE:HE1  | 1.98                     | 0.62              |
| 1:G:818:TYR:CZ  | 2:H:127:ARG:NH1  | 2.67                     | 0.62              |
| 2:H:146:GLY:O   | 2:H:147:ASN:CB   | 2.46                     | 0.62              |
| 2:H:144:VAL:HA  | 2:H:153:ILE:HD11 | 1.80                     | 0.62              |
| 1:A:730:SER:C   | 1:A:733:PRO:HD2  | 2.20                     | 0.62              |
| 1:J:724:TYR:HB3 | 1:J:727:LEU:HD12 | 1.80                     | 0.62              |
| 1:M:537:GLU:HB3 | 1:M:648:THR:HB   | 1.80                     | 0.62              |
| 1:J:541:MET:HE1 | 4:W:346:LEU:HD12 | 1.81                     | 0.62              |
| 1:P:578:HIS:CB  | 1:P:592:ILE:HD12 | 2.30                     | 0.62              |
| 1:A:529:PRO:C   | 4:8:354:GLN:CB   | 2.49                     | 0.62              |
| 1:A:551:MLY:C   | 4:V:46:GLY:O     | 2.47                     | 0.62              |
| 1:A:643:GLY:H   | 4:8:23:GLY:C     | 2.02                     | 0.62              |
| 4:2:322:PRO:CB  | 4:4:244:ASP:HB2  | 2.26                     | 0.62              |
| 3:O:49:ILE:HA   | 3:O:52:ASN:ND2   | 2.06                     | 0.62              |
| 1:A:800:ARG:O   | 3:C:149:VAL:HG21 | 1.91                     | 0.62              |
| 2:B:149:ASP:OD2 | 2:B:150:TYR:C    | 2.37                     | 0.62              |
| 1:J:278:GLN:HG3 | 1:J:318:GLY:N    | 2.15                     | 0.62              |
| 1:J:544:LYS:HB2 | 4:W:147:ARG:HA   | 1.80                     | 0.62              |
| 4:7:190:MET:SD  | 4:7:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:P:251:ARG:HB2 | 1:P:264:ASP:CB   | 2.29                     | 0.62              |
| 4:1:190:MET:SD  | 4:1:209:VAL:HG11 | 2.38                     | 0.62              |
| 4:Z:190:MET:SD  | 4:Z:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:A:302:MET:HG2 | 1:A:303:LEU:CD1  | 2.30                     | 0.62              |
| 4:5:190:MET:SD  | 4:5:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:P:819:ASN:OD1 | 2:Q:92:ASP:HB2   | 1.93                     | 0.62              |
| 1:P:541:MET:HE2 | 4:0:346:LEU:HD12 | 1.82                     | 0.62              |
| 1:P:537:GLU:HB3 | 1:P:648:THR:HB   | 1.80                     | 0.62              |
| 1:A:542:PHE:N   | 4:8:143:TYR:OH   | 2.33                     | 0.62              |
| 1:A:578:HIS:CB  | 1:A:592:ILE:HD12 | 2.30                     | 0.62              |
| 1:J:641:LYS:CE  | 1:J:647:GLN:CB   | 2.75                     | 0.62              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:713:SER:HB3 | 1:D:772:LEU:HD12 | 1.79                     | 0.62              |
| 1:M:804:ARG:O   | 1:M:808:GLU:CB   | 2.47                     | 0.62              |
| 1:G:830:PRO:HB2 | 2:H:67:MET:HE1   | 1.73                     | 0.62              |
| 3:F:24:LYS:HB3  | 3:F:63:ILE:H     | 1.64                     | 0.62              |
| 1:P:278:GLN:HG3 | 1:P:318:GLY:N    | 2.15                     | 0.62              |
| 1:D:755:HIS:HA  | 1:D:758:TYR:HE1  | 1.65                     | 0.62              |
| 4:V:190:MET:SD  | 4:V:209:VAL:HG11 | 2.38                     | 0.62              |
| 1:G:771:LEU:O   | 1:G:774:LEU:N    | 2.32                     | 0.62              |
| 1:A:505:MLY:HB3 | 1:A:762:HIS:H    | 1.65                     | 0.62              |
| 1:J:730:SER:C   | 1:J:733:PRO:HD2  | 2.19                     | 0.62              |
| 2:K:121:LEU:HA  | 2:K:128:PHE:CG   | 2.34                     | 0.62              |
| 1:J:538:GLU:HA  | 4:W:349:LEU:CG   | 2.28                     | 0.62              |
| 1:D:541:MET:HE2 | 4:9:346:LEU:HD12 | 1.82                     | 0.62              |
| 1:A:797:PHE:HE1 | 3:C:146:ILE:CA   | 1.92                     | 0.62              |
| 1:M:724:TYR:HD1 | 1:M:727:LEU:HD11 | 1.64                     | 0.62              |
| 1:M:35:MLY:HH23 | 1:M:778:MET:CG   | 2.21                     | 0.62              |
| 1:J:757:GLN:N   | 1:J:776:GLU:HB3  | 2.14                     | 0.62              |
| 1:P:771:LEU:O   | 1:P:774:LEU:N    | 2.32                     | 0.62              |
| 1:M:94:MET:O    | 1:M:713:SER:CA   | 2.46                     | 0.62              |
| 1:G:580:SER:HA  | 1:G:588:VAL:O    | 2.00                     | 0.62              |
| 1:M:98:HIS:HB3  | 1:M:100:PRO:CD   | 2.25                     | 0.62              |
| 1:D:278:GLN:CG  | 1:D:317:GLU:HB2  | 2.27                     | 0.62              |
| 4:V:361:GLU:HB3 | 4:V:369:ILE:HG12 | 1.82                     | 0.62              |
| 2:E:114:LYS:HG3 | 2:E:146:GLY:HA2  | 1.82                     | 0.62              |
| 1:P:730:SER:C   | 1:P:733:PRO:HD2  | 2.19                     | 0.62              |
| 2:H:117:LEU:CG  | 2:H:147:ASN:CB   | 2.76                     | 0.62              |
| 1:J:724:TYR:HD1 | 1:J:727:LEU:HD11 | 1.64                     | 0.62              |
| 1:D:542:PHE:CZ  | 1:D:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:G:730:SER:C   | 1:G:733:PRO:HD2  | 2.20                     | 0.62              |
| 1:A:791:GLN:NE2 | 3:C:115:GLY:CA   | 2.51                     | 0.62              |
| 1:A:543:PRO:HG2 | 4:8:143:TYR:O    | 1.98                     | 0.62              |
| 1:M:797:PHE:HD1 | 3:O:149:VAL:HG13 | 1.60                     | 0.62              |
| 1:D:642:LYS:CA  | 4:9:21:PHE:O     | 2.46                     | 0.62              |
| 1:M:643:GLY:H   | 4:Z:23:GLY:C     | 2.02                     | 0.62              |
| 1:D:831:TRP:CG  | 2:E:51:PHE:CZ    | 2.85                     | 0.62              |
| 1:J:756:THR:CG2 | 1:J:776:GLU:O    | 2.27                     | 0.62              |
| 1:G:544:LYS:HB2 | 4:V:147:ARG:HA   | 1.81                     | 0.62              |
| 1:A:544:LYS:HB2 | 4:8:147:ARG:HA   | 1.80                     | 0.62              |
| 1:M:278:GLN:HG3 | 1:M:318:GLY:N    | 2.15                     | 0.62              |
| 1:D:251:ARG:HB2 | 1:D:264:ASP:CB   | 2.29                     | 0.62              |
| 4:8:257:CYS:HB3 | 4:8:258:PRO:HD3  | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:580:SER:HA   | 1:D:588:VAL:O    | 2.00                     | 0.62              |
| 1:J:771:LEU:O    | 1:J:774:LEU:N    | 2.32                     | 0.62              |
| 1:D:725:ARG:C    | 1:D:782:MLY:CH2  | 2.63                     | 0.62              |
| 1:G:541:MET:C    | 4:V:143:TYR:CZ   | 2.73                     | 0.62              |
| 1:G:542:PHE:N    | 4:V:143:TYR:OH   | 2.33                     | 0.62              |
| 2:E:121:LEU:HA   | 2:E:128:PHE:CG   | 2.34                     | 0.62              |
| 2:H:132:GLU:O    | 2:H:136:MET:HG2  | 1.99                     | 0.62              |
| 2:H:111:SER:OG   | 2:H:148:VAL:CG1  | 2.47                     | 0.62              |
| 1:A:537:GLU:HB3  | 1:A:648:THR:HB   | 1.80                     | 0.62              |
| 1:D:771:LEU:O    | 1:D:774:LEU:N    | 2.32                     | 0.62              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:HE1  | 1.80                     | 0.62              |
| 1:M:35:MLY:HG3   | 1:M:777:GLU:CD   | 2.19                     | 0.62              |
| 1:P:724:TYR:HD1  | 1:P:727:LEU:HD11 | 1.64                     | 0.62              |
| 3:O:24:LYS:HB3   | 3:O:63:ILE:H     | 1.64                     | 0.62              |
| 1:J:161:ASN:HA   | 1:J:164:GLN:HE21 | 1.63                     | 0.62              |
| 4:X:361:GLU:HB3  | 4:X:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:520:ALA:O    | 1:A:524:GLU:HG2  | 2.00                     | 0.62              |
| 1:J:580:SER:HA   | 1:J:588:VAL:O    | 2.00                     | 0.62              |
| 4:Z:361:GLU:HB3  | 4:Z:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:D:735:GLY:O    | 1:D:743:ALA:HA   | 1.94                     | 0.62              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:CB   | 2.25                     | 0.62              |
| 2:Q:121:LEU:HA   | 2:Q:128:PHE:CG   | 2.34                     | 0.62              |
| 1:J:817:GLN:HB3  | 2:K:127:ARG:HD2  | 1.76                     | 0.62              |
| 1:M:542:PHE:CZ   | 1:M:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:J:542:PHE:CZ   | 1:J:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:D:542:PHE:CB   | 4:9:143:TYR:HE1  | 2.13                     | 0.62              |
| 1:P:580:SER:HA   | 1:P:588:VAL:O    | 2.00                     | 0.62              |
| 1:A:530:MET:CG   | 4:8:354:GLN:CG   | 2.71                     | 0.62              |
| 1:M:782:MLY:O    | 1:M:786:ILE:CD1  | 2.48                     | 0.62              |
| 1:M:730:SER:C    | 1:M:733:PRO:HD2  | 2.20                     | 0.62              |
| 3:R:49:ILE:CA    | 3:R:52:ASN:ND2   | 2.53                     | 0.62              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:CD2  | 2.88                     | 0.62              |
| 1:A:141:LEU:HD12 | 1:A:141:LEU:H    | 1.64                     | 0.62              |
| 1:D:161:ASN:HA   | 1:D:164:GLN:HE21 | 1.64                     | 0.62              |
| 4:V:257:CYS:HB3  | 4:V:258:PRO:HD3  | 1.81                     | 0.62              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:HB3  | 2.35                     | 0.62              |
| 1:A:717:TYR:HD1  | 1:A:744:SER:HG   | 1.47                     | 0.62              |
| 2:K:111:SER:OG   | 2:K:148:VAL:CG1  | 2.47                     | 0.62              |
| 1:P:542:PHE:CB   | 4:0:143:TYR:HE1  | 2.13                     | 0.62              |
| 1:M:406:VAL:HG12 | 1:M:407:GLY:N    | 2.13                     | 0.62              |
| 1:D:578:HIS:CB   | 1:D:592:ILE:HD12 | 2.30                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:541:MET:HE2  | 4:8:346:LEU:HD12 | 1.82                     | 0.62              |
| 4:0:288:ASP:HB3  | 4:2:63:GLY:H     | 1.62                     | 0.62              |
| 1:J:756:THR:HG23 | 1:J:779:ARG:CD   | 2.30                     | 0.62              |
| 1:J:94:MET:O     | 1:J:713:SER:CA   | 2.46                     | 0.62              |
| 1:G:829:TRP:CZ3  | 2:H:84:PHE:CZ    | 2.87                     | 0.62              |
| 3:I:50:LEU:O     | 3:I:53:PRO:HD2   | 2.00                     | 0.62              |
| 3:L:50:LEU:O     | 3:L:53:PRO:HD2   | 2.00                     | 0.62              |
| 1:G:98:HIS:HB3   | 1:G:100:PRO:CD   | 2.25                     | 0.62              |
| 1:A:98:HIS:HB3   | 1:A:100:PRO:CD   | 2.25                     | 0.62              |
| 4:8:361:GLU:HB3  | 4:8:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:2:361:GLU:HB3  | 4:2:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:W:361:GLU:HB3  | 4:W:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:M:251:ARG:HB2  | 1:M:264:ASP:CB   | 2.29                     | 0.62              |
| 4:3:190:MET:SD   | 4:3:209:VAL:HG11 | 2.38                     | 0.62              |
| 4:Y:361:GLU:HB3  | 4:Y:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:A:707:CYS:SG   | 1:A:714:ARG:CZ   | 2.88                     | 0.62              |
| 1:A:771:LEU:O    | 1:A:774:LEU:N    | 2.32                     | 0.62              |
| 1:G:542:PHE:CZ   | 1:G:553:MLY:HH11 | 2.34                     | 0.62              |
| 1:P:538:GLU:HA   | 4:0:349:LEU:CG   | 2.28                     | 0.62              |
| 1:M:543:PRO:HG2  | 4:Z:143:TYR:O    | 1.98                     | 0.62              |
| 1:M:541:MET:HE2  | 4:Z:346:LEU:HD12 | 1.81                     | 0.62              |
| 1:J:541:MET:C    | 4:W:143:TYR:CZ   | 2.72                     | 0.62              |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:N    | 2.13                     | 0.62              |
| 1:D:520:ALA:O    | 1:D:524:GLU:HG2  | 2.00                     | 0.62              |
| 1:D:541:MET:SD   | 4:9:346:LEU:O    | 2.48                     | 0.62              |
| 1:D:636:LYS:N    | 4:9:334:GLU:OE1  | 2.31                     | 0.62              |
| 1:M:839:MLY:HH21 | 2:N:158:THR:HG22 | 1.82                     | 0.62              |
| 1:A:642:LYS:CG   | 4:8:22:ALA:C     | 2.67                     | 0.62              |
| 1:P:767:PHE:HB3  | 1:P:772:LEU:HD22 | 1.82                     | 0.62              |
| 1:J:557:GLU:O    | 1:J:557:GLU:HG3  | 2.00                     | 0.62              |
| 1:G:578:HIS:CB   | 1:G:592:ILE:HD12 | 2.30                     | 0.62              |
| 1:D:544:LYS:HB2  | 4:9:147:ARG:HA   | 1.80                     | 0.62              |
| 1:G:127:ASN:HD22 | 1:G:128:PRO:CD   | 2.11                     | 0.62              |
| 1:A:161:ASN:HA   | 1:A:164:GLN:HE21 | 1.63                     | 0.62              |
| 1:M:161:ASN:HA   | 1:M:164:GLN:HE21 | 1.63                     | 0.62              |
| 4:0:361:GLU:HB3  | 4:0:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:M:302:MET:HG2  | 1:M:303:LEU:CD1  | 2.30                     | 0.62              |
| 4:9:361:GLU:HB3  | 4:9:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:3:361:GLU:HB3  | 4:3:369:ILE:HG12 | 1.82                     | 0.62              |
| 1:G:543:PRO:HG2  | 4:V:143:TYR:O    | 1.99                     | 0.62              |
| 4:1:288:ASP:CB   | 4:3:203:THR:HG21 | 2.29                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:642:LYS:CG   | 4:0:22:ALA:C     | 2.67                     | 0.62              |
| 1:M:541:MET:SD   | 4:Z:346:LEU:O    | 2.48                     | 0.62              |
| 1:P:785:GLU:C    | 1:P:786:ILE:HA   | 2.18                     | 0.62              |
| 1:D:541:MET:CA   | 4:9:143:TYR:OH   | 2.47                     | 0.62              |
| 1:A:797:PHE:CE2  | 3:C:126:LEU:CD2  | 2.58                     | 0.62              |
| 1:A:553:MLY:O    | 4:V:48:GLY:HA2   | 1.99                     | 0.62              |
| 1:M:797:PHE:CZ   | 3:O:146:ILE:CD1  | 2.75                     | 0.62              |
| 1:M:798:LEU:HD21 | 3:O:126:LEU:HD12 | 1.78                     | 0.62              |
| 1:M:508:ILE:HD11 | 1:M:759:ALA:HB1  | 1.80                     | 0.62              |
| 1:P:707:CYS:SG   | 1:P:714:ARG:NH2  | 2.73                     | 0.62              |
| 1:A:643:GLY:O    | 1:A:644:SER:CB   | 2.48                     | 0.62              |
| 1:D:278:GLN:HG3  | 1:D:318:GLY:N    | 2.15                     | 0.62              |
| 1:G:799:MET:SD   | 3:I:32:ASP:OD2   | 2.58                     | 0.62              |
| 1:M:154:HIS:CE1  | 1:M:156:PHE:CD2  | 2.88                     | 0.62              |
| 1:P:161:ASN:HA   | 1:P:164:GLN:HE21 | 1.64                     | 0.62              |
| 4:7:361:GLU:HB3  | 4:7:369:ILE:HG12 | 1.82                     | 0.62              |
| 4:3:257:CYS:HB3  | 4:3:258:PRO:HD3  | 1.81                     | 0.62              |
| 1:G:302:MET:HG2  | 1:G:303:LEU:CD1  | 2.30                     | 0.62              |
| 4:1:257:CYS:HB3  | 4:1:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:Z:257:CYS:HB3  | 4:Z:258:PRO:HD3  | 1.81                     | 0.62              |
| 4:X:257:CYS:HB3  | 4:X:258:PRO:HD3  | 1.81                     | 0.62              |
| 1:G:557:GLU:HB2  | 4:X:47:MET:N     | 2.11                     | 0.61              |
| 2:Q:114:LYS:HG3  | 2:Q:146:GLY:HA2  | 1.82                     | 0.61              |
| 2:Q:144:VAL:HA   | 2:Q:153:ILE:HD11 | 1.80                     | 0.61              |
| 4:X:324:THR:HG21 | 4:Z:247:VAL:CA   | 2.22                     | 0.61              |
| 1:P:530:MET:HE3  | 4:0:354:GLN:HG2  | 1.79                     | 0.61              |
| 1:M:520:ALA:O    | 1:M:524:GLU:HG2  | 2.00                     | 0.61              |
| 1:M:544:LYS:C    | 4:1:45:VAL:HG11  | 2.20                     | 0.61              |
| 1:J:542:PHE:CB   | 4:W:143:TYR:HE1  | 2.13                     | 0.61              |
| 1:M:730:SER:HB2  | 3:O:96:LYS:HB3   | 1.82                     | 0.61              |
| 1:A:81:ASN:OD1   | 1:A:96:HIS:HB2   | 2.00                     | 0.61              |
| 3:R:50:LEU:O     | 3:R:53:PRO:HD2   | 2.00                     | 0.61              |
| 1:A:278:GLN:HG3  | 1:A:318:GLY:N    | 2.15                     | 0.61              |
| 1:P:274:ARG:HB2  | 1:P:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:A:580:SER:HA   | 1:A:588:VAL:O    | 2.00                     | 0.61              |
| 1:D:302:MET:HG2  | 1:D:303:LEU:CD1  | 2.30                     | 0.61              |
| 2:Q:111:SER:OG   | 2:Q:148:VAL:CG1  | 2.47                     | 0.61              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:N    | 2.13                     | 0.61              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:C    | 2.69                     | 0.61              |
| 2:K:114:LYS:HG3  | 2:K:146:GLY:HA2  | 1.82                     | 0.61              |
| 1:P:643:GLY:H    | 4:0:23:GLY:C     | 2.02                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:578:HIS:CB   | 1:M:592:ILE:HD12 | 2.30                     | 0.61              |
| 1:M:580:SER:HA   | 1:M:588:VAL:O    | 2.00                     | 0.61              |
| 1:J:411:GLU:N    | 4:W:333:PRO:HB2  | 2.11                     | 0.61              |
| 1:A:541:MET:C    | 4:8:143:TYR:CZ   | 2.73                     | 0.61              |
| 1:A:579:PHE:CE1  | 1:A:581:LEU:HD13 | 2.35                     | 0.61              |
| 4:X:291:LYS:CE   | 4:Z:243:PRO:HB2  | 2.30                     | 0.61              |
| 3:C:24:LYS:HB3   | 3:C:63:ILE:H     | 1.64                     | 0.61              |
| 1:A:99:GLU:OE2   | 1:A:696:ARG:NH2  | 2.31                     | 0.61              |
| 1:G:278:GLN:HG3  | 1:G:318:GLY:N    | 2.15                     | 0.61              |
| 1:G:274:ARG:HB2  | 1:G:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:G:639:GLY:N    | 4:V:344:SER:C    | 2.54                     | 0.61              |
| 2:E:111:SER:OG   | 2:E:148:VAL:CG1  | 2.47                     | 0.61              |
| 2:H:144:VAL:CG1  | 2:H:153:ILE:HD13 | 2.20                     | 0.61              |
| 1:M:639:GLY:N    | 4:Z:344:SER:C    | 2.54                     | 0.61              |
| 1:J:530:MET:CG   | 4:W:354:GLN:CG   | 2.72                     | 0.61              |
| 1:P:795:ARG:CZ   | 3:R:116:GLU:CB   | 2.57                     | 0.61              |
| 1:A:798:LEU:CG   | 3:C:126:LEU:HD11 | 2.29                     | 0.61              |
| 1:G:148:ARG:HH21 | 1:G:764:MLY:CH2  | 2.12                     | 0.61              |
| 1:G:829:TRP:CH2  | 2:H:87:LYS:CE    | 2.83                     | 0.61              |
| 1:G:94:MET:HE1   | 1:G:101:ALA:HB1  | 1.80                     | 0.61              |
| 1:J:99:GLU:OE2   | 1:J:696:ARG:NH2  | 2.30                     | 0.61              |
| 1:D:708:ARG:O    | 1:D:710:GLY:N    | 2.33                     | 0.61              |
| 1:P:302:MET:HG2  | 1:P:303:LEU:CD1  | 2.30                     | 0.61              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:ND1  | 2.63                     | 0.61              |
| 1:G:643:GLY:O    | 1:G:644:SER:CB   | 2.48                     | 0.61              |
| 1:G:541:MET:HE2  | 4:V:346:LEU:HD12 | 1.82                     | 0.61              |
| 1:J:813:ILE:O    | 1:J:817:GLN:N    | 2.30                     | 0.61              |
| 1:P:541:MET:C    | 4:0:143:TYR:CZ   | 2.73                     | 0.61              |
| 1:P:542:PHE:CZ   | 1:P:553:MLY:HH11 | 2.34                     | 0.61              |
| 1:M:551:MLY:O    | 4:1:48:GLY:CA    | 2.46                     | 0.61              |
| 1:D:543:PRO:HG2  | 4:9:143:TYR:O    | 1.98                     | 0.61              |
| 1:D:576:GLU:CG   | 1:D:577:ALA:N    | 2.44                     | 0.61              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:OE1  | 2.29                     | 0.61              |
| 1:A:798:LEU:HD21 | 3:C:126:LEU:HD11 | 1.82                     | 0.61              |
| 1:M:793:ARG:HH11 | 3:O:40:ASN:HD22  | 0.63                     | 0.61              |
| 1:A:834:LEU:HD23 | 2:B:54:MET:HE3   | 1.73                     | 0.61              |
| 3:O:52:ASN:N     | 3:O:53:PRO:HD2   | 2.15                     | 0.61              |
| 1:M:623:PHE:CG   | 1:M:623:PHE:HA   | 2.35                     | 0.61              |
| 3:I:24:LYS:HB3   | 3:I:63:ILE:H     | 1.64                     | 0.61              |
| 1:M:81:ASN:OD1   | 1:M:96:HIS:HB2   | 2.00                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:81:ASN:OD1   | 1:G:96:HIS:HB2   | 2.00                     | 0.61              |
| 1:G:579:PHE:CE1  | 1:G:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:A:278:GLN:CG   | 1:A:317:GLU:HB2  | 2.27                     | 0.61              |
| 1:P:154:HIS:CE1  | 1:P:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:D:730:SER:C    | 1:D:733:PRO:HD2  | 2.20                     | 0.61              |
| 1:G:797:PHE:CZ   | 3:I:146:ILE:HD11 | 2.25                     | 0.61              |
| 1:G:553:MLY:HB2  | 4:X:46:GLY:HA3   | 1.83                     | 0.61              |
| 1:J:732:ILE:HG22 | 1:J:747:LEU:CD1  | 1.55                     | 0.61              |
| 2:B:111:SER:OG   | 2:B:148:VAL:CG1  | 2.47                     | 0.61              |
| 1:D:557:GLU:O    | 1:D:557:GLU:HG3  | 2.00                     | 0.61              |
| 1:M:797:PHE:CE2  | 3:O:126:LEU:CD2  | 2.82                     | 0.61              |
| 1:G:724:TYR:HB3  | 1:G:727:LEU:HD12 | 1.80                     | 0.61              |
| 2:Q:34:ILE:O     | 2:Q:46:ASP:HB3   | 2.01                     | 0.61              |
| 1:D:838:ILE:HD13 | 2:E:54:MET:CE    | 2.30                     | 0.61              |
| 1:D:202:SER:HA   | 1:D:207:LYS:HE3  | 1.72                     | 0.61              |
| 2:E:34:ILE:O     | 2:E:46:ASP:HB3   | 2.01                     | 0.61              |
| 1:J:578:HIS:CB   | 1:J:592:ILE:HD12 | 2.30                     | 0.61              |
| 1:M:99:GLU:OE2   | 1:M:696:ARG:NH2  | 2.30                     | 0.61              |
| 4:V:286:ASP:OD2  | 4:X:203:THR:CG2  | 2.47                     | 0.61              |
| 1:G:278:GLN:CG   | 1:G:317:GLU:HB2  | 2.26                     | 0.61              |
| 1:D:274:ARG:HB2  | 1:D:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:M:274:ARG:HB2  | 1:M:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:A:686:MET:HG3  | 1:A:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:D:686:MET:HG3  | 1:D:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:G:161:ASN:HA   | 1:G:164:GLN:HE21 | 1.63                     | 0.61              |
| 1:D:141:LEU:H    | 1:D:141:LEU:HD12 | 1.64                     | 0.61              |
| 4:4:361:GLU:HB3  | 4:4:369:ILE:HG12 | 1.82                     | 0.61              |
| 4:5:361:GLU:HB3  | 4:5:369:ILE:HG12 | 1.82                     | 0.61              |
| 1:A:149:GLN:HB2  | 1:A:718:ALA:HB3  | 0.96                     | 0.61              |
| 1:G:530:MET:HE3  | 4:V:354:GLN:CG   | 2.23                     | 0.61              |
| 2:H:114:LYS:HG3  | 2:H:146:GLY:HA2  | 1.82                     | 0.61              |
| 1:J:639:GLY:N    | 4:W:344:SER:C    | 2.54                     | 0.61              |
| 1:J:642:LYS:CD   | 4:W:24:ASP:O     | 2.43                     | 0.61              |
| 1:J:643:GLY:O    | 1:J:644:SER:CB   | 2.49                     | 0.61              |
| 1:D:541:MET:C    | 4:9:143:TYR:CZ   | 2.73                     | 0.61              |
| 1:D:410:ASN:CG   | 4:9:334:GLU:CA   | 2.47                     | 0.61              |
| 1:D:553:MLY:O    | 4:W:48:GLY:HA2   | 1.99                     | 0.61              |
| 3:I:52:ASN:N     | 3:I:53:PRO:HD2   | 2.16                     | 0.61              |
| 3:R:52:ASN:N     | 3:R:53:PRO:HD2   | 2.16                     | 0.61              |
| 1:J:623:PHE:CG   | 1:J:623:PHE:HA   | 2.35                     | 0.61              |
| 3:L:24:LYS:HB3   | 3:L:63:ILE:H     | 1.64                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:63:ILE:HG22  | 3:O:64:THR:O     | 2.01                     | 0.61              |
| 1:J:579:PHE:CE1  | 1:J:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:J:834:LEU:HD13 | 2:K:51:PHE:HE1   | 1.62                     | 0.61              |
| 1:J:302:MET:HG2  | 1:J:303:LEU:CD1  | 2.30                     | 0.61              |
| 1:P:81:ASN:OD1   | 1:P:96:HIS:HB2   | 2.00                     | 0.61              |
| 1:J:783:LEU:N    | 1:J:783:LEU:HD12 | 2.13                     | 0.61              |
| 1:G:797:PHE:HE2  | 3:I:126:LEU:HD13 | 1.66                     | 0.61              |
| 1:M:817:GLN:CG   | 2:N:127:ARG:HB2  | 2.28                     | 0.61              |
| 1:P:411:GLU:N    | 4:O:333:PRO:HB2  | 2.11                     | 0.61              |
| 1:P:643:GLY:O    | 1:P:644:SER:CB   | 2.48                     | 0.61              |
| 3:F:63:ILE:HG22  | 3:F:64:THR:O     | 2.01                     | 0.61              |
| 3:L:52:ASN:N     | 3:L:53:PRO:HD2   | 2.15                     | 0.61              |
| 3:I:63:ILE:HG22  | 3:I:64:THR:O     | 2.01                     | 0.61              |
| 1:P:40:VAL:HG22  | 1:P:41:VAL:N     | 2.16                     | 0.61              |
| 1:J:274:ARG:HB2  | 1:J:285:TYR:CE2  | 2.34                     | 0.61              |
| 1:P:686:MET:HG3  | 1:P:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:M:557:GLU:O    | 1:M:557:GLU:HG3  | 2.00                     | 0.61              |
| 1:D:798:LEU:CD2  | 3:F:122:GLU:HB3  | 2.31                     | 0.61              |
| 2:N:111:SER:OG   | 2:N:148:VAL:CG1  | 2.47                     | 0.61              |
| 2:N:114:LYS:HG3  | 2:N:146:GLY:HA2  | 1.82                     | 0.61              |
| 1:G:557:GLU:O    | 1:G:557:GLU:HG3  | 2.00                     | 0.61              |
| 1:J:820:VAL:CG1  | 2:K:136:MET:HE1  | 2.31                     | 0.61              |
| 1:P:639:GLY:N    | 4:O:344:SER:C    | 2.54                     | 0.61              |
| 1:M:579:PHE:CE1  | 1:M:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:J:643:GLY:H    | 4:W:23:GLY:C     | 2.02                     | 0.61              |
| 1:G:732:ILE:HG22 | 1:G:747:LEU:CD1  | 1.55                     | 0.61              |
| 1:A:542:PHE:CB   | 4:8:143:TYR:HE1  | 2.13                     | 0.61              |
| 1:M:786:ILE:C    | 1:M:789:ALA:HB3  | 2.21                     | 0.61              |
| 2:N:34:ILE:O     | 2:N:46:ASP:HB3   | 2.01                     | 0.61              |
| 1:M:202:SER:CA   | 1:M:207:LYS:HE3  | 2.27                     | 0.61              |
| 1:P:803:TYR:CE2  | 3:R:17:PHE:CZ    | 2.88                     | 0.61              |
| 1:D:634:GLY:N    | 4:9:25:ASP:O     | 2.31                     | 0.61              |
| 1:P:623:PHE:CG   | 1:P:623:PHE:HA   | 2.35                     | 0.61              |
| 1:M:686:MET:HG3  | 1:M:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:P:520:ALA:O    | 1:P:524:GLU:HG2  | 2.00                     | 0.61              |
| 1:D:508:ILE:HD12 | 1:D:766:PHE:CZ   | 2.17                     | 0.61              |
| 1:G:524:GLU:O    | 1:G:528:MLY:HB3  | 2.01                     | 0.61              |
| 1:A:721:LYS:HG2  | 1:A:736:GLN:CD   | 1.86                     | 0.61              |
| 1:J:524:GLU:O    | 1:J:528:MLY:HB3  | 2.01                     | 0.61              |
| 1:D:217:THR:C    | 1:D:221:GLN:HG2  | 2.21                     | 0.61              |
| 1:M:217:THR:C    | 1:M:221:GLN:HG2  | 2.21                     | 0.61              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:P:579:PHE:CE1 | 1:P:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:A:799:MET:SD  | 3:C:32:ASP:O     | 2.59                     | 0.61              |
| 1:M:805:ALA:O   | 1:M:809:ARG:HB2  | 1.99                     | 0.61              |
| 1:M:34:ALA:CB   | 1:M:777:GLU:CD   | 2.56                     | 0.61              |
| 3:C:52:ASN:N    | 3:C:53:PRO:HD2   | 2.15                     | 0.61              |
| 1:G:94:MET:O    | 1:G:713:SER:CA   | 2.49                     | 0.61              |
| 1:G:686:MET:HG3 | 1:G:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:J:154:HIS:CE1 | 1:J:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:D:154:HIS:CE1 | 1:D:156:PHE:CD2  | 2.88                     | 0.61              |
| 1:P:524:GLU:O   | 1:P:528:MLY:HB3  | 2.01                     | 0.61              |
| 1:G:91:MET:HE3  | 1:G:119:SER:HB2  | 1.83                     | 0.61              |
| 1:D:727:LEU:HB2 | 1:D:782:MLY:HH13 | 0.61                     | 0.61              |
| 2:E:144:VAL:CG1 | 2:E:153:ILE:HD13 | 2.19                     | 0.61              |
| 2:B:114:LYS:HG3 | 2:B:146:GLY:HA2  | 1.82                     | 0.61              |
| 1:D:579:PHE:CE1 | 1:D:581:LEU:HD13 | 2.35                     | 0.61              |
| 1:G:730:SER:OG  | 3:I:113:THR:CB   | 2.48                     | 0.61              |
| 1:A:95:THR:HB   | 1:A:772:LEU:HD22 | 1.83                     | 0.61              |
| 1:P:665:ARG:C   | 1:P:667:THR:H    | 2.05                     | 0.61              |
| 4:5:223:PHE:HD2 | 4:5:312:ARG:NH2  | 1.99                     | 0.61              |
| 4:4:223:PHE:HD2 | 4:4:312:ARG:NH2  | 1.99                     | 0.61              |
| 1:J:686:MET:HG3 | 1:J:691:VAL:HG21 | 1.83                     | 0.61              |
| 1:A:524:GLU:O   | 1:A:528:MLY:HB3  | 2.01                     | 0.61              |
| 1:P:735:GLY:O   | 1:P:743:ALA:HA   | 1.94                     | 0.60              |
| 1:M:578:HIS:CD2 | 1:M:591:ASN:HA   | 2.31                     | 0.60              |
| 1:D:530:MET:CG  | 4:9:354:GLN:HG3  | 2.30                     | 0.60              |
| 1:D:578:HIS:CD2 | 1:D:591:ASN:HA   | 2.31                     | 0.60              |
| 1:A:553:MLY:NZ  | 4:V:45:VAL:HG13  | 2.16                     | 0.60              |
| 1:G:724:TYR:HD1 | 1:G:727:LEU:HD11 | 1.64                     | 0.60              |
| 1:D:643:GLY:H   | 4:9:23:GLY:C     | 2.02                     | 0.60              |
| 1:G:829:TRP:CH2 | 2:H:83:MET:HE3   | 2.33                     | 0.60              |
| 1:G:769:ALA:O   | 1:G:773:GLY:HA2  | 2.01                     | 0.60              |
| 3:F:50:LEU:O    | 3:F:53:PRO:HD2   | 2.00                     | 0.60              |
| 3:C:50:LEU:O    | 3:C:53:PRO:HD2   | 2.00                     | 0.60              |
| 1:A:40:VAL:HG22 | 1:A:41:VAL:N     | 2.16                     | 0.60              |
| 1:J:665:ARG:C   | 1:J:667:THR:H    | 2.05                     | 0.60              |
| 4:9:223:PHE:HD2 | 4:9:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:G:795:ARG:NE  | 3:I:116:GLU:OE2  | 2.33                     | 0.60              |
| 2:Q:130:PRO:HA  | 2:Q:133:ILE:HD12 | 1.83                     | 0.60              |
| 1:D:813:ILE:O   | 1:D:817:GLN:N    | 2.30                     | 0.60              |
| 2:K:130:PRO:HA  | 2:K:133:ILE:HD12 | 1.83                     | 0.60              |
| 1:P:530:MET:HE3 | 4:0:355:MET:SD   | 2.41                     | 0.60              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:P:542:PHE:N   | 4:0:143:TYR:OH   | 2.33                     | 0.60              |
| 1:A:736:GLN:HA  | 1:A:743:ALA:HB1  | 1.27                     | 0.60              |
| 1:J:553:MLY:HE3 | 4:Y:45:VAL:HG12  | 1.80                     | 0.60              |
| 1:D:81:ASN:OD1  | 1:D:96:HIS:HB2   | 2.00                     | 0.60              |
| 1:M:717:TYR:HD1 | 1:M:744:SER:HG   | 1.47                     | 0.60              |
| 1:D:643:GLY:O   | 1:D:644:SER:CB   | 2.48                     | 0.60              |
| 1:M:643:GLY:O   | 1:M:644:SER:CB   | 2.49                     | 0.60              |
| 1:P:724:TYR:CE1 | 1:P:776:GLU:CD   | 2.67                     | 0.60              |
| 1:M:834:LEU:CD1 | 2:N:51:PHE:CD1   | 2.83                     | 0.60              |
| 1:A:665:ARG:C   | 1:A:667:THR:H    | 2.04                     | 0.60              |
| 4:8:223:PHE:HD2 | 4:8:312:ARG:NH2  | 2.00                     | 0.60              |
| 4:X:223:PHE:HD2 | 4:X:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:A:156:PHE:CD1 | 1:A:195:TYR:CD1  | 2.89                     | 0.60              |
| 4:1:361:GLU:HB3 | 4:1:369:ILE:HG12 | 1.82                     | 0.60              |
| 1:J:797:PHE:CZ  | 3:L:126:LEU:HD22 | 2.36                     | 0.60              |
| 1:G:797:PHE:CE2 | 3:I:126:LEU:HD13 | 2.36                     | 0.60              |
| 2:N:130:PRO:HA  | 2:N:133:ILE:HD12 | 1.83                     | 0.60              |
| 1:G:520:ALA:O   | 1:G:524:GLU:HG2  | 2.00                     | 0.60              |
| 1:J:28:GLN:OE1  | 1:J:723:ARG:CG   | 2.49                     | 0.60              |
| 1:M:550:PHE:CE2 | 1:M:592:ILE:HG23 | 2.37                     | 0.60              |
| 1:M:542:PHE:CB  | 4:Z:143:TYR:HE1  | 2.13                     | 0.60              |
| 1:J:530:MET:CG  | 4:W:354:GLN:HG3  | 2.30                     | 0.60              |
| 1:G:503:TYR:CZ  | 1:G:711:PHE:HE2  | 2.07                     | 0.60              |
| 4:0:245:GLY:N   | 4:Y:291:LYS:HB2  | 2.16                     | 0.60              |
| 1:A:837:MLY:O   | 1:A:840:PRO:HD2  | 2.02                     | 0.60              |
| 1:J:202:SER:HA  | 1:J:207:LYS:HE3  | 1.72                     | 0.60              |
| 1:J:95:THR:HA   | 1:J:713:SER:HG   | 1.63                     | 0.60              |
| 1:J:95:THR:HG23 | 1:J:96:HIS:ND1   | 2.17                     | 0.60              |
| 1:G:829:TRP:HH2 | 2:H:83:MET:CE    | 2.14                     | 0.60              |
| 1:D:623:PHE:HA  | 1:D:623:PHE:CG   | 2.36                     | 0.60              |
| 1:G:40:VAL:HG22 | 1:G:41:VAL:N     | 2.16                     | 0.60              |
| 1:J:769:ALA:CB  | 1:J:770:GLY:HA3  | 2.30                     | 0.60              |
| 4:Y:223:PHE:HD2 | 4:Y:312:ARG:NH2  | 1.99                     | 0.60              |
| 4:0:223:PHE:HD2 | 4:0:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:D:38:VAL:HB   | 1:D:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:P:38:VAL:HB   | 1:P:52:ILE:HD11  | 1.83                     | 0.60              |
| 1:A:292:MET:HE3 | 1:A:309:PRO:HA   | 1.82                     | 0.60              |
| 1:D:124:VAL:CG1 | 1:D:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:P:544:LYS:NZ  | 4:2:45:VAL:HG21  | 2.16                     | 0.60              |
| 1:J:217:THR:C   | 1:J:221:GLN:HG2  | 2.21                     | 0.60              |
| 1:J:520:ALA:O   | 1:J:524:GLU:HG2  | 2.00                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:542:PHE:N    | 4:W:143:TYR:OH   | 2.33                     | 0.60              |
| 1:D:524:GLU:O    | 1:D:528:MLY:HB3  | 2.01                     | 0.60              |
| 1:A:546:THR:HG22 | 1:A:547:ASP:N    | 2.17                     | 0.60              |
| 1:A:557:GLU:O    | 1:A:557:GLU:HG3  | 2.00                     | 0.60              |
| 1:M:837:MLY:O    | 1:M:840:PRO:HD2  | 2.01                     | 0.60              |
| 1:G:623:PHE:HA   | 1:G:623:PHE:CG   | 2.36                     | 0.60              |
| 1:M:768:MLY:O    | 1:M:770:GLY:N    | 2.35                     | 0.60              |
| 1:P:40:VAL:HG22  | 1:P:41:VAL:H     | 1.67                     | 0.60              |
| 1:M:40:VAL:HG22  | 1:M:41:VAL:N     | 2.16                     | 0.60              |
| 1:M:278:GLN:CG   | 1:M:317:GLU:HB2  | 2.27                     | 0.60              |
| 1:M:127:ASN:ND2  | 1:M:128:PRO:HD2  | 2.16                     | 0.60              |
| 4:1:223:PHE:HD2  | 4:1:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:J:38:VAL:HB    | 1:J:52:ILE:HD11  | 1.83                     | 0.60              |
| 1:G:124:VAL:CG1  | 1:G:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:P:91:MET:HE3   | 1:P:119:SER:HB2  | 1.83                     | 0.60              |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:HH21 | 1.82                     | 0.60              |
| 1:G:792:ALA:N    | 3:I:42:THR:HG22  | 2.16                     | 0.60              |
| 1:A:707:CYS:CB   | 1:A:714:ARG:NH1  | 2.64                     | 0.60              |
| 1:D:507:GLY:CA   | 1:D:762:HIS:CD2  | 2.84                     | 0.60              |
| 1:A:217:THR:C    | 1:A:221:GLN:HG2  | 2.21                     | 0.60              |
| 1:J:543:PRO:HG2  | 4:W:143:TYR:O    | 1.98                     | 0.60              |
| 1:D:639:GLY:N    | 4:9:344:SER:C    | 2.54                     | 0.60              |
| 1:G:837:MLY:O    | 1:G:840:PRO:HD2  | 2.02                     | 0.60              |
| 1:D:837:MLY:O    | 1:D:840:PRO:HD2  | 2.02                     | 0.60              |
| 4:2:324:THR:CG2  | 4:4:243:PRO:O    | 2.49                     | 0.60              |
| 3:O:50:LEU:O     | 3:O:53:PRO:HD2   | 2.00                     | 0.60              |
| 1:J:546:THR:HG22 | 1:J:547:ASP:N    | 2.17                     | 0.60              |
| 4:V:223:PHE:HD2  | 4:V:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:M:156:PHE:CD1  | 1:M:195:TYR:CD1  | 2.90                     | 0.60              |
| 1:D:166:MET:HE3  | 1:D:254:PHE:HD2  | 1.66                     | 0.60              |
| 1:A:38:VAL:HB    | 1:A:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:P:95:THR:HG23  | 1:P:96:HIS:ND1   | 2.17                     | 0.60              |
| 1:M:124:VAL:CG1  | 1:M:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:J:793:ARG:HH21 | 3:L:147:MET:HE1  | 1.66                     | 0.60              |
| 1:P:530:MET:CG   | 4:0:354:GLN:HG3  | 2.30                     | 0.60              |
| 1:G:217:THR:C    | 1:G:221:GLN:HG2  | 2.21                     | 0.60              |
| 1:M:538:GLU:HA   | 4:Z:349:LEU:CG   | 2.28                     | 0.60              |
| 1:J:81:ASN:OD1   | 1:J:96:HIS:HB2   | 2.00                     | 0.60              |
| 4:9:287:ILE:H    | 4:9:287:ILE:HD12 | 1.67                     | 0.60              |
| 1:P:829:TRP:CZ3  | 2:Q:84:PHE:CE1   | 2.89                     | 0.60              |
| 3:F:52:ASN:N     | 3:F:53:PRO:HD2   | 2.16                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:63:ILE:HG22  | 3:L:64:THR:O     | 2.01                     | 0.60              |
| 1:M:95:THR:HG23  | 1:M:96:HIS:ND1   | 2.17                     | 0.60              |
| 1:G:60:VAL:O     | 1:G:71:THR:HA    | 2.02                     | 0.60              |
| 1:P:60:VAL:O     | 1:P:71:THR:HA    | 2.02                     | 0.60              |
| 1:A:40:VAL:HG22  | 1:A:41:VAL:H     | 1.67                     | 0.60              |
| 4:7:223:PHE:HD2  | 4:7:312:ARG:NH2  | 1.99                     | 0.60              |
| 1:M:38:VAL:HB    | 1:M:52:ILE:HD11  | 1.83                     | 0.60              |
| 1:A:124:VAL:CG1  | 1:A:675:ILE:HD13 | 2.31                     | 0.60              |
| 1:G:542:PHE:CB   | 4:V:143:TYR:HE1  | 2.13                     | 0.60              |
| 1:P:817:GLN:OE1  | 2:Q:127:ARG:HD2  | 2.00                     | 0.60              |
| 1:J:735:GLY:O    | 1:J:743:ALA:HA   | 1.94                     | 0.60              |
| 1:P:544:LYS:HZ3  | 4:2:45:VAL:CG2   | 2.14                     | 0.60              |
| 1:D:530:MET:HA   | 4:9:354:GLN:CB   | 2.29                     | 0.60              |
| 1:A:411:GLU:N    | 4:8:333:PRO:HB2  | 2.11                     | 0.60              |
| 1:M:831:TRP:CZ2  | 2:N:47:LEU:HD21  | 2.24                     | 0.60              |
| 1:M:805:ALA:O    | 1:M:809:ARG:CA   | 2.46                     | 0.60              |
| 3:R:63:ILE:HG22  | 3:R:64:THR:O     | 2.01                     | 0.60              |
| 1:A:60:VAL:O     | 1:A:71:THR:HA    | 2.02                     | 0.60              |
| 1:D:40:VAL:HG22  | 1:D:41:VAL:N     | 2.16                     | 0.60              |
| 1:M:60:VAL:O     | 1:M:71:THR:HA    | 2.02                     | 0.60              |
| 1:D:665:ARG:C    | 1:D:667:THR:H    | 2.05                     | 0.60              |
| 3:O:3:SER:HG     | 3:O:5:ALA:N      | 1.98                     | 0.60              |
| 1:G:38:VAL:HB    | 1:G:52:ILE:HD11  | 1.84                     | 0.60              |
| 1:P:557:GLU:HG3  | 1:P:557:GLU:O    | 2.00                     | 0.60              |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:HD13 | 1.84                     | 0.60              |
| 1:M:524:GLU:O    | 1:M:528:MLY:HB3  | 2.01                     | 0.60              |
| 1:D:553:MLY:NZ   | 4:W:45:VAL:HG13  | 2.16                     | 0.60              |
| 1:A:787:ILE:O    | 1:A:790:THR:N    | 2.35                     | 0.60              |
| 1:P:546:THR:HG22 | 1:P:547:ASP:N    | 2.17                     | 0.60              |
| 1:P:217:THR:C    | 1:P:221:GLN:HG2  | 2.21                     | 0.60              |
| 4:7:287:ILE:HD12 | 4:7:287:ILE:H    | 1.67                     | 0.60              |
| 3:C:63:ILE:HG22  | 3:C:64:THR:O     | 2.01                     | 0.60              |
| 1:J:578:HIS:CD2  | 1:J:591:ASN:HA   | 2.31                     | 0.60              |
| 1:J:40:VAL:HG22  | 1:J:41:VAL:N     | 2.16                     | 0.60              |
| 1:J:60:VAL:O     | 1:J:71:THR:HA    | 2.02                     | 0.60              |
| 1:G:578:HIS:CD2  | 1:G:591:ASN:HA   | 2.31                     | 0.60              |
| 2:E:163:ALA:C    | 2:K:21:GLU:HB3   | 2.22                     | 0.60              |
| 1:G:156:PHE:CD1  | 1:G:195:TYR:CD1  | 2.90                     | 0.60              |
| 3:I:3:SER:HG     | 3:I:5:ALA:N      | 1.99                     | 0.60              |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:HD13 | 1.84                     | 0.60              |
| 1:M:91:MET:HE3   | 1:M:119:SER:HB2  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:798:LEU:HD12 | 3:F:126:LEU:CD2  | 2.20                     | 0.60              |
| 2:Q:117:LEU:HD11 | 2:Q:147:ASN:HB3  | 1.76                     | 0.60              |
| 1:P:543:PRO:HG2  | 4:O:143:TYR:O    | 1.98                     | 0.60              |
| 1:D:542:PHE:N    | 4:9:143:TYR:OH   | 2.33                     | 0.60              |
| 2:B:34:ILE:O     | 2:B:46:ASP:HB3   | 2.01                     | 0.60              |
| 1:A:791:GLN:CD   | 3:C:116:GLU:N    | 2.38                     | 0.60              |
| 1:M:776:GLU:O    | 1:M:779:ARG:HB3  | 2.02                     | 0.60              |
| 1:A:836:PHE:HE1  | 2:B:159:HIS:CB   | 2.13                     | 0.60              |
| 2:K:34:ILE:O     | 2:K:46:ASP:HB3   | 2.01                     | 0.60              |
| 1:J:829:TRP:HH2  | 2:K:84:PHE:CE1   | 2.14                     | 0.60              |
| 1:P:166:MET:HE3  | 1:P:254:PHE:HD2  | 1.65                     | 0.60              |
| 1:J:124:VAL:CG1  | 1:J:675:ILE:HD13 | 2.32                     | 0.60              |
| 1:M:818:TYR:CE1  | 2:N:127:ARG:CZ   | 2.83                     | 0.60              |
| 1:A:542:PHE:CD1  | 4:8:143:TYR:CE1  | 2.90                     | 0.60              |
| 1:M:839:MLY:HH13 | 2:N:159:HIS:HD2  | 1.67                     | 0.60              |
| 1:A:95:THR:HG23  | 1:A:96:HIS:ND1   | 2.16                     | 0.60              |
| 3:R:52:ASN:HB2   | 3:R:53:PRO:CD    | 2.28                     | 0.60              |
| 1:G:536:LEU:HD13 | 1:G:550:PHE:CE1  | 2.37                     | 0.60              |
| 1:G:546:THR:HG22 | 1:G:547:ASP:N    | 2.17                     | 0.60              |
| 1:J:834:LEU:HD12 | 2:K:51:PHE:HE1   | 1.65                     | 0.60              |
| 1:D:7:MET:HE3    | 1:D:14:ALA:HB1   | 1.84                     | 0.60              |
| 1:D:49:MLY:HH13  | 1:D:108:GLU:OE2  | 2.02                     | 0.60              |
| 1:A:757:GLN:HG3  | 1:A:771:LEU:CD1  | 2.25                     | 0.59              |
| 1:A:768:MLY:C    | 1:A:771:LEU:HB2  | 2.30                     | 0.59              |
| 1:P:791:GLN:HE22 | 3:R:115:GLY:CA   | 2.01                     | 0.59              |
| 1:P:536:LEU:HD13 | 1:P:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:A:550:PHE:CE2  | 1:A:592:ILE:HG23 | 2.37                     | 0.59              |
| 1:J:776:GLU:O    | 1:J:779:ARG:HB3  | 2.02                     | 0.59              |
| 1:G:834:LEU:HD12 | 2:H:51:PHE:HE1   | 1.50                     | 0.59              |
| 4:8:287:ILE:HD12 | 4:8:287:ILE:H    | 1.67                     | 0.59              |
| 1:G:665:ARG:C    | 1:G:667:THR:H    | 2.04                     | 0.59              |
| 1:J:7:MET:HE3    | 1:J:14:ALA:HB1   | 1.84                     | 0.59              |
| 1:P:49:MLY:HH13  | 1:P:108:GLU:OE2  | 2.02                     | 0.59              |
| 1:P:124:VAL:HG13 | 1:P:675:ILE:HD13 | 1.84                     | 0.59              |
| 1:P:124:VAL:CG1  | 1:P:675:ILE:HD13 | 2.31                     | 0.59              |
| 1:J:784:ALA:O    | 1:J:788:THR:HB   | 2.02                     | 0.59              |
| 1:G:541:MET:SD   | 4:V:346:LEU:O    | 2.48                     | 0.59              |
| 1:M:546:THR:HG22 | 1:M:547:ASP:N    | 2.17                     | 0.59              |
| 1:M:542:PHE:CD1  | 4:Z:143:TYR:CE1  | 2.91                     | 0.59              |
| 1:J:553:MLY:HG3  | 4:Y:45:VAL:O     | 2.02                     | 0.59              |
| 1:D:536:LEU:HD13 | 1:D:550:PHE:CE1  | 2.37                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:787:ILE:O    | 1:M:790:THR:N    | 2.35                     | 0.59              |
| 1:J:202:SER:CA   | 1:J:207:LYS:HE3  | 2.27                     | 0.59              |
| 1:J:756:THR:HG23 | 1:J:779:ARG:HD2  | 1.84                     | 0.59              |
| 1:A:623:PHE:HA   | 1:A:623:PHE:CG   | 2.36                     | 0.59              |
| 1:M:95:THR:N     | 1:M:713:SER:HB3  | 2.17                     | 0.59              |
| 1:G:550:PHE:CE2  | 1:G:592:ILE:HG23 | 2.37                     | 0.59              |
| 1:A:116:TYR:HB2  | 1:A:153:PRO:O    | 2.03                     | 0.59              |
| 1:D:91:MET:HE3   | 1:D:119:SER:HB2  | 1.84                     | 0.59              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:CG   | 2.28                     | 0.59              |
| 1:G:813:ILE:O    | 1:G:817:GLN:N    | 2.30                     | 0.59              |
| 1:P:578:HIS:CD2  | 1:P:591:ASN:HA   | 2.31                     | 0.59              |
| 1:A:530:MET:CG   | 4:8:354:GLN:HG3  | 2.30                     | 0.59              |
| 1:D:95:THR:HG23  | 1:D:96:HIS:ND1   | 2.17                     | 0.59              |
| 1:G:599:ASN:CB   | 1:G:649:VAL:HB   | 2.32                     | 0.59              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:HG22 | 1.80                     | 0.59              |
| 1:D:599:ASN:CB   | 1:D:649:VAL:HB   | 2.32                     | 0.59              |
| 1:A:634:GLY:N    | 4:8:25:ASP:O     | 2.31                     | 0.59              |
| 2:H:34:ILE:O     | 2:H:46:ASP:HB3   | 2.01                     | 0.59              |
| 1:P:99:GLU:OE2   | 1:P:696:ARG:NH2  | 2.30                     | 0.59              |
| 1:G:789:ALA:HB2  | 3:I:81:GLN:OE1   | 2.02                     | 0.59              |
| 1:M:665:ARG:C    | 1:M:667:THR:H    | 2.05                     | 0.59              |
| 4:V:286:ASP:OD1  | 4:X:202:THR:HB   | 2.02                     | 0.59              |
| 1:P:7:MET:HE3    | 1:P:14:ALA:HB1   | 1.84                     | 0.59              |
| 1:A:776:GLU:O    | 1:A:779:ARG:HB3  | 2.03                     | 0.59              |
| 1:A:707:CYS:SG   | 1:A:714:ARG:CD   | 2.90                     | 0.59              |
| 2:E:117:LEU:CB   | 2:E:147:ASN:ND2  | 2.35                     | 0.59              |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:HD11 | 1.75                     | 0.59              |
| 1:J:553:MLY:CH1  | 4:Y:45:VAL:HG11  | 2.32                     | 0.59              |
| 1:P:787:ILE:O    | 1:P:790:THR:N    | 2.35                     | 0.59              |
| 1:P:795:ARG:HE   | 3:R:116:GLU:HB3  | 1.67                     | 0.59              |
| 1:D:549:SER:OG   | 1:D:550:PHE:N    | 2.36                     | 0.59              |
| 1:A:797:PHE:CD1  | 3:C:146:ILE:CA   | 2.83                     | 0.59              |
| 1:P:550:PHE:CE2  | 1:P:592:ILE:HG23 | 2.37                     | 0.59              |
| 1:A:536:LEU:HD13 | 1:A:550:PHE:CE1  | 2.37                     | 0.59              |
| 4:2:287:ILE:H    | 4:2:287:ILE:HD12 | 1.67                     | 0.59              |
| 1:G:707:CYS:SG   | 1:G:714:ARG:NH1  | 2.75                     | 0.59              |
| 1:J:599:ASN:CB   | 1:J:649:VAL:HB   | 2.32                     | 0.59              |
| 1:G:830:PRO:HB2  | 2:H:67:MET:CE    | 2.30                     | 0.59              |
| 1:J:549:SER:OG   | 1:J:550:PHE:N    | 2.36                     | 0.59              |
| 4:Z:223:PHE:HD2  | 4:Z:312:ARG:NH2  | 1.99                     | 0.59              |
| 1:J:156:PHE:CD1  | 1:J:195:TYR:CD1  | 2.90                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:124:VAL:HG13 | 1:M:675:ILE:HD13 | 1.84                     | 0.59              |
| 1:M:135:TYR:N    | 1:M:135:TYR:CD1  | 2.69                     | 0.59              |
| 4:5:287:ILE:H    | 4:5:287:ILE:HD12 | 1.67                     | 0.59              |
| 1:A:135:TYR:N    | 1:A:135:TYR:CD1  | 2.70                     | 0.59              |
| 1:D:507:GLY:HA2  | 1:D:762:HIS:ND1  | 2.16                     | 0.59              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:CB   | 2.33                     | 0.59              |
| 1:P:826:VAL:HG21 | 2:Q:88:LEU:HD23  | 1.84                     | 0.59              |
| 1:P:542:PHE:CD1  | 4:O:143:TYR:CE1  | 2.91                     | 0.59              |
| 1:P:642:LYS:CG   | 4:O:22:ALA:CA    | 2.80                     | 0.59              |
| 1:M:545:ALA:CA   | 4:1:45:VAL:HG13  | 2.26                     | 0.59              |
| 1:P:800:ARG:HB3  | 3:R:149:VAL:CG2  | 2.32                     | 0.59              |
| 1:A:578:HIS:CD2  | 1:A:591:ASN:HA   | 2.31                     | 0.59              |
| 1:M:831:TRP:CH2  | 2:N:47:LEU:HD23  | 2.15                     | 0.59              |
| 1:A:818:TYR:HB3  | 2:B:90:GLY:H     | 1.67                     | 0.59              |
| 1:G:195:TYR:O    | 1:G:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:A:195:TYR:O    | 1:A:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:J:210:GLN:O    | 1:J:211:SER:OG   | 2.15                     | 0.59              |
| 1:D:732:ILE:HG22 | 1:D:747:LEU:CD1  | 1.55                     | 0.59              |
| 1:D:787:ILE:O    | 1:D:790:THR:N    | 2.35                     | 0.59              |
| 1:G:795:ARG:CZ   | 3:I:116:GLU:HB3  | 2.31                     | 0.59              |
| 1:P:817:GLN:CB   | 2:Q:127:ARG:NH1  | 2.47                     | 0.59              |
| 1:D:827:MLY:HH21 | 2:E:139:ALA:CB   | 2.32                     | 0.59              |
| 1:J:542:PHE:CD1  | 4:W:143:TYR:CE1  | 2.91                     | 0.59              |
| 1:M:599:ASN:CB   | 1:M:649:VAL:HB   | 2.32                     | 0.59              |
| 1:D:831:TRP:CD2  | 2:E:51:PHE:CE1   | 2.91                     | 0.59              |
| 1:P:776:GLU:O    | 1:P:779:ARG:HB3  | 2.02                     | 0.59              |
| 3:F:52:ASN:HB2   | 3:F:53:PRO:CD    | 2.28                     | 0.59              |
| 3:F:52:ASN:N     | 3:F:53:PRO:CD    | 2.65                     | 0.59              |
| 1:D:60:VAL:O     | 1:D:71:THR:HA    | 2.02                     | 0.59              |
| 1:M:97:LEU:HD23  | 1:M:712:PRO:CB   | 2.18                     | 0.59              |
| 1:G:549:SER:OG   | 1:G:550:PHE:N    | 2.36                     | 0.59              |
| 1:D:156:PHE:CD1  | 1:D:195:TYR:CD1  | 2.90                     | 0.59              |
| 1:J:265:ILE:HG22 | 1:J:266:GLU:N    | 2.18                     | 0.59              |
| 1:D:464:ILE:HG22 | 1:D:465:ALA:N    | 2.18                     | 0.59              |
| 1:J:49:MLY:HH13  | 1:J:108:GLU:OE2  | 2.02                     | 0.59              |
| 1:J:787:ILE:O    | 1:J:790:THR:N    | 2.35                     | 0.59              |
| 1:G:646:PHE:CD2  | 1:G:652:LEU:CD1  | 2.85                     | 0.59              |
| 1:G:530:MET:CG   | 4:V:354:GLN:HG3  | 2.30                     | 0.59              |
| 2:B:130:PRO:HA   | 2:B:133:ILE:HD12 | 1.84                     | 0.59              |
| 1:J:84:MLY:CH1   | 1:J:724:TYR:CD2  | 2.82                     | 0.59              |
| 1:J:530:MET:HA   | 4:W:354:GLN:CB   | 2.28                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:549:SER:OG   | 1:P:550:PHE:N    | 2.36                     | 0.59              |
| 1:J:837:MLY:O    | 1:J:840:PRO:HD2  | 2.02                     | 0.59              |
| 1:G:97:LEU:CD2   | 1:G:712:PRO:HB2  | 2.22                     | 0.59              |
| 4:0:110:LEU:C    | 4:1:195:GLU:HG3  | 2.23                     | 0.59              |
| 1:M:642:LYS:CD   | 4:Z:340:TRP:CZ3  | 2.79                     | 0.59              |
| 1:D:799:MET:SD   | 3:F:32:ASP:CG    | 2.79                     | 0.59              |
| 3:I:52:ASN:N     | 3:I:53:PRO:CD    | 2.65                     | 0.59              |
| 1:G:40:VAL:HG22  | 1:G:41:VAL:H     | 1.67                     | 0.59              |
| 1:J:536:LEU:HD13 | 1:J:550:PHE:CE1  | 2.37                     | 0.59              |
| 1:J:550:PHE:CE2  | 1:J:592:ILE:HG23 | 2.37                     | 0.59              |
| 3:L:102:VAL:HG11 | 3:L:107:LEU:HB2  | 1.85                     | 0.59              |
| 1:P:755:HIS:HA   | 1:P:758:TYR:HE1  | 1.64                     | 0.59              |
| 1:M:195:TYR:O    | 1:M:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:J:230:GLU:O    | 1:J:234:ASN:HB2  | 2.03                     | 0.59              |
| 4:4:287:ILE:H    | 4:4:287:ILE:HD12 | 1.67                     | 0.59              |
| 1:A:505:MLY:HB3  | 1:A:762:HIS:HD2  | 0.43                     | 0.59              |
| 4:1:287:ILE:HB   | 4:3:203:THR:CA   | 2.33                     | 0.59              |
| 2:H:130:PRO:HA   | 2:H:133:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:813:ILE:O    | 1:A:817:GLN:N    | 2.30                     | 0.59              |
| 1:A:529:PRO:HG3  | 4:8:353:GLN:OE1  | 2.03                     | 0.59              |
| 1:G:708:ARG:HA   | 1:G:712:PRO:HG3  | 1.83                     | 0.59              |
| 1:A:599:ASN:CB   | 1:A:649:VAL:HB   | 2.32                     | 0.59              |
| 1:M:806:MET:N    | 1:M:807:VAL:N    | 2.51                     | 0.59              |
| 1:P:599:ASN:CB   | 1:P:649:VAL:HB   | 2.32                     | 0.59              |
| 1:J:649:VAL:HG22 | 1:J:649:VAL:HA   | 1.80                     | 0.59              |
| 1:J:755:HIS:HA   | 1:J:758:TYR:HE1  | 1.65                     | 0.59              |
| 3:I:49:ILE:HA    | 3:I:52:ASN:ND2   | 2.06                     | 0.59              |
| 1:P:116:TYR:HB2  | 1:P:153:PRO:O    | 2.03                     | 0.59              |
| 1:G:116:TYR:HB2  | 1:G:153:PRO:O    | 2.03                     | 0.59              |
| 1:P:135:TYR:N    | 1:P:135:TYR:CD1  | 2.70                     | 0.59              |
| 1:D:601:ASP:N    | 1:D:602:PRO:HD3  | 2.18                     | 0.59              |
| 1:G:776:GLU:O    | 1:G:779:ARG:HB3  | 2.03                     | 0.59              |
| 1:A:149:GLN:HB3  | 1:A:719:ASP:CA   | 2.32                     | 0.59              |
| 1:D:508:ILE:HA   | 1:D:761:GLY:HA3  | 1.85                     | 0.59              |
| 1:D:506:GLU:CG   | 1:D:764:MLY:HE3  | 2.32                     | 0.59              |
| 1:M:818:TYR:C    | 2:N:90:GLY:HA3   | 2.23                     | 0.59              |
| 1:M:545:ALA:CB   | 4:1:45:VAL:HG13  | 2.32                     | 0.59              |
| 1:A:799:MET:SD   | 3:C:32:ASP:C     | 2.80                     | 0.59              |
| 4:X:325:MET:CE   | 4:Z:244:ASP:CG   | 2.69                     | 0.59              |
| 3:O:52:ASN:N     | 3:O:53:PRO:CD    | 2.65                     | 0.59              |
| 1:G:95:THR:HG23  | 1:G:96:HIS:ND1   | 2.17                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:195:TYR:O    | 1:P:199:ILE:HG23 | 2.03                     | 0.59              |
| 1:A:230:GLU:O    | 1:A:234:ASN:HB2  | 2.03                     | 0.59              |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:HD13 | 1.84                     | 0.59              |
| 1:J:798:LEU:HG   | 3:L:126:LEU:HD11 | 1.83                     | 0.59              |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:HD1  | 1.68                     | 0.59              |
| 2:E:130:PRO:HA   | 2:E:133:ILE:HD12 | 1.84                     | 0.59              |
| 1:P:538:GLU:O    | 1:P:541:MET:HB2  | 2.03                     | 0.59              |
| 1:D:542:PHE:CD1  | 4:9:143:TYR:CE1  | 2.90                     | 0.59              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:HD11 | 1.79                     | 0.59              |
| 1:M:646:PHE:CD2  | 1:M:652:LEU:CD1  | 2.85                     | 0.59              |
| 1:M:634:GLY:N    | 4:Z:25:ASP:O     | 2.31                     | 0.59              |
| 1:P:834:LEU:CD1  | 2:Q:51:PHE:CD1   | 2.86                     | 0.59              |
| 1:D:40:VAL:HG22  | 1:D:41:VAL:H     | 1.67                     | 0.59              |
| 1:M:753:VAL:HG13 | 1:M:775:LEU:HD23 | 1.83                     | 0.59              |
| 1:P:156:PHE:CD1  | 1:P:195:TYR:CD1  | 2.90                     | 0.59              |
| 1:G:230:GLU:O    | 1:G:234:ASN:HB2  | 2.03                     | 0.59              |
| 1:A:48:VAL:HG22  | 1:A:49:MLY:N     | 2.18                     | 0.59              |
| 1:A:601:ASP:N    | 1:A:602:PRO:HD3  | 2.18                     | 0.59              |
| 1:A:265:ILE:HG22 | 1:A:266:GLU:N    | 2.18                     | 0.59              |
| 1:G:510:TRP:CZ2  | 1:G:768:MLY:HH11 | 2.38                     | 0.58              |
| 1:G:542:PHE:CD1  | 4:V:143:TYR:CE1  | 2.91                     | 0.58              |
| 1:P:529:PRO:HG3  | 4:0:353:GLN:OE1  | 2.03                     | 0.58              |
| 1:A:538:GLU:O    | 1:A:541:MET:HB2  | 2.03                     | 0.58              |
| 1:M:782:MLY:C    | 1:M:786:ILE:HD11 | 2.32                     | 0.58              |
| 1:M:732:ILE:HG22 | 1:M:747:LEU:CD1  | 1.55                     | 0.58              |
| 1:A:837:MLY:CH2  | 2:H:20:ASP:HA    | 2.30                     | 0.58              |
| 4:3:287:ILE:H    | 4:3:287:ILE:HD12 | 1.67                     | 0.58              |
| 1:P:806:MET:HA   | 1:P:809:ARG:HB2  | 1.85                     | 0.58              |
| 1:P:769:ALA:C    | 1:P:771:LEU:CB   | 2.70                     | 0.58              |
| 4:3:223:PHE:HD2  | 4:3:312:ARG:NH2  | 1.99                     | 0.58              |
| 1:J:195:TYR:O    | 1:J:199:ILE:HG23 | 2.03                     | 0.58              |
| 1:P:124:VAL:HG13 | 1:P:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:M:48:VAL:HG22  | 1:M:49:MLY:N     | 2.18                     | 0.58              |
| 1:P:601:ASP:N    | 1:P:602:PRO:HD3  | 2.18                     | 0.58              |
| 1:M:536:LEU:HD13 | 1:M:550:PHE:CE1  | 2.37                     | 0.58              |
| 1:D:529:PRO:HG3  | 4:9:353:GLN:OE1  | 2.03                     | 0.58              |
| 1:P:715:VAL:HG11 | 1:P:720:PHE:HD1  | 1.68                     | 0.58              |
| 1:D:629:GLU:HB3  | 1:D:645:SER:N    | 2.18                     | 0.58              |
| 1:G:829:TRP:CZ2  | 2:H:83:MET:HE1   | 2.37                     | 0.58              |
| 4:3:322:PRO:CB   | 4:5:244:ASP:CG   | 2.54                     | 0.58              |
| 1:M:829:TRP:CZ3  | 2:N:84:PHE:CE1   | 2.91                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:150:TYR:C    | 2:E:151:LYS:CG   | 2.48                     | 0.58              |
| 1:D:127:ASN:ND2  | 1:D:128:PRO:HD2  | 2.16                     | 0.58              |
| 1:M:141:LEU:O    | 1:M:144:ARG:HB3  | 2.03                     | 0.58              |
| 1:D:141:LEU:O    | 1:D:144:ARG:HB3  | 2.03                     | 0.58              |
| 1:M:124:VAL:HG13 | 1:M:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:D:135:TYR:N    | 1:D:135:TYR:CD1  | 2.70                     | 0.58              |
| 1:G:265:ILE:HG22 | 1:G:266:GLU:N    | 2.18                     | 0.58              |
| 1:J:601:ASP:N    | 1:J:602:PRO:HD3  | 2.18                     | 0.58              |
| 1:D:798:LEU:HD21 | 3:F:122:GLU:HB3  | 1.85                     | 0.58              |
| 1:G:795:ARG:N    | 3:I:118:MET:CE   | 2.65                     | 0.58              |
| 1:P:643:GLY:HA2  | 4:O:24:ASP:OD1   | 2.04                     | 0.58              |
| 1:M:530:MET:CG   | 4:Z:354:GLN:HG3  | 2.30                     | 0.58              |
| 1:J:643:GLY:HA2  | 4:W:24:ASP:OD1   | 2.04                     | 0.58              |
| 1:J:646:PHE:CD2  | 1:J:652:LEU:CD1  | 2.85                     | 0.58              |
| 1:J:529:PRO:HG3  | 4:W:353:GLN:OE1  | 2.04                     | 0.58              |
| 1:D:534:SER:C    | 4:9:351:THR:CA   | 2.47                     | 0.58              |
| 1:A:530:MET:HE3  | 4:8:355:MET:SD   | 2.43                     | 0.58              |
| 1:A:549:SER:OG   | 1:A:550:PHE:N    | 2.36                     | 0.58              |
| 3:I:52:ASN:HB2   | 3:I:53:PRO:CD    | 2.28                     | 0.58              |
| 3:L:52:ASN:N     | 3:L:53:PRO:CD    | 2.65                     | 0.58              |
| 1:J:127:ASN:ND2  | 1:J:128:PRO:HD2  | 2.16                     | 0.58              |
| 1:M:116:TYR:HB2  | 1:M:153:PRO:O    | 2.03                     | 0.58              |
| 1:G:124:VAL:HG13 | 1:G:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:J:135:TYR:N    | 1:J:135:TYR:CD1  | 2.69                     | 0.58              |
| 1:M:265:ILE:HG22 | 1:M:266:GLU:N    | 2.18                     | 0.58              |
| 1:M:464:ILE:HG22 | 1:M:465:ALA:N    | 2.18                     | 0.58              |
| 1:G:135:TYR:CD1  | 1:G:135:TYR:N    | 2.70                     | 0.58              |
| 1:A:505:MLY:CG   | 1:A:741:LYS:HZ3  | 2.14                     | 0.58              |
| 1:G:629:GLU:HB3  | 1:G:645:SER:N    | 2.18                     | 0.58              |
| 1:G:642:LYS:CG   | 4:V:22:ALA:CA    | 2.80                     | 0.58              |
| 4:1:287:ILE:H    | 4:1:287:ILE:HD12 | 1.67                     | 0.58              |
| 1:G:818:TYR:CE1  | 2:H:127:ARG:NH1  | 2.72                     | 0.58              |
| 1:P:797:PHE:CG   | 3:R:146:ILE:HG23 | 2.39                     | 0.58              |
| 1:D:550:PHE:CE2  | 1:D:592:ILE:HG23 | 2.37                     | 0.58              |
| 1:D:218:LEU:N    | 1:D:221:GLN:HE21 | 2.01                     | 0.58              |
| 4:Y:287:ILE:HD12 | 4:Y:287:ILE:H    | 1.67                     | 0.58              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:CA   | 2.86                     | 0.58              |
| 4:Z:287:ILE:H    | 4:Z:287:ILE:HD12 | 1.67                     | 0.58              |
| 1:P:649:VAL:HA   | 1:P:649:VAL:HG22 | 1.80                     | 0.58              |
| 1:J:831:TRP:CZ3  | 2:K:34:ILE:HG21  | 2.38                     | 0.58              |
| 3:C:46:ILE:O     | 3:C:50:LEU:CG    | 2.47                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:175:ILE:HA   | 1:M:670:HIS:O    | 2.03                     | 0.58              |
| 3:C:102:VAL:HG11 | 3:C:107:LEU:HB2  | 1.85                     | 0.58              |
| 1:A:809:ARG:HH12 | 2:B:124:GLY:HA2  | 1.67                     | 0.58              |
| 1:J:116:TYR:HB2  | 1:J:153:PRO:O    | 2.03                     | 0.58              |
| 1:M:601:ASP:N    | 1:M:602:PRO:HD3  | 2.18                     | 0.58              |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:N    | 2.18                     | 0.58              |
| 1:G:787:ILE:O    | 1:G:790:THR:N    | 2.35                     | 0.58              |
| 1:J:819:ASN:CG   | 2:K:92:ASP:HB3   | 2.14                     | 0.58              |
| 1:J:218:LEU:N    | 1:J:221:GLN:HE21 | 2.01                     | 0.58              |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:HD1  | 1.68                     | 0.58              |
| 1:M:553:MLY:HG3  | 4:1:43:VAL:CG1   | 2.31                     | 0.58              |
| 1:M:553:MLY:CG   | 4:1:43:VAL:CG1   | 2.81                     | 0.58              |
| 1:P:794:CYS:O    | 1:P:798:LEU:N    | 2.37                     | 0.58              |
| 4:0:287:ILE:HD12 | 4:0:287:ILE:H    | 1.67                     | 0.58              |
| 1:M:629:GLU:HB3  | 1:M:645:SER:N    | 2.18                     | 0.58              |
| 1:A:818:TYR:CD2  | 2:B:89:LYS:O     | 2.57                     | 0.58              |
| 3:F:46:ILE:O     | 3:F:50:LEU:CG    | 2.47                     | 0.58              |
| 3:R:52:ASN:N     | 3:R:53:PRO:CD    | 2.65                     | 0.58              |
| 1:G:99:GLU:OE2   | 1:G:696:ARG:NH2  | 2.30                     | 0.58              |
| 3:F:102:VAL:HG11 | 3:F:107:LEU:HB2  | 1.85                     | 0.58              |
| 4:2:223:PHE:HD2  | 4:2:312:ARG:NH2  | 1.99                     | 0.58              |
| 1:P:230:GLU:O    | 1:P:234:ASN:HB2  | 2.03                     | 0.58              |
| 1:D:230:GLU:O    | 1:D:234:ASN:HB2  | 2.03                     | 0.58              |
| 1:P:141:LEU:O    | 1:P:144:ARG:HB3  | 2.04                     | 0.58              |
| 1:D:124:VAL:HG13 | 1:D:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:CD1  | 2.33                     | 0.58              |
| 1:A:124:VAL:HG13 | 1:A:675:ILE:HD13 | 1.84                     | 0.58              |
| 1:D:727:LEU:CB   | 1:D:782:MLY:CE   | 2.81                     | 0.58              |
| 1:D:747:LEU:HD11 | 1:D:782:MLY:HH22 | 1.80                     | 0.58              |
| 1:D:724:TYR:HD1  | 1:D:782:MLY:HD3  | 1.61                     | 0.58              |
| 1:G:538:GLU:O    | 1:G:541:MET:HB2  | 2.04                     | 0.58              |
| 1:G:552:ASN:C    | 4:X:47:MET:HE1   | 2.24                     | 0.58              |
| 1:P:629:GLU:HB3  | 1:P:645:SER:N    | 2.18                     | 0.58              |
| 1:M:529:PRO:HG3  | 4:Z:353:GLN:OE1  | 2.03                     | 0.58              |
| 1:A:410:ASN:CG   | 4:8:334:GLU:CA   | 2.48                     | 0.58              |
| 1:P:837:MLY:O    | 1:P:840:PRO:HD2  | 2.02                     | 0.58              |
| 1:G:717:TYR:HD1  | 1:G:744:SER:HG   | 1.51                     | 0.58              |
| 1:M:804:ARG:O    | 1:M:808:GLU:N    | 2.35                     | 0.58              |
| 1:P:804:ARG:O    | 1:P:808:GLU:CG   | 2.51                     | 0.58              |
| 1:J:40:VAL:HG22  | 1:J:41:VAL:H     | 1.67                     | 0.58              |
| 1:P:418:THR:HG22 | 1:P:419:VAL:H    | 1.69                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:48:VAL:HG22  | 1:D:49:MLY:N     | 2.18                     | 0.58              |
| 1:G:601:ASP:N    | 1:G:602:PRO:HD3  | 2.18                     | 0.58              |
| 1:A:817:GLN:CD   | 2:B:127:ARG:HE   | 1.99                     | 0.58              |
| 1:J:506:GLU:CG   | 1:J:760:PHE:O    | 2.52                     | 0.58              |
| 1:J:629:GLU:HB3  | 1:J:645:SER:N    | 2.18                     | 0.58              |
| 4:2:290:ARG:NE   | 4:4:202:THR:HG21 | 2.15                     | 0.58              |
| 1:D:643:GLY:HA2  | 4:9:24:ASP:OD1   | 2.04                     | 0.58              |
| 1:P:767:PHE:HD1  | 1:P:772:LEU:HD21 | 1.59                     | 0.58              |
| 4:X:286:ASP:CG   | 4:Z:203:THR:HG22 | 2.24                     | 0.58              |
| 1:G:831:TRP:HE1  | 2:H:67:MET:CG    | 2.17                     | 0.58              |
| 3:C:52:ASN:HB2   | 3:C:53:PRO:CD    | 2.28                     | 0.58              |
| 3:C:52:ASN:N     | 3:C:53:PRO:CD    | 2.65                     | 0.58              |
| 1:J:567:LYS:HZ1  | 4:Y:92:ASN:HD22  | 1.50                     | 0.58              |
| 4:W:285:CYS:O    | 4:Y:202:THR:CG2  | 2.52                     | 0.58              |
| 1:M:418:THR:HG22 | 1:M:419:VAL:H    | 1.69                     | 0.58              |
| 1:J:279:LEU:HB3  | 1:J:280:PRO:HD2  | 1.86                     | 0.58              |
| 1:G:64:THR:HG22  | 1:G:65:GLU:N     | 2.19                     | 0.58              |
| 1:M:64:THR:HG22  | 1:M:65:GLU:N     | 2.19                     | 0.58              |
| 1:J:48:VAL:HG22  | 1:J:49:MLY:N     | 2.18                     | 0.58              |
| 1:A:49:MLY:HH13  | 1:A:108:GLU:OE2  | 2.02                     | 0.58              |
| 1:G:48:VAL:HG22  | 1:G:49:MLY:N     | 2.18                     | 0.58              |
| 1:P:464:ILE:HG22 | 1:P:465:ALA:N    | 2.18                     | 0.58              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:CD1  | 2.85                     | 0.58              |
| 1:G:411:GLU:N    | 4:V:333:PRO:HB2  | 2.10                     | 0.58              |
| 1:G:553:MLY:HH13 | 4:X:45:VAL:CG1   | 2.25                     | 0.58              |
| 1:P:646:PHE:CD2  | 1:P:652:LEU:CD1  | 2.85                     | 0.58              |
| 1:M:538:GLU:O    | 1:M:541:MET:HB2  | 2.03                     | 0.58              |
| 1:M:568:PRO:HG3  | 1:M:578:HIS:H    | 1.69                     | 0.58              |
| 1:D:538:GLU:O    | 1:D:541:MET:HB2  | 2.04                     | 0.58              |
| 1:P:548:THR:HG23 | 4:2:49:GLN:CB    | 2.03                     | 0.58              |
| 1:G:148:ARG:HH21 | 1:G:764:MLY:HH11 | 1.67                     | 0.58              |
| 1:A:642:LYS:CG   | 4:8:22:ALA:CA    | 2.81                     | 0.58              |
| 1:A:818:TYR:HD2  | 2:B:89:LYS:O     | 1.87                     | 0.58              |
| 1:D:800:ARG:HD3  | 3:F:149:VAL:O    | 2.03                     | 0.58              |
| 1:M:40:VAL:HG22  | 1:M:41:VAL:H     | 1.67                     | 0.58              |
| 1:D:175:ILE:HA   | 1:D:670:HIS:O    | 2.03                     | 0.58              |
| 1:P:175:ILE:HA   | 1:P:670:HIS:O    | 2.04                     | 0.58              |
| 4:W:286:ASP:OD1  | 4:Y:203:THR:HG22 | 2.04                     | 0.58              |
| 1:D:254:PHE:CE2  | 1:D:459:ILE:HD12 | 2.39                     | 0.58              |
| 1:G:254:PHE:CE2  | 1:G:459:ILE:HD12 | 2.39                     | 0.58              |
| 1:A:141:LEU:O    | 1:A:144:ARG:HB3  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:676:ILE:HG23 | 1:D:676:ILE:O    | 2.03                     | 0.58              |
| 1:P:48:VAL:HG22  | 1:P:49:MLY:N     | 2.18                     | 0.58              |
| 1:J:464:ILE:HG22 | 1:J:465:ALA:N    | 2.18                     | 0.58              |
| 1:D:265:ILE:HG22 | 1:D:266:GLU:N    | 2.18                     | 0.58              |
| 1:M:813:ILE:O    | 1:M:817:GLN:N    | 2.30                     | 0.58              |
| 1:G:529:PRO:HG3  | 4:V:353:GLN:OE1  | 2.04                     | 0.58              |
| 1:D:546:THR:HG22 | 1:D:547:ASP:N    | 2.17                     | 0.58              |
| 1:A:541:MET:SD   | 4:8:346:LEU:O    | 2.48                     | 0.58              |
| 1:M:795:ARG:HB2  | 3:O:35:ARG:NH1   | 2.19                     | 0.58              |
| 1:J:175:ILE:HA   | 1:J:670:HIS:O    | 2.03                     | 0.58              |
| 1:M:612:GLN:HE22 | 1:M:627:GLY:HA2  | 1.66                     | 0.58              |
| 1:M:799:MET:SD   | 3:O:32:ASP:CG    | 2.81                     | 0.58              |
| 1:P:279:LEU:HB3  | 1:P:280:PRO:HD2  | 1.86                     | 0.58              |
| 1:A:64:THR:HG22  | 1:A:65:GLU:N     | 2.19                     | 0.58              |
| 1:M:49:MLY:HH13  | 1:M:108:GLU:OE2  | 2.02                     | 0.58              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:NH2   | 2.65                     | 0.58              |
| 1:A:93:MET:HE1   | 1:A:716:LEU:H    | 1.65                     | 0.58              |
| 1:P:732:ILE:HG22 | 1:P:747:LEU:CD1  | 1.55                     | 0.58              |
| 3:R:102:VAL:HG11 | 3:R:107:LEU:HB2  | 1.85                     | 0.58              |
| 1:D:220:ASP:O    | 1:D:224:SER:N    | 2.27                     | 0.58              |
| 1:M:218:LEU:N    | 1:M:221:GLN:HE21 | 2.01                     | 0.58              |
| 1:A:409:GLY:HA3  | 4:8:333:PRO:CD   | 2.34                     | 0.58              |
| 1:D:823:PHE:CZ   | 2:E:156:VAL:HG12 | 2.38                     | 0.58              |
| 1:A:819:ASN:OD1  | 2:B:92:ASP:N     | 2.32                     | 0.58              |
| 3:R:49:ILE:HA    | 3:R:52:ASN:ND2   | 2.06                     | 0.58              |
| 1:D:800:ARG:CD   | 3:F:149:VAL:O    | 2.52                     | 0.58              |
| 1:G:568:PRO:HG3  | 1:G:578:HIS:H    | 1.69                     | 0.58              |
| 1:A:175:ILE:HA   | 1:A:670:HIS:O    | 2.04                     | 0.58              |
| 3:O:102:VAL:HG11 | 3:O:107:LEU:HB2  | 1.85                     | 0.58              |
| 1:P:127:ASN:ND2  | 1:P:128:PRO:HD2  | 2.16                     | 0.58              |
| 1:J:481:ASN:N    | 1:J:481:ASN:ND2  | 2.51                     | 0.58              |
| 1:G:823:PHE:HE1  | 2:H:160:GLY:HA2  | 1.69                     | 0.58              |
| 1:P:64:THR:HG22  | 1:P:65:GLU:N     | 2.19                     | 0.58              |
| 1:M:230:GLU:O    | 1:M:234:ASN:HB2  | 2.03                     | 0.58              |
| 1:A:676:ILE:O    | 1:A:676:ILE:HG23 | 2.03                     | 0.58              |
| 1:G:49:MLY:HH13  | 1:G:108:GLU:OE2  | 2.02                     | 0.58              |
| 1:D:794:CYS:O    | 1:D:798:LEU:N    | 2.36                     | 0.57              |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CE2  | 2.33                     | 0.57              |
| 2:Q:144:VAL:CG1  | 2:Q:153:ILE:HD13 | 2.20                     | 0.57              |
| 2:Q:117:LEU:CG   | 2:Q:147:ASN:CB   | 2.76                     | 0.57              |
| 1:J:93:MET:HA    | 1:J:714:ARG:H    | 1.68                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:797:PHE:HE1  | 3:O:149:VAL:HG12 | 1.64                     | 0.57              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CD2   | 2.20                     | 0.57              |
| 1:D:279:LEU:HB3  | 1:D:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:M:279:LEU:HB3  | 1:M:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:D:322:VAL:HG11 | 1:D:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:J:676:ILE:O    | 1:J:676:ILE:HG23 | 2.03                     | 0.57              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:HH12  | 1.67                     | 0.57              |
| 1:D:776:GLU:O    | 1:D:779:ARG:HB3  | 2.03                     | 0.57              |
| 1:G:792:ALA:H    | 3:I:42:THR:HG22  | 1.68                     | 0.57              |
| 1:A:149:GLN:CG   | 1:A:719:ASP:N    | 2.63                     | 0.57              |
| 1:D:507:GLY:HA3  | 1:D:762:HIS:CD2  | 2.36                     | 0.57              |
| 1:P:747:LEU:O    | 1:P:747:LEU:HD23 | 2.04                     | 0.57              |
| 1:J:538:GLU:O    | 1:J:541:MET:HB2  | 2.03                     | 0.57              |
| 4:0:110:LEU:O    | 4:1:195:GLU:HG3  | 2.04                     | 0.57              |
| 1:P:506:GLU:CD   | 1:P:760:PHE:N    | 2.50                     | 0.57              |
| 1:D:643:GLY:N    | 4:9:23:GLY:C     | 2.55                     | 0.57              |
| 1:A:629:GLU:HB3  | 1:A:645:SER:N    | 2.18                     | 0.57              |
| 1:P:634:GLY:N    | 4:0:25:ASP:O     | 2.31                     | 0.57              |
| 1:P:727:LEU:HD21 | 1:P:779:ARG:HE   | 1.68                     | 0.57              |
| 1:A:418:THR:HG22 | 1:A:419:VAL:H    | 1.69                     | 0.57              |
| 1:J:64:THR:HG22  | 1:J:65:GLU:N     | 2.19                     | 0.57              |
| 1:J:254:PHE:CE2  | 1:J:459:ILE:HD12 | 2.39                     | 0.57              |
| 1:J:141:LEU:O    | 1:J:144:ARG:HB3  | 2.03                     | 0.57              |
| 1:J:124:VAL:HG13 | 1:J:675:ILE:CD1  | 2.33                     | 0.57              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:HH12  | 1.64                     | 0.57              |
| 1:A:707:CYS:CB   | 1:A:714:ARG:CZ   | 2.66                     | 0.57              |
| 1:P:813:ILE:O    | 1:P:817:GLN:N    | 2.30                     | 0.57              |
| 2:Q:112:ILE:C    | 2:Q:147:ASN:O    | 2.42                     | 0.57              |
| 1:M:409:GLY:HA3  | 4:Z:333:PRO:CD   | 2.35                     | 0.57              |
| 1:M:797:PHE:CE2  | 3:O:146:ILE:HD13 | 2.28                     | 0.57              |
| 1:M:735:GLY:O    | 1:M:743:ALA:HA   | 1.94                     | 0.57              |
| 1:G:148:ARG:NH2  | 1:G:764:MLY:CH1  | 2.66                     | 0.57              |
| 1:P:707:CYS:SG   | 1:P:714:ARG:CZ   | 2.93                     | 0.57              |
| 1:M:642:LYS:CG   | 4:Z:22:ALA:CA    | 2.80                     | 0.57              |
| 1:G:769:ALA:HB3  | 1:G:770:GLY:N    | 2.10                     | 0.57              |
| 1:D:64:THR:HG22  | 1:D:65:GLU:N     | 2.19                     | 0.57              |
| 1:D:809:ARG:NH2  | 2:E:120:LEU:HD11 | 2.19                     | 0.57              |
| 1:A:254:PHE:CE2  | 1:A:459:ILE:HD12 | 2.39                     | 0.57              |
| 1:M:254:PHE:CE2  | 1:M:459:ILE:HD12 | 2.39                     | 0.57              |
| 1:G:141:LEU:O    | 1:G:144:ARG:HB3  | 2.03                     | 0.57              |
| 1:P:676:ILE:HG23 | 1:P:676:ILE:O    | 2.03                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:265:ILE:HG22 | 1:P:266:GLU:N    | 2.18                     | 0.57              |
| 1:P:813:ILE:O    | 1:P:816:ILE:N    | 2.37                     | 0.57              |
| 1:D:813:ILE:O    | 1:D:816:ILE:N    | 2.38                     | 0.57              |
| 2:E:112:ILE:C    | 2:E:147:ASN:O    | 2.42                     | 0.57              |
| 1:P:792:ALA:CB   | 3:R:42:THR:HG23  | 2.24                     | 0.57              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:CG2  | 2.35                     | 0.57              |
| 4:X:291:LYS:HB3  | 4:Z:244:ASP:CA   | 2.32                     | 0.57              |
| 1:G:279:LEU:HB3  | 1:G:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:A:279:LEU:HB3  | 1:A:280:PRO:HD2  | 1.86                     | 0.57              |
| 1:A:7:MET:HE3    | 1:A:14:ALA:HB1   | 1.84                     | 0.57              |
| 1:J:322:VAL:HG11 | 1:J:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:P:322:VAL:HG11 | 1:P:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:N    | 2.18                     | 0.57              |
| 1:G:797:PHE:HZ   | 3:I:146:ILE:HD11 | 1.62                     | 0.57              |
| 1:G:409:GLY:HA3  | 4:V:333:PRO:CD   | 2.35                     | 0.57              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:P:218:LEU:N    | 1:P:221:GLN:HE21 | 2.02                     | 0.57              |
| 1:M:715:VAL:HG11 | 1:M:720:PHE:HD1  | 1.68                     | 0.57              |
| 1:P:726:VAL:HB   | 1:P:779:ARG:HH22 | 1.69                     | 0.57              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:HE1  | 1.87                     | 0.57              |
| 1:G:95:THR:HA    | 1:G:713:SER:HB3  | 1.87                     | 0.57              |
| 1:G:612:GLN:HE22 | 1:G:627:GLY:HA2  | 1.66                     | 0.57              |
| 1:G:175:ILE:HA   | 1:G:670:HIS:O    | 2.03                     | 0.57              |
| 1:D:418:THR:HG22 | 1:D:419:VAL:H    | 1.69                     | 0.57              |
| 3:I:102:VAL:HG23 | 3:I:139:TYR:CD1  | 2.39                     | 0.57              |
| 1:D:116:TYR:HB2  | 1:D:153:PRO:O    | 2.03                     | 0.57              |
| 1:J:82:PRO:HD2   | 1:J:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:A:218:LEU:N    | 1:A:221:GLN:HE21 | 2.01                     | 0.57              |
| 1:G:813:ILE:O    | 1:G:816:ILE:N    | 2.37                     | 0.57              |
| 1:M:541:MET:HG2  | 4:Z:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:M:411:GLU:N    | 4:Z:333:PRO:HB2  | 2.11                     | 0.57              |
| 1:P:789:ALA:HB1  | 3:R:81:GLN:NE2   | 2.20                     | 0.57              |
| 1:D:409:GLY:HA3  | 4:9:333:PRO:CD   | 2.35                     | 0.57              |
| 1:D:579:PHE:CD2  | 1:D:592:ILE:HD11 | 2.39                     | 0.57              |
| 1:A:783:LEU:O    | 1:A:787:ILE:N    | 2.28                     | 0.57              |
| 1:M:797:PHE:CD1  | 3:O:149:VAL:HG13 | 2.29                     | 0.57              |
| 1:D:646:PHE:CD2  | 1:D:652:LEU:CD1  | 2.85                     | 0.57              |
| 1:A:643:GLY:HA2  | 4:8:24:ASP:OD1   | 2.04                     | 0.57              |
| 1:D:173:GLN:C    | 1:D:667:THR:HG23 | 2.25                     | 0.57              |
| 1:P:173:GLN:C    | 1:P:667:THR:HG23 | 2.25                     | 0.57              |
| 1:G:173:GLN:C    | 1:G:667:THR:HG23 | 2.25                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:102:VAL:HG23 | 3:F:139:TYR:CD1  | 2.39                     | 0.57              |
| 1:D:195:TYR:O    | 1:D:199:ILE:HG23 | 2.03                     | 0.57              |
| 1:G:7:MET:HE3    | 1:G:14:ALA:HB1   | 1.85                     | 0.57              |
| 1:G:752:ASP:OD1  | 1:G:783:LEU:CB   | 2.52                     | 0.57              |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:HD1  | 1.68                     | 0.57              |
| 1:A:813:ILE:O    | 1:A:816:ILE:N    | 2.37                     | 0.57              |
| 1:P:541:MET:HG2  | 4:0:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:P:541:MET:SD   | 4:0:346:LEU:O    | 2.48                     | 0.57              |
| 1:A:747:LEU:HD23 | 1:A:747:LEU:O    | 2.05                     | 0.57              |
| 1:G:218:LEU:N    | 1:G:221:GLN:HE21 | 2.01                     | 0.57              |
| 1:A:639:GLY:N    | 4:8:344:SER:C    | 2.54                     | 0.57              |
| 1:D:823:PHE:CZ   | 2:E:156:VAL:CG1  | 2.88                     | 0.57              |
| 1:P:506:GLU:HG2  | 1:P:759:ALA:C    | 2.24                     | 0.57              |
| 1:M:599:ASN:CG   | 1:M:649:VAL:HB   | 2.25                     | 0.57              |
| 1:J:579:PHE:CD2  | 1:J:592:ILE:HD11 | 2.40                     | 0.57              |
| 1:A:173:GLN:C    | 1:A:667:THR:HG23 | 2.25                     | 0.57              |
| 1:J:800:ARG:CD   | 3:L:149:VAL:C    | 2.72                     | 0.57              |
| 1:D:724:TYR:CD1  | 1:D:782:MLY:CD   | 2.86                     | 0.57              |
| 1:D:717:TYR:HD1  | 1:D:744:SER:HG   | 1.52                     | 0.57              |
| 1:J:747:LEU:HD23 | 1:J:747:LEU:O    | 2.05                     | 0.57              |
| 1:J:93:MET:HG2   | 1:J:715:VAL:HA   | 1.85                     | 0.57              |
| 1:J:409:GLY:HA3  | 4:W:333:PRO:CD   | 2.35                     | 0.57              |
| 1:G:747:LEU:HD23 | 1:G:747:LEU:O    | 2.05                     | 0.57              |
| 1:M:747:LEU:O    | 1:M:747:LEU:HD23 | 2.05                     | 0.57              |
| 1:D:82:PRO:HD2   | 1:D:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:P:502:GLU:CD   | 1:P:761:GLY:HA3  | 2.24                     | 0.57              |
| 1:M:630:ALA:CA   | 4:Z:25:ASP:OD2   | 2.53                     | 0.57              |
| 1:A:322:VAL:HG11 | 1:A:325:ILE:HD11 | 1.86                     | 0.57              |
| 1:A:109:ARG:O    | 1:A:114:MET:N    | 2.37                     | 0.57              |
| 1:A:149:GLN:CG   | 1:A:716:LEU:HD23 | 2.34                     | 0.57              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:CG2  | 2.35                     | 0.57              |
| 1:J:530:MET:CA   | 4:W:354:GLN:HB3  | 2.35                     | 0.57              |
| 1:M:794:CYS:O    | 1:M:798:LEU:N    | 2.37                     | 0.57              |
| 1:P:202:SER:CA   | 1:P:207:LYS:HE3  | 2.27                     | 0.57              |
| 1:G:599:ASN:CG   | 1:G:649:VAL:HB   | 2.25                     | 0.57              |
| 1:M:643:GLY:N    | 4:Z:23:GLY:C     | 2.55                     | 0.57              |
| 1:A:640:LYS:C    | 4:8:23:GLY:CA    | 2.64                     | 0.57              |
| 1:M:173:GLN:C    | 1:M:667:THR:HG23 | 2.25                     | 0.57              |
| 1:P:254:PHE:CE2  | 1:P:459:ILE:HD12 | 2.39                     | 0.57              |
| 1:P:677:PRO:HB2  | 1:P:678:ASN:ND2  | 2.20                     | 0.57              |
| 1:G:798:LEU:HD23 | 3:I:118:MET:HB3  | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:287:ILE:HG22 | 4:3:204:ALA:H    | 1.69                     | 0.57              |
| 1:A:220:ASP:O    | 1:A:224:SER:N    | 2.27                     | 0.57              |
| 1:J:638:GLY:CA   | 4:W:345:ILE:H    | 2.18                     | 0.57              |
| 1:D:530:MET:CA   | 4:9:354:GLN:HB3  | 2.35                     | 0.57              |
| 1:A:635:GLY:HA3  | 4:8:334:GLU:CG   | 2.30                     | 0.57              |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:HD1  | 1.68                     | 0.57              |
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:HZ1  | 1.69                     | 0.57              |
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:NZ   | 2.20                     | 0.57              |
| 1:D:768:MLY:N    | 1:D:771:LEU:CD1  | 2.63                     | 0.57              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:HB   | 2.25                     | 0.57              |
| 1:J:561:LYS:HE3  | 4:Y:48:GLY:CA    | 2.29                     | 0.57              |
| 1:J:173:GLN:C    | 1:J:667:THR:HG23 | 2.25                     | 0.57              |
| 1:G:82:PRO:HD2   | 1:G:85:TYR:CD2   | 2.40                     | 0.57              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:CG2  | 2.35                     | 0.56              |
| 1:M:411:GLU:H    | 4:Z:333:PRO:HG2  | 1.71                     | 0.56              |
| 1:P:793:ARG:CZ   | 3:R:40:ASN:HD22  | 2.07                     | 0.56              |
| 1:P:568:PRO:HG3  | 1:P:578:HIS:H    | 1.69                     | 0.56              |
| 1:A:529:PRO:CG   | 4:8:353:GLN:OE1  | 2.53                     | 0.56              |
| 1:A:649:VAL:HG22 | 1:A:649:VAL:HA   | 1.80                     | 0.56              |
| 1:M:295:MLY:HG3  | 1:M:332:MET:HE1  | 1.86                     | 0.56              |
| 1:A:800:ARG:HD3  | 3:C:149:VAL:C    | 2.25                     | 0.56              |
| 3:C:102:VAL:HG23 | 3:C:139:TYR:CD1  | 2.39                     | 0.56              |
| 1:J:418:THR:HG22 | 1:J:419:VAL:H    | 1.69                     | 0.56              |
| 1:D:481:ASN:N    | 1:D:481:ASN:ND2  | 2.51                     | 0.56              |
| 1:M:676:ILE:O    | 1:M:676:ILE:HG23 | 2.03                     | 0.56              |
| 1:J:783:LEU:O    | 1:J:787:ILE:CB   | 2.52                     | 0.56              |
| 1:J:784:ALA:O    | 1:J:788:THR:CB   | 2.52                     | 0.56              |
| 1:D:797:PHE:CD1  | 3:F:146:ILE:HA   | 2.33                     | 0.56              |
| 1:G:642:LYS:CA   | 4:V:22:ALA:C     | 2.70                     | 0.56              |
| 1:D:411:GLU:H    | 4:9:333:PRO:HG2  | 1.70                     | 0.56              |
| 1:M:217:THR:HG22 | 1:M:218:LEU:O    | 2.05                     | 0.56              |
| 1:P:506:GLU:HG2  | 1:P:759:ALA:HB1  | 1.85                     | 0.56              |
| 1:M:643:GLY:HA2  | 4:Z:24:ASP:OD1   | 2.04                     | 0.56              |
| 1:D:22:LYS:HA    | 1:D:25:ILE:HB    | 1.87                     | 0.56              |
| 1:A:82:PRO:HD2   | 1:A:85:TYR:CD2   | 2.40                     | 0.56              |
| 1:M:82:PRO:HD2   | 1:M:85:TYR:CD2   | 2.40                     | 0.56              |
| 1:J:801:VAL:HG21 | 3:L:126:LEU:HD21 | 1.84                     | 0.56              |
| 1:J:797:PHE:HE2  | 3:L:126:LEU:HD22 | 1.62                     | 0.56              |
| 1:D:724:TYR:HA   | 1:D:782:MLY:HD2  | 0.62                     | 0.56              |
| 1:A:93:MET:HE2   | 1:A:715:VAL:HA   | 0.69                     | 0.56              |
| 1:G:642:LYS:CD   | 4:V:340:TRP:CZ3  | 2.80                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:817:GLN:HB3  | 2:Q:127:ARG:CZ   | 2.34                     | 0.56              |
| 1:J:813:ILE:O    | 1:J:816:ILE:N    | 2.37                     | 0.56              |
| 2:B:112:ILE:C    | 2:B:147:ASN:O    | 2.42                     | 0.56              |
| 1:A:733:PRO:CB   | 1:A:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:M:530:MET:CA   | 4:Z:354:GLN:HB3  | 2.35                     | 0.56              |
| 1:J:541:MET:SD   | 4:W:346:LEU:O    | 2.48                     | 0.56              |
| 1:A:831:TRP:CD1  | 2:B:51:PHE:CE1   | 2.91                     | 0.56              |
| 1:A:797:PHE:CD1  | 3:C:146:ILE:C    | 2.77                     | 0.56              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:HB3  | 2.08                     | 0.56              |
| 1:M:642:LYS:CA   | 4:Z:22:ALA:C     | 2.70                     | 0.56              |
| 1:P:804:ARG:O    | 1:P:808:GLU:N    | 2.38                     | 0.56              |
| 1:A:630:ALA:CA   | 4:8:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:J:568:PRO:HG3  | 1:J:578:HIS:H    | 1.69                     | 0.56              |
| 1:D:99:GLU:OE2   | 1:D:696:ARG:NH2  | 2.30                     | 0.56              |
| 3:I:102:VAL:HG11 | 3:I:107:LEU:HB2  | 1.85                     | 0.56              |
| 1:A:481:ASN:ND2  | 1:A:481:ASN:N    | 2.51                     | 0.56              |
| 1:D:22:LYS:O     | 1:D:26:GLU:N     | 2.29                     | 0.56              |
| 1:G:338:ILE:HG21 | 1:G:348:MLY:HB3  | 1.87                     | 0.56              |
| 1:M:322:VAL:HG11 | 1:M:325:ILE:HD11 | 1.86                     | 0.56              |
| 1:A:302:MET:HG2  | 1:A:303:LEU:HD13 | 1.87                     | 0.56              |
| 4:3:365:ALA:HB3  | 4:3:369:ILE:HB   | 1.88                     | 0.56              |
| 4:1:365:ALA:HB3  | 4:1:369:ILE:HB   | 1.88                     | 0.56              |
| 1:A:135:TYR:N    | 1:A:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:A:210:GLN:O    | 1:A:211:SER:OG   | 2.15                     | 0.56              |
| 1:J:677:PRO:HB2  | 1:J:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:G:643:GLY:HA2  | 4:V:24:ASP:OD1   | 2.04                     | 0.56              |
| 1:G:643:GLY:N    | 4:V:23:GLY:C     | 2.55                     | 0.56              |
| 2:H:112:ILE:C    | 2:H:147:ASN:O    | 2.42                     | 0.56              |
| 2:B:140:PHE:O    | 2:B:141:PRO:C    | 2.33                     | 0.56              |
| 1:M:553:MLY:HG3  | 4:1:43:VAL:CG2   | 2.31                     | 0.56              |
| 1:P:783:LEU:O    | 1:P:786:ILE:HG13 | 2.05                     | 0.56              |
| 1:P:789:ALA:HB1  | 3:R:81:GLN:CG    | 2.35                     | 0.56              |
| 1:A:797:PHE:CD2  | 3:C:146:ILE:HD12 | 2.37                     | 0.56              |
| 4:2:287:ILE:HB   | 4:4:204:ALA:N    | 2.21                     | 0.56              |
| 1:D:95:THR:HG1   | 1:D:771:LEU:H    | 1.52                     | 0.56              |
| 1:A:646:PHE:CD2  | 1:A:652:LEU:CD1  | 2.85                     | 0.56              |
| 1:D:215:GLN:CA   | 1:D:340:ILE:CG2  | 2.63                     | 0.56              |
| 1:G:769:ALA:HB2  | 1:G:770:GLY:N    | 2.20                     | 0.56              |
| 1:M:755:HIS:HA   | 1:M:758:TYR:HE1  | 1.64                     | 0.56              |
| 1:P:97:LEU:HD23  | 1:P:712:PRO:HB3  | 1.83                     | 0.56              |
| 3:O:102:VAL:HG23 | 3:O:139:TYR:CD1  | 2.39                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:755:HIS:HA   | 1:A:758:TYR:HE1  | 1.64                     | 0.56              |
| 1:M:556:ASP:CG   | 4:1:49:GLN:OE1   | 2.44                     | 0.56              |
| 1:G:322:VAL:HG11 | 1:G:325:ILE:HD11 | 1.86                     | 0.56              |
| 1:G:676:ILE:O    | 1:G:676:ILE:HG23 | 2.03                     | 0.56              |
| 1:M:135:TYR:N    | 1:M:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:D:135:TYR:N    | 1:D:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:G:677:PRO:HB2  | 1:G:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:A:677:PRO:HB2  | 1:A:678:ASN:ND2  | 2.20                     | 0.56              |
| 1:G:792:ALA:HB1  | 3:I:41:PRO:C     | 2.24                     | 0.56              |
| 1:P:733:PRO:CB   | 1:P:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:P:530:MET:HA   | 4:0:354:GLN:CD   | 2.11                     | 0.56              |
| 1:M:534:SER:C    | 4:Z:351:THR:CA   | 2.47                     | 0.56              |
| 1:D:406:VAL:HG12 | 1:D:407:GLY:H    | 1.71                     | 0.56              |
| 1:D:568:PRO:HG3  | 1:D:578:HIS:H    | 1.69                     | 0.56              |
| 1:G:733:PRO:CB   | 1:G:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:A:411:GLU:H    | 4:8:333:PRO:HG2  | 1.71                     | 0.56              |
| 1:A:546:THR:HG21 | 1:A:548:THR:HB   | 1.88                     | 0.56              |
| 1:A:568:PRO:HG3  | 1:A:578:HIS:H    | 1.69                     | 0.56              |
| 1:M:783:LEU:CD1  | 1:M:786:ILE:CD1  | 2.64                     | 0.56              |
| 1:M:506:GLU:OE2  | 1:M:761:GLY:CA   | 2.50                     | 0.56              |
| 1:G:838:ILE:CG1  | 2:H:54:MET:HE3   | 2.27                     | 0.56              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:HB   | 2.25                     | 0.56              |
| 4:X:287:ILE:HG23 | 4:Z:201:VAL:HG23 | 1.87                     | 0.56              |
| 4:W:223:PHE:HD2  | 4:W:312:ARG:NH2  | 1.99                     | 0.56              |
| 1:D:116:TYR:CE2  | 1:D:154:HIS:CD2  | 2.94                     | 0.56              |
| 1:M:7:MET:HE3    | 1:M:14:ALA:HB1   | 1.86                     | 0.56              |
| 1:A:338:ILE:HG21 | 1:A:348:MLY:HB3  | 1.87                     | 0.56              |
| 1:G:302:MET:HG2  | 1:G:303:LEU:HD13 | 1.88                     | 0.56              |
| 1:G:135:TYR:N    | 1:G:135:TYR:HD1  | 2.04                     | 0.56              |
| 1:J:794:CYS:O    | 1:J:798:LEU:N    | 2.37                     | 0.56              |
| 1:D:733:PRO:CB   | 1:D:737:PHE:HE1  | 2.19                     | 0.56              |
| 1:G:795:ARG:CZ   | 3:I:116:GLU:CG   | 2.82                     | 0.56              |
| 4:1:287:ILE:HG21 | 4:3:203:THR:N    | 2.19                     | 0.56              |
| 1:P:530:MET:CA   | 4:0:354:GLN:HB3  | 2.35                     | 0.56              |
| 1:M:546:THR:HG21 | 1:M:548:THR:HB   | 1.88                     | 0.56              |
| 1:G:725:ARG:HG3  | 1:G:733:PRO:CA   | 2.36                     | 0.56              |
| 1:P:839:MLY:HH21 | 2:Q:158:THR:CG2  | 2.35                     | 0.56              |
| 1:P:206:LYS:HB3  | 1:P:217:THR:OG1  | 2.06                     | 0.56              |
| 4:1:204:ALA:H    | 4:Z:287:ILE:HG21 | 1.67                     | 0.56              |
| 1:G:649:VAL:HG22 | 1:G:649:VAL:HA   | 1.80                     | 0.56              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:CB   | 2.53                     | 0.56              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 3:L:102:VAL:HG23 | 3:L:139:TYR:CD1 | 2.39                     | 0.56              |
| 1:J:769:ALA:HB3  | 1:J:770:GLY:HA3 | 1.87                     | 0.56              |
| 1:P:116:TYR:CE2  | 1:P:154:HIS:CD2 | 2.94                     | 0.56              |
| 1:J:116:TYR:CE2  | 1:J:154:HIS:CD2 | 2.94                     | 0.56              |
| 1:P:22:LYS:HA    | 1:P:25:ILE:HB   | 1.87                     | 0.56              |
| 1:J:338:ILE:HG21 | 1:J:348:MLY:HB3 | 1.87                     | 0.56              |
| 1:M:109:ARG:O    | 1:M:114:MET:N   | 2.37                     | 0.56              |
| 1:D:677:PRO:HB2  | 1:D:678:ASN:ND2 | 2.20                     | 0.56              |
| 1:D:795:ARG:CZ   | 3:F:116:GLU:HB3 | 2.35                     | 0.56              |
| 1:A:93:MET:CE    | 1:A:715:VAL:CB  | 2.83                     | 0.56              |
| 1:A:217:THR:HG22 | 1:A:218:LEU:O   | 2.05                     | 0.56              |
| 1:A:206:LYS:HB3  | 1:A:217:THR:OG1 | 2.06                     | 0.56              |
| 1:P:638:GLY:CA   | 4:0:345:ILE:H   | 2.18                     | 0.56              |
| 1:M:206:LYS:HB3  | 1:M:217:THR:OG1 | 2.06                     | 0.56              |
| 1:A:530:MET:CA   | 4:8:354:GLN:HB3 | 2.35                     | 0.56              |
| 4:1:203:THR:CG2  | 4:Z:287:ILE:HB  | 2.35                     | 0.56              |
| 1:M:649:VAL:CG1  | 1:M:649:VAL:HA  | 2.35                     | 0.56              |
| 1:D:831:TRP:CZ3  | 2:E:50:THR:HG21 | 2.38                     | 0.56              |
| 1:A:116:TYR:CE2  | 1:A:154:HIS:CD2 | 2.94                     | 0.56              |
| 1:G:7:MET:HE3    | 1:G:14:ALA:CB   | 2.36                     | 0.56              |
| 1:J:135:TYR:HD1  | 1:J:135:TYR:N   | 2.04                     | 0.56              |
| 1:M:813:ILE:O    | 1:M:816:ILE:N   | 2.38                     | 0.56              |
| 1:P:725:ARG:HG3  | 1:P:733:PRO:CA  | 2.36                     | 0.56              |
| 1:P:733:PRO:CA   | 1:P:737:PHE:HE1 | 2.19                     | 0.56              |
| 1:P:629:GLU:O    | 1:P:643:GLY:HA3 | 2.06                     | 0.56              |
| 1:M:410:ASN:CG   | 4:Z:334:GLU:C   | 2.65                     | 0.56              |
| 1:D:529:PRO:CG   | 4:9:353:GLN:OE1 | 2.53                     | 0.56              |
| 1:A:649:VAL:HG23 | 1:A:649:VAL:HA  | 1.83                     | 0.56              |
| 1:P:599:ASN:CG   | 1:P:649:VAL:HB  | 2.25                     | 0.56              |
| 1:P:806:MET:HB2  | 1:P:807:VAL:N   | 2.21                     | 0.56              |
| 1:G:418:THR:HG22 | 1:G:419:VAL:H   | 1.69                     | 0.56              |
| 1:D:435:GLU:O    | 1:D:438:PHE:HB3 | 2.06                     | 0.56              |
| 1:M:435:GLU:O    | 1:M:438:PHE:HB3 | 2.06                     | 0.56              |
| 1:P:338:ILE:HG21 | 1:P:348:MLY:HB3 | 1.87                     | 0.56              |
| 1:P:32:PHE:CG    | 1:P:83:PRO:HD3  | 2.41                     | 0.56              |
| 1:P:82:PRO:HD2   | 1:P:85:TYR:CD2  | 2.40                     | 0.56              |
| 1:D:727:LEU:CA   | 1:D:782:MLY:HE2 | 2.36                     | 0.56              |
| 1:G:783:LEU:HA   | 1:G:786:ILE:HB  | 1.87                     | 0.56              |
| 1:A:502:GLU:O    | 1:A:761:GLY:CA  | 2.54                     | 0.56              |
| 1:G:537:GLU:HB3  | 1:G:648:THR:CB  | 2.36                     | 0.56              |
| 1:P:640:LYS:C    | 1:P:645:SER:OG  | 2.44                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:217:THR:HG22 | 1:G:218:LEU:O    | 2.06                     | 0.56              |
| 1:P:783:LEU:O    | 1:P:786:ILE:N    | 2.38                     | 0.56              |
| 1:D:638:GLY:CA   | 4:9:345:ILE:H    | 2.19                     | 0.56              |
| 1:G:649:VAL:CG1  | 1:G:649:VAL:HA   | 2.35                     | 0.56              |
| 1:A:599:ASN:CG   | 1:A:649:VAL:HB   | 2.25                     | 0.56              |
| 1:J:756:THR:HG22 | 1:J:776:GLU:HA   | 1.77                     | 0.56              |
| 1:J:630:ALA:CA   | 4:W:25:ASP:OD2   | 2.53                     | 0.56              |
| 1:P:630:ALA:CA   | 4:0:25:ASP:OD2   | 2.53                     | 0.56              |
| 4:0:173:HIS:CD2  | 4:1:268:GLY:CA   | 2.88                     | 0.56              |
| 1:G:22:LYS:O     | 1:G:26:GLU:HG3   | 2.06                     | 0.56              |
| 1:G:435:GLU:O    | 1:G:438:PHE:HB3  | 2.06                     | 0.56              |
| 4:V:288:ASP:N    | 4:X:204:ALA:H    | 2.03                     | 0.56              |
| 1:G:109:ARG:O    | 1:G:114:MET:N    | 2.37                     | 0.56              |
| 1:D:725:ARG:HG3  | 1:D:733:PRO:CA   | 2.36                     | 0.56              |
| 1:G:410:ASN:CG   | 4:V:334:GLU:C    | 2.64                     | 0.56              |
| 1:G:538:GLU:CG   | 4:V:351:THR:C    | 2.73                     | 0.56              |
| 1:G:530:MET:CA   | 4:V:354:GLN:HB3  | 2.35                     | 0.56              |
| 1:P:409:GLY:HA3  | 4:0:333:PRO:CD   | 2.35                     | 0.56              |
| 1:P:530:MET:CB   | 4:0:354:GLN:HG3  | 2.36                     | 0.56              |
| 1:G:206:LYS:HB3  | 1:G:217:THR:OG1  | 2.06                     | 0.56              |
| 1:J:217:THR:HG22 | 1:J:218:LEU:O    | 2.05                     | 0.56              |
| 1:M:529:PRO:CG   | 4:Z:353:GLN:OE1  | 2.54                     | 0.56              |
| 1:M:546:THR:HB   | 1:M:549:SER:H    | 1.71                     | 0.56              |
| 1:J:530:MET:CB   | 4:W:354:GLN:HG3  | 2.37                     | 0.56              |
| 1:P:217:THR:HG22 | 1:P:218:LEU:O    | 2.05                     | 0.56              |
| 1:D:640:LYS:C    | 1:D:645:SER:OG   | 2.44                     | 0.56              |
| 1:M:629:GLU:O    | 1:M:643:GLY:HA3  | 2.06                     | 0.56              |
| 1:M:806:MET:HA   | 1:M:809:ARG:HB2  | 1.88                     | 0.56              |
| 1:A:22:LYS:O     | 1:A:26:GLU:HG3   | 2.06                     | 0.56              |
| 4:4:365:ALA:HB3  | 4:4:369:ILE:HB   | 1.88                     | 0.56              |
| 1:D:733:PRO:CA   | 1:D:737:PHE:HE1  | 2.18                     | 0.55              |
| 1:D:795:ARG:CD   | 3:F:43:ASN:CG    | 2.69                     | 0.55              |
| 1:D:795:ARG:HD2  | 3:F:35:ARG:NH1   | 2.16                     | 0.55              |
| 1:D:798:LEU:HD13 | 3:F:126:LEU:HD13 | 1.82                     | 0.55              |
| 1:D:795:ARG:HB2  | 3:F:35:ARG:NH1   | 2.17                     | 0.55              |
| 2:N:112:ILE:C    | 2:N:147:ASN:O    | 2.42                     | 0.55              |
| 1:G:529:PRO:CG   | 4:V:353:GLN:OE1  | 2.54                     | 0.55              |
| 1:G:638:GLY:CA   | 4:V:345:ILE:H    | 2.18                     | 0.55              |
| 4:1:287:ILE:HB   | 4:3:203:THR:CB   | 2.35                     | 0.55              |
| 3:R:102:VAL:HG23 | 3:R:139:TYR:CD1  | 2.39                     | 0.55              |
| 1:J:725:ARG:HG3  | 1:J:733:PRO:CA   | 2.36                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:529:PRO:CG   | 4:O:353:GLN:OE1  | 2.54                     | 0.55              |
| 1:M:530:MET:HE3  | 4:Z:355:MET:SD   | 2.46                     | 0.55              |
| 1:P:792:ALA:CB   | 3:R:42:THR:CA    | 2.84                     | 0.55              |
| 1:D:819:ASN:OD1  | 2:E:91:ALA:HA    | 1.87                     | 0.55              |
| 1:P:549:SER:HA   | 4:2:49:GLN:HG3   | 1.88                     | 0.55              |
| 1:M:733:PRO:CA   | 1:M:737:PHE:HE1  | 2.19                     | 0.55              |
| 4:X:286:ASP:CB   | 4:Z:202:THR:HB   | 2.26                     | 0.55              |
| 1:D:290:GLN:HG2  | 1:D:331:LEU:HA   | 1.87                     | 0.55              |
| 1:J:406:VAL:HG12 | 1:J:407:GLY:H    | 1.71                     | 0.55              |
| 4:Y:365:ALA:HB3  | 4:Y:369:ILE:HB   | 1.88                     | 0.55              |
| 1:D:32:PHE:CG    | 1:D:83:PRO:HD3   | 2.41                     | 0.55              |
| 1:M:604:ASN:OD1  | 1:M:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:747:LEU:O    | 1:D:747:LEU:HD23 | 2.05                     | 0.55              |
| 1:G:753:VAL:O    | 1:G:779:ARG:HD3  | 2.06                     | 0.55              |
| 1:G:411:GLU:H    | 4:V:333:PRO:HG2  | 1.70                     | 0.55              |
| 1:P:406:VAL:HG12 | 1:P:407:GLY:H    | 1.71                     | 0.55              |
| 1:A:733:PRO:CA   | 1:A:737:PHE:HE1  | 2.19                     | 0.55              |
| 1:J:629:GLU:O    | 1:J:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:D:529:PRO:CB   | 4:9:354:GLN:HA   | 2.36                     | 0.55              |
| 1:D:530:MET:HE3  | 4:9:355:MET:SD   | 2.46                     | 0.55              |
| 1:A:752:ASP:OD2  | 1:A:782:MLY:HG2  | 2.06                     | 0.55              |
| 1:P:546:THR:HG21 | 1:P:548:THR:HB   | 1.88                     | 0.55              |
| 1:A:546:THR:HB   | 1:A:549:SER:H    | 1.71                     | 0.55              |
| 1:M:730:SER:OG   | 3:O:96:LYS:HB3   | 2.06                     | 0.55              |
| 1:A:612:GLN:HE22 | 1:A:627:GLY:HA2  | 1.66                     | 0.55              |
| 1:G:116:TYR:CE2  | 1:G:154:HIS:CD2  | 2.94                     | 0.55              |
| 1:A:290:GLN:HG2  | 1:A:331:LEU:HA   | 1.87                     | 0.55              |
| 1:A:7:MET:HE3    | 1:A:14:ALA:CB    | 2.36                     | 0.55              |
| 1:M:7:MET:HE3    | 1:M:14:ALA:CB    | 2.36                     | 0.55              |
| 1:A:32:PHE:CG    | 1:A:83:PRO:HD3   | 2.42                     | 0.55              |
| 4:V:291:LYS:HD2  | 4:X:243:PRO:HB2  | 1.87                     | 0.55              |
| 1:D:795:ARG:NE   | 3:F:116:GLU:HB3  | 2.20                     | 0.55              |
| 3:I:35:ARG:HA    | 3:I:39:GLN:O     | 2.07                     | 0.55              |
| 1:G:557:GLU:HB2  | 4:X:47:MET:O     | 2.04                     | 0.55              |
| 4:1:287:ILE:CG2  | 4:3:202:THR:CA   | 2.82                     | 0.55              |
| 1:G:819:ASN:ND2  | 2:H:90:GLY:O     | 2.39                     | 0.55              |
| 1:A:735:GLY:O    | 1:A:743:ALA:HA   | 1.94                     | 0.55              |
| 1:M:529:PRO:CB   | 4:Z:354:GLN:HA   | 2.36                     | 0.55              |
| 1:P:791:GLN:NE2  | 3:R:116:GLU:H    | 2.05                     | 0.55              |
| 1:D:537:GLU:HB3  | 1:D:648:THR:CB   | 2.36                     | 0.55              |
| 1:G:730:SER:HG   | 3:I:113:THR:CG2  | 2.09                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:579:PHE:HE1  | 1:P:581:LEU:HD13 | 1.72                     | 0.55              |
| 1:A:537:GLU:HB3  | 1:A:648:THR:CB   | 2.36                     | 0.55              |
| 1:M:84:MLY:CD    | 1:M:723:ARG:CD   | 2.75                     | 0.55              |
| 1:M:649:VAL:HA   | 1:M:649:VAL:HG22 | 1.80                     | 0.55              |
| 1:P:727:LEU:CD2  | 1:P:779:ARG:HE   | 2.19                     | 0.55              |
| 1:D:630:ALA:CA   | 4:9:25:ASP:OD2   | 2.53                     | 0.55              |
| 1:J:831:TRP:HZ2  | 2:K:47:LEU:HD21  | 1.67                     | 0.55              |
| 3:O:46:ILE:O     | 3:O:50:LEU:CG    | 2.47                     | 0.55              |
| 3:R:46:ILE:O     | 3:R:50:LEU:CG    | 2.47                     | 0.55              |
| 1:G:127:ASN:ND2  | 1:G:128:PRO:HD2  | 2.17                     | 0.55              |
| 1:M:290:GLN:HG2  | 1:M:331:LEU:HA   | 1.87                     | 0.55              |
| 1:A:406:VAL:HG12 | 1:A:407:GLY:H    | 1.71                     | 0.55              |
| 1:A:345:ALA:O    | 1:A:349:THR:N    | 2.40                     | 0.55              |
| 1:M:338:ILE:HG21 | 1:M:348:MLY:HB3  | 1.87                     | 0.55              |
| 4:0:365:ALA:HB3  | 4:0:369:ILE:HB   | 1.88                     | 0.55              |
| 4:5:365:ALA:HB3  | 4:5:369:ILE:HB   | 1.88                     | 0.55              |
| 1:M:677:PRO:HB2  | 1:M:678:ASN:ND2  | 2.20                     | 0.55              |
| 3:O:123:VAL:O    | 3:O:127:MET:HG2  | 2.07                     | 0.55              |
| 1:M:32:PHE:CG    | 1:M:83:PRO:HD3   | 2.42                     | 0.55              |
| 1:G:530:MET:HE3  | 4:V:354:GLN:CB   | 2.37                     | 0.55              |
| 4:1:287:ILE:CA   | 4:3:202:THR:HB   | 2.35                     | 0.55              |
| 1:J:821:ARG:HH22 | 2:K:127:ARG:CD   | 2.10                     | 0.55              |
| 1:P:411:GLU:H    | 4:0:333:PRO:HG2  | 1.70                     | 0.55              |
| 1:P:646:PHE:CE2  | 1:P:652:LEU:CG   | 2.90                     | 0.55              |
| 1:J:646:PHE:CE2  | 1:J:652:LEU:CG   | 2.90                     | 0.55              |
| 1:G:735:GLY:C    | 1:G:743:ALA:HB1  | 1.84                     | 0.55              |
| 1:D:217:THR:HG22 | 1:D:218:LEU:O    | 2.06                     | 0.55              |
| 1:P:579:PHE:CD2  | 1:P:592:ILE:HD11 | 2.40                     | 0.55              |
| 1:A:538:GLU:CG   | 4:8:351:THR:C    | 2.74                     | 0.55              |
| 2:E:156:VAL:HA   | 2:E:159:HIS:O    | 2.07                     | 0.55              |
| 1:M:640:LYS:C    | 1:M:645:SER:OG   | 2.44                     | 0.55              |
| 4:X:287:ILE:CG2  | 4:Z:201:VAL:HG23 | 2.37                     | 0.55              |
| 1:M:630:ALA:HA   | 4:Z:25:ASP:OD2   | 2.07                     | 0.55              |
| 1:J:829:TRP:CH2  | 2:K:83:MET:HE2   | 2.41                     | 0.55              |
| 1:J:579:PHE:HE1  | 1:J:581:LEU:HD13 | 1.72                     | 0.55              |
| 1:A:290:GLN:NE2  | 1:A:334:THR:OG1  | 2.40                     | 0.55              |
| 4:X:365:ALA:HB3  | 4:X:369:ILE:HB   | 1.88                     | 0.55              |
| 1:G:752:ASP:OD1  | 1:G:783:LEU:CA   | 2.54                     | 0.55              |
| 1:J:733:PRO:CB   | 1:J:737:PHE:HE1  | 2.19                     | 0.55              |
| 1:P:635:GLY:HA3  | 4:0:334:GLU:CG   | 2.30                     | 0.55              |
| 1:A:725:ARG:HG3  | 1:A:733:PRO:CA   | 2.36                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:640:LYS:C    | 1:J:645:SER:OG   | 2.44                     | 0.55              |
| 1:D:546:THR:HG21 | 1:D:548:THR:HB   | 1.88                     | 0.55              |
| 3:C:35:ARG:HA    | 3:C:39:GLN:O     | 2.07                     | 0.55              |
| 1:A:529:PRO:CB   | 4:8:354:GLN:HA   | 2.36                     | 0.55              |
| 1:M:806:MET:HB2  | 1:M:807:VAL:N    | 2.21                     | 0.55              |
| 1:A:629:GLU:O    | 1:A:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:A:640:LYS:C    | 1:A:645:SER:OG   | 2.44                     | 0.55              |
| 1:G:546:THR:HB   | 1:G:549:SER:H    | 1.71                     | 0.55              |
| 1:G:579:PHE:HE1  | 1:G:581:LEU:HD13 | 1.72                     | 0.55              |
| 1:M:481:ASN:N    | 1:M:481:ASN:ND2  | 2.51                     | 0.55              |
| 1:M:826:VAL:HG21 | 2:N:88:LEU:HD23  | 1.89                     | 0.55              |
| 1:M:22:LYS:HA    | 1:M:25:ILE:HB    | 1.87                     | 0.55              |
| 4:W:365:ALA:HB3  | 4:W:369:ILE:HB   | 1.88                     | 0.55              |
| 1:M:302:MET:HG2  | 1:M:303:LEU:HD13 | 1.87                     | 0.55              |
| 3:R:123:VAL:O    | 3:R:127:MET:HG2  | 2.07                     | 0.55              |
| 1:A:604:ASN:OD1  | 1:A:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:604:ASN:OD1  | 1:D:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:727:LEU:CD1  | 1:D:782:MLY:NZ   | 2.53                     | 0.55              |
| 1:J:821:ARG:HH12 | 2:K:127:ARG:NE   | 2.03                     | 0.55              |
| 1:J:206:LYS:HB3  | 1:J:217:THR:OG1  | 2.06                     | 0.55              |
| 1:J:32:PHE:CG    | 1:J:83:PRO:HD3   | 2.41                     | 0.55              |
| 1:M:406:VAL:HG12 | 1:M:407:GLY:H    | 1.71                     | 0.55              |
| 1:J:529:PRO:CB   | 4:W:354:GLN:HA   | 2.36                     | 0.55              |
| 1:D:206:LYS:HB3  | 1:D:217:THR:OG1  | 2.06                     | 0.55              |
| 1:P:546:THR:HB   | 1:P:549:SER:H    | 1.71                     | 0.55              |
| 1:M:783:LEU:N    | 1:M:786:ILE:HD11 | 2.22                     | 0.55              |
| 1:M:84:MLY:HH12  | 1:M:715:VAL:CG2  | 2.37                     | 0.55              |
| 1:D:629:GLU:O    | 1:D:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:J:834:LEU:HD12 | 2:K:51:PHE:CE1   | 2.41                     | 0.55              |
| 1:M:116:TYR:CE2  | 1:M:154:HIS:CD2  | 2.94                     | 0.55              |
| 1:J:22:LYS:HA    | 1:J:25:ILE:HB    | 1.87                     | 0.55              |
| 1:J:302:MET:HG2  | 1:J:303:LEU:HD13 | 1.87                     | 0.55              |
| 1:P:135:TYR:N    | 1:P:135:TYR:HD1  | 2.04                     | 0.55              |
| 3:I:123:VAL:O    | 3:I:127:MET:HG2  | 2.07                     | 0.55              |
| 1:G:629:GLU:O    | 1:G:643:GLY:HA3  | 2.06                     | 0.55              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CG   | 2.90                     | 0.55              |
| 1:J:733:PRO:CA   | 1:J:737:PHE:HE1  | 2.19                     | 0.55              |
| 1:J:529:PRO:CG   | 4:W:353:GLN:OE1  | 2.54                     | 0.55              |
| 1:D:530:MET:CB   | 4:9:354:GLN:HG3  | 2.36                     | 0.55              |
| 1:G:733:PRO:CA   | 1:G:737:PHE:HE1  | 2.19                     | 0.55              |
| 1:M:795:ARG:CB   | 3:O:35:ARG:NH1   | 2.70                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:646:PHE:CE2  | 1:D:652:LEU:CG   | 2.90                     | 0.55              |
| 1:M:646:PHE:CE2  | 1:M:652:LEU:CG   | 2.90                     | 0.55              |
| 1:M:35:MLY:CH2   | 1:M:778:MET:HA   | 2.37                     | 0.55              |
| 1:J:95:THR:CA    | 1:J:713:SER:CB   | 2.75                     | 0.55              |
| 1:G:739:ASP:CB   | 1:G:742:LYS:CB   | 2.81                     | 0.55              |
| 1:G:290:GLN:NE2  | 1:G:334:THR:OG1  | 2.40                     | 0.55              |
| 1:G:22:LYS:HA    | 1:G:25:ILE:HB    | 1.87                     | 0.55              |
| 1:P:22:LYS:O     | 1:P:26:GLU:HG3   | 2.07                     | 0.55              |
| 1:J:7:MET:HE3    | 1:J:14:ALA:CB    | 2.36                     | 0.55              |
| 1:D:338:ILE:HG21 | 1:D:348:MLY:HB3  | 1.87                     | 0.55              |
| 1:J:82:PRO:HD2   | 1:J:85:TYR:HD2   | 1.72                     | 0.55              |
| 1:G:797:PHE:CE2  | 3:I:126:LEU:HD21 | 2.29                     | 0.55              |
| 1:G:826:VAL:HG21 | 2:H:88:LEU:CD2   | 2.37                     | 0.55              |
| 1:M:638:GLY:CA   | 4:Z:345:ILE:H    | 2.18                     | 0.55              |
| 1:J:410:ASN:CG   | 4:W:334:GLU:C    | 2.65                     | 0.55              |
| 1:J:411:GLU:H    | 4:W:333:PRO:HG2  | 1.71                     | 0.55              |
| 2:Q:156:VAL:HA   | 2:Q:159:HIS:O    | 2.07                     | 0.55              |
| 2:B:156:VAL:HA   | 2:B:159:HIS:O    | 2.07                     | 0.55              |
| 1:A:642:LYS:CA   | 4:8:22:ALA:C     | 2.71                     | 0.55              |
| 1:J:649:VAL:CG1  | 1:J:649:VAL:HA   | 2.35                     | 0.55              |
| 1:D:831:TRP:CZ2  | 2:E:47:LEU:HD22  | 2.42                     | 0.55              |
| 1:D:831:TRP:HZ2  | 2:E:47:LEU:CB    | 2.20                     | 0.55              |
| 1:D:830:PRO:HB2  | 2:E:51:PHE:CE1   | 2.42                     | 0.55              |
| 1:J:97:LEU:HD22  | 1:J:712:PRO:HB2  | 1.89                     | 0.55              |
| 1:M:832:MET:SD   | 2:N:84:PHE:HE2   | 2.30                     | 0.55              |
| 1:M:290:GLN:NE2  | 1:M:334:THR:OG1  | 2.40                     | 0.55              |
| 1:J:345:ALA:O    | 1:J:349:THR:N    | 2.40                     | 0.55              |
| 1:J:435:GLU:O    | 1:J:438:PHE:HB3  | 2.06                     | 0.55              |
| 1:P:435:GLU:O    | 1:P:438:PHE:HB3  | 2.06                     | 0.55              |
| 1:M:22:LYS:O     | 1:M:26:GLU:N     | 2.30                     | 0.55              |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CE2  | 2.42                     | 0.55              |
| 1:P:7:MET:HE3    | 1:P:14:ALA:CB    | 2.36                     | 0.55              |
| 4:9:365:ALA:HB3  | 4:9:369:ILE:HB   | 1.88                     | 0.55              |
| 4:7:365:ALA:HB3  | 4:7:369:ILE:HB   | 1.88                     | 0.55              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:CD   | 2.37                     | 0.55              |
| 3:F:123:VAL:O    | 3:F:127:MET:HG2  | 2.07                     | 0.55              |
| 1:D:470:PHE:O    | 1:D:473:ASN:ND2  | 2.40                     | 0.55              |
| 3:C:123:VAL:O    | 3:C:127:MET:HG2  | 2.06                     | 0.55              |
| 1:P:813:ILE:HG23 | 2:Q:128:PHE:CE1  | 2.42                     | 0.55              |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD11 | 1.75                     | 0.55              |
| 1:M:537:GLU:HB3  | 1:M:648:THR:CB   | 2.36                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:530:MET:CB   | 4:Z:354:GLN:HG3  | 2.36                     | 0.55              |
| 1:J:538:GLU:CG   | 4:W:351:THR:C    | 2.73                     | 0.55              |
| 1:J:643:GLY:N    | 4:W:23:GLY:C     | 2.55                     | 0.55              |
| 1:D:726:VAL:O    | 1:D:785:GLU:CG   | 2.52                     | 0.55              |
| 2:K:156:VAL:HA   | 2:K:159:HIS:O    | 2.07                     | 0.55              |
| 4:3:287:ILE:HG21 | 4:5:204:ALA:H    | 1.67                     | 0.55              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:CG1  | 2.35                     | 0.55              |
| 1:J:546:THR:HG21 | 1:J:548:THR:HB   | 1.88                     | 0.55              |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:CG   | 2.20                     | 0.55              |
| 1:J:290:GLN:HG2  | 1:J:331:LEU:HA   | 1.87                     | 0.55              |
| 1:P:290:GLN:NE2  | 1:P:334:THR:OG1  | 2.40                     | 0.55              |
| 1:G:290:GLN:HG2  | 1:G:331:LEU:HA   | 1.87                     | 0.55              |
| 1:D:7:MET:HE3    | 1:D:14:ALA:CB    | 2.36                     | 0.55              |
| 4:2:365:ALA:HB3  | 4:2:369:ILE:HB   | 1.88                     | 0.55              |
| 1:D:302:MET:HG2  | 1:D:303:LEU:HD13 | 1.88                     | 0.55              |
| 1:J:604:ASN:OD1  | 1:J:607:VAL:HG23 | 2.06                     | 0.55              |
| 3:F:35:ARG:HA    | 3:F:39:GLN:O     | 2.07                     | 0.55              |
| 1:G:791:GLN:HE22 | 3:I:115:GLY:HA2  | 1.62                     | 0.55              |
| 1:A:765:VAL:HG12 | 1:A:766:PHE:N    | 2.22                     | 0.55              |
| 1:G:640:LYS:C    | 1:G:645:SER:OG   | 2.44                     | 0.55              |
| 1:G:638:GLY:HA2  | 4:V:345:ILE:H    | 1.72                     | 0.55              |
| 1:A:813:ILE:HG12 | 2:B:128:PHE:HE1  | 1.72                     | 0.55              |
| 1:P:529:PRO:CB   | 4:0:354:GLN:HA   | 2.36                     | 0.55              |
| 1:J:530:MET:HE3  | 4:W:354:GLN:CG   | 2.31                     | 0.55              |
| 1:A:638:GLY:CA   | 4:8:345:ILE:H    | 2.19                     | 0.55              |
| 3:O:35:ARG:HA    | 3:O:39:GLN:O     | 2.07                     | 0.55              |
| 1:M:84:MLY:HH12  | 1:M:715:VAL:HG21 | 1.88                     | 0.55              |
| 1:M:723:ARG:HH11 | 1:M:723:ARG:CG   | 2.20                     | 0.55              |
| 1:P:503:TYR:HH   | 1:P:711:PHE:HD2  | 0.64                     | 0.55              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CG   | 2.90                     | 0.55              |
| 1:P:295:MLY:HG3  | 1:P:332:MET:HE1  | 1.89                     | 0.55              |
| 1:J:561:LYS:CE   | 4:Y:48:GLY:CA    | 2.82                     | 0.55              |
| 1:A:630:ALA:HA   | 4:8:25:ASP:OD2   | 2.07                     | 0.55              |
| 1:J:829:TRP:CZ2  | 2:K:83:MET:HE3   | 2.38                     | 0.55              |
| 1:A:800:ARG:CG   | 3:C:149:VAL:HG22 | 2.35                     | 0.55              |
| 3:I:49:ILE:CA    | 3:I:52:ASN:ND2   | 2.53                     | 0.55              |
| 1:P:612:GLN:HE22 | 1:P:627:GLY:HA2  | 1.66                     | 0.55              |
| 1:A:127:ASN:ND2  | 1:A:128:PRO:HD2  | 2.16                     | 0.55              |
| 1:P:799:MET:SD   | 3:R:32:ASP:OD2   | 2.65                     | 0.55              |
| 2:H:156:VAL:HA   | 2:H:159:HIS:O    | 2.07                     | 0.55              |
| 1:P:290:GLN:HG2  | 1:P:331:LEU:HA   | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:22:LYS:HA    | 1:A:25:ILE:HB    | 1.88                     | 0.55              |
| 1:A:435:GLU:O    | 1:A:438:PHE:HB3  | 2.06                     | 0.55              |
| 4:2:148:THR:HG21 | 4:4:45:VAL:HG21  | 1.89                     | 0.55              |
| 1:M:135:TYR:HD2  | 1:M:191:ARG:HG2  | 1.72                     | 0.55              |
| 1:P:135:TYR:HD2  | 1:P:191:ARG:HG2  | 1.72                     | 0.55              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:HG2  | 1.72                     | 0.55              |
| 1:G:604:ASN:OD1  | 1:G:607:VAL:HG23 | 2.06                     | 0.55              |
| 1:P:109:ARG:O    | 1:P:114:MET:N    | 2.37                     | 0.55              |
| 1:J:797:PHE:CE2  | 3:L:126:LEU:CD2  | 2.80                     | 0.54              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:HD11 | 1.26                     | 0.54              |
| 1:D:797:PHE:CD1  | 3:F:146:ILE:CB   | 2.87                     | 0.54              |
| 1:G:791:GLN:CD   | 3:I:116:GLU:H    | 2.09                     | 0.54              |
| 1:A:149:GLN:CB   | 1:A:718:ALA:CA   | 2.85                     | 0.54              |
| 1:A:93:MET:O     | 1:A:713:SER:HB3  | 2.06                     | 0.54              |
| 1:P:537:GLU:HB3  | 1:P:648:THR:CB   | 2.36                     | 0.54              |
| 1:A:831:TRP:CZ3  | 2:B:34:ILE:CG2   | 2.87                     | 0.54              |
| 1:M:795:ARG:HD2  | 3:O:35:ARG:HH12  | 1.72                     | 0.54              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:HE1  | 1.89                     | 0.54              |
| 1:G:831:TRP:CZ3  | 2:H:34:ILE:HG21  | 2.41                     | 0.54              |
| 1:G:78:PHE:HB3   | 1:G:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:M:345:ALA:O    | 1:M:349:THR:N    | 2.40                     | 0.54              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:CD   | 2.37                     | 0.54              |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:CZ   | 2.42                     | 0.54              |
| 4:Z:365:ALA:HB3  | 4:Z:369:ILE:HB   | 1.88                     | 0.54              |
| 1:P:302:MET:HG2  | 1:P:303:LEU:HD13 | 1.87                     | 0.54              |
| 1:P:82:PRO:HD2   | 1:P:85:TYR:HD2   | 1.72                     | 0.54              |
| 4:V:291:LYS:HD2  | 4:X:243:PRO:CB   | 2.38                     | 0.54              |
| 1:A:10:PHE:O     | 1:A:12:GLU:N     | 2.41                     | 0.54              |
| 1:G:754:ASP:HA   | 1:G:779:ARG:CZ   | 2.35                     | 0.54              |
| 1:G:530:MET:CB   | 4:V:354:GLN:HG3  | 2.37                     | 0.54              |
| 1:J:721:LYS:C    | 1:J:736:GLN:OE1  | 2.46                     | 0.54              |
| 1:D:553:MLY:HG3  | 4:W:44:MET:O     | 2.07                     | 0.54              |
| 1:A:638:GLY:HA2  | 4:8:345:ILE:H    | 1.72                     | 0.54              |
| 1:M:797:PHE:CZ   | 3:O:146:ILE:HA   | 2.41                     | 0.54              |
| 1:M:733:PRO:CB   | 1:M:737:PHE:HE1  | 2.19                     | 0.54              |
| 1:M:806:MET:HA   | 1:M:809:ARG:CD   | 2.37                     | 0.54              |
| 1:J:561:LYS:HE2  | 4:Y:48:GLY:HA3   | 1.88                     | 0.54              |
| 1:G:834:LEU:HD21 | 2:H:34:ILE:HG12  | 1.87                     | 0.54              |
| 1:P:832:MET:SD   | 2:Q:84:PHE:HE2   | 2.30                     | 0.54              |
| 4:W:286:ASP:OD2  | 4:Y:203:THR:CG2  | 2.47                     | 0.54              |
| 1:D:290:GLN:NE2  | 1:D:334:THR:OG1  | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:22:LYS:O     | 1:D:26:GLU:HG3   | 2.07                     | 0.54              |
| 1:P:305:ILE:HG22 | 1:P:312:TYR:CE2  | 2.43                     | 0.54              |
| 1:P:305:ILE:HG22 | 1:P:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CE2  | 2.43                     | 0.54              |
| 1:G:126:VAL:HG13 | 1:G:675:ILE:HG22 | 1.89                     | 0.54              |
| 1:G:82:PRO:HD2   | 1:G:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:G:32:PHE:CG    | 1:G:83:PRO:HD3   | 2.41                     | 0.54              |
| 1:A:508:ILE:HD13 | 1:A:759:ALA:HB3  | 1.75                     | 0.54              |
| 1:A:505:MLY:HH21 | 1:A:762:HIS:O    | 2.03                     | 0.54              |
| 1:G:406:VAL:HG12 | 1:G:407:GLY:H    | 1.71                     | 0.54              |
| 1:G:817:GLN:HG3  | 2:H:128:PHE:CE1  | 2.41                     | 0.54              |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:CG   | 2.20                     | 0.54              |
| 1:J:537:GLU:HB3  | 1:J:648:THR:CB   | 2.36                     | 0.54              |
| 1:D:638:GLY:HA2  | 4:9:345:ILE:H    | 1.72                     | 0.54              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:HG3  | 1.71                     | 0.54              |
| 1:A:579:PHE:HE1  | 1:A:581:LEU:HD13 | 1.72                     | 0.54              |
| 1:M:785:GLU:O    | 1:M:789:ALA:CB   | 2.53                     | 0.54              |
| 1:D:82:PRO:HD2   | 1:D:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:M:84:MLY:HB3   | 1:M:723:ARG:HE   | 1.61                     | 0.54              |
| 1:P:759:ALA:O    | 1:P:766:PHE:N    | 2.32                     | 0.54              |
| 1:J:634:GLY:N    | 4:W:25:ASP:O     | 2.31                     | 0.54              |
| 1:P:84:MLY:CH1   | 1:P:724:TYR:OH   | 2.55                     | 0.54              |
| 1:P:727:LEU:CG   | 1:P:779:ARG:HH21 | 2.09                     | 0.54              |
| 1:J:546:THR:HB   | 1:J:549:SER:H    | 1.71                     | 0.54              |
| 1:M:78:PHE:HB3   | 1:M:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:P:345:ALA:O    | 1:P:349:THR:N    | 2.40                     | 0.54              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CE2  | 2.43                     | 0.54              |
| 1:P:126:VAL:HG13 | 1:P:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:A:82:PRO:HD2   | 1:A:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:D:10:PHE:O     | 1:D:12:GLU:N     | 2.41                     | 0.54              |
| 1:M:629:GLU:CB   | 1:M:643:GLY:C    | 2.76                     | 0.54              |
| 1:G:546:THR:HG21 | 1:G:548:THR:HB   | 1.88                     | 0.54              |
| 1:J:290:GLN:NE2  | 1:J:334:THR:OG1  | 2.40                     | 0.54              |
| 1:D:345:ALA:O    | 1:D:349:THR:N    | 2.40                     | 0.54              |
| 1:G:345:ALA:O    | 1:G:349:THR:N    | 2.40                     | 0.54              |
| 1:M:38:VAL:CB    | 1:M:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:G:38:VAL:CB    | 1:G:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:J:126:VAL:HG13 | 1:J:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:P:10:PHE:O     | 1:P:12:GLU:N     | 2.40                     | 0.54              |
| 1:P:723:ARG:CG   | 1:P:723:ARG:HH11 | 2.20                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:819:ASN:OD1  | 2:N:90:GLY:O     | 2.24                     | 0.54              |
| 2:K:146:GLY:O    | 2:K:147:ASN:ND2  | 2.41                     | 0.54              |
| 1:M:538:GLU:CG   | 4:Z:351:THR:C    | 2.73                     | 0.54              |
| 1:J:635:GLY:HA3  | 4:W:334:GLU:CG   | 2.30                     | 0.54              |
| 1:J:710:GLY:O    | 1:J:772:LEU:CD2  | 2.55                     | 0.54              |
| 1:G:765:VAL:HG12 | 1:G:766:PHE:N    | 2.22                     | 0.54              |
| 1:J:839:MLY:HH21 | 2:K:158:THR:HG22 | 1.89                     | 0.54              |
| 1:D:640:LYS:C    | 4:9:23:GLY:CA    | 2.64                     | 0.54              |
| 1:A:642:LYS:HG2  | 4:8:22:ALA:C     | 2.27                     | 0.54              |
| 1:P:215:GLN:CA   | 1:P:340:ILE:CG2  | 2.62                     | 0.54              |
| 1:M:34:ALA:HB3   | 1:M:777:GLU:HG3  | 1.87                     | 0.54              |
| 1:J:305:ILE:HG22 | 1:J:312:TYR:CZ   | 2.42                     | 0.54              |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:CE2  | 2.43                     | 0.54              |
| 1:D:126:VAL:HG13 | 1:D:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:A:126:VAL:HG13 | 1:A:675:ILE:HG22 | 1.90                     | 0.54              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:HG2  | 1.72                     | 0.54              |
| 1:P:604:ASN:OD1  | 1:P:607:VAL:HG23 | 2.06                     | 0.54              |
| 1:G:640:LYS:C    | 4:V:23:GLY:CA    | 2.64                     | 0.54              |
| 1:G:629:GLU:CB   | 1:G:643:GLY:C    | 2.75                     | 0.54              |
| 1:P:642:LYS:HG2  | 4:0:22:ALA:C     | 2.27                     | 0.54              |
| 3:R:35:ARG:HA    | 3:R:39:GLN:O     | 2.07                     | 0.54              |
| 1:M:721:LYS:C    | 1:M:736:GLN:OE1  | 2.46                     | 0.54              |
| 1:M:733:PRO:O    | 1:M:737:PHE:CE1  | 2.53                     | 0.54              |
| 1:G:649:VAL:HA   | 1:G:649:VAL:HG23 | 1.83                     | 0.54              |
| 1:D:630:ALA:HA   | 4:9:25:ASP:OD2   | 2.07                     | 0.54              |
| 4:3:324:THR:H    | 4:5:244:ASP:HA   | 1.73                     | 0.54              |
| 1:D:571:ALA:O    | 1:D:572:LYS:CB   | 2.56                     | 0.54              |
| 1:M:769:ALA:C    | 1:M:770:GLY:CA   | 2.76                     | 0.54              |
| 1:G:576:GLU:CG   | 1:G:577:ALA:N    | 2.43                     | 0.54              |
| 1:P:78:PHE:HB3   | 1:P:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:A:78:PHE:HB3   | 1:A:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:A:418:THR:CB   | 1:A:421:GLU:HG3  | 2.37                     | 0.54              |
| 1:P:493:HIS:ND1  | 1:P:514:ASP:OD2  | 2.41                     | 0.54              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:CD   | 2.37                     | 0.54              |
| 1:J:791:GLN:O    | 1:J:794:CYS:HB2  | 2.08                     | 0.54              |
| 1:A:97:LEU:HD21  | 1:A:712:PRO:C    | 2.28                     | 0.54              |
| 1:D:765:VAL:HG12 | 1:D:766:PHE:N    | 2.22                     | 0.54              |
| 1:G:529:PRO:CB   | 4:V:354:GLN:HA   | 2.37                     | 0.54              |
| 1:P:818:TYR:CD1  | 2:Q:127:ARG:NH1  | 2.76                     | 0.54              |
| 1:G:817:GLN:CB   | 2:H:127:ARG:HD3  | 2.21                     | 0.54              |
| 2:H:117:LEU:CG   | 2:H:147:ASN:OD1  | 2.53                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:820:VAL:CG1  | 2:K:136:MET:CE   | 2.85                     | 0.54              |
| 1:P:538:GLU:CG   | 4:O:351:THR:C    | 2.73                     | 0.54              |
| 1:M:579:PHE:HE1  | 1:M:581:LEU:HD13 | 1.72                     | 0.54              |
| 1:J:629:GLU:CB   | 1:J:643:GLY:C    | 2.76                     | 0.54              |
| 1:D:218:LEU:CD2  | 1:D:222:ILE:CG1  | 2.86                     | 0.54              |
| 1:D:819:ASN:CB   | 2:E:90:GLY:O     | 2.55                     | 0.54              |
| 1:A:530:MET:CB   | 4:8:354:GLN:HG3  | 2.36                     | 0.54              |
| 1:G:148:ARG:NE   | 1:G:764:MLY:HH21 | 2.23                     | 0.54              |
| 1:G:97:LEU:CD2   | 1:G:712:PRO:CA   | 2.83                     | 0.54              |
| 4:X:291:LYS:CB   | 4:Z:244:ASP:CA   | 2.86                     | 0.54              |
| 1:J:78:PHE:HB3   | 1:J:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:D:78:PHE:HB3   | 1:D:98:HIS:NE2   | 2.22                     | 0.54              |
| 1:M:493:HIS:ND1  | 1:M:514:ASP:OD2  | 2.41                     | 0.54              |
| 1:J:493:HIS:ND1  | 1:J:514:ASP:OD2  | 2.41                     | 0.54              |
| 1:D:305:ILE:HG22 | 1:D:312:TYR:CZ   | 2.43                     | 0.54              |
| 1:D:38:VAL:CB    | 1:D:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:J:22:LYS:O     | 1:J:26:GLU:HG3   | 2.07                     | 0.54              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:CD   | 2.37                     | 0.54              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:CE2  | 2.42                     | 0.54              |
| 1:P:292:MET:HE1  | 1:P:309:PRO:CD   | 2.37                     | 0.54              |
| 4:V:365:ALA:HB3  | 4:V:369:ILE:HB   | 1.88                     | 0.54              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:HG2  | 1.72                     | 0.54              |
| 1:G:470:PHE:O    | 1:G:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:A:470:PHE:O    | 1:A:473:ASN:ND2  | 2.40                     | 0.54              |
| 3:L:35:ARG:HA    | 3:L:39:GLN:O     | 2.07                     | 0.54              |
| 1:D:723:ARG:HH11 | 1:D:723:ARG:CG   | 2.20                     | 0.54              |
| 1:A:508:ILE:HD11 | 1:A:759:ALA:HB1  | 0.54                     | 0.54              |
| 1:P:629:GLU:CB   | 1:P:643:GLY:C    | 2.76                     | 0.54              |
| 1:G:220:ASP:O    | 1:G:224:SER:N    | 2.27                     | 0.54              |
| 1:J:642:LYS:HG2  | 4:W:22:ALA:C     | 2.27                     | 0.54              |
| 1:D:635:GLY:HA3  | 4:9:334:GLU:CG   | 2.30                     | 0.54              |
| 4:O:202:THR:CB   | 4:Y:287:ILE:N    | 2.69                     | 0.54              |
| 1:J:836:PHE:CE2  | 2:K:160:GLY:CA   | 2.90                     | 0.54              |
| 1:P:831:TRP:HE1  | 2:Q:67:MET:CG    | 2.20                     | 0.54              |
| 4:3:287:ILE:HB   | 4:5:203:THR:CG2  | 2.35                     | 0.54              |
| 3:L:46:ILE:O     | 3:L:50:LEU:CG    | 2.47                     | 0.54              |
| 1:G:571:ALA:O    | 1:G:572:LYS:CB   | 2.56                     | 0.54              |
| 1:G:493:HIS:ND1  | 1:G:514:ASP:OD2  | 2.41                     | 0.54              |
| 1:M:22:LYS:O     | 1:M:26:GLU:HG3   | 2.07                     | 0.54              |
| 1:P:38:VAL:CB    | 1:P:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:J:10:PHE:O     | 1:J:12:GLU:N     | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:470:PHE:O    | 1:M:473:ASN:ND2  | 2.40                     | 0.54              |
| 1:J:791:GLN:HE22 | 3:L:115:GLY:CA   | 2.20                     | 0.54              |
| 1:D:791:GLN:O    | 1:D:794:CYS:HB2  | 2.08                     | 0.54              |
| 1:G:754:ASP:C    | 1:G:776:GLU:OE1  | 2.46                     | 0.54              |
| 1:J:765:VAL:HG12 | 1:J:766:PHE:N    | 2.22                     | 0.54              |
| 1:J:638:GLY:HA2  | 4:W:345:ILE:H    | 1.72                     | 0.54              |
| 2:N:156:VAL:HA   | 2:N:159:HIS:O    | 2.07                     | 0.54              |
| 1:A:629:GLU:CB   | 1:A:643:GLY:C    | 2.75                     | 0.54              |
| 1:P:805:ALA:O    | 1:P:809:ARG:HB2  | 2.07                     | 0.54              |
| 1:J:757:GLN:HA   | 1:J:776:GLU:CB   | 2.37                     | 0.54              |
| 1:A:571:ALA:O    | 1:A:572:LYS:CB   | 2.56                     | 0.54              |
| 1:A:38:VAL:CB    | 1:A:52:ILE:HD11  | 2.38                     | 0.54              |
| 1:M:292:MET:HE1  | 1:M:309:PRO:CD   | 2.37                     | 0.54              |
| 1:A:305:ILE:HG22 | 1:A:312:TYR:CZ   | 2.43                     | 0.54              |
| 3:L:123:VAL:O    | 3:L:127:MET:HG2  | 2.07                     | 0.54              |
| 1:G:404:PRO:CG   | 1:G:417:GLU:HG3  | 2.38                     | 0.54              |
| 1:G:10:PHE:O     | 1:G:12:GLU:N     | 2.41                     | 0.54              |
| 1:J:109:ARG:O    | 1:J:114:MET:N    | 2.37                     | 0.54              |
| 1:G:757:GLN:OE1  | 1:G:772:LEU:CB   | 2.55                     | 0.54              |
| 2:E:146:GLY:O    | 2:E:147:ASN:ND2  | 2.41                     | 0.54              |
| 2:H:146:GLY:O    | 2:H:147:ASN:ND2  | 2.41                     | 0.54              |
| 1:M:551:MLY:N    | 4:1:46:GLY:O     | 2.41                     | 0.54              |
| 1:M:638:GLY:HA2  | 4:Z:345:ILE:H    | 1.72                     | 0.54              |
| 1:J:640:LYS:C    | 4:W:23:GLY:CA    | 2.64                     | 0.54              |
| 1:A:410:ASN:CG   | 4:8:334:GLU:C    | 2.65                     | 0.54              |
| 1:A:538:GLU:HG3  | 4:8:352:PHE:CA   | 2.38                     | 0.54              |
| 1:P:839:MLY:HH13 | 2:Q:159:HIS:CD2  | 2.43                     | 0.54              |
| 1:D:98:HIS:HB3   | 1:D:100:PRO:CD   | 2.25                     | 0.54              |
| 4:8:365:ALA:HB3  | 4:8:369:ILE:HB   | 1.88                     | 0.54              |
| 1:M:135:TYR:HD2  | 1:M:191:ARG:HD3  | 1.73                     | 0.54              |
| 1:M:82:PRO:HD2   | 1:M:85:TYR:HD2   | 1.72                     | 0.54              |
| 1:D:721:LYS:C    | 1:D:736:GLN:OE1  | 2.46                     | 0.53              |
| 1:G:791:GLN:NE2  | 3:I:115:GLY:C    | 2.60                     | 0.53              |
| 1:G:794:CYS:O    | 1:G:798:LEU:N    | 2.37                     | 0.53              |
| 2:N:114:LYS:O    | 2:N:147:ASN:ND2  | 2.42                     | 0.53              |
| 2:N:146:GLY:O    | 2:N:147:ASN:ND2  | 2.41                     | 0.53              |
| 1:J:817:GLN:CD   | 2:K:127:ARG:CD   | 2.65                     | 0.53              |
| 1:P:643:GLY:N    | 4:0:23:GLY:C     | 2.55                     | 0.53              |
| 1:P:638:GLY:HA2  | 4:0:345:ILE:H    | 1.72                     | 0.53              |
| 1:P:538:GLU:HG3  | 4:0:352:PHE:CA   | 2.38                     | 0.53              |
| 1:D:579:PHE:HE1  | 1:D:581:LEU:HD13 | 1.72                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:725:ARG:HG3  | 1:M:733:PRO:CA   | 2.36                     | 0.53              |
| 1:G:503:TYR:CZ   | 1:G:711:PHE:HD2  | 2.11                     | 0.53              |
| 1:A:649:VAL:CG1  | 1:A:649:VAL:HA   | 2.35                     | 0.53              |
| 1:D:649:VAL:HA   | 1:D:649:VAL:HG23 | 1.82                     | 0.53              |
| 1:J:630:ALA:HA   | 4:W:25:ASP:OD2   | 2.07                     | 0.53              |
| 3:I:92:ARG:HA    | 3:I:139:TYR:OH   | 2.08                     | 0.53              |
| 1:A:493:HIS:ND1  | 1:A:514:ASP:OD2  | 2.41                     | 0.53              |
| 1:P:154:HIS:CE1  | 1:P:156:PHE:HD2  | 2.26                     | 0.53              |
| 1:J:38:VAL:CB    | 1:J:52:ILE:HD11  | 2.38                     | 0.53              |
| 1:M:126:VAL:HG13 | 1:M:675:ILE:HG22 | 1.90                     | 0.53              |
| 1:P:135:TYR:HD2  | 1:P:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:HG2  | 1.73                     | 0.53              |
| 4:4:185:LEU:HD23 | 4:4:306:TYR:OH   | 2.08                     | 0.53              |
| 1:P:819:ASN:OD1  | 2:Q:90:GLY:O     | 2.25                     | 0.53              |
| 1:P:721:LYS:C    | 1:P:736:GLN:OE1  | 2.46                     | 0.53              |
| 1:A:813:ILE:CG2  | 2:B:127:ARG:CG   | 2.85                     | 0.53              |
| 2:B:146:GLY:O    | 2:B:147:ASN:ND2  | 2.41                     | 0.53              |
| 1:P:410:ASN:CG   | 4:0:334:GLU:C    | 2.65                     | 0.53              |
| 1:J:218:LEU:CD2  | 1:J:222:ILE:CG1  | 2.86                     | 0.53              |
| 1:J:538:GLU:HG3  | 4:W:352:PHE:CA   | 2.38                     | 0.53              |
| 1:A:752:ASP:CB   | 1:A:782:MLY:HD3  | 2.38                     | 0.53              |
| 4:0:202:THR:HG23 | 4:Y:287:ILE:H    | 1.72                     | 0.53              |
| 1:A:553:MLY:O    | 4:V:48:GLY:CA    | 2.56                     | 0.53              |
| 1:M:791:GLN:OE1  | 3:O:116:GLU:HG3  | 2.08                     | 0.53              |
| 1:P:502:GLU:OE2  | 1:P:760:PHE:O    | 2.25                     | 0.53              |
| 1:D:629:GLU:CB   | 1:D:643:GLY:C    | 2.75                     | 0.53              |
| 1:M:571:ALA:O    | 1:M:572:LYS:CB   | 2.56                     | 0.53              |
| 1:J:612:GLN:HE22 | 1:J:627:GLY:HA2  | 1.66                     | 0.53              |
| 3:F:92:ARG:HA    | 3:F:139:TYR:OH   | 2.08                     | 0.53              |
| 3:C:92:ARG:HA    | 3:C:139:TYR:OH   | 2.09                     | 0.53              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:P:32:PHE:CD1   | 1:P:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:A:584:TYR:CD1  | 1:A:585:ALA:N    | 2.77                     | 0.53              |
| 1:P:584:TYR:CD1  | 1:P:585:ALA:N    | 2.77                     | 0.53              |
| 1:G:754:ASP:O    | 1:G:776:GLU:OE1  | 2.25                     | 0.53              |
| 1:G:791:GLN:O    | 1:G:794:CYS:HB2  | 2.08                     | 0.53              |
| 1:G:795:ARG:CB   | 3:I:35:ARG:CZ    | 2.86                     | 0.53              |
| 2:Q:146:GLY:O    | 2:Q:147:ASN:ND2  | 2.41                     | 0.53              |
| 1:G:734:GLU:OE2  | 3:I:109:HIS:CE1  | 2.61                     | 0.53              |
| 1:D:768:MLY:O    | 1:D:771:LEU:CG   | 2.55                     | 0.53              |
| 1:G:838:ILE:HG13 | 2:H:54:MET:CE    | 2.38                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:506:GLU:HG2  | 1:P:759:ALA:CA   | 2.38                     | 0.53              |
| 1:M:599:ASN:CG   | 1:M:649:VAL:H    | 2.12                     | 0.53              |
| 4:V:324:THR:HG22 | 4:X:247:VAL:HG13 | 1.91                     | 0.53              |
| 1:P:571:ALA:O    | 1:P:572:LYS:CB   | 2.56                     | 0.53              |
| 1:P:277:PHE:CG   | 1:P:278:GLN:N    | 2.76                     | 0.53              |
| 1:M:277:PHE:CG   | 1:M:278:GLN:N    | 2.76                     | 0.53              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:HD3  | 1.73                     | 0.53              |
| 1:M:32:PHE:CD1   | 1:M:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:A:404:PRO:CG   | 1:A:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:M:10:PHE:O     | 1:M:12:GLU:N     | 2.40                     | 0.53              |
| 1:M:404:PRO:CG   | 1:M:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:G:795:ARG:HG2  | 3:I:118:MET:HE2  | 1.76                     | 0.53              |
| 1:A:149:GLN:HG2  | 1:A:719:ASP:N    | 2.15                     | 0.53              |
| 1:A:218:LEU:N    | 1:A:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:J:733:PRO:O    | 1:J:737:PHE:CE1  | 2.53                     | 0.53              |
| 1:G:815:CYS:SG   | 2:H:92:ASP:OD1   | 2.66                     | 0.53              |
| 1:P:791:GLN:O    | 1:P:794:CYS:HB2  | 2.08                     | 0.53              |
| 1:P:795:ARG:HH22 | 3:R:116:GLU:HG2  | 1.62                     | 0.53              |
| 1:D:546:THR:HB   | 1:D:549:SER:H    | 1.71                     | 0.53              |
| 1:D:553:MLY:O    | 4:W:48:GLY:CA    | 2.56                     | 0.53              |
| 1:D:819:ASN:CA   | 2:E:90:GLY:O     | 2.56                     | 0.53              |
| 1:P:548:THR:CB   | 4:2:49:GLN:N     | 2.64                     | 0.53              |
| 1:P:552:ASN:HD22 | 4:2:49:GLN:CD    | 2.02                     | 0.53              |
| 1:M:791:GLN:O    | 1:M:794:CYS:HB2  | 2.08                     | 0.53              |
| 1:G:723:ARG:CG   | 1:G:723:ARG:HH11 | 2.20                     | 0.53              |
| 4:X:291:LYS:HB3  | 4:Z:244:ASP:HB3  | 0.64                     | 0.53              |
| 1:A:295:MLY:HE2  | 1:A:332:MET:HE1  | 1.91                     | 0.53              |
| 1:J:571:ALA:O    | 1:J:572:LYS:CB   | 2.56                     | 0.53              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:HB2  | 1.91                     | 0.53              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:HD3  | 1.74                     | 0.53              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:CD1  | 1.04                     | 0.53              |
| 1:G:754:ASP:CG   | 1:G:779:ARG:CB   | 2.72                     | 0.53              |
| 1:G:795:ARG:NE   | 3:I:116:GLU:CD   | 2.62                     | 0.53              |
| 1:G:538:GLU:HG3  | 4:V:352:PHE:CA   | 2.38                     | 0.53              |
| 1:G:556:ASP:OD2  | 4:X:44:MET:HG3   | 2.08                     | 0.53              |
| 1:P:640:LYS:C    | 4:0:23:GLY:CA    | 2.64                     | 0.53              |
| 1:A:721:LYS:C    | 1:A:736:GLN:OE1  | 2.46                     | 0.53              |
| 1:J:149:GLN:HG2  | 1:J:716:LEU:HD11 | 1.89                     | 0.53              |
| 1:J:530:MET:HE3  | 4:W:355:MET:SD   | 2.48                     | 0.53              |
| 1:D:529:PRO:HB2  | 4:9:354:GLN:HA   | 1.91                     | 0.53              |
| 1:G:721:LYS:C    | 1:G:736:GLN:OE1  | 2.46                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:552:ASN:HB3  | 4:2:41:GLN:NE2   | 2.23                     | 0.53              |
| 1:M:786:ILE:C    | 1:M:787:ILE:N    | 2.62                     | 0.53              |
| 1:P:220:ASP:O    | 1:P:224:SER:N    | 2.27                     | 0.53              |
| 1:M:732:ILE:CG2  | 1:M:747:LEU:HD11 | 1.26                     | 0.53              |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:CD1  | 1.05                     | 0.53              |
| 1:M:765:VAL:HG12 | 1:M:766:PHE:N    | 2.22                     | 0.53              |
| 1:M:643:GLY:N    | 4:Z:24:ASP:CA    | 2.46                     | 0.53              |
| 1:P:599:ASN:CG   | 1:P:649:VAL:H    | 2.12                     | 0.53              |
| 1:J:295:MLY:CG   | 1:J:332:MET:HE1  | 2.39                     | 0.53              |
| 1:P:739:ASP:CB   | 1:P:742:LYS:CB   | 2.81                     | 0.53              |
| 1:D:661:MET:O    | 1:D:665:ARG:HG3  | 2.09                     | 0.53              |
| 1:M:661:MET:O    | 1:M:665:ARG:HG3  | 2.09                     | 0.53              |
| 4:W:288:ASP:H    | 4:Y:204:ALA:H    | 1.56                     | 0.53              |
| 4:7:185:LEU:HD23 | 4:7:306:TYR:OH   | 2.09                     | 0.53              |
| 1:D:584:TYR:CD1  | 1:D:585:ALA:N    | 2.77                     | 0.53              |
| 1:P:404:PRO:CG   | 1:P:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:J:404:PRO:CG   | 1:J:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:J:795:ARG:HE   | 3:L:116:GLU:HB3  | 1.73                     | 0.53              |
| 1:D:723:ARG:NH2  | 1:D:779:ARG:HH21 | 2.06                     | 0.53              |
| 1:G:796:GLY:HA2  | 3:I:35:ARG:CZ    | 2.36                     | 0.53              |
| 2:Q:114:LYS:O    | 2:Q:147:ASN:ND2  | 2.41                     | 0.53              |
| 4:X:324:THR:CB   | 4:Z:247:VAL:N    | 2.66                     | 0.53              |
| 1:A:217:THR:C    | 1:A:221:GLN:NE2  | 2.62                     | 0.53              |
| 1:J:218:LEU:N    | 1:J:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:A:529:PRO:HB2  | 4:8:354:GLN:HA   | 1.91                     | 0.53              |
| 1:A:836:PHE:CE1  | 2:B:159:HIS:HA   | 2.43                     | 0.53              |
| 1:D:642:LYS:HG2  | 4:9:22:ALA:C     | 2.27                     | 0.53              |
| 1:J:295:MLY:HE2  | 1:J:332:MET:HE1  | 1.91                     | 0.53              |
| 1:P:769:ALA:CA   | 1:P:770:GLY:N    | 2.71                     | 0.53              |
| 1:G:831:TRP:NE1  | 2:H:67:MET:CG    | 2.72                     | 0.53              |
| 3:I:46:ILE:O     | 3:I:50:LEU:CG    | 2.47                     | 0.53              |
| 1:A:42:HIS:HB3   | 1:A:45:GLN:O     | 2.09                     | 0.53              |
| 1:G:661:MET:O    | 1:G:665:ARG:HG3  | 2.09                     | 0.53              |
| 1:D:277:PHE:CG   | 1:D:278:GLN:N    | 2.76                     | 0.53              |
| 1:M:584:TYR:CD1  | 1:M:585:ALA:N    | 2.77                     | 0.53              |
| 4:0:246:GLN:HG2  | 4:Y:325:MET:CE   | 2.38                     | 0.53              |
| 4:8:185:LEU:HD23 | 4:8:306:TYR:OH   | 2.08                     | 0.53              |
| 4:2:185:LEU:HD23 | 4:2:306:TYR:OH   | 2.09                     | 0.53              |
| 1:D:404:PRO:CG   | 1:D:417:GLU:HG3  | 2.38                     | 0.53              |
| 1:D:783:LEU:O    | 1:D:787:ILE:N    | 2.28                     | 0.53              |
| 1:G:820:VAL:HG11 | 2:H:136:MET:HE1  | 1.86                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:32:PHE:CD1   | 1:J:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:M:529:PRO:HB2  | 4:Z:354:GLN:HA   | 1.91                     | 0.53              |
| 1:A:794:CYS:O    | 1:A:798:LEU:N    | 2.37                     | 0.53              |
| 1:P:218:LEU:N    | 1:P:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:P:148:ARG:HH21 | 1:P:764:MLY:HH21 | 1.72                     | 0.53              |
| 1:P:649:VAL:CG1  | 1:P:649:VAL:HA   | 2.35                     | 0.53              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:H    | 2.12                     | 0.53              |
| 1:P:630:ALA:HA   | 4:0:25:ASP:OD2   | 2.07                     | 0.53              |
| 1:J:830:PRO:HB3  | 2:K:67:MET:HE1   | 1.91                     | 0.53              |
| 1:D:42:HIS:HB3   | 1:D:45:GLN:O     | 2.09                     | 0.53              |
| 1:M:42:HIS:HB3   | 1:M:45:GLN:O     | 2.09                     | 0.53              |
| 1:G:95:THR:HA    | 1:G:713:SER:CB   | 2.39                     | 0.53              |
| 1:G:277:PHE:CG   | 1:G:278:GLN:N    | 2.76                     | 0.53              |
| 1:D:135:TYR:CD2  | 1:D:191:ARG:HG2  | 2.44                     | 0.53              |
| 1:G:32:PHE:CD1   | 1:G:83:PRO:HD3   | 2.44                     | 0.53              |
| 4:9:185:LEU:HD23 | 4:9:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:121:LEU:HG   | 1:A:764:MLY:HH21 | 1.91                     | 0.53              |
| 1:A:505:MLY:CD   | 1:A:762:HIS:CB   | 2.70                     | 0.53              |
| 1:D:507:GLY:O    | 1:D:761:GLY:CA   | 2.57                     | 0.53              |
| 1:G:636:LYS:HB2  | 4:V:334:GLU:OE1  | 2.09                     | 0.53              |
| 1:G:642:LYS:HG2  | 4:V:22:ALA:C     | 2.27                     | 0.53              |
| 2:E:129:THR:O    | 2:E:133:ILE:HG13 | 2.09                     | 0.53              |
| 1:D:538:GLU:CG   | 4:9:351:THR:C    | 2.74                     | 0.53              |
| 1:A:539:GLU:OE2  | 4:V:45:VAL:C     | 2.47                     | 0.53              |
| 4:0:287:ILE:CG2  | 4:2:203:THR:HG21 | 2.32                     | 0.53              |
| 1:P:765:VAL:HG12 | 1:P:766:PHE:N    | 2.22                     | 0.53              |
| 3:L:52:ASN:HB2   | 3:L:53:PRO:CD    | 2.28                     | 0.53              |
| 1:A:753:VAL:HG12 | 1:A:775:LEU:CD2  | 2.39                     | 0.53              |
| 1:J:661:MET:O    | 1:J:665:ARG:HG3  | 2.09                     | 0.53              |
| 1:D:493:HIS:ND1  | 1:D:514:ASP:OD2  | 2.41                     | 0.53              |
| 1:G:292:MET:CE   | 1:G:309:PRO:HA   | 2.39                     | 0.53              |
| 4:Y:185:LEU:HD23 | 4:Y:306:TYR:OH   | 2.09                     | 0.53              |
| 4:0:185:LEU:HD23 | 4:0:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:505:MLY:HG3  | 1:A:741:LYS:HZ3  | 1.58                     | 0.53              |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CG   | 2.44                     | 0.53              |
| 1:G:642:LYS:CG   | 4:V:22:ALA:HA    | 2.37                     | 0.53              |
| 2:K:114:LYS:O    | 2:K:147:ASN:ND2  | 2.41                     | 0.53              |
| 2:K:129:THR:O    | 2:K:133:ILE:HG13 | 2.09                     | 0.53              |
| 1:P:529:PRO:HB2  | 4:0:354:GLN:HA   | 1.91                     | 0.53              |
| 1:P:795:ARG:HD2  | 3:R:35:ARG:HH12  | 1.73                     | 0.53              |
| 1:A:831:TRP:CZ2  | 2:B:50:THR:HB    | 2.34                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:831:TRP:CE2  | 2:B:51:PHE:CZ    | 2.96                     | 0.53              |
| 4:0:205:GLU:HG3  | 4:Y:287:ILE:HD13 | 1.88                     | 0.53              |
| 1:M:732:ILE:HG21 | 1:M:747:LEU:CD1  | 0.63                     | 0.53              |
| 1:M:84:MLY:HB3   | 1:M:723:ARG:CZ   | 2.31                     | 0.53              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:H    | 2.12                     | 0.53              |
| 1:P:806:MET:HA   | 1:P:809:ARG:CD   | 2.39                     | 0.53              |
| 1:G:295:MLY:HE2  | 1:G:332:MET:HE1  | 1.91                     | 0.53              |
| 3:O:52:ASN:HB2   | 3:O:53:PRO:CD    | 2.28                     | 0.53              |
| 1:D:739:ASP:CB   | 1:D:742:LYS:CB   | 2.81                     | 0.53              |
| 4:1:244:ASP:HA   | 4:Z:324:THR:H    | 1.73                     | 0.53              |
| 3:L:92:ARG:HA    | 3:L:139:TYR:OH   | 2.08                     | 0.53              |
| 1:P:418:THR:CB   | 1:P:421:GLU:HG3  | 2.37                     | 0.53              |
| 1:P:481:ASN:N    | 1:P:481:ASN:ND2  | 2.51                     | 0.53              |
| 1:P:156:PHE:HD1  | 1:P:195:TYR:CD1  | 2.27                     | 0.53              |
| 1:A:156:PHE:HD1  | 1:A:195:TYR:CD1  | 2.27                     | 0.53              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:HB2  | 1.91                     | 0.53              |
| 1:A:135:TYR:CD2  | 1:A:191:ARG:HG2  | 2.44                     | 0.53              |
| 1:D:32:PHE:CD1   | 1:D:83:PRO:HD3   | 2.43                     | 0.53              |
| 1:A:32:PHE:CD1   | 1:A:83:PRO:HD3   | 2.44                     | 0.53              |
| 1:M:404:PRO:HG3  | 1:M:417:GLU:HG3  | 1.91                     | 0.53              |
| 1:P:404:PRO:HG3  | 1:P:417:GLU:HG3  | 1.91                     | 0.53              |
| 1:J:404:PRO:HG3  | 1:J:417:GLU:HG3  | 1.91                     | 0.53              |
| 1:J:584:TYR:CD1  | 1:J:585:ALA:N    | 2.77                     | 0.53              |
| 4:3:185:LEU:HD23 | 4:3:306:TYR:OH   | 2.09                     | 0.53              |
| 1:G:218:LEU:N    | 1:G:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:P:796:GLY:CA   | 3:R:35:ARG:CD    | 2.71                     | 0.53              |
| 1:D:218:LEU:N    | 1:D:221:GLN:HG2  | 2.24                     | 0.53              |
| 1:M:800:ARG:HD2  | 3:O:149:VAL:HG22 | 1.91                     | 0.53              |
| 1:G:506:GLU:HG2  | 1:G:759:ALA:HB1  | 1.89                     | 0.53              |
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:HE3  | 1.90                     | 0.53              |
| 1:M:642:LYS:HG2  | 4:Z:22:ALA:C     | 2.27                     | 0.53              |
| 1:M:295:MLY:HE2  | 1:M:332:MET:HE1  | 1.91                     | 0.53              |
| 1:J:98:HIS:HB3   | 1:J:100:PRO:CD   | 2.25                     | 0.53              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:HD3  | 1.73                     | 0.53              |
| 3:C:104:GLY:HA2  | 3:C:137:ILE:HD11 | 1.91                     | 0.53              |
| 4:X:185:LEU:HD23 | 4:X:306:TYR:OH   | 2.09                     | 0.53              |
| 1:A:92:ALA:O     | 1:A:714:ARG:N    | 2.37                     | 0.52              |
| 2:N:129:THR:O    | 2:N:133:ILE:HG13 | 2.09                     | 0.52              |
| 2:Q:114:LYS:HA   | 2:Q:147:ASN:HD22 | 1.74                     | 0.52              |
| 1:J:529:PRO:HB2  | 4:W:354:GLN:HA   | 1.91                     | 0.52              |
| 1:D:538:GLU:HG3  | 4:9:352:PHE:CA   | 2.38                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:599:ASN:CG   | 1:A:649:VAL:H    | 2.12                     | 0.52              |
| 1:D:831:TRP:NE1  | 2:E:67:MET:SD    | 2.80                     | 0.52              |
| 1:J:739:ASP:CB   | 1:J:742:LYS:CB   | 2.81                     | 0.52              |
| 3:F:53:PRO:HB2   | 3:F:55:LYS:HG3   | 1.91                     | 0.52              |
| 1:P:63:MLY:HG3   | 1:P:64:THR:H     | 1.75                     | 0.52              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:HD2  | 2.27                     | 0.52              |
| 1:A:22:LYS:O     | 1:A:26:GLU:N     | 2.29                     | 0.52              |
| 1:D:556:ASP:HB3  | 4:W:43:VAL:HG12  | 1.91                     | 0.52              |
| 1:P:135:TYR:CD2  | 1:P:191:ARG:HG2  | 2.44                     | 0.52              |
| 1:D:404:PRO:HG3  | 1:D:417:GLU:HG3  | 1.91                     | 0.52              |
| 4:5:185:LEU:HD23 | 4:5:306:TYR:OH   | 2.09                     | 0.52              |
| 1:G:584:TYR:CD1  | 1:G:585:ALA:N    | 2.77                     | 0.52              |
| 4:7:180:LEU:HD22 | 4:7:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:Z:185:LEU:HD23 | 4:Z:306:TYR:OH   | 2.09                     | 0.52              |
| 1:A:505:MLY:H    | 1:A:762:HIS:CD2  | 2.25                     | 0.52              |
| 1:A:768:MLY:CA   | 1:A:771:LEU:HB2  | 2.26                     | 0.52              |
| 2:Q:129:THR:O    | 2:Q:133:ILE:HG13 | 2.09                     | 0.52              |
| 2:E:114:LYS:O    | 2:E:147:ASN:ND2  | 2.41                     | 0.52              |
| 3:R:92:ARG:HA    | 3:R:139:TYR:OH   | 2.08                     | 0.52              |
| 2:B:114:LYS:O    | 2:B:147:ASN:ND2  | 2.41                     | 0.52              |
| 1:P:544:LYS:HZ1  | 4:2:45:VAL:HG21  | 1.73                     | 0.52              |
| 1:G:217:THR:C    | 1:G:221:GLN:NE2  | 2.62                     | 0.52              |
| 1:J:642:LYS:CG   | 4:W:22:ALA:CA    | 2.80                     | 0.52              |
| 1:P:797:PHE:CZ   | 3:R:146:ILE:HG23 | 2.44                     | 0.52              |
| 1:A:791:GLN:O    | 1:A:794:CYS:HB2  | 2.08                     | 0.52              |
| 1:A:555:TYR:N    | 4:V:48:GLY:N     | 2.58                     | 0.52              |
| 1:P:197:ALA:O    | 1:P:201:ALA:HB2  | 2.09                     | 0.52              |
| 1:J:197:ALA:O    | 1:J:201:ALA:HB2  | 2.10                     | 0.52              |
| 1:G:599:ASN:CG   | 1:G:649:VAL:H    | 2.12                     | 0.52              |
| 1:M:642:LYS:CG   | 4:Z:22:ALA:HA    | 2.37                     | 0.52              |
| 1:P:727:LEU:CG   | 1:P:779:ARG:HE   | 2.23                     | 0.52              |
| 3:I:53:PRO:HB2   | 3:I:55:LYS:HG3   | 1.91                     | 0.52              |
| 3:R:53:PRO:HB2   | 3:R:55:LYS:HG3   | 1.91                     | 0.52              |
| 3:L:53:PRO:HB2   | 3:L:55:LYS:HG3   | 1.91                     | 0.52              |
| 1:P:661:MET:O    | 1:P:665:ARG:HG3  | 2.09                     | 0.52              |
| 3:O:92:ARG:HA    | 3:O:139:TYR:OH   | 2.08                     | 0.52              |
| 1:G:63:MLY:HG3   | 1:G:64:THR:H     | 1.75                     | 0.52              |
| 1:M:154:HIS:CE1  | 1:M:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:J:135:TYR:CD2  | 1:J:191:ARG:HG2  | 2.44                     | 0.52              |
| 4:V:180:LEU:HD22 | 4:V:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:V:185:LEU:HD23 | 4:V:306:TYR:OH   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:93:MET:O     | 1:A:713:SER:CB   | 2.57                     | 0.52              |
| 1:M:545:ALA:CB   | 4:1:45:VAL:CG1   | 2.85                     | 0.52              |
| 1:M:538:GLU:HG3  | 4:Z:352:PHE:CA   | 2.38                     | 0.52              |
| 1:A:579:PHE:CD2  | 1:A:592:ILE:HD11 | 2.40                     | 0.52              |
| 1:M:649:VAL:HG23 | 1:M:649:VAL:HA   | 1.83                     | 0.52              |
| 1:P:295:MLY:HG3  | 1:P:332:MET:HE2  | 1.90                     | 0.52              |
| 4:3:322:PRO:C    | 4:5:244:ASP:HB2  | 2.30                     | 0.52              |
| 1:J:277:PHE:CG   | 1:J:278:GLN:N    | 2.76                     | 0.52              |
| 1:D:128:PRO:O    | 1:D:129:TYR:HB2  | 2.09                     | 0.52              |
| 1:A:556:ASP:HB3  | 4:V:43:VAL:HG12  | 1.91                     | 0.52              |
| 1:P:251:ARG:HB2  | 1:P:264:ASP:HB2  | 1.91                     | 0.52              |
| 1:G:404:PRO:HG3  | 1:G:417:GLU:HG3  | 1.91                     | 0.52              |
| 4:W:185:LEU:HD23 | 4:W:306:TYR:OH   | 2.09                     | 0.52              |
| 4:1:185:LEU:HD23 | 4:1:306:TYR:OH   | 2.09                     | 0.52              |
| 1:D:494:HIS:O    | 1:D:498:LEU:HB2  | 2.09                     | 0.52              |
| 4:4:180:LEU:HD22 | 4:4:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:795:ARG:CG   | 3:F:118:MET:HE1  | 2.27                     | 0.52              |
| 1:A:149:GLN:CD   | 1:A:718:ALA:CB   | 2.54                     | 0.52              |
| 1:D:506:GLU:O    | 1:D:762:HIS:HB2  | 2.09                     | 0.52              |
| 1:G:530:MET:HG2  | 4:V:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:CD1  | 1.05                     | 0.52              |
| 1:G:818:TYR:CB   | 2:H:90:GLY:HA3   | 2.37                     | 0.52              |
| 2:H:114:LYS:HA   | 2:H:147:ASN:HD22 | 1.75                     | 0.52              |
| 2:H:114:LYS:O    | 2:H:147:ASN:ND2  | 2.41                     | 0.52              |
| 2:K:121:LEU:CA   | 2:K:128:PHE:CG   | 2.89                     | 0.52              |
| 1:P:544:LYS:NZ   | 4:2:45:VAL:HG22  | 2.23                     | 0.52              |
| 1:D:636:LYS:HB2  | 4:9:334:GLU:OE1  | 2.09                     | 0.52              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:HD11 | 1.26                     | 0.52              |
| 1:A:636:LYS:HB2  | 4:8:334:GLU:OE1  | 2.08                     | 0.52              |
| 1:M:839:MLY:HH21 | 2:N:158:THR:CG2  | 2.40                     | 0.52              |
| 1:D:642:LYS:CG   | 4:9:22:ALA:CA    | 2.80                     | 0.52              |
| 1:A:295:MLY:HG3  | 1:A:332:MET:HE2  | 1.90                     | 0.52              |
| 3:C:53:PRO:HB2   | 3:C:55:LYS:HG3   | 1.91                     | 0.52              |
| 1:P:42:HIS:HB3   | 1:P:45:GLN:O     | 2.09                     | 0.52              |
| 1:G:579:PHE:CD2  | 1:G:592:ILE:HD11 | 2.40                     | 0.52              |
| 1:A:277:PHE:CG   | 1:A:278:GLN:N    | 2.76                     | 0.52              |
| 1:J:418:THR:CB   | 1:J:421:GLU:HG3  | 2.37                     | 0.52              |
| 1:J:156:PHE:HD1  | 1:J:195:TYR:CD1  | 2.27                     | 0.52              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:A:109:ARG:HD3  | 1:A:117:THR:HB   | 1.92                     | 0.52              |
| 4:8:180:LEU:HD22 | 4:8:267:ILE:HD11 | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:3:180:LEU:HD22 | 4:3:267:ILE:HD11 | 1.92                     | 0.52              |
| 3:C:110:VAL:HG13 | 3:C:114:LEU:HD12 | 1.91                     | 0.52              |
| 1:P:491:PHE:HD1  | 1:P:671:PHE:CE2  | 2.27                     | 0.52              |
| 3:L:110:VAL:HG13 | 3:L:114:LEU:HD12 | 1.92                     | 0.52              |
| 1:D:732:ILE:H    | 1:D:733:PRO:HD2  | 1.74                     | 0.52              |
| 1:J:817:GLN:OE1  | 2:K:127:ARG:HD2  | 2.06                     | 0.52              |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CE1  | 2.44                     | 0.52              |
| 1:P:636:LYS:HB2  | 4:0:334:GLU:OE1  | 2.09                     | 0.52              |
| 1:J:642:LYS:CA   | 4:W:22:ALA:C     | 2.70                     | 0.52              |
| 4:9:287:ILE:HG22 | 4:W:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:A:661:MET:O    | 1:A:665:ARG:HG3  | 2.09                     | 0.52              |
| 4:V:285:CYS:O    | 4:V:290:ARG:NH1  | 2.43                     | 0.52              |
| 4:1:180:LEU:HD22 | 4:1:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:G:836:PHE:CZ   | 2:H:159:HIS:HA   | 2.44                     | 0.52              |
| 1:J:22:LYS:O     | 1:J:26:GLU:N     | 2.30                     | 0.52              |
| 1:P:292:MET:CE   | 1:P:309:PRO:HA   | 2.39                     | 0.52              |
| 4:0:180:LEU:HD22 | 4:0:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:9:180:LEU:HD22 | 4:9:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:3:285:CYS:O    | 4:3:290:ARG:NH1  | 2.43                     | 0.52              |
| 3:I:104:GLY:HA2  | 3:I:137:ILE:HD11 | 1.92                     | 0.52              |
| 3:L:104:GLY:HA2  | 3:L:137:ILE:HD11 | 1.92                     | 0.52              |
| 4:5:180:LEU:HD22 | 4:5:267:ILE:HD11 | 1.92                     | 0.52              |
| 2:N:114:LYS:N    | 2:N:146:GLY:O    | 2.40                     | 0.52              |
| 2:E:121:LEU:CA   | 2:E:128:PHE:CG   | 2.89                     | 0.52              |
| 1:P:725:ARG:O    | 1:P:729:ALA:HA   | 2.10                     | 0.52              |
| 1:P:733:PRO:O    | 1:P:737:PHE:CE1  | 2.53                     | 0.52              |
| 1:A:218:LEU:CD2  | 1:A:222:ILE:CG1  | 2.85                     | 0.52              |
| 2:H:129:THR:O    | 2:H:133:ILE:HG13 | 2.09                     | 0.52              |
| 4:0:205:GLU:HB2  | 4:Y:287:ILE:HD13 | 1.91                     | 0.52              |
| 1:D:831:TRP:CZ3  | 2:E:34:ILE:HG12  | 2.44                     | 0.52              |
| 1:P:41:VAL:HG13  | 1:P:42:HIS:N     | 2.25                     | 0.52              |
| 1:J:41:VAL:HG13  | 1:J:42:HIS:N     | 2.25                     | 0.52              |
| 4:W:285:CYS:O    | 4:W:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:63:MLY:HG3   | 1:A:64:THR:H     | 1.75                     | 0.52              |
| 1:D:156:PHE:HD1  | 1:D:195:TYR:CD1  | 2.27                     | 0.52              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:M:494:HIS:O    | 1:M:498:LEU:HB2  | 2.09                     | 0.52              |
| 4:X:180:LEU:HD22 | 4:X:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:491:PHE:HD1  | 1:D:671:PHE:CE2  | 2.27                     | 0.52              |
| 4:5:285:CYS:O    | 4:5:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:G:795:ARG:N    | 3:I:118:MET:HE1  | 2.21                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:507:GLY:CA   | 1:D:762:HIS:CE1  | 2.88                     | 0.52              |
| 1:D:506:GLU:CG   | 1:D:764:MLY:CE   | 2.87                     | 0.52              |
| 1:G:529:PRO:HB2  | 4:V:354:GLN:HA   | 1.92                     | 0.52              |
| 2:K:117:LEU:CG   | 2:K:147:ASN:OD1  | 2.52                     | 0.52              |
| 1:M:553:MLY:CG   | 4:1:43:VAL:CB    | 2.85                     | 0.52              |
| 1:M:530:MET:HE3  | 4:Z:354:GLN:CG   | 2.32                     | 0.52              |
| 1:J:530:MET:HG2  | 4:W:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:D:538:GLU:HA   | 4:9:349:LEU:CB   | 2.40                     | 0.52              |
| 1:D:818:TYR:CG   | 2:E:90:GLY:CA    | 2.82                     | 0.52              |
| 1:M:84:MLY:HH13  | 1:M:724:TYR:CE2  | 2.42                     | 0.52              |
| 1:G:830:PRO:CG   | 2:H:67:MET:CE    | 2.80                     | 0.52              |
| 4:7:287:ILE:HG22 | 4:9:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:G:40:VAL:HG13  | 1:G:41:VAL:O     | 2.10                     | 0.52              |
| 1:G:42:HIS:HB3   | 1:G:45:GLN:O     | 2.09                     | 0.52              |
| 1:D:41:VAL:HG13  | 1:D:42:HIS:N     | 2.25                     | 0.52              |
| 1:D:708:ARG:HA   | 1:D:710:GLY:N    | 2.25                     | 0.52              |
| 1:D:418:THR:CB   | 1:D:421:GLU:HG3  | 2.37                     | 0.52              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:HB2  | 1.91                     | 0.52              |
| 1:M:251:ARG:HB2  | 1:M:264:ASP:HB2  | 1.91                     | 0.52              |
| 1:A:404:PRO:HG3  | 1:A:417:GLU:HG3  | 1.91                     | 0.52              |
| 3:R:104:GLY:HA2  | 3:R:137:ILE:HD11 | 1.92                     | 0.52              |
| 4:Y:180:LEU:HD22 | 4:Y:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:Z:285:CYS:O    | 4:Z:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:D:727:LEU:N    | 1:D:782:MLY:CE   | 2.59                     | 0.52              |
| 1:A:494:HIS:O    | 1:A:498:LEU:HB2  | 2.09                     | 0.52              |
| 1:G:534:SER:C    | 4:V:351:THR:CA   | 2.48                     | 0.52              |
| 1:A:212:GLY:O    | 1:A:213:LYS:HB2  | 2.10                     | 0.52              |
| 1:J:642:LYS:HG2  | 4:W:21:PHE:C     | 2.29                     | 0.52              |
| 1:D:836:PHE:HD2  | 2:E:161:GLU:OE1  | 1.92                     | 0.52              |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:HB3  | 1.91                     | 0.52              |
| 1:G:197:ALA:O    | 1:G:201:ALA:HB2  | 2.09                     | 0.52              |
| 1:A:642:LYS:CG   | 4:8:22:ALA:HA    | 2.38                     | 0.52              |
| 4:9:285:CYS:O    | 4:9:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:G:41:VAL:HG13  | 1:G:42:HIS:N     | 2.25                     | 0.52              |
| 1:P:40:VAL:HG13  | 1:P:41:VAL:O     | 2.10                     | 0.52              |
| 1:A:40:VAL:HG13  | 1:A:41:VAL:O     | 2.10                     | 0.52              |
| 1:J:42:HIS:HB3   | 1:J:45:GLN:O     | 2.09                     | 0.52              |
| 1:J:128:PRO:O    | 1:J:129:TYR:HB2  | 2.10                     | 0.52              |
| 1:P:195:TYR:CE2  | 1:P:199:ILE:CD1  | 2.93                     | 0.52              |
| 1:J:154:HIS:CE1  | 1:J:156:PHE:HD2  | 2.26                     | 0.52              |
| 1:G:135:TYR:CD2  | 1:G:191:ARG:HG2  | 2.44                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:491:PHE:HD1  | 1:A:671:PHE:CE2  | 2.27                     | 0.52              |
| 1:G:491:PHE:HD1  | 1:G:671:PHE:CE2  | 2.27                     | 0.52              |
| 4:W:180:LEU:HD22 | 4:W:267:ILE:HD11 | 1.92                     | 0.52              |
| 4:Z:180:LEU:HD22 | 4:Z:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:D:725:ARG:O    | 1:D:729:ALA:HA   | 2.10                     | 0.52              |
| 1:A:97:LEU:HD23  | 1:A:712:PRO:HA   | 1.90                     | 0.52              |
| 1:J:725:ARG:O    | 1:J:729:ALA:HA   | 2.10                     | 0.52              |
| 2:H:114:LYS:N    | 2:H:146:GLY:O    | 2.40                     | 0.52              |
| 2:K:114:LYS:HA   | 2:K:147:ASN:HD22 | 1.74                     | 0.52              |
| 1:M:530:MET:HG2  | 4:Z:354:GLN:HB2  | 0.57                     | 0.52              |
| 1:M:538:GLU:HA   | 4:Z:349:LEU:CB   | 2.40                     | 0.52              |
| 1:M:579:PHE:CD2  | 1:M:592:ILE:HD11 | 2.40                     | 0.52              |
| 1:D:555:TYR:N    | 4:W:48:GLY:N     | 2.58                     | 0.52              |
| 1:M:218:LEU:N    | 1:M:221:GLN:HG2  | 2.24                     | 0.52              |
| 1:A:538:GLU:HA   | 4:8:349:LEU:CB   | 2.39                     | 0.52              |
| 1:M:791:GLN:CD   | 3:O:116:GLU:H    | 2.11                     | 0.52              |
| 1:D:642:LYS:HG2  | 4:9:21:PHE:C     | 2.30                     | 0.52              |
| 4:1:244:ASP:HB2  | 4:Z:322:PRO:C    | 2.30                     | 0.52              |
| 1:P:98:HIS:HB3   | 1:P:100:PRO:CD   | 2.25                     | 0.52              |
| 1:G:128:PRO:O    | 1:G:129:TYR:HB2  | 2.09                     | 0.52              |
| 1:M:63:MLY:HG3   | 1:M:64:THR:H     | 1.74                     | 0.52              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:CD1  | 2.93                     | 0.52              |
| 1:G:156:PHE:HD1  | 1:G:195:TYR:CD1  | 2.27                     | 0.52              |
| 1:A:292:MET:CE   | 1:A:309:PRO:HA   | 2.39                     | 0.52              |
| 1:M:135:TYR:HD2  | 1:M:191:ARG:CD   | 2.23                     | 0.52              |
| 1:G:109:ARG:HD3  | 1:G:117:THR:HB   | 1.92                     | 0.52              |
| 1:J:494:HIS:O    | 1:J:498:LEU:HB2  | 2.09                     | 0.52              |
| 4:2:180:LEU:HD22 | 4:2:267:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:742:LYS:O    | 1:A:745:GLU:HB2  | 2.10                     | 0.52              |
| 2:N:114:LYS:HA   | 2:N:147:ASN:HD22 | 1.74                     | 0.52              |
| 1:P:730:SER:CA   | 3:R:93:VAL:HG22  | 2.39                     | 0.52              |
| 1:M:636:LYS:HB2  | 4:Z:334:GLU:OE1  | 2.09                     | 0.52              |
| 1:J:636:LYS:HB2  | 4:W:334:GLU:OE1  | 2.09                     | 0.52              |
| 1:M:221:GLN:HB2  | 1:M:449:LEU:HD11 | 1.92                     | 0.52              |
| 4:2:285:CYS:O    | 4:2:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:M:725:ARG:O    | 1:M:729:ALA:HA   | 2.10                     | 0.52              |
| 1:M:732:ILE:H    | 1:M:733:PRO:CD   | 2.23                     | 0.52              |
| 1:D:295:MLY:HE2  | 1:D:332:MET:HE1  | 1.91                     | 0.52              |
| 4:7:285:CYS:O    | 4:7:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:P:742:LYS:O    | 1:P:745:GLU:HB2  | 2.10                     | 0.52              |
| 1:G:94:MET:O     | 1:G:713:SER:HA   | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:232:PHE:CE1  | 1:P:287:ILE:HD13 | 2.45                     | 0.52              |
| 1:J:232:PHE:CE1  | 1:J:287:ILE:HD13 | 2.44                     | 0.52              |
| 1:J:63:MLY:HG3   | 1:J:64:THR:H     | 1.74                     | 0.52              |
| 1:D:63:MLY:HG3   | 1:D:64:THR:H     | 1.75                     | 0.52              |
| 1:M:292:MET:CE   | 1:M:309:PRO:HA   | 2.40                     | 0.52              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:HB2  | 1.91                     | 0.52              |
| 1:J:135:TYR:HD2  | 1:J:191:ARG:CD   | 2.23                     | 0.52              |
| 1:M:491:PHE:HD1  | 1:M:671:PHE:CE2  | 2.27                     | 0.52              |
| 3:F:100:GLY:O    | 3:F:138:ASN:HA   | 2.10                     | 0.52              |
| 1:D:109:ARG:HD3  | 1:D:117:THR:HB   | 1.92                     | 0.52              |
| 4:4:285:CYS:O    | 4:4:290:ARG:NH1  | 2.43                     | 0.52              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:HG11 | 1.91                     | 0.51              |
| 2:E:112:ILE:HG23 | 2:E:147:ASN:HB3  | 1.93                     | 0.51              |
| 1:P:732:ILE:CG2  | 1:P:747:LEU:HD11 | 1.26                     | 0.51              |
| 1:P:642:LYS:CA   | 4:0:22:ALA:C     | 2.70                     | 0.51              |
| 1:P:642:LYS:HG2  | 4:0:21:PHE:C     | 2.30                     | 0.51              |
| 1:J:220:ASP:O    | 1:J:224:SER:N    | 2.27                     | 0.51              |
| 1:J:221:GLN:HB2  | 1:J:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:P:798:LEU:CD1  | 3:R:126:LEU:HD22 | 2.30                     | 0.51              |
| 1:P:795:ARG:HE   | 3:R:118:MET:HE2  | 1.74                     | 0.51              |
| 1:A:578:HIS:O    | 1:A:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:D:767:PHE:O    | 1:D:771:LEU:HD13 | 1.98                     | 0.51              |
| 4:X:285:CYS:O    | 4:X:290:ARG:NH1  | 2.43                     | 0.51              |
| 4:8:287:ILE:HG22 | 4:V:204:ALA:HB3  | 1.91                     | 0.51              |
| 1:D:41:VAL:HG21  | 1:D:76:GLN:HG3   | 1.92                     | 0.51              |
| 1:J:40:VAL:HG13  | 1:J:41:VAL:O     | 2.10                     | 0.51              |
| 1:M:135:TYR:CD2  | 1:M:191:ARG:HG2  | 2.44                     | 0.51              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:CD   | 2.23                     | 0.51              |
| 1:P:135:TYR:HD2  | 1:P:191:ARG:CD   | 2.23                     | 0.51              |
| 1:G:634:GLY:N    | 4:V:25:ASP:O     | 2.31                     | 0.51              |
| 1:G:494:HIS:O    | 1:G:498:LEU:HB2  | 2.09                     | 0.51              |
| 1:J:491:PHE:HD1  | 1:J:671:PHE:CE2  | 2.27                     | 0.51              |
| 1:D:732:ILE:H    | 1:D:733:PRO:CD   | 2.23                     | 0.51              |
| 2:N:121:LEU:O    | 2:N:128:PHE:CG   | 2.61                     | 0.51              |
| 1:P:640:LYS:CA   | 1:P:645:SER:OG   | 2.58                     | 0.51              |
| 1:J:83:PRO:C     | 1:J:723:ARG:HH21 | 2.13                     | 0.51              |
| 1:J:538:GLU:HA   | 4:W:349:LEU:CB   | 2.40                     | 0.51              |
| 1:M:212:GLY:O    | 1:M:213:LYS:HB2  | 2.11                     | 0.51              |
| 1:M:218:LEU:CD2  | 1:M:222:ILE:CG1  | 2.86                     | 0.51              |
| 1:A:408:VAL:CG1  | 4:8:332:PRO:HB3  | 2.40                     | 0.51              |
| 1:A:530:MET:HG2  | 4:8:354:GLN:HB2  | 0.57                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:592:ILE:O    | 1:A:592:ILE:HG22 | 2.11                     | 0.51              |
| 1:P:221:GLN:HB2  | 1:P:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:M:640:LYS:CA   | 1:M:645:SER:OG   | 2.58                     | 0.51              |
| 1:A:41:VAL:HG13  | 1:A:42:HIS:N     | 2.25                     | 0.51              |
| 1:M:232:PHE:CE1  | 1:M:287:ILE:HD13 | 2.44                     | 0.51              |
| 1:G:232:PHE:CE1  | 1:G:287:ILE:HD13 | 2.45                     | 0.51              |
| 1:A:232:PHE:CE1  | 1:A:287:ILE:HD13 | 2.45                     | 0.51              |
| 3:F:110:VAL:HG13 | 3:F:114:LEU:HD12 | 1.91                     | 0.51              |
| 1:G:801:VAL:CG2  | 3:I:126:LEU:HD21 | 2.40                     | 0.51              |
| 1:A:757:GLN:O    | 1:A:771:LEU:HD22 | 2.10                     | 0.51              |
| 1:A:221:GLN:HB2  | 1:A:449:LEU:HD11 | 1.93                     | 0.51              |
| 1:J:817:GLN:CG   | 2:K:127:ARG:HB2  | 2.35                     | 0.51              |
| 2:K:112:ILE:C    | 2:K:147:ASN:O    | 2.42                     | 0.51              |
| 1:J:212:GLY:O    | 1:J:213:LYS:HB2  | 2.10                     | 0.51              |
| 1:D:410:ASN:CG   | 4:9:334:GLU:C    | 2.65                     | 0.51              |
| 1:D:217:THR:C    | 1:D:221:GLN:NE2  | 2.62                     | 0.51              |
| 1:D:221:GLN:HB2  | 1:D:449:LEU:HD11 | 1.92                     | 0.51              |
| 1:A:546:THR:CG2  | 1:A:548:THR:HB   | 2.41                     | 0.51              |
| 1:M:84:MLY:CA    | 1:M:723:ARG:CZ   | 2.85                     | 0.51              |
| 1:D:40:VAL:HG13  | 1:D:41:VAL:O     | 2.10                     | 0.51              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:M:156:PHE:HD1  | 1:M:195:TYR:CD1  | 2.27                     | 0.51              |
| 1:J:248:MLY:N    | 1:J:463:ASP:O    | 2.44                     | 0.51              |
| 1:G:559:LEU:C    | 1:G:559:LEU:HD23 | 2.31                     | 0.51              |
| 3:R:110:VAL:HG13 | 3:R:114:LEU:HD12 | 1.92                     | 0.51              |
| 1:P:248:MLY:N    | 1:P:463:ASP:O    | 2.44                     | 0.51              |
| 1:A:501:GLU:HB3  | 1:A:762:HIS:ND1  | 2.19                     | 0.51              |
| 1:G:538:GLU:HA   | 4:V:349:LEU:CB   | 2.40                     | 0.51              |
| 2:E:114:LYS:HA   | 2:E:147:ASN:HD22 | 1.74                     | 0.51              |
| 1:J:821:ARG:NH1  | 2:K:127:ARG:NE   | 2.59                     | 0.51              |
| 1:M:553:MLY:HG2  | 4:I:43:VAL:HB    | 1.93                     | 0.51              |
| 1:P:789:ALA:CB   | 3:R:81:GLN:NE2   | 2.74                     | 0.51              |
| 1:M:839:MLY:HH13 | 2:N:159:HIS:CD2  | 2.46                     | 0.51              |
| 3:O:110:VAL:HG13 | 3:O:114:LEU:HD12 | 1.92                     | 0.51              |
| 1:D:742:LYS:O    | 1:D:745:GLU:HB2  | 2.10                     | 0.51              |
| 1:G:742:LYS:O    | 1:G:745:GLU:HB2  | 2.10                     | 0.51              |
| 1:G:546:THR:CG2  | 1:G:548:THR:HB   | 2.41                     | 0.51              |
| 1:P:128:PRO:O    | 1:P:129:TYR:HB2  | 2.10                     | 0.51              |
| 1:G:481:ASN:ND2  | 1:G:481:ASN:N    | 2.51                     | 0.51              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:M:109:ARG:HD3  | 1:M:117:THR:HB   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:1:285:CYS:O    | 4:1:290:ARG:NH1  | 2.43                     | 0.51              |
| 3:C:100:GLY:O    | 3:C:138:ASN:HA   | 2.11                     | 0.51              |
| 1:D:248:MLY:N    | 1:D:463:ASP:O    | 2.44                     | 0.51              |
| 1:G:411:GLU:H    | 4:V:333:PRO:CG   | 2.24                     | 0.51              |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:CD1  | 1.04                     | 0.51              |
| 1:G:820:VAL:CG1  | 2:H:136:MET:CE   | 2.79                     | 0.51              |
| 2:B:114:LYS:HA   | 2:B:147:ASN:HD22 | 1.75                     | 0.51              |
| 1:D:538:GLU:CD   | 4:9:355:MET:HE3  | 2.29                     | 0.51              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:O    | 2.62                     | 0.51              |
| 4:Y:285:CYS:O    | 4:Y:290:ARG:NH1  | 2.43                     | 0.51              |
| 1:P:212:GLY:O    | 1:P:213:LYS:HB2  | 2.11                     | 0.51              |
| 1:M:804:ARG:C    | 1:M:808:GLU:H    | 2.14                     | 0.51              |
| 1:P:310:TYR:CE2  | 1:P:320:ILE:CD1  | 2.94                     | 0.51              |
| 1:G:418:THR:O    | 1:G:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:D:232:PHE:CE1  | 1:D:287:ILE:HD13 | 2.45                     | 0.51              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:G:13:ALA:C     | 1:G:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:J:13:ALA:C     | 1:J:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:G:675:ILE:CG2  | 1:G:676:ILE:N    | 2.74                     | 0.51              |
| 1:P:494:HIS:O    | 1:P:498:LEU:HB2  | 2.09                     | 0.51              |
| 1:A:759:ALA:O    | 1:A:766:PHE:N    | 2.32                     | 0.51              |
| 1:A:502:GLU:C    | 1:A:761:GLY:HA2  | 2.30                     | 0.51              |
| 1:G:221:GLN:HB2  | 1:G:449:LEU:HD11 | 1.93                     | 0.51              |
| 1:J:93:MET:CE    | 1:J:716:LEU:HD12 | 2.41                     | 0.51              |
| 1:J:640:LYS:CA   | 1:J:645:SER:OG   | 2.58                     | 0.51              |
| 1:D:411:GLU:H    | 4:9:333:PRO:CG   | 2.24                     | 0.51              |
| 1:G:732:ILE:HG23 | 1:G:747:LEU:CD1  | 1.04                     | 0.51              |
| 1:J:202:SER:HB2  | 1:J:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:D:197:ALA:O    | 1:D:201:ALA:HB2  | 2.10                     | 0.51              |
| 1:A:818:TYR:CB   | 2:B:89:LYS:C     | 2.78                     | 0.51              |
| 1:D:831:TRP:CE3  | 2:E:34:ILE:HD13  | 2.46                     | 0.51              |
| 1:J:592:ILE:HG22 | 1:J:592:ILE:O    | 2.10                     | 0.51              |
| 1:M:128:PRO:O    | 1:M:129:TYR:HB2  | 2.10                     | 0.51              |
| 1:J:687:GLU:O    | 1:J:691:VAL:HG23 | 2.11                     | 0.51              |
| 1:D:237:THR:O    | 1:D:240:ASN:O    | 2.29                     | 0.51              |
| 1:P:13:ALA:C     | 1:P:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:A:248:MLY:N    | 1:A:463:ASP:O    | 2.44                     | 0.51              |
| 4:0:285:CYS:O    | 4:0:290:ARG:NH1  | 2.43                     | 0.51              |
| 3:F:104:GLY:HA2  | 3:F:137:ILE:HD11 | 1.92                     | 0.51              |
| 1:M:817:GLN:OE1  | 2:N:127:ARG:HD2  | 2.02                     | 0.51              |
| 1:J:84:MLY:HH23  | 1:J:719:ASP:O    | 2.08                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:592:ILE:O    | 1:M:592:ILE:HG22 | 2.11                     | 0.51              |
| 1:A:831:TRP:CE3  | 2:B:34:ILE:HD13  | 2.46                     | 0.51              |
| 3:I:110:VAL:HG13 | 3:I:114:LEU:HD12 | 1.92                     | 0.51              |
| 1:M:836:PHE:CD2  | 2:N:160:GLY:N    | 2.79                     | 0.51              |
| 1:M:732:ILE:H    | 1:M:733:PRO:HD2  | 1.74                     | 0.51              |
| 1:G:84:MLY:CB    | 1:G:723:ARG:HD2  | 2.41                     | 0.51              |
| 3:O:53:PRO:HB2   | 3:O:55:LYS:HG3   | 1.91                     | 0.51              |
| 1:J:578:HIS:O    | 1:J:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:M:40:VAL:HG13  | 1:M:41:VAL:O     | 2.10                     | 0.51              |
| 1:G:578:HIS:O    | 1:G:579:PHE:HB3  | 2.11                     | 0.51              |
| 1:P:418:THR:O    | 1:P:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:J:418:THR:O    | 1:J:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:M:418:THR:O    | 1:M:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:A:418:THR:O    | 1:A:422:VAL:HG23 | 2.11                     | 0.51              |
| 1:M:195:TYR:CE2  | 1:M:199:ILE:CD1  | 2.93                     | 0.51              |
| 1:A:38:VAL:CG1   | 1:A:39:PHE:N     | 2.74                     | 0.51              |
| 1:G:38:VAL:CG1   | 1:G:39:PHE:N     | 2.74                     | 0.51              |
| 1:J:292:MET:CE   | 1:J:309:PRO:HA   | 2.40                     | 0.51              |
| 3:O:100:GLY:O    | 3:O:138:ASN:HA   | 2.10                     | 0.51              |
| 1:P:559:LEU:HD23 | 1:P:559:LEU:C    | 2.31                     | 0.51              |
| 1:G:400:ALA:HB1  | 1:G:606:THR:HG22 | 1.93                     | 0.51              |
| 1:G:248:MLY:N    | 1:G:463:ASP:O    | 2.44                     | 0.51              |
| 1:A:559:LEU:HD23 | 1:A:559:LEU:C    | 2.31                     | 0.51              |
| 2:K:114:LYS:N    | 2:K:146:GLY:O    | 2.40                     | 0.51              |
| 1:D:592:ILE:O    | 1:D:592:ILE:HG22 | 2.10                     | 0.51              |
| 1:A:791:GLN:OE1  | 3:C:116:GLU:N    | 2.42                     | 0.51              |
| 1:P:592:ILE:O    | 1:P:592:ILE:HG22 | 2.10                     | 0.51              |
| 1:M:798:LEU:HD21 | 3:O:126:LEU:CG   | 2.38                     | 0.51              |
| 4:O:287:ILE:HG12 | 4:2:203:THR:HB   | 1.93                     | 0.51              |
| 4:1:204:ALA:HB3  | 4:Z:287:ILE:HG22 | 1.91                     | 0.51              |
| 1:D:202:SER:HB2  | 1:D:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:M:197:ALA:O    | 1:M:201:ALA:HB2  | 2.10                     | 0.51              |
| 1:M:806:MET:CA   | 1:M:809:ARG:HD2  | 2.40                     | 0.51              |
| 1:A:646:PHE:CE2  | 1:A:652:LEU:CD2  | 2.87                     | 0.51              |
| 1:J:755:HIS:N    | 1:J:780:ASP:OD2  | 2.43                     | 0.51              |
| 1:A:631:GLU:C    | 4:8:25:ASP:HB2   | 2.32                     | 0.51              |
| 2:E:163:ALA:O    | 2:K:21:GLU:CA    | 2.58                     | 0.51              |
| 1:A:128:PRO:O    | 1:A:129:TYR:HB2  | 2.09                     | 0.51              |
| 1:G:267:THR:HG21 | 1:G:438:PHE:HE2  | 1.76                     | 0.51              |
| 1:G:311:ASP:HB2  | 1:G:312:TYR:CE1  | 2.46                     | 0.51              |
| 1:A:400:ALA:HB1  | 1:A:606:THR:HG22 | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:400:ALA:HB1  | 1:D:606:THR:HG22 | 1.92                     | 0.51              |
| 1:D:723:ARG:NE   | 1:D:779:ARG:HG3  | 2.25                     | 0.51              |
| 1:G:795:ARG:C    | 3:I:35:ARG:HH22  | 2.09                     | 0.51              |
| 1:G:632:GLY:HA3  | 1:G:643:GLY:N    | 2.17                     | 0.51              |
| 2:K:140:PHE:O    | 2:K:141:PRO:C    | 2.33                     | 0.51              |
| 1:D:218:LEU:N    | 1:D:221:GLN:CG   | 2.74                     | 0.51              |
| 1:P:217:THR:C    | 1:P:221:GLN:NE2  | 2.62                     | 0.51              |
| 1:G:97:LEU:HD21  | 1:G:712:PRO:CA   | 2.41                     | 0.51              |
| 4:1:204:ALA:N    | 4:Z:287:ILE:CG2  | 2.68                     | 0.51              |
| 1:A:197:ALA:O    | 1:A:201:ALA:HB2  | 2.09                     | 0.51              |
| 1:D:642:LYS:CA   | 4:9:22:ALA:C     | 2.71                     | 0.51              |
| 1:D:831:TRP:CE2  | 2:E:51:PHE:CE1   | 2.94                     | 0.51              |
| 4:X:287:ILE:HG13 | 4:Z:202:THR:HG23 | 1.93                     | 0.51              |
| 4:8:285:CYS:O    | 4:8:290:ARG:NH1  | 2.43                     | 0.51              |
| 1:M:742:LYS:O    | 1:M:745:GLU:HB2  | 2.10                     | 0.51              |
| 1:G:41:VAL:HG21  | 1:G:76:GLN:HG3   | 1.93                     | 0.51              |
| 1:J:41:VAL:HG21  | 1:J:76:GLN:HG3   | 1.93                     | 0.51              |
| 1:M:41:VAL:HG13  | 1:M:42:HIS:N     | 2.25                     | 0.51              |
| 1:D:687:GLU:O    | 1:D:691:VAL:HG23 | 2.11                     | 0.51              |
| 1:M:291:ILE:HA   | 1:M:331:LEU:CD1  | 2.39                     | 0.51              |
| 1:G:631:GLU:C    | 4:V:25:ASP:HB2   | 2.31                     | 0.51              |
| 1:J:169:ASP:OD1  | 1:J:169:ASP:N    | 2.44                     | 0.51              |
| 1:M:169:ASP:OD1  | 1:M:169:ASP:N    | 2.44                     | 0.51              |
| 1:P:732:ILE:O    | 1:P:736:GLN:HG3  | 2.11                     | 0.51              |
| 1:P:408:VAL:CG1  | 4:O:332:PRO:HB3  | 2.40                     | 0.51              |
| 1:J:218:LEU:N    | 1:J:221:GLN:CG   | 2.74                     | 0.51              |
| 1:M:546:THR:CG2  | 1:M:548:THR:HB   | 2.41                     | 0.51              |
| 1:J:408:VAL:CG1  | 4:W:332:PRO:HB3  | 2.40                     | 0.51              |
| 1:D:578:HIS:O    | 1:D:579:PHE:HB3  | 2.10                     | 0.51              |
| 1:G:725:ARG:O    | 1:G:729:ALA:HA   | 2.10                     | 0.51              |
| 1:M:218:LEU:N    | 1:M:221:GLN:CG   | 2.74                     | 0.51              |
| 1:M:202:SER:HB2  | 1:M:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:M:629:GLU:CB   | 1:M:645:SER:N    | 2.73                     | 0.51              |
| 1:P:631:GLU:C    | 4:O:25:ASP:HB2   | 2.32                     | 0.51              |
| 1:J:742:LYS:O    | 1:J:745:GLU:HB2  | 2.10                     | 0.51              |
| 1:D:38:VAL:CG1   | 1:D:39:PHE:N     | 2.74                     | 0.51              |
| 1:M:237:THR:O    | 1:M:240:ASN:O    | 2.29                     | 0.51              |
| 1:M:13:ALA:C     | 1:M:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:D:13:ALA:C     | 1:D:15:PRO:HD2   | 2.31                     | 0.51              |
| 1:M:311:ASP:HB2  | 1:M:312:TYR:CE1  | 2.46                     | 0.51              |
| 1:A:311:ASP:HB2  | 1:A:312:TYR:CE1  | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:135:TYR:HD2  | 1:G:191:ARG:CD   | 2.23                     | 0.51              |
| 1:P:400:ALA:HB1  | 1:P:606:THR:HG22 | 1.93                     | 0.51              |
| 1:J:732:ILE:H    | 1:J:733:PRO:HD2  | 1.74                     | 0.50              |
| 1:J:732:ILE:H    | 1:J:733:PRO:CD   | 2.23                     | 0.50              |
| 1:G:212:GLY:O    | 1:G:213:LYS:HB2  | 2.10                     | 0.50              |
| 1:D:530:MET:HG2  | 4:9:354:GLN:HB2  | 0.56                     | 0.50              |
| 1:D:212:GLY:O    | 1:D:213:LYS:HB2  | 2.11                     | 0.50              |
| 4:0:110:LEU:O    | 4:1:195:GLU:CG   | 2.59                     | 0.50              |
| 1:P:202:SER:HB2  | 1:P:207:LYS:NZ   | 2.26                     | 0.50              |
| 1:A:640:LYS:CA   | 1:A:645:SER:OG   | 2.58                     | 0.50              |
| 1:P:295:MLY:HE2  | 1:P:332:MET:HE1  | 1.91                     | 0.50              |
| 1:D:830:PRO:HB2  | 2:E:51:PHE:CZ    | 2.46                     | 0.50              |
| 1:J:567:LYS:NZ   | 4:Y:92:ASN:ND2   | 2.36                     | 0.50              |
| 1:M:267:THR:HG21 | 1:M:438:PHE:HE2  | 1.76                     | 0.50              |
| 1:M:38:VAL:CG1   | 1:M:39:PHE:N     | 2.74                     | 0.50              |
| 1:J:237:THR:O    | 1:J:240:ASN:O    | 2.29                     | 0.50              |
| 1:P:22:LYS:O     | 1:P:26:GLU:N     | 2.29                     | 0.50              |
| 3:O:104:GLY:HA2  | 3:O:137:ILE:HD11 | 1.92                     | 0.50              |
| 1:D:559:LEU:HD23 | 1:D:559:LEU:C    | 2.31                     | 0.50              |
| 1:G:429:LEU:O    | 1:G:433:VAL:HG23 | 2.11                     | 0.50              |
| 1:G:795:ARG:NH2  | 3:I:116:GLU:CB   | 2.73                     | 0.50              |
| 1:J:732:ILE:O    | 1:J:736:GLN:HG3  | 2.12                     | 0.50              |
| 2:H:137:TRP:CA   | 2:H:145:ALA:CB   | 2.82                     | 0.50              |
| 1:A:725:ARG:O    | 1:A:729:ALA:HA   | 2.10                     | 0.50              |
| 1:G:218:LEU:N    | 1:G:221:GLN:CG   | 2.74                     | 0.50              |
| 1:J:646:PHE:HE2  | 1:J:652:LEU:CG   | 2.25                     | 0.50              |
| 1:J:411:GLU:H    | 4:W:333:PRO:CG   | 2.24                     | 0.50              |
| 1:J:553:MLY:CE   | 4:Y:45:VAL:HG11  | 2.32                     | 0.50              |
| 1:D:546:THR:CG2  | 1:D:548:THR:HB   | 2.40                     | 0.50              |
| 1:M:732:ILE:O    | 1:M:736:GLN:HG3  | 2.11                     | 0.50              |
| 1:J:836:PHE:CE2  | 2:K:160:GLY:HA3  | 2.45                     | 0.50              |
| 1:P:502:GLU:OE2  | 1:P:760:PHE:C    | 2.50                     | 0.50              |
| 1:G:202:SER:HB2  | 1:G:207:LYS:NZ   | 2.26                     | 0.50              |
| 1:J:631:GLU:C    | 4:W:25:ASP:HB2   | 2.31                     | 0.50              |
| 1:G:830:PRO:HG2  | 2:H:67:MET:HE2   | 1.92                     | 0.50              |
| 1:G:829:TRP:CH2  | 2:H:83:MET:HE1   | 2.47                     | 0.50              |
| 1:D:800:ARG:CB   | 3:F:149:VAL:CG2  | 2.80                     | 0.50              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:HG13 | 1.92                     | 0.50              |
| 1:A:41:VAL:HG21  | 1:A:76:GLN:HG3   | 1.93                     | 0.50              |
| 1:A:687:GLU:O    | 1:A:691:VAL:HG23 | 2.11                     | 0.50              |
| 1:P:687:GLU:O    | 1:P:691:VAL:HG23 | 2.11                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:154:HIS:CD2  | 1:P:155:ILE:H    | 2.30                     | 0.50              |
| 1:J:346:ASP:O    | 1:J:349:THR:HB   | 2.11                     | 0.50              |
| 1:A:675:ILE:CG2  | 1:A:676:ILE:N    | 2.74                     | 0.50              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:CD   | 2.23                     | 0.50              |
| 1:D:109:ARG:O    | 1:D:114:MET:N    | 2.37                     | 0.50              |
| 1:J:400:ALA:HB1  | 1:J:606:THR:HG22 | 1.93                     | 0.50              |
| 3:R:100:GLY:O    | 3:R:138:ASN:HA   | 2.11                     | 0.50              |
| 1:M:248:MLY:N    | 1:M:463:ASP:O    | 2.44                     | 0.50              |
| 1:D:795:ARG:CG   | 3:F:35:ARG:HH12  | 2.25                     | 0.50              |
| 2:N:112:ILE:HG23 | 2:N:147:ASN:HB3  | 1.92                     | 0.50              |
| 1:G:538:GLU:OE1  | 4:V:351:THR:HB   | 2.12                     | 0.50              |
| 1:P:818:TYR:C    | 2:Q:90:GLY:HA3   | 2.31                     | 0.50              |
| 2:B:117:LEU:HG   | 2:B:147:ASN:HB3  | 1.93                     | 0.50              |
| 2:B:129:THR:O    | 2:B:133:ILE:HG13 | 2.09                     | 0.50              |
| 1:J:506:GLU:HG3  | 1:J:760:PHE:O    | 2.11                     | 0.50              |
| 1:D:819:ASN:OD1  | 2:E:91:ALA:CA    | 2.56                     | 0.50              |
| 1:P:578:HIS:O    | 1:P:579:PHE:HB3  | 2.11                     | 0.50              |
| 1:A:530:MET:HE3  | 4:8:354:GLN:CG   | 2.36                     | 0.50              |
| 1:A:576:GLU:CG   | 1:A:577:ALA:N    | 2.44                     | 0.50              |
| 1:P:836:PHE:CD2  | 2:Q:160:GLY:N    | 2.79                     | 0.50              |
| 1:G:592:ILE:O    | 1:G:592:ILE:HG22 | 2.11                     | 0.50              |
| 4:W:285:CYS:O    | 4:Y:202:THR:HG22 | 2.12                     | 0.50              |
| 1:D:346:ASP:O    | 1:D:349:THR:HB   | 2.11                     | 0.50              |
| 1:A:267:THR:HG21 | 1:A:438:PHE:HE2  | 1.76                     | 0.50              |
| 1:J:311:ASP:HB2  | 1:J:312:TYR:CE1  | 2.46                     | 0.50              |
| 1:D:169:ASP:N    | 1:D:169:ASP:OD1  | 2.44                     | 0.50              |
| 1:M:400:ALA:HB1  | 1:M:606:THR:HG22 | 1.93                     | 0.50              |
| 1:M:559:LEU:C    | 1:M:559:LEU:HD23 | 2.31                     | 0.50              |
| 1:P:429:LEU:O    | 1:P:433:VAL:HG23 | 2.12                     | 0.50              |
| 1:P:818:TYR:HE1  | 2:Q:127:ARG:NH2  | 1.93                     | 0.50              |
| 1:P:530:MET:HG2  | 4:0:354:GLN:HB2  | 0.57                     | 0.50              |
| 1:M:548:THR:O    | 4:1:47:MET:HG3   | 2.04                     | 0.50              |
| 1:A:553:MLY:HG3  | 4:V:44:MET:O     | 2.07                     | 0.50              |
| 1:P:148:ARG:CZ   | 1:P:764:MLY:HH21 | 2.41                     | 0.50              |
| 4:X:291:LYS:HD2  | 4:Z:243:PRO:C    | 2.31                     | 0.50              |
| 1:A:629:GLU:CB   | 1:A:645:SER:N    | 2.74                     | 0.50              |
| 1:M:35:MLY:HH21  | 1:M:778:MET:HA   | 1.93                     | 0.50              |
| 1:J:756:THR:HA   | 1:J:776:GLU:OE1  | 2.11                     | 0.50              |
| 1:D:631:GLU:C    | 4:9:25:ASP:HB2   | 2.31                     | 0.50              |
| 1:M:631:GLU:C    | 4:Z:25:ASP:HB2   | 2.32                     | 0.50              |
| 1:P:278:GLN:HG3  | 1:P:318:GLY:H    | 1.75                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:418:THR:O    | 1:D:422:VAL:HG23 | 2.11                     | 0.50              |
| 1:P:237:THR:O    | 1:P:240:ASN:O    | 2.29                     | 0.50              |
| 1:J:109:ARG:HD3  | 1:J:117:THR:HB   | 1.92                     | 0.50              |
| 1:D:429:LEU:O    | 1:D:433:VAL:HG23 | 2.11                     | 0.50              |
| 1:M:429:LEU:O    | 1:M:433:VAL:HG23 | 2.12                     | 0.50              |
| 1:A:501:GLU:CB   | 1:A:762:HIS:CE1  | 2.85                     | 0.50              |
| 1:A:505:MLY:HB3  | 1:A:762:HIS:N    | 2.25                     | 0.50              |
| 2:E:114:LYS:N    | 2:E:146:GLY:O    | 2.40                     | 0.50              |
| 1:P:733:PRO:CA   | 1:P:737:PHE:CE1  | 2.94                     | 0.50              |
| 1:J:733:PRO:CA   | 1:J:737:PHE:CE1  | 2.95                     | 0.50              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:CD1  | 1.04                     | 0.50              |
| 1:M:578:HIS:O    | 1:M:579:PHE:HB3  | 2.11                     | 0.50              |
| 1:J:553:MLY:CE   | 4:Y:45:VAL:CG1   | 2.78                     | 0.50              |
| 1:G:732:ILE:H    | 1:G:733:PRO:HD2  | 1.74                     | 0.50              |
| 1:P:546:THR:CG2  | 1:P:548:THR:HB   | 2.41                     | 0.50              |
| 4:0:287:ILE:HG22 | 4:2:203:THR:CG2  | 2.28                     | 0.50              |
| 4:1:204:ALA:H    | 4:Z:287:ILE:CB   | 2.24                     | 0.50              |
| 1:D:646:PHE:HE2  | 1:D:652:LEU:CG   | 2.25                     | 0.50              |
| 1:M:41:VAL:HG21  | 1:M:76:GLN:HG3   | 1.93                     | 0.50              |
| 1:J:769:ALA:HB2  | 1:J:770:GLY:HA2  | 1.78                     | 0.50              |
| 1:M:687:GLU:O    | 1:M:691:VAL:HG23 | 2.11                     | 0.50              |
| 1:J:154:HIS:CD2  | 1:J:155:ILE:H    | 2.30                     | 0.50              |
| 1:G:237:THR:O    | 1:G:240:ASN:O    | 2.29                     | 0.50              |
| 1:A:13:ALA:C     | 1:A:15:PRO:HD2   | 2.31                     | 0.50              |
| 1:A:169:ASP:OD1  | 1:A:169:ASP:N    | 2.44                     | 0.50              |
| 3:L:100:GLY:O    | 3:L:138:ASN:HA   | 2.11                     | 0.50              |
| 1:J:788:THR:O    | 3:L:42:THR:CG2   | 2.52                     | 0.50              |
| 1:D:797:PHE:CD1  | 3:F:146:ILE:O    | 2.62                     | 0.50              |
| 1:G:646:PHE:CE2  | 1:G:652:LEU:CD2  | 2.87                     | 0.50              |
| 1:P:411:GLU:H    | 4:0:333:PRO:CG   | 2.24                     | 0.50              |
| 1:P:538:GLU:HA   | 4:0:349:LEU:CB   | 2.40                     | 0.50              |
| 1:A:732:ILE:O    | 1:A:736:GLN:HG3  | 2.12                     | 0.50              |
| 1:G:218:LEU:CD2  | 1:G:222:ILE:CG1  | 2.85                     | 0.50              |
| 1:J:538:GLU:CD   | 4:W:355:MET:HE3  | 2.30                     | 0.50              |
| 1:J:629:GLU:CB   | 1:J:645:SER:N    | 2.74                     | 0.50              |
| 1:D:408:VAL:CG1  | 4:9:332:PRO:HB3  | 2.41                     | 0.50              |
| 1:P:839:MLY:N    | 1:P:840:PRO:CD   | 2.75                     | 0.50              |
| 1:G:687:GLU:O    | 1:G:691:VAL:HG23 | 2.11                     | 0.50              |
| 1:G:291:ILE:HA   | 1:G:331:LEU:CD1  | 2.39                     | 0.50              |
| 1:D:154:HIS:CD2  | 1:D:155:ILE:H    | 2.30                     | 0.50              |
| 1:M:154:HIS:CD2  | 1:M:155:ILE:H    | 2.30                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:346:ASP:O    | 1:P:349:THR:HB   | 2.11                     | 0.50              |
| 1:D:311:ASP:HB2  | 1:D:312:TYR:CE1  | 2.46                     | 0.50              |
| 1:P:762:HIS:CD2  | 1:P:762:HIS:N    | 2.78                     | 0.50              |
| 1:J:675:ILE:CG2  | 1:J:676:ILE:N    | 2.74                     | 0.50              |
| 3:I:100:GLY:O    | 3:I:138:ASN:HA   | 2.11                     | 0.50              |
| 1:D:732:ILE:HD13 | 1:D:782:MLY:CH2  | 2.40                     | 0.50              |
| 1:G:795:ARG:N    | 3:I:118:MET:HE3  | 2.27                     | 0.50              |
| 1:D:506:GLU:OE2  | 1:D:764:MLY:CE   | 2.59                     | 0.50              |
| 2:H:112:ILE:HG23 | 2:H:147:ASN:HB3  | 1.93                     | 0.50              |
| 1:P:629:GLU:CB   | 1:P:645:SER:N    | 2.73                     | 0.50              |
| 1:M:545:ALA:CA   | 4:1:45:VAL:HG11  | 2.19                     | 0.50              |
| 1:M:547:ASP:O    | 1:M:550:PHE:HB3  | 2.12                     | 0.50              |
| 1:D:553:MLY:CE   | 4:W:45:VAL:CA    | 2.49                     | 0.50              |
| 1:G:715:VAL:O    | 1:G:764:MLY:HB3  | 2.12                     | 0.50              |
| 1:J:839:MLY:N    | 1:J:840:PRO:CD   | 2.75                     | 0.50              |
| 1:J:836:PHE:CE1  | 2:K:160:GLY:N    | 2.78                     | 0.50              |
| 1:P:93:MET:HE2   | 1:P:764:MLY:HD3  | 1.94                     | 0.50              |
| 1:D:629:GLU:CA   | 1:D:643:GLY:C    | 2.73                     | 0.50              |
| 1:P:805:ALA:O    | 1:P:809:ARG:CA   | 2.54                     | 0.50              |
| 1:J:546:THR:CG2  | 1:J:548:THR:HB   | 2.41                     | 0.50              |
| 1:G:310:TYR:CE2  | 1:G:320:ILE:CD1  | 2.94                     | 0.50              |
| 1:P:38:VAL:CG1   | 1:P:39:PHE:N     | 2.74                     | 0.50              |
| 1:A:601:ASP:N    | 1:A:602:PRO:CD   | 2.75                     | 0.50              |
| 1:J:559:LEU:HD23 | 1:J:559:LEU:C    | 2.31                     | 0.50              |
| 4:8:70:PRO:HG3   | 4:8:81:ASP:HB3   | 1.94                     | 0.50              |
| 1:J:429:LEU:O    | 1:J:433:VAL:HG23 | 2.12                     | 0.50              |
| 1:D:733:PRO:CA   | 1:D:737:PHE:CE1  | 2.94                     | 0.50              |
| 1:A:508:ILE:HD13 | 1:A:759:ALA:HB2  | 1.78                     | 0.50              |
| 1:D:715:VAL:O    | 1:D:764:MLY:HB3  | 2.12                     | 0.50              |
| 1:A:218:LEU:N    | 1:A:221:GLN:CG   | 2.74                     | 0.50              |
| 1:P:642:LYS:CG   | 4:0:22:ALA:HA    | 2.37                     | 0.50              |
| 1:J:538:GLU:OE1  | 4:W:351:THR:HB   | 2.12                     | 0.50              |
| 1:D:538:GLU:OE1  | 4:9:351:THR:HB   | 2.12                     | 0.50              |
| 1:M:217:THR:C    | 1:M:221:GLN:NE2  | 2.62                     | 0.50              |
| 4:0:202:THR:N    | 4:Y:287:ILE:H    | 2.10                     | 0.50              |
| 1:M:836:PHE:CE2  | 2:N:160:GLY:H    | 1.68                     | 0.50              |
| 1:M:733:PRO:CA   | 1:M:737:PHE:CE1  | 2.95                     | 0.50              |
| 4:0:287:ILE:CB   | 4:2:203:THR:CG2  | 2.90                     | 0.50              |
| 4:3:287:ILE:CB   | 4:5:204:ALA:H    | 2.24                     | 0.50              |
| 1:M:805:ALA:O    | 1:M:809:ARG:HG3  | 2.12                     | 0.50              |
| 1:J:649:VAL:HG23 | 1:J:649:VAL:HA   | 1.83                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:237:THR:O    | 1:A:240:ASN:O    | 2.29                     | 0.50              |
| 1:P:109:ARG:HD3  | 1:P:117:THR:HB   | 1.92                     | 0.50              |
| 1:G:471:ASP:HB3  | 1:G:573:GLY:O    | 2.12                     | 0.50              |
| 1:D:471:ASP:HB3  | 1:D:573:GLY:O    | 2.12                     | 0.50              |
| 1:D:732:ILE:O    | 1:D:736:GLN:HG3  | 2.12                     | 0.50              |
| 2:N:117:LEU:HG   | 2:N:147:ASN:HB3  | 1.93                     | 0.50              |
| 1:G:640:LYS:CA   | 1:G:645:SER:OG   | 2.58                     | 0.50              |
| 2:Q:112:ILE:HG23 | 2:Q:147:ASN:HB3  | 1.92                     | 0.50              |
| 2:Q:114:LYS:N    | 2:Q:146:GLY:O    | 2.40                     | 0.50              |
| 4:1:288:ASP:CB   | 4:3:203:THR:CG2  | 2.87                     | 0.50              |
| 2:K:117:LEU:HG   | 2:K:147:ASN:HB3  | 1.93                     | 0.50              |
| 2:B:121:LEU:HA   | 2:B:128:PHE:CD2  | 2.46                     | 0.50              |
| 1:M:530:MET:CE   | 4:Z:354:GLN:HG3  | 2.35                     | 0.50              |
| 1:P:795:ARG:HE   | 3:R:116:GLU:CB   | 2.24                     | 0.50              |
| 1:P:547:ASP:O    | 1:P:550:PHE:HB3  | 2.12                     | 0.50              |
| 1:A:530:MET:HA   | 4:8:354:GLN:CD   | 2.11                     | 0.50              |
| 1:A:409:GLY:N    | 1:A:636:LYS:CD   | 2.70                     | 0.50              |
| 1:A:547:ASP:O    | 1:A:550:PHE:HB3  | 2.12                     | 0.50              |
| 4:0:243:PRO:CD   | 4:Y:291:LYS:HE3  | 2.42                     | 0.50              |
| 1:J:762:HIS:N    | 1:J:762:HIS:CD2  | 2.78                     | 0.50              |
| 1:D:640:LYS:CA   | 1:D:645:SER:OG   | 2.58                     | 0.50              |
| 1:M:739:ASP:CB   | 1:M:742:LYS:CB   | 2.81                     | 0.50              |
| 1:P:41:VAL:HG21  | 1:P:76:GLN:HG3   | 1.93                     | 0.50              |
| 1:D:612:GLN:HE22 | 1:D:627:GLY:HA2  | 1.66                     | 0.50              |
| 1:J:278:GLN:HG3  | 1:J:318:GLY:H    | 1.75                     | 0.50              |
| 1:G:278:GLN:HG3  | 1:G:318:GLY:H    | 1.75                     | 0.50              |
| 1:A:278:GLN:HG3  | 1:A:318:GLY:H    | 1.75                     | 0.50              |
| 1:G:346:ASP:O    | 1:G:349:THR:HB   | 2.11                     | 0.50              |
| 1:M:346:ASP:O    | 1:M:349:THR:HB   | 2.11                     | 0.50              |
| 1:M:675:ILE:CG2  | 1:M:676:ILE:N    | 2.74                     | 0.50              |
| 1:P:169:ASP:OD1  | 1:P:169:ASP:N    | 2.44                     | 0.50              |
| 1:A:471:ASP:HB3  | 1:A:573:GLY:O    | 2.12                     | 0.50              |
| 4:Z:318:THR:HA   | 4:Z:327:ILE:HG12 | 1.94                     | 0.50              |
| 4:0:318:THR:HA   | 4:0:327:ILE:HG12 | 1.94                     | 0.50              |
| 1:P:646:PHE:HE2  | 1:P:652:LEU:CG   | 2.25                     | 0.49              |
| 1:J:715:VAL:O    | 1:J:764:MLY:HB3  | 2.12                     | 0.49              |
| 1:J:642:LYS:CG   | 4:W:22:ALA:HA    | 2.37                     | 0.49              |
| 1:G:732:ILE:O    | 1:G:736:GLN:HG3  | 2.12                     | 0.49              |
| 1:G:733:PRO:CA   | 1:G:737:PHE:CE1  | 2.95                     | 0.49              |
| 1:M:715:VAL:HG12 | 1:M:716:LEU:O    | 2.12                     | 0.49              |
| 1:A:839:MLY:HB2  | 1:A:840:PRO:HD3  | 1.94                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:839:MLY:N    | 1:D:840:PRO:CD   | 2.75                     | 0.49              |
| 1:P:502:GLU:OE2  | 1:P:761:GLY:N    | 2.44                     | 0.49              |
| 1:M:806:MET:CB   | 1:M:807:VAL:N    | 2.75                     | 0.49              |
| 1:A:310:TYR:CE2  | 1:A:320:ILE:CD1  | 2.94                     | 0.49              |
| 1:M:128:PRO:O    | 1:M:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:HD3  | 1.94                     | 0.49              |
| 4:W:318:THR:HA   | 4:W:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:M:471:ASP:HB3  | 1:M:573:GLY:O    | 2.12                     | 0.49              |
| 4:9:318:THR:HA   | 4:9:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:X:318:THR:HA   | 4:X:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:5:70:PRO:HG3   | 4:5:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:V:318:THR:HA   | 4:V:327:ILE:HG12 | 1.94                     | 0.49              |
| 2:E:140:PHE:HB3  | 2:E:144:VAL:HG12 | 1.94                     | 0.49              |
| 1:P:629:GLU:CA   | 1:P:643:GLY:C    | 2.73                     | 0.49              |
| 1:J:217:THR:C    | 1:J:221:GLN:NE2  | 2.62                     | 0.49              |
| 1:M:409:GLY:N    | 1:M:636:LYS:CD   | 2.70                     | 0.49              |
| 1:J:543:PRO:CD   | 4:W:146:GLY:O    | 2.61                     | 0.49              |
| 1:D:539:GLU:OE2  | 4:W:45:VAL:C     | 2.47                     | 0.49              |
| 1:A:411:GLU:H    | 4:8:333:PRO:CG   | 2.24                     | 0.49              |
| 1:M:839:MLY:HB2  | 1:M:840:PRO:HD3  | 1.94                     | 0.49              |
| 1:G:148:ARG:NH2  | 1:G:764:MLY:CH2  | 2.73                     | 0.49              |
| 1:G:715:VAL:HG12 | 1:G:716:LEU:O    | 2.12                     | 0.49              |
| 1:G:759:ALA:O    | 1:G:766:PHE:N    | 2.32                     | 0.49              |
| 1:A:202:SER:HB2  | 1:A:207:LYS:NZ   | 2.26                     | 0.49              |
| 1:P:715:VAL:HG12 | 1:P:716:LEU:O    | 2.12                     | 0.49              |
| 1:D:642:LYS:CG   | 4:9:22:ALA:HA    | 2.37                     | 0.49              |
| 1:M:642:LYS:HG2  | 4:Z:21:PHE:C     | 2.29                     | 0.49              |
| 1:P:214:MET:HA   | 1:P:340:ILE:CD1  | 2.41                     | 0.49              |
| 1:M:35:MLY:HG3   | 1:M:777:GLU:OE2  | 2.11                     | 0.49              |
| 4:V:322:PRO:HB3  | 4:X:246:GLN:HG2  | 1.92                     | 0.49              |
| 4:1:324:THR:CB   | 4:3:244:ASP:CA   | 2.82                     | 0.49              |
| 1:A:51:THR:C     | 1:A:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:J:192:VAL:O    | 1:J:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:J:38:VAL:CG1   | 1:J:39:PHE:N     | 2.74                     | 0.49              |
| 4:3:318:THR:HA   | 4:3:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:G:169:ASP:N    | 1:G:169:ASP:OD1  | 2.44                     | 0.49              |
| 4:7:318:THR:HA   | 4:7:327:ILE:HG12 | 1.94                     | 0.49              |
| 2:E:123:THR:HA   | 3:F:19:ARG:HH12  | 1.77                     | 0.49              |
| 1:J:801:VAL:CG2  | 3:L:126:LEU:HD21 | 2.39                     | 0.49              |
| 1:A:715:VAL:O    | 1:A:764:MLY:HB3  | 2.12                     | 0.49              |
| 1:G:553:MLY:O    | 4:X:46:GLY:HA3   | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:CB   | 4:V:24:ASP:O     | 2.60                     | 0.49              |
| 2:K:114:LYS:HG3  | 2:K:137:TRP:CZ2  | 2.48                     | 0.49              |
| 2:B:114:LYS:HG3  | 2:B:137:TRP:CZ2  | 2.48                     | 0.49              |
| 2:B:140:PHE:HB3  | 2:B:144:VAL:HG12 | 1.94                     | 0.49              |
| 1:A:733:PRO:CA   | 1:A:737:PHE:CE1  | 2.95                     | 0.49              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:HG3  | 1.71                     | 0.49              |
| 1:M:543:PRO:CD   | 4:Z:146:GLY:O    | 2.61                     | 0.49              |
| 1:M:411:GLU:H    | 4:Z:333:PRO:CG   | 2.24                     | 0.49              |
| 1:J:642:LYS:HA   | 4:W:22:ALA:C     | 2.33                     | 0.49              |
| 1:P:797:PHE:CD1  | 3:R:149:VAL:HG13 | 2.45                     | 0.49              |
| 1:G:839:MLY:HB2  | 1:G:840:PRO:HD3  | 1.94                     | 0.49              |
| 1:G:739:ASP:OD1  | 1:G:740:SER:N    | 2.45                     | 0.49              |
| 1:P:128:PRO:O    | 1:P:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:D:291:ILE:HA   | 1:D:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:P:311:ASP:HB2  | 1:P:312:TYR:CE1  | 2.46                     | 0.49              |
| 1:J:251:ARG:O    | 1:J:263:ALA:HA   | 2.12                     | 0.49              |
| 1:P:251:ARG:O    | 1:P:263:ALA:HA   | 2.12                     | 0.49              |
| 1:D:251:ARG:O    | 1:D:263:ALA:HA   | 2.12                     | 0.49              |
| 1:J:601:ASP:N    | 1:J:602:PRO:CD   | 2.75                     | 0.49              |
| 1:M:601:ASP:N    | 1:M:602:PRO:CD   | 2.75                     | 0.49              |
| 4:Y:318:THR:HA   | 4:Y:327:ILE:HG12 | 1.95                     | 0.49              |
| 4:5:318:THR:HA   | 4:5:327:ILE:HG12 | 1.94                     | 0.49              |
| 2:N:93:PRO:O     | 2:N:97:ILE:HG13  | 2.12                     | 0.49              |
| 1:G:754:ASP:CG   | 1:G:776:GLU:HA   | 2.32                     | 0.49              |
| 2:N:121:LEU:HA   | 2:N:128:PHE:CD2  | 2.46                     | 0.49              |
| 1:G:543:PRO:CD   | 4:V:146:GLY:O    | 2.61                     | 0.49              |
| 2:E:121:LEU:HA   | 2:E:128:PHE:CD2  | 2.46                     | 0.49              |
| 2:K:112:ILE:HG23 | 2:K:147:ASN:HB3  | 1.92                     | 0.49              |
| 1:P:538:GLU:OE1  | 4:0:351:THR:HB   | 2.12                     | 0.49              |
| 1:M:762:HIS:CD2  | 1:M:762:HIS:N    | 2.78                     | 0.49              |
| 1:M:84:MLY:HH21  | 1:M:719:ASP:C    | 2.29                     | 0.49              |
| 1:D:839:MLY:HB2  | 1:D:840:PRO:HD3  | 1.94                     | 0.49              |
| 1:M:629:GLU:CA   | 1:M:643:GLY:C    | 2.73                     | 0.49              |
| 1:P:806:MET:CB   | 1:P:807:VAL:N    | 2.74                     | 0.49              |
| 2:Q:149:ASP:CG   | 2:Q:150:TYR:N    | 2.49                     | 0.49              |
| 1:D:278:GLN:HG3  | 1:D:318:GLY:H    | 1.75                     | 0.49              |
| 1:M:555:TYR:HB2  | 4:1:49:GLN:O     | 2.12                     | 0.49              |
| 1:D:128:PRO:O    | 1:D:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:P:192:VAL:O    | 1:P:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:A:291:ILE:HA   | 1:A:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:A:154:HIS:CD2  | 1:A:155:ILE:H    | 2.30                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:4:70:PRO:HG3   | 4:4:81:ASP:HB3   | 1.94                     | 0.49              |
| 2:B:93:PRO:O     | 2:B:97:ILE:HG13  | 2.12                     | 0.49              |
| 1:A:20:SER:HB3   | 1:A:23:GLU:OE1   | 2.13                     | 0.49              |
| 4:8:124:PHE:CZ   | 4:8:132:MET:HG3  | 2.48                     | 0.49              |
| 1:G:756:THR:O    | 1:G:758:TYR:N    | 2.45                     | 0.49              |
| 1:J:813:ILE:HG23 | 2:K:128:PHE:CZ   | 2.48                     | 0.49              |
| 1:P:543:PRO:CD   | 4:0:146:GLY:O    | 2.61                     | 0.49              |
| 1:A:795:ARG:CG   | 3:C:35:ARG:NH1   | 2.49                     | 0.49              |
| 1:A:543:PRO:CD   | 4:8:146:GLY:O    | 2.61                     | 0.49              |
| 1:M:715:VAL:O    | 1:M:764:MLY:HB3  | 2.12                     | 0.49              |
| 4:1:204:ALA:H    | 4:Z:287:ILE:HG22 | 1.74                     | 0.49              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:HB3  | 2.43                     | 0.49              |
| 1:J:214:MET:HA   | 1:J:340:ILE:CD1  | 2.41                     | 0.49              |
| 1:J:756:THR:O    | 1:J:758:TYR:N    | 2.45                     | 0.49              |
| 1:J:739:ASP:OD1  | 1:J:740:SER:N    | 2.45                     | 0.49              |
| 3:O:50:LEU:O     | 3:O:55:LYS:HB2   | 2.13                     | 0.49              |
| 1:M:739:ASP:OD1  | 1:M:740:SER:N    | 2.45                     | 0.49              |
| 1:M:103:LEU:C    | 1:M:103:LEU:HD12 | 2.33                     | 0.49              |
| 1:D:173:GLN:OE1  | 1:D:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:M:756:THR:O    | 1:M:758:TYR:N    | 2.46                     | 0.49              |
| 1:M:278:GLN:HG3  | 1:M:318:GLY:H    | 1.75                     | 0.49              |
| 1:A:756:THR:O    | 1:A:758:TYR:N    | 2.45                     | 0.49              |
| 1:J:128:PRO:O    | 1:J:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:J:291:ILE:HA   | 1:J:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:G:290:GLN:HG2  | 1:G:331:LEU:CA   | 2.43                     | 0.49              |
| 1:D:192:VAL:O    | 1:D:195:TYR:HB3  | 2.13                     | 0.49              |
| 1:A:346:ASP:O    | 1:A:349:THR:HB   | 2.11                     | 0.49              |
| 1:D:251:ARG:HB2  | 1:D:264:ASP:HB3  | 1.95                     | 0.49              |
| 1:A:429:LEU:O    | 1:A:433:VAL:HG23 | 2.11                     | 0.49              |
| 4:V:70:PRO:HG3   | 4:V:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:V:124:PHE:CZ   | 4:V:132:MET:HG3  | 2.48                     | 0.49              |
| 4:2:70:PRO:HG3   | 4:2:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:2:124:PHE:CZ   | 4:2:132:MET:HG3  | 2.48                     | 0.49              |
| 4:X:124:PHE:CZ   | 4:X:132:MET:HG3  | 2.48                     | 0.49              |
| 1:D:732:ILE:CG2  | 1:D:782:MLY:CH2  | 2.68                     | 0.49              |
| 1:G:754:ASP:HB3  | 1:G:757:GLN:HG2  | 1.72                     | 0.49              |
| 1:G:754:ASP:N    | 1:G:779:ARG:HD2  | 2.12                     | 0.49              |
| 1:A:720:PHE:CD2  | 1:A:744:SER:HB3  | 2.48                     | 0.49              |
| 1:A:97:LEU:N     | 1:A:97:LEU:HD13  | 2.28                     | 0.49              |
| 1:D:507:GLY:O    | 1:D:762:HIS:CD2  | 2.66                     | 0.49              |
| 4:1:287:ILE:HD13 | 4:3:203:THR:CA   | 2.41                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:821:ARG:NH1  | 2:K:127:ARG:CZ   | 2.71                     | 0.49              |
| 1:M:538:GLU:OE1  | 4:Z:351:THR:HB   | 2.12                     | 0.49              |
| 1:P:839:MLY:HB2  | 1:P:840:PRO:HD3  | 1.94                     | 0.49              |
| 1:M:642:LYS:HA   | 4:Z:22:ALA:C     | 2.33                     | 0.49              |
| 1:P:805:ALA:O    | 1:P:808:GLU:N    | 2.45                     | 0.49              |
| 1:J:95:THR:N     | 1:J:713:SER:HB3  | 2.24                     | 0.49              |
| 1:P:103:LEU:C    | 1:P:103:LEU:HD12 | 2.33                     | 0.49              |
| 1:P:51:THR:C     | 1:P:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:G:154:HIS:CD2  | 1:G:155:ILE:H    | 2.30                     | 0.49              |
| 1:P:237:THR:HG22 | 1:P:238:VAL:N    | 2.28                     | 0.49              |
| 1:P:312:TYR:N    | 1:P:312:TYR:CD1  | 2.81                     | 0.49              |
| 1:J:251:ARG:HB2  | 1:J:264:ASP:HB3  | 1.94                     | 0.49              |
| 4:X:70:PRO:HG3   | 4:X:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:P:20:SER:HB3   | 1:P:23:GLU:OE1   | 2.13                     | 0.49              |
| 4:Z:124:PHE:CZ   | 4:Z:132:MET:HG3  | 2.48                     | 0.49              |
| 2:H:93:PRO:O     | 2:H:97:ILE:HG13  | 2.12                     | 0.49              |
| 1:P:314:TYR:CZ   | 1:P:362:GLY:HA2  | 2.48                     | 0.49              |
| 4:1:318:THR:HA   | 4:1:327:ILE:HG12 | 1.95                     | 0.49              |
| 4:8:318:THR:HA   | 4:8:327:ILE:HG12 | 1.95                     | 0.49              |
| 1:D:793:ARG:O    | 1:D:797:PHE:N    | 2.39                     | 0.49              |
| 2:N:140:PHE:HB3  | 2:N:144:VAL:HG12 | 1.94                     | 0.49              |
| 2:E:128:PHE:O    | 2:E:133:ILE:HD11 | 2.13                     | 0.49              |
| 1:A:813:ILE:HG21 | 2:B:127:ARG:CG   | 2.41                     | 0.49              |
| 2:B:112:ILE:HG23 | 2:B:147:ASN:HB3  | 1.93                     | 0.49              |
| 1:P:544:LYS:HD2  | 4:0:147:ARG:CB   | 2.36                     | 0.49              |
| 1:D:543:PRO:CD   | 4:9:146:GLY:O    | 2.61                     | 0.49              |
| 1:M:839:MLY:N    | 1:M:840:PRO:CD   | 2.75                     | 0.49              |
| 4:0:243:PRO:HB2  | 4:Y:291:LYS:CE   | 2.43                     | 0.49              |
| 1:A:839:MLY:N    | 1:A:840:PRO:CD   | 2.75                     | 0.49              |
| 1:G:839:MLY:N    | 1:G:840:PRO:CD   | 2.75                     | 0.49              |
| 1:M:640:LYS:C    | 4:Z:23:GLY:CA    | 2.64                     | 0.49              |
| 1:A:642:LYS:HG2  | 4:8:21:PHE:C     | 2.30                     | 0.49              |
| 1:D:214:MET:HA   | 1:D:340:ILE:CD1  | 2.41                     | 0.49              |
| 1:J:97:LEU:HD13  | 1:J:97:LEU:N     | 2.28                     | 0.49              |
| 1:D:739:ASP:OD1  | 1:D:740:SER:N    | 2.45                     | 0.49              |
| 1:J:64:THR:CG2   | 1:J:65:GLU:N     | 2.75                     | 0.49              |
| 1:G:51:THR:C     | 1:G:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:M:192:VAL:O    | 1:M:195:TYR:HB3  | 2.13                     | 0.49              |
| 4:5:198:TYR:CZ   | 4:5:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:Z:198:TYR:CZ   | 4:Z:248:ILE:HG13 | 2.48                     | 0.49              |
| 1:J:237:THR:HG22 | 1:J:238:VAL:N    | 2.28                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:251:ARG:O    | 1:M:263:ALA:HA   | 2.12                     | 0.49              |
| 1:D:601:ASP:N    | 1:D:602:PRO:CD   | 2.75                     | 0.49              |
| 4:3:70:PRO:HG3   | 4:3:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:J:471:ASP:HB3  | 1:J:573:GLY:O    | 2.12                     | 0.49              |
| 4:4:318:THR:HA   | 4:4:327:ILE:HG12 | 1.94                     | 0.49              |
| 4:7:70:PRO:HG3   | 4:7:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:2:318:THR:HA   | 4:2:327:ILE:HG12 | 1.94                     | 0.49              |
| 1:A:739:ASP:OD1  | 1:A:740:SER:N    | 2.45                     | 0.49              |
| 1:G:530:MET:HA   | 4:V:354:GLN:CD   | 2.11                     | 0.49              |
| 2:K:121:LEU:O    | 2:K:128:PHE:CG   | 2.61                     | 0.49              |
| 1:M:553:MLY:HH22 | 4:1:43:VAL:HG23  | 1.95                     | 0.49              |
| 1:D:538:GLU:HA   | 4:9:351:THR:H    | 1.77                     | 0.49              |
| 1:M:798:LEU:CD2  | 3:O:122:GLU:HB3  | 2.37                     | 0.49              |
| 1:J:839:MLY:HH21 | 2:K:158:THR:CG2  | 2.42                     | 0.49              |
| 1:D:712:PRO:CG   | 1:D:771:LEU:CB   | 2.71                     | 0.49              |
| 1:D:768:MLY:HA   | 1:D:771:LEU:HD13 | 1.94                     | 0.49              |
| 1:D:834:LEU:HD23 | 2:E:54:MET:HE3   | 1.95                     | 0.49              |
| 1:D:642:LYS:HA   | 4:9:22:ALA:C     | 2.33                     | 0.49              |
| 1:G:41:VAL:CG1   | 1:G:42:HIS:N     | 2.75                     | 0.49              |
| 1:J:173:GLN:OE1  | 1:J:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:A:173:GLN:OE1  | 1:A:668:HIS:HB3  | 2.13                     | 0.49              |
| 1:P:291:ILE:HA   | 1:P:331:LEU:CD1  | 2.39                     | 0.49              |
| 1:P:290:GLN:HG2  | 1:P:331:LEU:CA   | 2.43                     | 0.49              |
| 1:M:64:THR:CG2   | 1:M:65:GLU:N     | 2.75                     | 0.49              |
| 1:A:192:VAL:O    | 1:A:195:TYR:HB3  | 2.13                     | 0.49              |
| 4:X:198:TYR:CZ   | 4:X:248:ILE:HG13 | 2.48                     | 0.49              |
| 1:D:237:THR:HG22 | 1:D:238:VAL:N    | 2.28                     | 0.49              |
| 1:J:312:TYR:N    | 1:J:312:TYR:CD1  | 2.81                     | 0.49              |
| 1:A:312:TYR:N    | 1:A:312:TYR:CD1  | 2.81                     | 0.49              |
| 1:G:601:ASP:N    | 1:G:602:PRO:CD   | 2.75                     | 0.49              |
| 1:J:20:SER:HB3   | 1:J:23:GLU:OE1   | 2.13                     | 0.49              |
| 4:Z:70:PRO:HG3   | 4:Z:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:P:470:PHE:O    | 1:P:473:ASN:ND2  | 2.40                     | 0.49              |
| 1:D:20:SER:HB3   | 1:D:23:GLU:OE1   | 2.13                     | 0.49              |
| 1:G:20:SER:HB3   | 1:G:23:GLU:OE1   | 2.12                     | 0.49              |
| 4:1:148:THR:OG1  | 4:3:45:VAL:CG2   | 2.61                     | 0.49              |
| 1:J:795:ARG:CB   | 3:L:35:ARG:CZ    | 2.56                     | 0.49              |
| 1:A:715:VAL:HG12 | 1:A:716:LEU:O    | 2.13                     | 0.49              |
| 1:D:507:GLY:O    | 1:D:761:GLY:HA2  | 2.13                     | 0.49              |
| 1:A:757:GLN:CA   | 1:A:771:LEU:CD1  | 2.80                     | 0.49              |
| 1:G:642:LYS:HA   | 4:V:22:ALA:C     | 2.33                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:HG2  | 4:V:21:PHE:C     | 2.30                     | 0.49              |
| 1:G:553:MLY:CB   | 4:X:45:VAL:O     | 2.57                     | 0.49              |
| 1:G:817:GLN:NE2  | 2:H:128:PHE:CE1  | 2.81                     | 0.49              |
| 1:J:720:PHE:CD2  | 1:J:744:SER:HB3  | 2.48                     | 0.49              |
| 1:D:547:ASP:O    | 1:D:550:PHE:HB3  | 2.12                     | 0.49              |
| 1:G:732:ILE:H    | 1:G:733:PRO:CD   | 2.23                     | 0.49              |
| 1:D:818:TYR:CD2  | 2:E:90:GLY:CA    | 2.96                     | 0.49              |
| 1:A:538:GLU:OE1  | 4:8:351:THR:HB   | 2.12                     | 0.49              |
| 1:M:783:LEU:CB   | 1:M:786:ILE:HD12 | 2.33                     | 0.49              |
| 1:P:218:LEU:N    | 1:P:221:GLN:CG   | 2.74                     | 0.49              |
| 1:J:839:MLY:HB2  | 1:J:840:PRO:HD3  | 1.94                     | 0.49              |
| 1:D:834:LEU:CD2  | 2:E:54:MET:SD    | 3.00                     | 0.49              |
| 1:P:715:VAL:O    | 1:P:764:MLY:HB3  | 2.12                     | 0.49              |
| 1:A:332:MET:O    | 1:A:336:SER:OG   | 2.27                     | 0.49              |
| 1:D:800:ARG:C    | 3:F:149:VAL:CG2  | 2.74                     | 0.49              |
| 1:P:97:LEU:CD2   | 1:P:712:PRO:CB   | 2.86                     | 0.49              |
| 1:D:290:GLN:HG2  | 1:D:331:LEU:CA   | 2.43                     | 0.49              |
| 1:G:192:VAL:O    | 1:G:195:TYR:HB3  | 2.13                     | 0.49              |
| 4:V:198:TYR:CZ   | 4:V:248:ILE:HG13 | 2.48                     | 0.49              |
| 1:D:168:THR:HG22 | 1:D:169:ASP:OD1  | 2.12                     | 0.49              |
| 4:4:213:LYS:O    | 4:4:217:CYS:HB2  | 2.13                     | 0.49              |
| 1:P:471:ASP:HB3  | 1:P:573:GLY:O    | 2.12                     | 0.49              |
| 4:1:124:PHE:CZ   | 4:1:132:MET:HG3  | 2.48                     | 0.49              |
| 4:9:124:PHE:CZ   | 4:9:132:MET:HG3  | 2.48                     | 0.49              |
| 4:9:70:PRO:HG3   | 4:9:81:ASP:HB3   | 1.94                     | 0.49              |
| 1:D:725:ARG:NE   | 1:D:733:PRO:CB   | 1.95                     | 0.49              |
| 1:D:727:LEU:HB2  | 1:D:782:MLY:CE   | 2.43                     | 0.49              |
| 1:D:733:PRO:O    | 1:D:737:PHE:CE1  | 2.53                     | 0.49              |
| 1:G:755:HIS:H    | 1:G:779:ARG:NH2  | 2.09                     | 0.49              |
| 1:G:792:ALA:O    | 3:I:35:ARG:NH1   | 2.46                     | 0.49              |
| 2:N:128:PHE:O    | 2:N:133:ILE:HD11 | 2.13                     | 0.49              |
| 2:N:114:LYS:HG3  | 2:N:137:TRP:CZ2  | 2.47                     | 0.49              |
| 1:J:723:ARG:HH11 | 1:J:723:ARG:HG3  | 1.78                     | 0.49              |
| 1:M:553:MLY:HG2  | 4:1:43:VAL:HG11  | 1.93                     | 0.49              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:C    | 2.86                     | 0.49              |
| 1:P:720:PHE:CD2  | 1:P:744:SER:HB3  | 2.48                     | 0.49              |
| 1:P:649:VAL:HG23 | 1:P:649:VAL:HA   | 1.83                     | 0.49              |
| 1:D:332:MET:O    | 1:D:336:SER:OG   | 2.27                     | 0.49              |
| 1:J:215:GLN:H    | 1:J:340:ILE:CD1  | 2.20                     | 0.49              |
| 1:P:739:ASP:OD1  | 1:P:740:SER:N    | 2.45                     | 0.49              |
| 1:P:173:GLN:OE1  | 1:P:668:HIS:HB3  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:97:LEU:N     | 1:P:97:LEU:HD13  | 2.27                     | 0.49              |
| 1:J:310:TYR:CE2  | 1:J:320:ILE:CD1  | 2.94                     | 0.49              |
| 1:G:128:PRO:O    | 1:G:683:PRO:HB3  | 2.12                     | 0.49              |
| 1:J:51:THR:C     | 1:J:62:VAL:HG13  | 2.32                     | 0.49              |
| 1:A:290:GLN:HG2  | 1:A:331:LEU:CA   | 2.43                     | 0.49              |
| 4:9:198:TYR:CZ   | 4:9:248:ILE:HG13 | 2.48                     | 0.49              |
| 4:7:198:TYR:CZ   | 4:7:248:ILE:HG13 | 2.48                     | 0.49              |
| 1:A:237:THR:HG22 | 1:A:238:VAL:N    | 2.28                     | 0.49              |
| 1:G:134:VAL:C    | 1:G:136:ASN:H    | 2.16                     | 0.49              |
| 1:A:168:THR:HG22 | 1:A:169:ASP:OD1  | 2.12                     | 0.49              |
| 1:G:168:THR:HG22 | 1:G:169:ASP:OD1  | 2.12                     | 0.49              |
| 1:P:595:TRP:CD1  | 1:P:595:TRP:N    | 2.80                     | 0.49              |
| 4:1:299:MET:HE2  | 4:1:331:ALA:HB2  | 1.94                     | 0.49              |
| 4:1:70:PRO:HG3   | 4:1:81:ASP:HB3   | 1.94                     | 0.49              |
| 4:7:124:PHE:CZ   | 4:7:132:MET:HG3  | 2.48                     | 0.49              |
| 4:W:124:PHE:CZ   | 4:W:132:MET:HG3  | 2.48                     | 0.49              |
| 1:D:724:TYR:CB   | 1:D:782:MLY:NZ   | 2.66                     | 0.48              |
| 2:Q:121:LEU:CA   | 2:Q:128:PHE:CG   | 2.89                     | 0.48              |
| 2:Q:128:PHE:O    | 2:Q:133:ILE:HD11 | 2.13                     | 0.48              |
| 2:E:114:LYS:HG3  | 2:E:137:TRP:CZ2  | 2.48                     | 0.48              |
| 1:A:218:LEU:HD22 | 1:A:222:ILE:HG13 | 1.95                     | 0.48              |
| 1:G:818:TYR:HB3  | 2:H:90:GLY:CA    | 2.38                     | 0.48              |
| 1:M:635:GLY:HA3  | 4:Z:334:GLU:CG   | 2.30                     | 0.48              |
| 1:P:789:ALA:HB1  | 3:R:81:GLN:HG2   | 1.94                     | 0.48              |
| 1:M:725:ARG:NE   | 1:M:733:PRO:CB   | 1.95                     | 0.48              |
| 1:M:723:ARG:HH11 | 1:M:723:ARG:HG3  | 1.78                     | 0.48              |
| 4:2:322:PRO:C    | 4:4:244:ASP:HB2  | 2.33                     | 0.48              |
| 3:R:50:LEU:O     | 3:R:55:LYS:HB2   | 2.13                     | 0.48              |
| 1:G:547:ASP:O    | 1:G:550:PHE:HB3  | 2.12                     | 0.48              |
| 1:P:64:THR:CG2   | 1:P:65:GLU:N     | 2.75                     | 0.48              |
| 1:P:251:ARG:HB2  | 1:P:264:ASP:HB3  | 1.95                     | 0.48              |
| 1:P:601:ASP:N    | 1:P:602:PRO:CD   | 2.75                     | 0.48              |
| 4:0:124:PHE:CZ   | 4:0:132:MET:HG3  | 2.48                     | 0.48              |
| 1:M:20:SER:HB3   | 1:M:23:GLU:OE1   | 2.13                     | 0.48              |
| 1:P:405:ARG:HB2  | 1:P:414:THR:OG1  | 2.13                     | 0.48              |
| 4:W:70:PRO:HG3   | 4:W:81:ASP:HB3   | 1.94                     | 0.48              |
| 2:Q:93:PRO:O     | 2:Q:97:ILE:HG13  | 2.12                     | 0.48              |
| 1:J:795:ARG:HE   | 3:L:116:GLU:CB   | 2.26                     | 0.48              |
| 1:D:715:VAL:HG12 | 1:D:716:LEU:O    | 2.12                     | 0.48              |
| 1:M:813:ILE:HG23 | 2:N:128:PHE:CE1  | 2.48                     | 0.48              |
| 2:H:114:LYS:HG3  | 2:H:137:TRP:CZ2  | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:117:LEU:HG   | 2:H:147:ASN:HB3  | 1.93                     | 0.48              |
| 1:J:813:ILE:CG2  | 2:K:128:PHE:CE1  | 2.96                     | 0.48              |
| 1:P:642:LYS:CB   | 4:0:24:ASP:O     | 2.60                     | 0.48              |
| 1:P:642:LYS:HA   | 4:0:22:ALA:C     | 2.33                     | 0.48              |
| 1:A:732:ILE:H    | 1:A:733:PRO:CD   | 2.22                     | 0.48              |
| 1:J:715:VAL:HG12 | 1:J:716:LEU:O    | 2.12                     | 0.48              |
| 1:M:576:GLU:CG   | 1:M:577:ALA:N    | 2.44                     | 0.48              |
| 1:P:793:ARG:O    | 1:P:797:PHE:N    | 2.39                     | 0.48              |
| 1:P:795:ARG:CZ   | 3:R:43:ASN:OD1   | 2.38                     | 0.48              |
| 1:A:542:PHE:CD2  | 4:8:143:TYR:CD1  | 3.02                     | 0.48              |
| 1:M:791:GLN:OE1  | 3:O:116:GLU:N    | 2.35                     | 0.48              |
| 4:3:287:ILE:HG22 | 4:5:204:ALA:H    | 1.74                     | 0.48              |
| 1:M:646:PHE:CE2  | 1:M:652:LEU:CD2  | 2.87                     | 0.48              |
| 4:0:166:TYR:CZ   | 4:2:64:ILE:HG22  | 2.42                     | 0.48              |
| 1:J:41:VAL:CG1   | 1:J:42:HIS:N     | 2.75                     | 0.48              |
| 1:M:97:LEU:HD22  | 1:M:712:PRO:HB2  | 1.95                     | 0.48              |
| 1:A:103:LEU:HD12 | 1:A:103:LEU:C    | 2.33                     | 0.48              |
| 1:A:128:PRO:O    | 1:A:683:PRO:HB3  | 2.12                     | 0.48              |
| 1:J:290:GLN:HG2  | 1:J:331:LEU:CA   | 2.43                     | 0.48              |
| 4:W:198:TYR:CZ   | 4:W:248:ILE:HG13 | 2.48                     | 0.48              |
| 1:D:267:THR:HG21 | 1:D:438:PHE:HE2  | 1.76                     | 0.48              |
| 1:P:267:THR:HG21 | 1:P:438:PHE:HE2  | 1.76                     | 0.48              |
| 1:M:312:TYR:CD1  | 1:M:312:TYR:N    | 2.81                     | 0.48              |
| 1:P:136:ASN:HA   | 1:P:137:PRO:HD3  | 1.50                     | 0.48              |
| 1:G:251:ARG:O    | 1:G:263:ALA:HA   | 2.12                     | 0.48              |
| 1:G:248:MLY:HE2  | 1:G:250:ILE:HD11 | 1.95                     | 0.48              |
| 1:J:168:THR:HG22 | 1:J:169:ASP:OD1  | 2.12                     | 0.48              |
| 1:M:168:THR:HG22 | 1:M:169:ASP:OD1  | 2.12                     | 0.48              |
| 1:M:405:ARG:HB2  | 1:M:414:THR:OG1  | 2.13                     | 0.48              |
| 2:E:93:PRO:O     | 2:E:97:ILE:HG13  | 2.13                     | 0.48              |
| 4:1:213:LYS:O    | 4:1:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:P:729:ALA:HB1  | 3:R:93:VAL:CB    | 2.39                     | 0.48              |
| 2:B:130:PRO:O    | 2:B:131:GLU:C    | 2.52                     | 0.48              |
| 2:B:114:LYS:N    | 2:B:146:GLY:O    | 2.40                     | 0.48              |
| 1:J:530:MET:HE3  | 4:W:354:GLN:CB   | 2.43                     | 0.48              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:HG23 | 2.45                     | 0.48              |
| 4:0:167:GLU:CD   | 4:2:42:GLY:CA    | 2.43                     | 0.48              |
| 1:P:206:LYS:HD2  | 1:P:217:THR:CG2  | 2.17                     | 0.48              |
| 1:G:765:VAL:CG1  | 1:G:766:PHE:N    | 2.77                     | 0.48              |
| 1:D:642:LYS:CB   | 4:9:24:ASP:O     | 2.59                     | 0.48              |
| 1:A:642:LYS:HA   | 4:8:22:ALA:C     | 2.33                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:829:TRP:HZ3  | 2:Q:84:PHE:CE2   | 2.30                     | 0.48              |
| 3:I:50:LEU:O     | 3:I:55:LYS:HB2   | 2.13                     | 0.48              |
| 1:M:97:LEU:N     | 1:M:97:LEU:HD13  | 2.28                     | 0.48              |
| 1:A:723:ARG:HH11 | 1:A:723:ARG:HG3  | 1.78                     | 0.48              |
| 1:J:103:LEU:C    | 1:J:103:LEU:HD12 | 2.33                     | 0.48              |
| 1:G:103:LEU:HD12 | 1:G:103:LEU:C    | 2.33                     | 0.48              |
| 1:J:544:LYS:HD2  | 4:W:147:ARG:CB   | 2.36                     | 0.48              |
| 1:D:310:TYR:CE2  | 1:D:320:ILE:CD1  | 2.94                     | 0.48              |
| 1:D:64:THR:CG2   | 1:D:65:GLU:N     | 2.75                     | 0.48              |
| 4:Z:253:GLU:HA   | 4:Z:256:ARG:CG   | 2.42                     | 0.48              |
| 4:8:198:TYR:CZ   | 4:8:248:ILE:HG13 | 2.48                     | 0.48              |
| 1:D:292:MET:CE   | 1:D:309:PRO:HA   | 2.39                     | 0.48              |
| 4:4:198:TYR:CZ   | 4:4:248:ILE:HG13 | 2.48                     | 0.48              |
| 1:G:237:THR:HG22 | 1:G:238:VAL:N    | 2.28                     | 0.48              |
| 1:A:251:ARG:O    | 1:A:263:ALA:HA   | 2.12                     | 0.48              |
| 4:3:120:THR:HG21 | 4:3:370:VAL:HG11 | 1.95                     | 0.48              |
| 1:P:675:ILE:CG2  | 1:P:676:ILE:N    | 2.74                     | 0.48              |
| 1:P:723:ARG:HG3  | 1:P:723:ARG:HH11 | 1.78                     | 0.48              |
| 1:J:404:PRO:HD2  | 1:J:415:MLY:O    | 2.13                     | 0.48              |
| 1:D:404:PRO:HD2  | 1:D:415:MLY:O    | 2.13                     | 0.48              |
| 1:G:405:ARG:HB2  | 1:G:414:THR:OG1  | 2.13                     | 0.48              |
| 1:M:499:GLU:OE1  | 1:M:499:GLU:HA   | 2.13                     | 0.48              |
| 4:Y:124:PHE:CZ   | 4:Y:132:MET:HG3  | 2.48                     | 0.48              |
| 1:J:405:ARG:HB2  | 1:J:414:THR:OG1  | 2.13                     | 0.48              |
| 1:D:405:ARG:HB2  | 1:D:414:THR:OG1  | 2.13                     | 0.48              |
| 1:D:727:LEU:HD11 | 1:D:782:MLY:HD3  | 1.78                     | 0.48              |
| 1:A:499:GLU:OE1  | 1:A:499:GLU:HA   | 2.13                     | 0.48              |
| 1:A:97:LEU:CD2   | 1:A:712:PRO:C    | 2.81                     | 0.48              |
| 1:G:530:MET:CE   | 4:V:354:GLN:HG3  | 2.34                     | 0.48              |
| 1:G:557:GLU:CB   | 4:X:47:MET:C     | 2.50                     | 0.48              |
| 2:Q:114:LYS:HG3  | 2:Q:137:TRP:CZ2  | 2.48                     | 0.48              |
| 2:Q:140:PHE:HB3  | 2:Q:144:VAL:HG12 | 1.94                     | 0.48              |
| 1:J:819:ASN:ND2  | 2:K:92:ASP:CG    | 2.66                     | 0.48              |
| 2:K:130:PRO:O    | 2:K:131:GLU:C    | 2.52                     | 0.48              |
| 2:K:128:PHE:O    | 2:K:133:ILE:HD11 | 2.13                     | 0.48              |
| 1:J:84:MLY:HH12  | 1:J:715:VAL:HG11 | 1.94                     | 0.48              |
| 1:M:35:MLY:CH2   | 1:M:778:MET:HG3  | 2.37                     | 0.48              |
| 1:J:756:THR:HG21 | 1:J:779:ARG:HB3  | 1.95                     | 0.48              |
| 1:G:834:LEU:CD2  | 2:H:34:ILE:HG12  | 2.43                     | 0.48              |
| 1:M:689:GLU:HG2  | 1:M:689:GLU:O    | 2.14                     | 0.48              |
| 1:M:173:GLN:OE1  | 1:M:668:HIS:HB3  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:173:GLN:OE1  | 1:G:668:HIS:HB3  | 2.13                     | 0.48              |
| 1:P:756:THR:O    | 1:P:758:TYR:N    | 2.45                     | 0.48              |
| 1:M:418:THR:CB   | 1:M:421:GLU:HG3  | 2.37                     | 0.48              |
| 1:A:556:ASP:CA   | 4:V:49:GLN:O     | 2.52                     | 0.48              |
| 1:G:64:THR:CG2   | 1:G:65:GLU:N     | 2.75                     | 0.48              |
| 1:M:51:THR:C     | 1:M:62:VAL:HG13  | 2.32                     | 0.48              |
| 1:J:267:THR:HG21 | 1:J:438:PHE:HE2  | 1.76                     | 0.48              |
| 1:J:136:ASN:O    | 1:J:139:VAL:N    | 2.47                     | 0.48              |
| 1:P:404:PRO:HD2  | 1:P:415:MLY:O    | 2.13                     | 0.48              |
| 1:P:168:THR:HG22 | 1:P:169:ASP:OD1  | 2.12                     | 0.48              |
| 4:5:124:PHE:CZ   | 4:5:132:MET:HG3  | 2.48                     | 0.48              |
| 4:0:70:PRO:HG3   | 4:0:81:ASP:HB3   | 1.94                     | 0.48              |
| 1:M:617:MLY:O    | 1:M:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:G:617:MLY:O    | 1:G:620:ALA:HB3  | 2.14                     | 0.48              |
| 1:J:314:TYR:CZ   | 1:J:362:GLY:HA2  | 2.48                     | 0.48              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:NH1   | 2.24                     | 0.48              |
| 1:A:765:VAL:CG1  | 1:A:766:PHE:N    | 2.77                     | 0.48              |
| 1:G:409:GLY:N    | 1:G:636:LYS:CD   | 2.71                     | 0.48              |
| 1:G:629:GLU:CA   | 1:G:643:GLY:C    | 2.73                     | 0.48              |
| 1:G:538:GLU:HA   | 4:V:351:THR:H    | 1.76                     | 0.48              |
| 2:E:121:LEU:O    | 2:E:128:PHE:CG   | 2.61                     | 0.48              |
| 1:P:732:ILE:H    | 1:P:733:PRO:HD2  | 1.74                     | 0.48              |
| 1:J:28:GLN:OE1   | 1:J:723:ARG:NH1  | 2.42                     | 0.48              |
| 1:J:410:ASN:HD22 | 4:W:336:LYS:HE2  | 1.78                     | 0.48              |
| 1:G:720:PHE:CD2  | 1:G:744:SER:HB3  | 2.48                     | 0.48              |
| 1:D:712:PRO:HB2  | 1:D:771:LEU:CG   | 2.42                     | 0.48              |
| 1:M:720:PHE:CD2  | 1:M:744:SER:HB3  | 2.48                     | 0.48              |
| 1:M:295:MLY:HG3  | 1:M:332:MET:HE2  | 1.94                     | 0.48              |
| 1:A:64:THR:CG2   | 1:A:65:GLU:N     | 2.76                     | 0.48              |
| 1:G:823:PHE:HE1  | 2:H:160:GLY:CA   | 2.27                     | 0.48              |
| 1:A:406:VAL:CG1  | 1:A:407:GLY:N    | 2.77                     | 0.48              |
| 4:4:120:THR:HG21 | 4:4:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:3:124:PHE:CZ   | 4:3:132:MET:HG3  | 2.48                     | 0.48              |
| 1:P:617:MLY:O    | 1:P:620:ALA:HB3  | 2.14                     | 0.48              |
| 4:0:213:LYS:O    | 4:0:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:D:314:TYR:CZ   | 1:D:362:GLY:HA2  | 2.48                     | 0.48              |
| 4:W:213:LYS:O    | 4:W:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:D:765:VAL:CG1  | 1:D:766:PHE:N    | 2.77                     | 0.48              |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:HD11 | 1.75                     | 0.48              |
| 1:P:410:ASN:HD22 | 4:0:336:LYS:HE2  | 1.78                     | 0.48              |
| 1:M:406:VAL:CG1  | 1:M:407:GLY:N    | 2.77                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:530:MET:HA   | 4:Z:354:GLN:CD   | 2.11                     | 0.48              |
| 1:M:544:LYS:HD2  | 4:Z:147:ARG:CB   | 2.36                     | 0.48              |
| 1:M:410:ASN:HD22 | 4:Z:336:LYS:HE2  | 1.78                     | 0.48              |
| 1:D:550:PHE:CE2  | 1:D:592:ILE:CG2  | 2.97                     | 0.48              |
| 1:D:818:TYR:HB3  | 2:E:90:GLY:H     | 1.72                     | 0.48              |
| 1:G:84:MLY:HB3   | 1:G:723:ARG:CD   | 2.42                     | 0.48              |
| 1:M:805:ALA:O    | 1:M:809:ARG:CG   | 2.61                     | 0.48              |
| 1:J:547:ASP:O    | 1:J:550:PHE:HB3  | 2.12                     | 0.48              |
| 1:D:756:THR:O    | 1:D:758:TYR:N    | 2.45                     | 0.48              |
| 4:3:198:TYR:CZ   | 4:3:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:3:253:GLU:HA   | 4:3:256:ARG:CG   | 2.42                     | 0.48              |
| 4:4:250:ILE:HG23 | 4:4:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:M:136:ASN:O    | 1:M:139:VAL:N    | 2.47                     | 0.48              |
| 1:D:617:MLY:O    | 1:D:620:ALA:HB3  | 2.14                     | 0.48              |
| 4:Y:70:PRO:HG3   | 4:Y:81:ASP:HB3   | 1.94                     | 0.48              |
| 1:G:499:GLU:OE1  | 1:G:499:GLU:HA   | 2.13                     | 0.48              |
| 1:A:405:ARG:HB2  | 1:A:414:THR:OG1  | 2.13                     | 0.48              |
| 4:4:124:PHE:CZ   | 4:4:132:MET:HG3  | 2.48                     | 0.48              |
| 1:J:795:ARG:HD2  | 3:L:35:ARG:NH1   | 2.28                     | 0.48              |
| 1:G:795:ARG:CG   | 3:I:118:MET:CE   | 2.54                     | 0.48              |
| 1:A:739:ASP:CB   | 1:A:742:LYS:CB   | 2.81                     | 0.48              |
| 1:D:720:PHE:CD2  | 1:D:744:SER:HB3  | 2.48                     | 0.48              |
| 2:N:130:PRO:O    | 2:N:131:GLU:C    | 2.52                     | 0.48              |
| 1:P:732:ILE:HG21 | 1:P:747:LEU:CD1  | 0.63                     | 0.48              |
| 1:M:544:LYS:O    | 4:1:45:VAL:CG1   | 2.57                     | 0.48              |
| 1:J:538:GLU:HA   | 4:W:351:THR:H    | 1.77                     | 0.48              |
| 1:G:733:PRO:O    | 1:G:737:PHE:CE1  | 2.53                     | 0.48              |
| 1:G:724:TYR:HD1  | 1:G:727:LEU:CD1  | 2.27                     | 0.48              |
| 1:A:836:PHE:CZ   | 2:B:159:HIS:C    | 2.87                     | 0.48              |
| 4:0:288:ASP:OD1  | 4:2:62:ARG:CG    | 2.62                     | 0.48              |
| 1:J:756:THR:C    | 1:J:776:GLU:CD   | 2.68                     | 0.48              |
| 3:F:50:LEU:O     | 3:F:55:LYS:HB2   | 2.13                     | 0.48              |
| 1:M:290:GLN:HG2  | 1:M:331:LEU:CA   | 2.43                     | 0.48              |
| 1:D:51:THR:C     | 1:D:62:VAL:HG13  | 2.32                     | 0.48              |
| 1:A:354:LEU:HA   | 1:A:354:LEU:HD12 | 1.56                     | 0.48              |
| 4:5:250:ILE:HG23 | 4:5:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:Y:250:ILE:HG23 | 4:Y:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:D:436:MLY:HE3  | 1:D:626:TYR:HE1  | 1.77                     | 0.48              |
| 4:V:120:THR:HG21 | 4:V:370:VAL:HG11 | 1.95                     | 0.48              |
| 1:J:10:PHE:CD2   | 1:J:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:A:248:MLY:HE2  | 1:A:250:ILE:HD11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:93:PRO:O     | 2:K:97:ILE:HG13  | 2.12                     | 0.48              |
| 1:J:617:MLY:O    | 1:J:620:ALA:HB3  | 2.14                     | 0.48              |
| 4:Y:213:LYS:O    | 4:Y:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:P:499:GLU:HA   | 1:P:499:GLU:OE1  | 2.13                     | 0.48              |
| 4:Z:213:LYS:O    | 4:Z:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:7:213:LYS:O    | 4:7:217:CYS:HB2  | 2.13                     | 0.48              |
| 4:X:213:LYS:O    | 4:X:217:CYS:HB2  | 2.13                     | 0.48              |
| 2:K:112:ILE:CG2  | 2:K:147:ASN:O    | 2.62                     | 0.48              |
| 1:M:546:THR:CG2  | 1:M:547:ASP:N    | 2.77                     | 0.48              |
| 1:P:546:THR:CG2  | 1:P:547:ASP:N    | 2.77                     | 0.48              |
| 1:A:546:THR:CG2  | 1:A:547:ASP:N    | 2.77                     | 0.48              |
| 1:P:839:MLY:HH11 | 2:Q:158:THR:HG22 | 1.96                     | 0.48              |
| 1:M:214:MET:HA   | 1:M:340:ILE:CD1  | 2.41                     | 0.48              |
| 1:G:834:LEU:CD2  | 2:H:34:ILE:CD1   | 2.92                     | 0.48              |
| 1:P:689:GLU:O    | 1:P:689:GLU:HG2  | 2.14                     | 0.48              |
| 1:D:689:GLU:O    | 1:D:689:GLU:HG2  | 2.14                     | 0.48              |
| 4:V:285:CYS:O    | 4:X:202:THR:HG22 | 2.14                     | 0.48              |
| 4:1:198:TYR:CZ   | 4:1:248:ILE:HG13 | 2.48                     | 0.48              |
| 4:0:250:ILE:HG23 | 4:0:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:7:250:ILE:HG23 | 4:7:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:2:250:ILE:HG23 | 4:2:253:GLU:HG2  | 1.96                     | 0.48              |
| 1:J:87:MLY:HH12  | 1:J:87:MLY:HD3   | 1.61                     | 0.48              |
| 1:G:312:TYR:N    | 1:G:312:TYR:CD1  | 2.80                     | 0.48              |
| 1:J:134:VAL:C    | 1:J:136:ASN:H    | 2.16                     | 0.48              |
| 1:A:10:PHE:CD2   | 1:A:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:G:10:PHE:CD2   | 1:G:17:LEU:HD23  | 2.49                     | 0.48              |
| 1:M:404:PRO:HD2  | 1:M:415:MLY:O    | 2.13                     | 0.48              |
| 1:D:106:LEU:HD12 | 1:D:117:THR:HG21 | 1.96                     | 0.48              |
| 4:5:213:LYS:O    | 4:5:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:J:470:PHE:O    | 1:J:473:ASN:ND2  | 2.40                     | 0.48              |
| 1:D:791:GLN:CD   | 3:F:115:GLY:HA3  | 2.22                     | 0.48              |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:HE   | 1.62                     | 0.48              |
| 2:N:144:VAL:HG12 | 2:N:153:ILE:HD13 | 1.92                     | 0.48              |
| 2:Q:121:LEU:HA   | 2:Q:128:PHE:CD2  | 2.46                     | 0.48              |
| 2:K:140:PHE:HB3  | 2:K:144:VAL:HG12 | 1.94                     | 0.48              |
| 1:D:546:THR:CG2  | 1:D:547:ASP:N    | 2.77                     | 0.48              |
| 1:M:785:GLU:HG3  | 3:O:81:GLN:HG3   | 1.95                     | 0.48              |
| 1:G:97:LEU:N     | 1:G:97:LEU:HD13  | 2.27                     | 0.48              |
| 1:P:154:HIS:CE1  | 1:P:156:PHE:CE2  | 3.02                     | 0.48              |
| 4:W:250:ILE:HG23 | 4:W:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:0:198:TYR:CZ   | 4:0:248:ILE:HG13 | 2.48                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:198:TYR:CZ   | 4:Y:248:ILE:HG13 | 2.48                     | 0.48              |
| 1:D:312:TYR:CD1  | 1:D:312:TYR:N    | 2.81                     | 0.48              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:HD3  | 1.96                     | 0.48              |
| 1:P:136:ASN:O    | 1:P:139:VAL:N    | 2.47                     | 0.48              |
| 1:M:595:TRP:CD1  | 1:M:595:TRP:N    | 2.80                     | 0.48              |
| 2:H:140:PHE:HB3  | 2:H:144:VAL:HG12 | 1.95                     | 0.48              |
| 1:M:550:PHE:CE2  | 1:M:592:ILE:CG2  | 2.97                     | 0.48              |
| 1:J:636:LYS:O    | 4:W:144:ALA:HB1  | 2.14                     | 0.48              |
| 1:P:786:ILE:O    | 1:P:790:THR:N    | 2.47                     | 0.48              |
| 1:P:793:ARG:HA   | 3:R:40:ASN:CB    | 2.42                     | 0.48              |
| 1:D:578:HIS:HB3  | 1:D:592:ILE:CD1  | 2.38                     | 0.48              |
| 1:A:550:PHE:CE2  | 1:A:592:ILE:CG2  | 2.97                     | 0.48              |
| 1:M:786:ILE:CG2  | 1:M:787:ILE:N    | 2.75                     | 0.48              |
| 1:D:712:PRO:HB2  | 1:D:771:LEU:CD2  | 2.44                     | 0.48              |
| 1:G:838:ILE:C    | 1:G:840:PRO:HD2  | 2.34                     | 0.48              |
| 1:D:831:TRP:HZ3  | 2:E:34:ILE:HG12  | 1.79                     | 0.48              |
| 1:A:544:LYS:HD2  | 4:8:147:ARG:CB   | 2.36                     | 0.48              |
| 1:D:544:LYS:HD2  | 4:9:147:ARG:CB   | 2.36                     | 0.48              |
| 4:9:250:ILE:HG23 | 4:9:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:V:250:ILE:HG23 | 4:V:253:GLU:HG2  | 1.96                     | 0.48              |
| 4:X:120:THR:HG21 | 4:X:370:VAL:HG11 | 1.95                     | 0.48              |
| 4:8:120:THR:HG21 | 4:8:370:VAL:HG11 | 1.95                     | 0.48              |
| 1:D:602:PRO:O    | 1:D:603:LEU:HD12 | 2.14                     | 0.48              |
| 1:M:564:ASN:HD22 | 1:M:582:VAL:HB   | 1.79                     | 0.48              |
| 1:D:554:LEU:HA   | 1:D:554:LEU:HD12 | 1.76                     | 0.48              |
| 1:A:617:MLY:O    | 1:A:620:ALA:HB3  | 2.14                     | 0.48              |
| 4:V:213:LYS:O    | 4:V:217:CYS:HB2  | 2.13                     | 0.48              |
| 1:G:792:ALA:HB2  | 3:I:42:THR:N     | 2.07                     | 0.47              |
| 1:A:149:GLN:CD   | 1:A:718:ALA:H    | 2.17                     | 0.47              |
| 2:Q:117:LEU:HG   | 2:Q:147:ASN:HB3  | 1.93                     | 0.47              |
| 2:H:128:PHE:O    | 2:H:133:ILE:HD11 | 2.13                     | 0.47              |
| 1:A:732:ILE:H    | 1:A:733:PRO:HD2  | 1.74                     | 0.47              |
| 1:J:629:GLU:CA   | 1:J:643:GLY:C    | 2.73                     | 0.47              |
| 1:J:542:PHE:CD2  | 4:W:143:TYR:CD1  | 3.02                     | 0.47              |
| 1:D:542:PHE:CD2  | 4:9:143:TYR:CD1  | 3.02                     | 0.47              |
| 1:D:568:PRO:HD3  | 1:D:579:PHE:HA   | 1.96                     | 0.47              |
| 1:M:206:LYS:HD2  | 1:M:217:THR:CG2  | 2.17                     | 0.47              |
| 1:P:550:PHE:CE2  | 1:P:592:ILE:CG2  | 2.97                     | 0.47              |
| 1:M:783:LEU:O    | 1:M:786:ILE:CG1  | 2.46                     | 0.47              |
| 1:P:218:LEU:CD2  | 1:P:222:ILE:CG1  | 2.86                     | 0.47              |
| 1:G:723:ARG:HG3  | 1:G:723:ARG:HH11 | 1.78                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:838:ILE:C    | 1:J:840:PRO:HD2  | 2.35                     | 0.47              |
| 1:M:92:ALA:O     | 1:M:714:ARG:CG   | 2.62                     | 0.47              |
| 1:A:640:LYS:HD2  | 1:A:646:PHE:O    | 2.15                     | 0.47              |
| 4:9:288:ASP:CA   | 4:W:204:ALA:HB2  | 2.31                     | 0.47              |
| 3:C:50:LEU:O     | 3:C:55:LYS:HB2   | 2.13                     | 0.47              |
| 3:L:50:LEU:O     | 3:L:55:LYS:HB2   | 2.13                     | 0.47              |
| 1:J:550:PHE:CE2  | 1:J:592:ILE:CG2  | 2.97                     | 0.47              |
| 1:G:550:PHE:CE2  | 1:G:592:ILE:CG2  | 2.97                     | 0.47              |
| 1:A:689:GLU:O    | 1:A:689:GLU:HG2  | 2.14                     | 0.47              |
| 1:M:310:TYR:CE2  | 1:M:320:ILE:CD1  | 2.94                     | 0.47              |
| 4:1:253:GLU:HA   | 4:1:256:ARG:CG   | 2.42                     | 0.47              |
| 4:3:250:ILE:HG23 | 4:3:253:GLU:HG2  | 1.96                     | 0.47              |
| 1:M:346:ASP:O    | 1:M:350:ALA:N    | 2.45                     | 0.47              |
| 4:2:198:TYR:CZ   | 4:2:248:ILE:HG13 | 2.48                     | 0.47              |
| 1:J:436:MLY:HE3  | 1:J:626:TYR:HE1  | 1.77                     | 0.47              |
| 1:M:237:THR:HG22 | 1:M:238:VAL:N    | 2.28                     | 0.47              |
| 4:Z:120:THR:HG21 | 4:Z:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:D:10:PHE:CD2   | 1:D:17:LEU:HD23  | 2.49                     | 0.47              |
| 1:M:314:TYR:CZ   | 1:M:362:GLY:HA2  | 2.48                     | 0.47              |
| 1:G:564:ASN:HD22 | 1:G:582:VAL:HB   | 1.79                     | 0.47              |
| 1:D:97:LEU:N     | 1:D:97:LEU:HD13  | 2.28                     | 0.47              |
| 1:A:314:TYR:CZ   | 1:A:362:GLY:HA2  | 2.48                     | 0.47              |
| 4:9:213:LYS:O    | 4:9:217:CYS:HB2  | 2.13                     | 0.47              |
| 1:D:759:ALA:O    | 1:D:766:PHE:N    | 2.32                     | 0.47              |
| 1:G:410:ASN:HD22 | 4:V:336:LYS:HE2  | 1.79                     | 0.47              |
| 1:G:538:GLU:CD   | 4:V:355:MET:HE1  | 2.25                     | 0.47              |
| 1:G:556:ASP:OD1  | 4:X:47:MET:CE    | 2.27                     | 0.47              |
| 1:P:732:ILE:H    | 1:P:733:PRO:CD   | 2.23                     | 0.47              |
| 2:H:130:PRO:O    | 2:H:131:GLU:C    | 2.52                     | 0.47              |
| 2:B:128:PHE:O    | 2:B:133:ILE:HD11 | 2.13                     | 0.47              |
| 1:P:636:LYS:O    | 4:0:144:ALA:HB1  | 2.14                     | 0.47              |
| 1:P:792:ALA:CB   | 3:R:42:THR:HA    | 2.44                     | 0.47              |
| 1:A:410:ASN:HD22 | 4:8:336:LYS:HE2  | 1.78                     | 0.47              |
| 4:0:110:LEU:CA   | 4:1:195:GLU:HG3  | 2.44                     | 0.47              |
| 1:D:838:ILE:C    | 1:D:840:PRO:HD2  | 2.34                     | 0.47              |
| 4:1:204:ALA:N    | 4:Z:287:ILE:HG21 | 2.28                     | 0.47              |
| 4:X:291:LYS:CA   | 4:Z:244:ASP:HB3  | 2.37                     | 0.47              |
| 4:X:325:MET:HE1  | 4:Z:244:ASP:OD2  | 2.06                     | 0.47              |
| 1:P:214:MET:C    | 1:P:340:ILE:CD1  | 2.82                     | 0.47              |
| 1:P:829:TRP:CH2  | 2:Q:84:PHE:CE1   | 3.02                     | 0.47              |
| 1:D:800:ARG:HH22 | 3:F:40:ASN:HD21  | 1.25                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:103:LEU:HD12 | 1:D:103:LEU:C    | 2.33                     | 0.47              |
| 4:V:285:CYS:O    | 4:X:202:THR:CG2  | 2.62                     | 0.47              |
| 4:1:250:ILE:HG23 | 4:1:253:GLU:HG2  | 1.96                     | 0.47              |
| 4:Z:250:ILE:HG23 | 4:Z:253:GLU:HG2  | 1.96                     | 0.47              |
| 4:X:250:ILE:HG23 | 4:X:253:GLU:HG2  | 1.96                     | 0.47              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:136:ASN:O    | 1:A:139:VAL:N    | 2.47                     | 0.47              |
| 4:5:120:THR:HG21 | 4:5:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:D:564:ASN:HD22 | 1:D:582:VAL:HB   | 1.79                     | 0.47              |
| 4:8:213:LYS:O    | 4:8:217:CYS:HB2  | 2.13                     | 0.47              |
| 4:3:213:LYS:O    | 4:3:217:CYS:HB2  | 2.13                     | 0.47              |
| 1:D:793:ARG:CZ   | 3:F:87:PHE:HE1   | 2.27                     | 0.47              |
| 1:G:640:LYS:HD2  | 1:G:646:PHE:O    | 2.15                     | 0.47              |
| 2:E:130:PRO:O    | 2:E:131:GLU:C    | 2.52                     | 0.47              |
| 1:P:542:PHE:CD2  | 4:0:143:TYR:CD1  | 3.02                     | 0.47              |
| 1:P:640:LYS:HD2  | 1:P:646:PHE:O    | 2.14                     | 0.47              |
| 1:M:542:PHE:CD2  | 4:Z:143:TYR:CD1  | 3.02                     | 0.47              |
| 1:M:786:ILE:C    | 1:M:790:THR:N    | 2.59                     | 0.47              |
| 1:M:84:MLY:HA    | 1:M:723:ARG:NH1  | 2.28                     | 0.47              |
| 1:A:838:ILE:C    | 1:A:840:PRO:HD2  | 2.35                     | 0.47              |
| 1:M:640:LYS:HD2  | 1:M:646:PHE:O    | 2.14                     | 0.47              |
| 3:R:53:PRO:O     | 3:R:55:LYS:HG3   | 2.15                     | 0.47              |
| 1:J:689:GLU:O    | 1:J:689:GLU:HG2  | 2.14                     | 0.47              |
| 1:D:154:HIS:CE1  | 1:D:156:PHE:CE2  | 3.02                     | 0.47              |
| 4:8:250:ILE:HG23 | 4:8:253:GLU:HG2  | 1.96                     | 0.47              |
| 1:M:134:VAL:C    | 1:M:136:ASN:H    | 2.16                     | 0.47              |
| 1:M:251:ARG:HB2  | 1:M:264:ASP:HB3  | 1.95                     | 0.47              |
| 4:1:120:THR:HG21 | 4:1:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:D:675:ILE:CG2  | 1:D:676:ILE:N    | 2.74                     | 0.47              |
| 1:A:602:PRO:O    | 1:A:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:P:10:PHE:CD2   | 1:P:17:LEU:HD23  | 2.49                     | 0.47              |
| 1:P:194:GLN:HB3  | 1:P:194:GLN:HE21 | 1.43                     | 0.47              |
| 1:G:314:TYR:CZ   | 1:G:362:GLY:HA2  | 2.48                     | 0.47              |
| 4:Y:162:ASN:OD1  | 4:Y:277:THR:HG22 | 2.15                     | 0.47              |
| 4:2:213:LYS:O    | 4:2:217:CYS:HB2  | 2.13                     | 0.47              |
| 1:P:821:ARG:NH2  | 2:Q:127:ARG:CD   | 2.77                     | 0.47              |
| 4:X:324:THR:OG1  | 4:Z:246:GLN:N    | 2.25                     | 0.47              |
| 2:H:121:LEU:O    | 2:H:128:PHE:CG   | 2.61                     | 0.47              |
| 2:B:121:LEU:CA   | 2:B:128:PHE:CG   | 2.89                     | 0.47              |
| 1:M:568:PRO:HD3  | 1:M:579:PHE:HA   | 1.96                     | 0.47              |
| 1:M:538:GLU:HA   | 4:Z:351:THR:H    | 1.77                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:553:MLY:CG   | 4:V:47:MET:N     | 2.54                     | 0.47              |
| 2:N:160:GLY:O    | 2:N:161:GLU:HG2  | 2.14                     | 0.47              |
| 1:P:206:LYS:CE   | 1:P:217:THR:HG23 | 2.30                     | 0.47              |
| 1:D:823:PHE:HD1  | 2:E:160:GLY:CA   | 2.23                     | 0.47              |
| 1:J:214:MET:C    | 1:J:340:ILE:CD1  | 2.82                     | 0.47              |
| 1:A:214:MET:C    | 1:A:340:ILE:CD1  | 2.82                     | 0.47              |
| 1:G:295:MLY:HG3  | 1:G:332:MET:HE2  | 1.94                     | 0.47              |
| 1:J:546:THR:CG2  | 1:J:547:ASP:N    | 2.77                     | 0.47              |
| 1:M:41:VAL:CG1   | 1:M:42:HIS:N     | 2.75                     | 0.47              |
| 1:G:544:LYS:HD2  | 4:V:147:ARG:CB   | 2.36                     | 0.47              |
| 2:H:160:GLY:O    | 2:H:161:GLU:HG2  | 2.15                     | 0.47              |
| 1:G:154:HIS:CE1  | 1:G:156:PHE:CE2  | 3.02                     | 0.47              |
| 4:5:253:GLU:HA   | 4:5:256:ARG:CG   | 2.42                     | 0.47              |
| 1:P:292:MET:HE1  | 1:P:309:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:136:ASN:HA   | 1:A:137:PRO:HD3  | 1.49                     | 0.47              |
| 4:2:120:THR:HG21 | 4:2:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:9:120:THR:HG21 | 4:9:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:7:120:THR:HG21 | 4:7:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:G:106:LEU:HD12 | 1:G:117:THR:HG21 | 1.96                     | 0.47              |
| 4:0:162:ASN:OD1  | 4:0:277:THR:HG22 | 2.15                     | 0.47              |
| 1:G:122:PHE:CE2  | 1:G:700:VAL:HA   | 2.50                     | 0.47              |
| 1:A:122:PHE:CE2  | 1:A:700:VAL:HA   | 2.49                     | 0.47              |
| 4:Z:162:ASN:OD1  | 4:Z:277:THR:HG22 | 2.15                     | 0.47              |
| 1:D:506:GLU:HG3  | 1:D:764:MLY:CE   | 2.44                     | 0.47              |
| 4:1:287:ILE:C    | 4:3:203:THR:HG22 | 2.35                     | 0.47              |
| 2:H:112:ILE:CG2  | 2:H:147:ASN:O    | 2.62                     | 0.47              |
| 1:J:724:TYR:HD1  | 1:J:727:LEU:CD1  | 2.27                     | 0.47              |
| 1:M:538:GLU:CD   | 4:Z:355:MET:HE1  | 2.24                     | 0.47              |
| 1:D:410:ASN:HD22 | 4:9:336:LYS:HE2  | 1.78                     | 0.47              |
| 1:D:524:GLU:HB3  | 1:D:528:MLY:HG2  | 1.97                     | 0.47              |
| 1:A:831:TRP:HZ2  | 2:B:47:LEU:CA    | 2.15                     | 0.47              |
| 1:M:218:LEU:HA   | 1:M:221:GLN:H    | 1.80                     | 0.47              |
| 1:A:538:GLU:HA   | 4:8:351:THR:H    | 1.78                     | 0.47              |
| 1:M:831:TRP:NE1  | 2:N:67:MET:CG    | 2.75                     | 0.47              |
| 1:D:769:ALA:C    | 1:D:774:LEU:CB   | 2.79                     | 0.47              |
| 1:D:640:LYS:HD2  | 1:D:646:PHE:O    | 2.15                     | 0.47              |
| 1:A:646:PHE:HE2  | 1:A:652:LEU:CG   | 2.24                     | 0.47              |
| 1:G:215:GLN:H    | 1:G:340:ILE:CD1  | 2.20                     | 0.47              |
| 3:F:53:PRO:O     | 3:F:55:LYS:HG3   | 2.14                     | 0.47              |
| 1:G:546:THR:CG2  | 1:G:547:ASP:N    | 2.77                     | 0.47              |
| 1:G:689:GLU:HG2  | 1:G:689:GLU:O    | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:814:PHE:CA   | 2:E:127:ARG:NH1  | 2.64                     | 0.47              |
| 1:J:406:VAL:CG1  | 1:J:407:GLY:N    | 2.77                     | 0.47              |
| 1:A:154:HIS:CE1  | 1:A:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:J:188:ASN:ND2  | 1:J:674:CYS:SG   | 2.88                     | 0.47              |
| 1:D:499:GLU:OE1  | 1:D:499:GLU:HA   | 2.13                     | 0.47              |
| 1:D:188:ASN:ND2  | 1:D:674:CYS:SG   | 2.88                     | 0.47              |
| 4:X:162:ASN:OD1  | 4:X:277:THR:HG22 | 2.15                     | 0.47              |
| 1:M:122:PHE:CE2  | 1:M:700:VAL:HA   | 2.50                     | 0.47              |
| 4:7:162:ASN:OD1  | 4:7:277:THR:HG22 | 2.15                     | 0.47              |
| 1:G:795:ARG:HB3  | 3:I:35:ARG:CZ    | 2.45                     | 0.47              |
| 2:Q:130:PRO:O    | 2:Q:131:GLU:C    | 2.52                     | 0.47              |
| 1:A:218:LEU:HA   | 1:A:221:GLN:H    | 1.79                     | 0.47              |
| 2:H:121:LEU:HA   | 2:H:128:PHE:CD2  | 2.47                     | 0.47              |
| 2:H:121:LEU:CA   | 2:H:128:PHE:CG   | 2.89                     | 0.47              |
| 2:K:121:LEU:HA   | 2:K:128:PHE:CD2  | 2.47                     | 0.47              |
| 1:M:220:ASP:O    | 1:M:224:SER:N    | 2.27                     | 0.47              |
| 1:A:783:LEU:HA   | 1:A:786:ILE:HB   | 1.96                     | 0.47              |
| 2:E:160:GLY:O    | 2:E:161:GLU:HG2  | 2.14                     | 0.47              |
| 4:3:287:ILE:HG21 | 4:5:204:ALA:N    | 2.28                     | 0.47              |
| 1:M:642:LYS:CB   | 4:Z:24:ASP:O     | 2.60                     | 0.47              |
| 1:J:568:PRO:HD3  | 1:J:579:PHE:HA   | 1.96                     | 0.47              |
| 2:E:163:ALA:C    | 2:K:22:THR:H     | 2.07                     | 0.47              |
| 1:M:436:MLY:HE3  | 1:M:626:TYR:HE1  | 1.77                     | 0.47              |
| 1:G:22:LYS:O     | 1:G:26:GLU:N     | 2.29                     | 0.47              |
| 1:M:10:PHE:CD2   | 1:M:17:LEU:HD23  | 2.49                     | 0.47              |
| 1:D:248:MLY:HE2  | 1:D:250:ILE:HD11 | 1.95                     | 0.47              |
| 1:P:400:ALA:HB1  | 1:P:606:THR:CG2  | 2.45                     | 0.47              |
| 1:M:559:LEU:HD23 | 1:M:560:GLY:N    | 2.30                     | 0.47              |
| 4:1:162:ASN:OD1  | 4:1:277:THR:HG22 | 2.15                     | 0.47              |
| 4:2:162:ASN:OD1  | 4:2:277:THR:HG22 | 2.15                     | 0.47              |
| 4:W:162:ASN:OD1  | 4:W:277:THR:HG22 | 2.15                     | 0.47              |
| 4:8:299:MET:HE2  | 4:8:331:ALA:HB2  | 1.95                     | 0.47              |
| 1:J:564:ASN:HD22 | 1:J:582:VAL:HB   | 1.79                     | 0.47              |
| 1:P:122:PHE:CE2  | 1:P:700:VAL:HA   | 2.50                     | 0.47              |
| 1:J:800:ARG:HB3  | 3:L:149:VAL:HG13 | 1.97                     | 0.47              |
| 1:D:783:LEU:HA   | 1:D:786:ILE:HB   | 1.96                     | 0.47              |
| 1:A:502:GLU:CA   | 1:A:761:GLY:HA2  | 2.37                     | 0.47              |
| 1:G:542:PHE:CD2  | 4:V:143:TYR:CD1  | 3.03                     | 0.47              |
| 1:G:553:MLY:HH12 | 4:X:45:VAL:CG1   | 2.29                     | 0.47              |
| 1:G:635:GLY:HA3  | 4:V:334:GLU:CG   | 2.30                     | 0.47              |
| 1:G:406:VAL:CG1  | 1:G:407:GLY:N    | 2.77                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:112:ILE:CG2  | 2:Q:147:ASN:O    | 2.62                     | 0.47              |
| 2:E:112:ILE:CG2  | 2:E:147:ASN:O    | 2.62                     | 0.47              |
| 1:J:732:ILE:CG2  | 1:J:747:LEU:CD1  | 0.65                     | 0.47              |
| 1:J:818:TYR:C    | 2:K:90:GLY:HA3   | 2.35                     | 0.47              |
| 2:K:139:ALA:C    | 2:K:141:PRO:HD3  | 2.33                     | 0.47              |
| 2:B:112:ILE:CG2  | 2:B:147:ASN:O    | 2.62                     | 0.47              |
| 1:P:538:GLU:HA   | 4:O:351:THR:H    | 1.77                     | 0.47              |
| 1:P:406:VAL:CG1  | 1:P:407:GLY:N    | 2.77                     | 0.47              |
| 1:M:637:LYS:HD2  | 4:Z:144:ALA:HB3  | 1.20                     | 0.47              |
| 1:M:530:MET:HE3  | 4:Z:354:GLN:CB   | 2.44                     | 0.47              |
| 1:J:524:GLU:HB3  | 1:J:528:MLY:HG2  | 1.97                     | 0.47              |
| 1:P:783:LEU:CD1  | 1:P:783:LEU:N    | 2.78                     | 0.47              |
| 1:P:786:ILE:N    | 1:P:787:ILE:N    | 2.63                     | 0.47              |
| 1:D:530:MET:HE3  | 4:9:354:GLN:CG   | 2.32                     | 0.47              |
| 1:D:636:LYS:O    | 4:9:144:ALA:HB1  | 2.15                     | 0.47              |
| 1:P:568:PRO:HD3  | 1:P:579:PHE:HA   | 1.96                     | 0.47              |
| 1:M:786:ILE:N    | 1:M:787:ILE:N    | 2.62                     | 0.47              |
| 1:P:218:LEU:HA   | 1:P:221:GLN:H    | 1.79                     | 0.47              |
| 1:M:707:CYS:SG   | 1:M:714:ARG:NH1  | 2.88                     | 0.47              |
| 1:M:724:TYR:HD1  | 1:M:727:LEU:CD1  | 2.27                     | 0.47              |
| 1:D:713:SER:HB2  | 1:D:775:LEU:HD21 | 1.92                     | 0.47              |
| 1:M:28:GLN:OE1   | 1:M:723:ARG:NH1  | 2.48                     | 0.47              |
| 1:M:765:VAL:CG1  | 1:M:766:PHE:N    | 2.77                     | 0.47              |
| 4:1:203:THR:OG1  | 4:Z:288:ASP:OD2  | 2.33                     | 0.47              |
| 1:G:202:SER:HA   | 1:G:207:LYS:NZ   | 2.22                     | 0.47              |
| 4:W:325:MET:SD   | 4:Y:244:ASP:OD2  | 2.73                     | 0.47              |
| 1:D:214:MET:C    | 1:D:340:ILE:CD1  | 2.82                     | 0.47              |
| 1:D:831:TRP:CZ3  | 2:E:50:THR:CG2   | 2.97                     | 0.47              |
| 1:P:84:MLY:CH1   | 1:P:724:TYR:CE2  | 2.95                     | 0.47              |
| 1:G:829:TRP:CZ2  | 2:H:83:MET:CE    | 2.97                     | 0.47              |
| 3:O:50:LEU:O     | 3:O:53:PRO:CD    | 2.63                     | 0.47              |
| 3:F:52:ASN:CB    | 3:F:53:PRO:CD    | 2.92                     | 0.47              |
| 3:L:53:PRO:O     | 3:L:55:LYS:HG3   | 2.14                     | 0.47              |
| 4:1:244:ASP:HA   | 4:Z:324:THR:N    | 2.22                     | 0.47              |
| 1:P:41:VAL:CG1   | 1:P:42:HIS:N     | 2.75                     | 0.47              |
| 1:J:664:LEU:HD12 | 1:J:664:LEU:HA   | 1.52                     | 0.47              |
| 1:A:176:LEU:CD1  | 1:A:176:LEU:N    | 2.74                     | 0.47              |
| 1:M:176:LEU:CD1  | 1:M:176:LEU:N    | 2.75                     | 0.47              |
| 4:W:286:ASP:HA   | 4:Y:202:THR:HG22 | 1.32                     | 0.47              |
| 1:J:406:VAL:CG1  | 1:J:407:GLY:H    | 2.28                     | 0.47              |
| 1:G:695:LEU:HB3  | 1:G:701:LEU:HD22 | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:154:HIS:CE1  | 1:J:156:PHE:CE2  | 3.02                     | 0.47              |
| 1:M:154:HIS:CE1  | 1:M:156:PHE:CE2  | 3.02                     | 0.47              |
| 4:2:253:GLU:HA   | 4:2:256:ARG:CG   | 2.42                     | 0.47              |
| 1:D:311:ASP:CB   | 1:D:312:TYR:CE1  | 2.98                     | 0.47              |
| 1:J:519:LEU:CD1  | 1:J:519:LEU:N    | 2.77                     | 0.47              |
| 1:D:556:ASP:CA   | 4:W:49:GLN:O     | 2.52                     | 0.47              |
| 1:A:724:TYR:HD1  | 1:A:727:LEU:CD1  | 2.27                     | 0.47              |
| 1:A:251:ARG:HB2  | 1:A:264:ASP:HB3  | 1.95                     | 0.47              |
| 1:G:251:ARG:HB2  | 1:G:264:ASP:HB3  | 1.95                     | 0.47              |
| 4:Y:120:THR:HG21 | 4:Y:370:VAL:HG11 | 1.95                     | 0.47              |
| 4:W:120:THR:HG21 | 4:W:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:CG   | 2.45                     | 0.47              |
| 1:J:602:PRO:O    | 1:J:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:M:602:PRO:O    | 1:M:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:G:602:PRO:O    | 1:G:603:LEU:HD12 | 2.14                     | 0.47              |
| 1:P:106:LEU:HD12 | 1:P:117:THR:HG21 | 1.96                     | 0.47              |
| 1:A:404:PRO:HD2  | 1:A:415:MLY:O    | 2.13                     | 0.47              |
| 1:D:400:ALA:HB1  | 1:D:606:THR:CG2  | 2.45                     | 0.47              |
| 1:J:400:ALA:HB1  | 1:J:606:THR:CG2  | 2.45                     | 0.47              |
| 1:M:248:MLY:HE2  | 1:M:250:ILE:HD11 | 1.95                     | 0.47              |
| 1:M:289:TYR:OH   | 1:M:315:VAL:O    | 2.27                     | 0.47              |
| 1:A:564:ASN:HD22 | 1:A:582:VAL:HB   | 1.79                     | 0.47              |
| 1:A:595:TRP:CD1  | 1:A:595:TRP:N    | 2.80                     | 0.47              |
| 4:X:299:MET:HE2  | 4:X:331:ALA:HB2  | 1.95                     | 0.47              |
| 4:3:162:ASN:OD1  | 4:3:277:THR:HG22 | 2.15                     | 0.47              |
| 1:G:784:ALA:O    | 1:G:788:THR:CA   | 2.61                     | 0.47              |
| 2:Q:137:TRP:CZ3  | 2:Q:145:ALA:N    | 2.81                     | 0.47              |
| 2:H:137:TRP:CZ3  | 2:H:145:ALA:N    | 2.81                     | 0.47              |
| 1:J:84:MLY:O     | 1:J:723:ARG:HD2  | 2.03                     | 0.47              |
| 1:D:543:PRO:HD2  | 4:9:146:GLY:O    | 2.15                     | 0.47              |
| 2:Q:160:GLY:O    | 2:Q:161:GLU:HG2  | 2.14                     | 0.47              |
| 1:D:823:PHE:CD1  | 2:E:156:VAL:O    | 2.67                     | 0.47              |
| 1:G:214:MET:C    | 1:G:340:ILE:CD1  | 2.82                     | 0.47              |
| 3:R:50:LEU:O     | 3:R:53:PRO:CD    | 2.63                     | 0.47              |
| 1:D:695:LEU:HB3  | 1:D:701:LEU:HD22 | 1.97                     | 0.47              |
| 1:A:406:VAL:CG1  | 1:A:407:GLY:H    | 2.28                     | 0.47              |
| 1:J:311:ASP:CB   | 1:J:312:TYR:CE1  | 2.98                     | 0.47              |
| 1:G:136:ASN:HA   | 1:G:137:PRO:HD3  | 1.49                     | 0.47              |
| 4:0:120:THR:HG21 | 4:0:370:VAL:HG11 | 1.95                     | 0.47              |
| 1:G:404:PRO:HD2  | 1:G:415:MLY:O    | 2.13                     | 0.47              |
| 4:9:162:ASN:OD1  | 4:9:277:THR:HG22 | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:162:ASN:OD1  | 4:8:277:THR:HG22 | 2.15                     | 0.47              |
| 4:4:299:MET:HE2  | 4:4:331:ALA:HB2  | 1.97                     | 0.47              |
| 1:P:188:ASN:ND2  | 1:P:674:CYS:SG   | 2.88                     | 0.47              |
| 1:J:795:ARG:HB2  | 3:L:35:ARG:HH11  | 1.74                     | 0.47              |
| 1:D:723:ARG:HG3  | 1:D:723:ARG:HH11 | 1.79                     | 0.47              |
| 1:D:732:ILE:HG23 | 1:D:747:LEU:HD12 | 0.95                     | 0.47              |
| 1:G:406:VAL:CG1  | 1:G:407:GLY:H    | 2.28                     | 0.47              |
| 2:E:117:LEU:HG   | 2:E:147:ASN:HB3  | 1.93                     | 0.47              |
| 1:P:411:GLU:H    | 4:0:333:PRO:HB2  | 1.80                     | 0.47              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:CD1  | 0.65                     | 0.47              |
| 1:G:218:LEU:HA   | 1:G:221:GLN:H    | 1.79                     | 0.47              |
| 1:P:786:ILE:C    | 1:P:787:ILE:C    | 2.73                     | 0.47              |
| 1:D:406:VAL:CG1  | 1:D:407:GLY:N    | 2.77                     | 0.47              |
| 1:G:148:ARG:CZ   | 1:G:764:MLY:HH21 | 2.45                     | 0.47              |
| 1:A:202:SER:HA   | 1:A:207:LYS:NZ   | 2.22                     | 0.47              |
| 1:M:202:SER:HA   | 1:M:207:LYS:NZ   | 2.22                     | 0.47              |
| 1:D:629:GLU:CB   | 1:D:645:SER:N    | 2.74                     | 0.47              |
| 1:A:629:GLU:CA   | 1:A:643:GLY:C    | 2.73                     | 0.47              |
| 4:8:287:ILE:CB   | 4:V:204:ALA:H    | 2.13                     | 0.47              |
| 3:I:53:PRO:O     | 3:I:55:LYS:HG3   | 2.15                     | 0.47              |
| 3:F:50:LEU:O     | 3:F:53:PRO:CD    | 2.63                     | 0.47              |
| 1:P:42:HIS:O     | 1:P:45:GLN:O     | 2.33                     | 0.47              |
| 1:J:578:HIS:HB3  | 1:J:592:ILE:CD1  | 2.38                     | 0.47              |
| 1:G:664:LEU:HD12 | 1:G:664:LEU:HA   | 1.53                     | 0.47              |
| 4:0:173:HIS:HB3  | 4:1:267:ILE:HA   | 1.97                     | 0.47              |
| 1:J:496:PHE:CE2  | 1:J:514:ASP:HA   | 2.50                     | 0.47              |
| 4:7:253:GLU:HA   | 4:7:256:ARG:CG   | 2.42                     | 0.47              |
| 4:V:253:GLU:HA   | 4:V:256:ARG:CG   | 2.42                     | 0.47              |
| 1:A:106:LEU:HD12 | 1:A:117:THR:HG21 | 1.96                     | 0.47              |
| 1:G:559:LEU:HD23 | 1:G:560:GLY:N    | 2.30                     | 0.47              |
| 1:J:122:PHE:CE2  | 1:J:700:VAL:HA   | 2.50                     | 0.47              |
| 1:M:194:GLN:HB3  | 1:M:194:GLN:HE21 | 1.44                     | 0.47              |
| 1:D:783:LEU:CD1  | 1:D:783:LEU:N    | 2.78                     | 0.47              |
| 1:D:715:VAL:HG11 | 1:D:720:PHE:CD1  | 2.50                     | 0.47              |
| 1:G:530:MET:HE3  | 4:V:355:MET:SD   | 2.54                     | 0.47              |
| 1:G:543:PRO:HD2  | 4:V:146:GLY:O    | 2.15                     | 0.47              |
| 1:G:646:PHE:HE2  | 1:G:652:LEU:CG   | 2.24                     | 0.47              |
| 1:P:629:GLU:HG2  | 1:P:643:GLY:C    | 2.35                     | 0.47              |
| 1:A:732:ILE:HG23 | 1:A:747:LEU:HD12 | 0.94                     | 0.47              |
| 1:J:218:LEU:HA   | 1:J:221:GLN:H    | 1.79                     | 0.47              |
| 1:M:543:PRO:HD2  | 4:Z:146:GLY:O    | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:732:ILE:HG21 | 1:G:747:LEU:CD1  | 0.64                     | 0.47              |
| 1:P:578:HIS:HB3  | 1:P:592:ILE:CD1  | 2.38                     | 0.47              |
| 1:A:538:GLU:OE1  | 4:8:355:MET:HE3  | 2.15                     | 0.47              |
| 1:A:636:LYS:O    | 4:8:144:ALA:HB1  | 2.15                     | 0.47              |
| 1:P:838:ILE:C    | 1:P:840:PRO:HD2  | 2.35                     | 0.47              |
| 1:D:726:VAL:C    | 1:D:785:GLU:HG2  | 2.35                     | 0.47              |
| 1:P:714:ARG:HD3  | 1:P:766:PHE:CE2  | 2.50                     | 0.47              |
| 1:M:643:GLY:CA   | 4:Z:24:ASP:OD1   | 2.62                     | 0.47              |
| 1:M:829:TRP:CE3  | 2:N:87:LYS:NZ    | 2.72                     | 0.47              |
| 1:P:134:VAL:C    | 1:P:136:ASN:H    | 2.16                     | 0.47              |
| 1:A:400:ALA:HB1  | 1:A:606:THR:CG2  | 2.45                     | 0.47              |
| 1:G:188:ASN:ND2  | 1:G:674:CYS:SG   | 2.88                     | 0.47              |
| 1:G:595:TRP:N    | 1:G:595:TRP:CD1  | 2.80                     | 0.47              |
| 1:J:554:LEU:HA   | 1:J:554:LEU:HD12 | 1.77                     | 0.47              |
| 1:D:30:MLY:HB3   | 1:D:31:PRO:HD2   | 1.97                     | 0.47              |
| 4:V:162:ASN:OD1  | 4:V:277:THR:HG22 | 2.15                     | 0.47              |
| 1:P:564:ASN:HD22 | 1:P:582:VAL:HB   | 1.79                     | 0.47              |
| 1:G:793:ARG:O    | 1:G:797:PHE:N    | 2.39                     | 0.46              |
| 1:D:714:ARG:HD3  | 1:D:766:PHE:CE2  | 2.50                     | 0.46              |
| 2:N:112:ILE:CG2  | 2:N:147:ASN:O    | 2.62                     | 0.46              |
| 1:G:637:LYS:HD2  | 4:V:144:ALA:HB3  | 1.20                     | 0.46              |
| 1:P:730:SER:H    | 3:R:93:VAL:HG23  | 1.73                     | 0.46              |
| 2:H:137:TRP:CA   | 2:H:145:ALA:HB2  | 2.37                     | 0.46              |
| 1:G:819:ASN:ND2  | 2:H:91:ALA:C     | 2.66                     | 0.46              |
| 1:J:821:ARG:CZ   | 2:K:127:ARG:CD   | 2.92                     | 0.46              |
| 2:K:137:TRP:CZ3  | 2:K:145:ALA:N    | 2.81                     | 0.46              |
| 1:P:640:LYS:C    | 4:0:23:GLY:C     | 2.74                     | 0.46              |
| 1:M:406:VAL:CG1  | 1:M:407:GLY:H    | 2.28                     | 0.46              |
| 1:J:640:LYS:C    | 4:W:23:GLY:C     | 2.74                     | 0.46              |
| 1:P:798:LEU:HD12 | 3:R:126:LEU:CD2  | 2.32                     | 0.46              |
| 1:D:406:VAL:CG1  | 1:D:407:GLY:H    | 2.28                     | 0.46              |
| 1:M:783:LEU:CD1  | 1:M:783:LEU:N    | 2.78                     | 0.46              |
| 1:G:506:GLU:OE2  | 1:G:760:PHE:C    | 2.52                     | 0.46              |
| 4:0:244:ASP:N    | 4:Y:291:LYS:HE2  | 0.24                     | 0.46              |
| 1:M:642:LYS:HA   | 4:Z:21:PHE:C     | 2.36                     | 0.46              |
| 1:G:214:MET:HA   | 1:G:340:ILE:CD1  | 2.41                     | 0.46              |
| 1:J:97:LEU:HD22  | 1:J:712:PRO:CB   | 2.42                     | 0.46              |
| 3:I:50:LEU:O     | 3:I:53:PRO:CD    | 2.63                     | 0.46              |
| 1:A:41:VAL:CG1   | 1:A:42:HIS:N     | 2.75                     | 0.46              |
| 1:J:42:HIS:O     | 1:J:45:GLN:O     | 2.33                     | 0.46              |
| 1:G:568:PRO:HD3  | 1:G:579:PHE:HA   | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:374:GLN:NE2  | 1:P:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:J:374:GLN:NE2  | 1:J:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:D:496:PHE:CE2  | 1:D:514:ASP:HA   | 2.50                     | 0.46              |
| 1:A:144:ARG:HA   | 1:A:144:ARG:HD2  | 1.78                     | 0.46              |
| 1:A:524:GLU:HB3  | 1:A:528:MLY:HG2  | 1.96                     | 0.46              |
| 1:P:602:PRO:O    | 1:P:603:LEU:HD12 | 2.14                     | 0.46              |
| 1:J:248:MLY:HE2  | 1:J:250:ILE:HD11 | 1.95                     | 0.46              |
| 4:5:299:MET:HE2  | 4:5:331:ALA:HB2  | 1.96                     | 0.46              |
| 1:P:554:LEU:HD12 | 1:P:554:LEU:HA   | 1.77                     | 0.46              |
| 1:J:499:GLU:OE1  | 1:J:499:GLU:HA   | 2.13                     | 0.46              |
| 2:B:88:LEU:HB3   | 2:B:91:ALA:HB2   | 1.97                     | 0.46              |
| 4:4:162:ASN:OD1  | 4:4:277:THR:HG22 | 2.15                     | 0.46              |
| 1:P:289:TYR:OH   | 1:P:315:VAL:O    | 2.27                     | 0.46              |
| 1:J:797:PHE:HE2  | 3:L:126:LEU:HD13 | 1.81                     | 0.46              |
| 1:G:408:VAL:HG22 | 1:G:636:LYS:HG2  | 1.51                     | 0.46              |
| 2:K:137:TRP:CA   | 2:K:145:ALA:CB   | 2.82                     | 0.46              |
| 2:B:139:ALA:C    | 2:B:141:PRO:HD3  | 2.33                     | 0.46              |
| 1:J:629:GLU:HG2  | 1:J:643:GLY:C    | 2.35                     | 0.46              |
| 1:J:640:LYS:HD2  | 1:J:646:PHE:O    | 2.15                     | 0.46              |
| 1:P:791:GLN:CD   | 3:R:116:GLU:H    | 2.17                     | 0.46              |
| 1:D:221:GLN:H    | 1:D:221:GLN:HG2  | 1.47                     | 0.46              |
| 1:A:795:ARG:CG   | 3:C:118:MET:CE   | 2.88                     | 0.46              |
| 1:M:783:LEU:C    | 1:M:786:ILE:CG1  | 2.58                     | 0.46              |
| 1:G:93:MET:HG3   | 1:G:714:ARG:HG3  | 1.98                     | 0.46              |
| 2:B:160:GLY:O    | 2:B:161:GLU:HG2  | 2.14                     | 0.46              |
| 1:P:503:TYR:OH   | 1:P:711:PHE:CD2  | 2.31                     | 0.46              |
| 4:0:166:TYR:OH   | 4:2:64:ILE:CD1   | 2.59                     | 0.46              |
| 1:P:712:PRO:HB2  | 1:P:713:SER:H    | 1.61                     | 0.46              |
| 1:P:496:PHE:CE2  | 1:P:514:ASP:HA   | 2.50                     | 0.46              |
| 1:A:87:MLY:HH12  | 1:A:87:MLY:HD3   | 1.62                     | 0.46              |
| 1:M:87:MLY:HH12  | 1:M:87:MLY:HD3   | 1.61                     | 0.46              |
| 1:P:311:ASP:CB   | 1:P:312:TYR:CE1  | 2.98                     | 0.46              |
| 1:A:265:ILE:CG2  | 1:A:266:GLU:N    | 2.78                     | 0.46              |
| 1:P:248:MLY:HE2  | 1:P:250:ILE:HD11 | 1.95                     | 0.46              |
| 1:P:559:LEU:HD23 | 1:P:560:GLY:N    | 2.30                     | 0.46              |
| 1:A:559:LEU:HD23 | 1:A:560:GLY:N    | 2.30                     | 0.46              |
| 4:Z:299:MET:HE2  | 4:Z:331:ALA:HB2  | 1.95                     | 0.46              |
| 1:D:122:PHE:CE2  | 1:D:700:VAL:HA   | 2.50                     | 0.46              |
| 4:V:299:MET:HE2  | 4:V:331:ALA:HB2  | 1.96                     | 0.46              |
| 1:A:504:MLY:C    | 1:A:762:HIS:HE2  | 2.26                     | 0.46              |
| 1:G:636:LYS:O    | 4:V:144:ALA:HB1  | 2.14                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:725:ARG:NE   | 1:P:733:PRO:CB   | 1.95                     | 0.46              |
| 1:J:819:ASN:CG   | 2:K:90:GLY:O     | 2.53                     | 0.46              |
| 1:J:765:VAL:CG1  | 1:J:766:PHE:N    | 2.77                     | 0.46              |
| 1:J:543:PRO:HD2  | 4:W:146:GLY:O    | 2.15                     | 0.46              |
| 1:J:529:PRO:HB2  | 4:W:354:GLN:HB3  | 1.97                     | 0.46              |
| 1:P:795:ARG:NE   | 3:R:116:GLU:CB   | 2.71                     | 0.46              |
| 1:D:540:CYS:N    | 4:9:349:LEU:HD11 | 2.31                     | 0.46              |
| 1:A:543:PRO:HD2  | 4:8:146:GLY:O    | 2.15                     | 0.46              |
| 1:A:568:PRO:HD3  | 1:A:579:PHE:HA   | 1.96                     | 0.46              |
| 1:M:838:ILE:C    | 1:M:840:PRO:HD2  | 2.35                     | 0.46              |
| 1:J:839:MLY:HH13 | 2:K:159:HIS:HD2  | 1.81                     | 0.46              |
| 1:D:768:MLY:O    | 1:D:771:LEU:HD11 | 2.05                     | 0.46              |
| 1:A:640:LYS:HB3  | 1:A:645:SER:CB   | 2.42                     | 0.46              |
| 1:P:804:ARG:C    | 1:P:808:GLU:H    | 2.17                     | 0.46              |
| 4:0:166:TYR:OH   | 4:2:64:ILE:CB    | 2.64                     | 0.46              |
| 3:C:53:PRO:O     | 3:C:55:LYS:HG3   | 2.15                     | 0.46              |
| 1:A:42:HIS:O     | 1:A:45:GLN:O     | 2.33                     | 0.46              |
| 1:D:42:HIS:O     | 1:D:45:GLN:O     | 2.33                     | 0.46              |
| 4:W:6:THR:HG22   | 4:W:101:HIS:HA   | 1.98                     | 0.46              |
| 4:0:6:THR:HG22   | 4:0:101:HIS:HA   | 1.98                     | 0.46              |
| 1:M:664:LEU:HA   | 1:M:664:LEU:HD12 | 1.52                     | 0.46              |
| 1:M:556:ASP:OD2  | 4:1:49:GLN:CD    | 2.51                     | 0.46              |
| 1:G:418:THR:CB   | 1:G:421:GLU:HG3  | 2.37                     | 0.46              |
| 1:G:139:VAL:HG12 | 1:G:143:TYR:HD2  | 1.81                     | 0.46              |
| 1:M:292:MET:HE1  | 1:M:309:PRO:CG   | 2.46                     | 0.46              |
| 1:M:265:ILE:CG2  | 1:M:266:GLU:N    | 2.78                     | 0.46              |
| 1:P:82:PRO:HG2   | 1:P:85:TYR:CE2   | 2.50                     | 0.46              |
| 1:J:106:LEU:HD12 | 1:J:117:THR:HG21 | 1.96                     | 0.46              |
| 1:J:559:LEU:HD23 | 1:J:560:GLY:N    | 2.30                     | 0.46              |
| 1:J:783:LEU:N    | 1:J:783:LEU:CD1  | 2.78                     | 0.46              |
| 1:D:732:ILE:CG2  | 1:D:747:LEU:CD1  | 0.65                     | 0.46              |
| 1:A:715:VAL:CG1  | 1:A:720:PHE:HB2  | 2.46                     | 0.46              |
| 1:G:411:GLU:H    | 4:V:333:PRO:HB2  | 1.80                     | 0.46              |
| 1:J:817:GLN:HG2  | 2:K:127:ARG:CG   | 2.44                     | 0.46              |
| 1:P:543:PRO:HD2  | 4:0:146:GLY:O    | 2.15                     | 0.46              |
| 1:P:797:PHE:CE1  | 3:R:149:VAL:HG11 | 2.48                     | 0.46              |
| 1:D:543:PRO:CD   | 4:9:143:TYR:O    | 2.64                     | 0.46              |
| 1:D:530:MET:HE3  | 4:9:354:GLN:CB   | 2.44                     | 0.46              |
| 1:A:411:GLU:H    | 4:8:333:PRO:HB2  | 1.80                     | 0.46              |
| 1:M:839:MLY:HH11 | 2:N:158:THR:HG22 | 1.96                     | 0.46              |
| 1:D:82:PRO:HG2   | 1:D:85:TYR:CE2   | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:503:TYR:CZ   | 1:P:711:PHE:CE2  | 3.01                     | 0.46              |
| 1:D:640:LYS:HB3  | 1:D:645:SER:CB   | 2.42                     | 0.46              |
| 1:D:642:LYS:HB2  | 4:9:24:ASP:O     | 1.88                     | 0.46              |
| 1:M:214:MET:C    | 1:M:340:ILE:CD1  | 2.82                     | 0.46              |
| 4:Y:6:THR:HG22   | 4:Y:101:HIS:HA   | 1.98                     | 0.46              |
| 4:9:6:THR:HG22   | 4:9:101:HIS:HA   | 1.98                     | 0.46              |
| 1:D:374:GLN:NE2  | 1:D:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:M:139:VAL:HG12 | 1:M:143:TYR:HD2  | 1.81                     | 0.46              |
| 1:J:82:PRO:HG2   | 1:J:85:TYR:CE2   | 2.50                     | 0.46              |
| 1:A:188:ASN:ND2  | 1:A:674:CYS:SG   | 2.88                     | 0.46              |
| 1:D:443:ILE:HG22 | 1:D:444:ARG:N    | 2.29                     | 0.46              |
| 1:D:725:ARG:CG   | 1:D:733:PRO:HA   | 2.43                     | 0.46              |
| 1:G:524:GLU:HB3  | 1:G:528:MLY:HG2  | 1.96                     | 0.46              |
| 1:G:640:LYS:HB3  | 1:G:645:SER:CB   | 2.42                     | 0.46              |
| 2:Q:140:PHE:HA   | 2:Q:141:PRO:HD2  | 1.56                     | 0.46              |
| 2:E:137:TRP:CZ3  | 2:E:145:ALA:N    | 2.81                     | 0.46              |
| 2:B:144:VAL:HG12 | 2:B:153:ILE:HD13 | 1.92                     | 0.46              |
| 1:J:206:LYS:HD3  | 1:J:217:THR:OG1  | 2.16                     | 0.46              |
| 1:J:93:MET:HG2   | 1:J:715:VAL:CA   | 2.41                     | 0.46              |
| 1:J:540:CYS:N    | 4:W:349:LEU:HD11 | 2.31                     | 0.46              |
| 1:J:642:LYS:HA   | 4:W:21:PHE:C     | 2.36                     | 0.46              |
| 1:J:534:SER:HB2  | 4:W:354:GLN:HE22 | 1.56                     | 0.46              |
| 1:D:529:PRO:HB2  | 4:9:354:GLN:HB3  | 1.98                     | 0.46              |
| 1:D:206:LYS:HD3  | 1:D:217:THR:OG1  | 2.16                     | 0.46              |
| 1:D:218:LEU:HA   | 1:D:221:GLN:H    | 1.79                     | 0.46              |
| 2:K:160:GLY:O    | 2:K:161:GLU:HG2  | 2.14                     | 0.46              |
| 1:M:714:ARG:HD3  | 1:M:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:G:835:PHE:CE1  | 2:H:30:ALA:HB2   | 2.51                     | 0.46              |
| 1:D:640:LYS:C    | 4:9:23:GLY:C     | 2.74                     | 0.46              |
| 1:M:640:LYS:C    | 4:Z:23:GLY:C     | 2.74                     | 0.46              |
| 1:A:642:LYS:CB   | 4:8:24:ASP:O     | 2.59                     | 0.46              |
| 1:D:831:TRP:HH2  | 2:E:47:LEU:HA    | 1.71                     | 0.46              |
| 4:8:324:THR:O    | 4:V:244:ASP:HA   | 2.08                     | 0.46              |
| 1:G:278:GLN:HB3  | 1:G:278:GLN:HE21 | 1.42                     | 0.46              |
| 1:A:695:LEU:HB3  | 1:A:701:LEU:HD22 | 1.97                     | 0.46              |
| 1:A:374:GLN:NE2  | 1:A:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:HG13 | 1.98                     | 0.46              |
| 1:M:188:ASN:ND2  | 1:M:674:CYS:SG   | 2.88                     | 0.46              |
| 1:P:448:GLN:C    | 1:P:450:ASP:H    | 2.19                     | 0.46              |
| 1:A:714:ARG:HD3  | 1:A:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:D:715:VAL:CG1  | 1:D:720:PHE:HB2  | 2.46                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:732:ILE:CG2  | 1:J:747:LEU:HD12 | 0.35                     | 0.46              |
| 1:G:820:VAL:CG1  | 2:H:136:MET:HE1  | 2.45                     | 0.46              |
| 1:J:83:PRO:O     | 1:J:723:ARG:CZ   | 2.62                     | 0.46              |
| 1:D:410:ASN:HA   | 4:9:334:GLU:HB3  | 1.29                     | 0.46              |
| 1:A:543:PRO:CD   | 4:8:143:TYR:O    | 2.64                     | 0.46              |
| 1:P:839:MLY:HH11 | 2:Q:158:THR:CG2  | 2.46                     | 0.46              |
| 1:G:715:VAL:CG1  | 1:G:720:PHE:HB2  | 2.45                     | 0.46              |
| 1:M:715:VAL:HG11 | 1:M:720:PHE:CD1  | 2.50                     | 0.46              |
| 1:M:715:VAL:CG1  | 1:M:720:PHE:HB2  | 2.45                     | 0.46              |
| 1:G:835:PHE:O    | 1:G:839:MLY:N    | 2.49                     | 0.46              |
| 1:J:202:SER:HA   | 1:J:207:LYS:NZ   | 2.22                     | 0.46              |
| 1:P:765:VAL:CG1  | 1:P:766:PHE:N    | 2.77                     | 0.46              |
| 1:M:640:LYS:C    | 1:M:645:SER:HG   | 2.11                     | 0.46              |
| 1:P:215:GLN:H    | 1:P:340:ILE:CD1  | 2.20                     | 0.46              |
| 1:A:796:GLY:HA3  | 3:C:40:ASN:OD1   | 2.16                     | 0.46              |
| 1:G:374:GLN:NE2  | 1:G:403:TYR:CE1  | 2.84                     | 0.46              |
| 4:0:366:GLY:O    | 4:0:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:G:400:ALA:HB1  | 1:G:606:THR:CG2  | 2.45                     | 0.46              |
| 1:G:752:ASP:CB   | 1:G:783:LEU:HB2  | 2.46                     | 0.46              |
| 1:G:410:ASN:HA   | 4:V:334:GLU:HB3  | 1.28                     | 0.46              |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:NE   | 2.14                     | 0.46              |
| 2:Q:114:LYS:CG   | 2:Q:146:GLY:HA2  | 2.46                     | 0.46              |
| 1:P:540:CYS:N    | 4:0:349:LEU:HD11 | 2.31                     | 0.46              |
| 1:P:529:PRO:HB2  | 4:0:354:GLN:HB3  | 1.98                     | 0.46              |
| 1:P:632:GLY:HA3  | 1:P:643:GLY:N    | 2.17                     | 0.46              |
| 1:J:218:LEU:HD22 | 1:J:222:ILE:HG13 | 1.95                     | 0.46              |
| 1:J:714:ARG:HD3  | 1:J:766:PHE:CE2  | 2.50                     | 0.46              |
| 1:M:529:PRO:HB2  | 4:Z:354:GLN:HB3  | 1.98                     | 0.46              |
| 1:J:530:MET:CE   | 4:W:354:GLN:HG3  | 2.35                     | 0.46              |
| 1:A:797:PHE:CE1  | 3:C:146:ILE:CB   | 2.98                     | 0.46              |
| 1:P:206:LYS:HD3  | 1:P:217:THR:OG1  | 2.16                     | 0.46              |
| 1:D:629:GLU:HG2  | 1:D:643:GLY:C    | 2.35                     | 0.46              |
| 1:D:642:LYS:HA   | 4:9:21:PHE:C     | 2.36                     | 0.46              |
| 1:A:640:LYS:C    | 4:8:23:GLY:C     | 2.74                     | 0.46              |
| 1:A:800:ARG:HH21 | 3:C:40:ASN:CG    | 2.12                     | 0.46              |
| 1:A:664:LEU:HD12 | 1:A:664:LEU:HA   | 1.53                     | 0.46              |
| 1:A:810:ARG:HG2  | 1:A:810:ARG:NH1  | 2.29                     | 0.46              |
| 1:G:311:ASP:CB   | 1:G:312:TYR:CE1  | 2.98                     | 0.46              |
| 1:P:335:ASP:OD1  | 1:P:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:D:335:ASP:OD1  | 1:D:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:A:335:ASP:OD1  | 1:A:348:MLY:NZ   | 2.49                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:136:ASN:O    | 1:D:139:VAL:N    | 2.47                     | 0.46              |
| 1:J:30:MLY:HB3   | 1:J:31:PRO:HD2   | 1.97                     | 0.46              |
| 1:G:326:ASP:O    | 1:G:330:GLU:HG2  | 2.16                     | 0.46              |
| 1:A:326:ASP:O    | 1:A:330:GLU:HG2  | 2.16                     | 0.46              |
| 1:D:508:ILE:HD13 | 1:D:766:PHE:CD2  | 2.51                     | 0.46              |
| 2:E:114:LYS:CG   | 2:E:146:GLY:HA2  | 2.46                     | 0.46              |
| 1:A:206:LYS:HD3  | 1:A:217:THR:OG1  | 2.16                     | 0.46              |
| 2:B:114:LYS:CG   | 2:B:146:GLY:HA2  | 2.46                     | 0.46              |
| 1:P:642:LYS:HA   | 4:O:21:PHE:C     | 2.36                     | 0.46              |
| 1:G:206:LYS:HD3  | 1:G:217:THR:OG1  | 2.16                     | 0.46              |
| 1:J:206:LYS:HD2  | 1:J:217:THR:CG2  | 2.17                     | 0.46              |
| 1:J:93:MET:CG    | 1:J:715:VAL:HA   | 2.45                     | 0.46              |
| 1:M:553:MLY:HG2  | 4:1:43:VAL:CG1   | 2.45                     | 0.46              |
| 1:M:732:ILE:CG2  | 1:M:747:LEU:CD1  | 0.65                     | 0.46              |
| 1:G:93:MET:CG    | 1:G:714:ARG:CA   | 2.76                     | 0.46              |
| 1:M:84:MLY:HD3   | 1:M:723:ARG:HD3  | 1.96                     | 0.46              |
| 1:P:715:VAL:CG1  | 1:P:720:PHE:HB2  | 2.45                     | 0.46              |
| 1:P:803:TYR:HE2  | 3:R:17:PHE:CZ    | 2.34                     | 0.46              |
| 1:D:831:TRP:CE2  | 2:E:47:LEU:HD22  | 2.51                     | 0.46              |
| 4:8:288:ASP:CA   | 4:V:204:ALA:HB2  | 2.31                     | 0.46              |
| 1:D:708:ARG:CA   | 1:D:710:GLY:N    | 2.78                     | 0.46              |
| 1:A:418:THR:CG2  | 1:A:419:VAL:N    | 2.79                     | 0.46              |
| 1:M:89:GLU:CD    | 1:M:153:PRO:HD2  | 2.36                     | 0.46              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:HG13 | 1.98                     | 0.46              |
| 1:G:335:ASP:OD1  | 1:G:348:MLY:NZ   | 2.49                     | 0.46              |
| 1:M:292:MET:HE1  | 1:M:309:PRO:HD3  | 1.98                     | 0.46              |
| 1:M:311:ASP:CB   | 1:M:312:TYR:CE1  | 2.98                     | 0.46              |
| 4:W:366:GLY:O    | 4:W:369:ILE:HG22 | 2.16                     | 0.46              |
| 4:Y:366:GLY:O    | 4:Y:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:M:659:MLY:HD2  | 1:M:659:MLY:HH22 | 1.42                     | 0.46              |
| 1:A:464:ILE:CG2  | 1:A:465:ALA:N    | 2.79                     | 0.46              |
| 1:G:82:PRO:HG2   | 1:G:85:TYR:CE2   | 2.50                     | 0.46              |
| 1:D:97:LEU:HD12  | 1:D:97:LEU:HA    | 1.67                     | 0.46              |
| 1:D:595:TRP:CD1  | 1:D:595:TRP:N    | 2.80                     | 0.46              |
| 1:A:361:TYR:O    | 1:A:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:G:754:ASP:O    | 1:G:776:GLU:CD   | 2.55                     | 0.46              |
| 1:G:642:LYS:HA   | 4:V:21:PHE:C     | 2.36                     | 0.46              |
| 1:M:524:GLU:HB3  | 1:M:528:MLY:HG2  | 1.97                     | 0.46              |
| 1:M:540:CYS:N    | 4:Z:349:LEU:HD11 | 2.31                     | 0.46              |
| 1:A:642:LYS:HA   | 4:8:21:PHE:C     | 2.36                     | 0.46              |
| 3:C:52:ASN:CB    | 3:C:53:PRO:HD3   | 2.28                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:6:THR:HG22   | 4:7:101:HIS:HA   | 1.98                     | 0.46              |
| 4:2:6:THR:HG22   | 4:2:101:HIS:HA   | 1.98                     | 0.46              |
| 4:4:6:THR:HG22   | 4:4:101:HIS:HA   | 1.97                     | 0.46              |
| 4:1:223:PHE:CD2  | 4:1:259:GLU:HG3  | 2.51                     | 0.46              |
| 1:G:89:GLU:CD    | 1:G:153:PRO:HD2  | 2.36                     | 0.46              |
| 1:P:322:VAL:HB   | 1:P:325:ILE:HG13 | 1.98                     | 0.46              |
| 4:4:190:MET:O    | 4:4:194:THR:HG23 | 2.16                     | 0.46              |
| 4:2:366:GLY:O    | 4:2:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:A:311:ASP:CB   | 1:A:312:TYR:CE1  | 2.98                     | 0.46              |
| 1:D:265:ILE:CG2  | 1:D:266:GLU:N    | 2.78                     | 0.46              |
| 4:5:162:ASN:OD1  | 4:5:277:THR:HG22 | 2.15                     | 0.46              |
| 4:7:299:MET:HE2  | 4:7:331:ALA:HB2  | 1.97                     | 0.46              |
| 1:J:361:TYR:O    | 1:J:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:J:791:GLN:NE2  | 3:L:116:GLU:H    | 2.13                     | 0.46              |
| 1:D:794:CYS:O    | 1:D:797:PHE:HB3  | 2.16                     | 0.46              |
| 1:A:505:MLY:CB   | 1:A:762:HIS:N    | 2.79                     | 0.46              |
| 2:H:88:LEU:HB3   | 2:H:91:ALA:HB2   | 1.98                     | 0.46              |
| 2:K:112:ILE:O    | 2:K:148:VAL:HA   | 2.17                     | 0.46              |
| 1:G:725:ARG:HH21 | 1:G:733:PRO:HB2  | 1.81                     | 0.46              |
| 1:G:750:GLY:HA3  | 3:I:114:LEU:HD22 | 1.96                     | 0.46              |
| 1:M:206:LYS:HD3  | 1:M:217:THR:OG1  | 2.16                     | 0.46              |
| 1:A:793:ARG:O    | 1:A:797:PHE:N    | 2.39                     | 0.46              |
| 1:A:797:PHE:CD2  | 3:C:146:ILE:HG23 | 2.46                     | 0.46              |
| 1:P:202:SER:HA   | 1:P:207:LYS:NZ   | 2.22                     | 0.46              |
| 1:M:642:LYS:HB3  | 4:Z:24:ASP:HB2   | 1.37                     | 0.46              |
| 2:K:88:LEU:HB3   | 2:K:91:ALA:HB2   | 1.98                     | 0.46              |
| 1:G:834:LEU:CD2  | 2:H:34:ILE:HD11  | 2.46                     | 0.46              |
| 3:L:50:LEU:O     | 3:L:53:PRO:CD    | 2.63                     | 0.46              |
| 4:5:6:THR:HG22   | 4:5:101:HIS:HA   | 1.97                     | 0.46              |
| 1:D:99:GLU:N     | 1:D:100:PRO:CD   | 2.79                     | 0.46              |
| 1:M:695:LEU:HB3  | 1:M:701:LEU:HD22 | 1.97                     | 0.46              |
| 1:M:374:GLN:NE2  | 1:M:403:TYR:CE1  | 2.84                     | 0.46              |
| 1:G:823:PHE:CE1  | 2:H:156:VAL:O    | 2.69                     | 0.46              |
| 1:A:496:PHE:CE2  | 1:A:514:ASP:HA   | 2.50                     | 0.46              |
| 1:M:496:PHE:CE2  | 1:M:514:ASP:HA   | 2.50                     | 0.46              |
| 2:N:88:LEU:HB3   | 2:N:91:ALA:HB2   | 1.98                     | 0.46              |
| 4:W:253:GLU:HA   | 4:W:256:ARG:CG   | 2.42                     | 0.46              |
| 1:G:436:MLY:HE3  | 1:G:626:TYR:HE1  | 1.77                     | 0.46              |
| 1:J:810:ARG:NH1  | 1:J:810:ARG:HG2  | 2.29                     | 0.46              |
| 1:A:322:VAL:HB   | 1:A:325:ILE:HG13 | 1.98                     | 0.46              |
| 4:5:190:MET:O    | 4:5:194:THR:HG23 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:9:366:GLY:O    | 4:9:369:ILE:HG22 | 2.16                     | 0.46              |
| 1:J:265:ILE:CG2  | 1:J:266:GLU:N    | 2.79                     | 0.46              |
| 1:G:265:ILE:CG2  | 1:G:266:GLU:N    | 2.78                     | 0.46              |
| 1:A:82:PRO:HG2   | 1:A:85:TYR:CE2   | 2.50                     | 0.46              |
| 1:D:559:LEU:HD23 | 1:D:560:GLY:N    | 2.30                     | 0.46              |
| 1:D:448:GLN:C    | 1:D:450:ASP:H    | 2.19                     | 0.46              |
| 1:P:361:TYR:O    | 1:P:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:G:361:TYR:O    | 1:G:364:LEU:HB2  | 2.16                     | 0.46              |
| 1:J:330:GLU:O    | 1:J:333:ALA:HB3  | 2.16                     | 0.46              |
| 1:G:543:PRO:CD   | 4:V:143:TYR:O    | 2.65                     | 0.45              |
| 1:J:725:ARG:HH21 | 1:J:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:G:206:LYS:HD2  | 1:G:217:THR:CG2  | 2.17                     | 0.45              |
| 1:M:639:GLY:CA   | 4:Z:344:SER:O    | 2.39                     | 0.45              |
| 1:A:783:LEU:N    | 1:A:783:LEU:CD1  | 2.79                     | 0.45              |
| 1:J:510:TRP:CZ2  | 1:J:772:LEU:HD11 | 2.51                     | 0.45              |
| 1:D:202:SER:HA   | 1:D:207:LYS:NZ   | 2.22                     | 0.45              |
| 1:M:640:LYS:HB3  | 1:M:645:SER:CB   | 2.42                     | 0.45              |
| 3:O:53:PRO:O     | 3:O:55:LYS:HG3   | 2.15                     | 0.45              |
| 3:C:50:LEU:O     | 3:C:53:PRO:CD    | 2.63                     | 0.45              |
| 1:G:42:HIS:O     | 1:G:45:GLN:O     | 2.33                     | 0.45              |
| 1:M:667:THR:O    | 1:M:669:PRO:HD3  | 2.17                     | 0.45              |
| 4:W:223:PHE:CD2  | 4:W:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:D:89:GLU:CD    | 1:D:153:PRO:HD2  | 2.36                     | 0.45              |
| 1:D:292:MET:HE3  | 1:D:309:PRO:CA   | 2.43                     | 0.45              |
| 1:G:144:ARG:HA   | 1:G:144:ARG:HD2  | 1.78                     | 0.45              |
| 1:G:322:VAL:HB   | 1:G:325:ILE:HG13 | 1.98                     | 0.45              |
| 4:2:190:MET:O    | 4:2:194:THR:HG23 | 2.16                     | 0.45              |
| 4:W:190:MET:O    | 4:W:194:THR:HG23 | 2.16                     | 0.45              |
| 4:3:190:MET:O    | 4:3:194:THR:HG23 | 2.16                     | 0.45              |
| 4:7:366:GLY:O    | 4:7:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:G:464:ILE:CG2  | 1:G:465:ALA:N    | 2.80                     | 0.45              |
| 1:P:723:ARG:CG   | 1:P:723:ARG:NH1  | 2.79                     | 0.45              |
| 1:M:361:TYR:O    | 1:M:364:LEU:HB2  | 2.16                     | 0.45              |
| 4:Z:32:PRO:HB2   | 4:Z:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:G:795:ARG:CZ   | 3:I:116:GLU:OE2  | 2.64                     | 0.45              |
| 2:N:139:ALA:C    | 2:N:141:PRO:HD3  | 2.33                     | 0.45              |
| 1:G:540:CYS:N    | 4:V:349:LEU:HD11 | 2.31                     | 0.45              |
| 1:P:543:PRO:CD   | 4:0:143:TYR:O    | 2.64                     | 0.45              |
| 1:P:544:LYS:CE   | 4:2:45:VAL:HG22  | 2.46                     | 0.45              |
| 1:P:406:VAL:CG1  | 1:P:407:GLY:H    | 2.28                     | 0.45              |
| 1:P:410:ASN:HA   | 4:0:334:GLU:HB3  | 1.29                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:725:ARG:NE   | 1:A:733:PRO:CB   | 1.95                     | 0.45              |
| 1:M:836:PHE:CD2  | 2:N:160:GLY:CA   | 2.99                     | 0.45              |
| 1:P:804:ARG:O    | 1:P:808:GLU:CB   | 2.64                     | 0.45              |
| 1:M:42:HIS:O     | 1:M:45:GLN:O     | 2.33                     | 0.45              |
| 4:W:287:ILE:HG13 | 4:Y:202:THR:HG23 | 1.72                     | 0.45              |
| 4:3:223:PHE:CD2  | 4:3:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:J:695:LEU:HB3  | 1:J:701:LEU:HD22 | 1.97                     | 0.45              |
| 1:J:186:THR:O    | 1:J:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:J:335:ASP:OD1  | 1:J:348:MLY:NZ   | 2.49                     | 0.45              |
| 1:A:139:VAL:HG12 | 1:A:143:TYR:HD2  | 1.81                     | 0.45              |
| 1:M:464:ILE:CG2  | 1:M:465:ALA:N    | 2.80                     | 0.45              |
| 1:M:82:PRO:HG2   | 1:M:85:TYR:CE2   | 2.50                     | 0.45              |
| 1:A:210:GLN:C    | 1:A:211:SER:HG   | 2.14                     | 0.45              |
| 1:M:106:LEU:HD12 | 1:M:117:THR:HG21 | 1.96                     | 0.45              |
| 1:M:485:GLU:OE1  | 1:M:583:HIS:ND1  | 2.49                     | 0.45              |
| 1:J:448:GLN:C    | 1:J:450:ASP:H    | 2.19                     | 0.45              |
| 1:D:476:GLU:OE2  | 1:D:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:G:448:GLN:C    | 1:G:450:ASP:H    | 2.19                     | 0.45              |
| 1:A:443:ILE:HG22 | 1:A:444:ARG:N    | 2.29                     | 0.45              |
| 1:G:30:MLY:HB3   | 1:G:31:PRO:HD2   | 1.97                     | 0.45              |
| 1:A:30:MLY:HB3   | 1:A:31:PRO:HD2   | 1.97                     | 0.45              |
| 1:D:724:TYR:CE1  | 1:D:778:MET:CB   | 2.99                     | 0.45              |
| 1:D:795:ARG:HD2  | 3:F:43:ASN:CG    | 2.36                     | 0.45              |
| 1:G:540:CYS:C    | 4:V:349:LEU:HD21 | 2.36                     | 0.45              |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:HE   | 1.62                     | 0.45              |
| 2:Q:112:ILE:O    | 2:Q:148:VAL:HA   | 2.17                     | 0.45              |
| 1:A:206:LYS:CE   | 1:A:217:THR:HG23 | 2.30                     | 0.45              |
| 1:J:725:ARG:HA   | 1:J:732:ILE:HG22 | 1.99                     | 0.45              |
| 2:B:121:LEU:O    | 2:B:128:PHE:CG   | 2.61                     | 0.45              |
| 1:J:759:ALA:O    | 1:J:766:PHE:N    | 2.32                     | 0.45              |
| 1:J:642:LYS:NZ   | 4:W:340:TRP:O    | 2.50                     | 0.45              |
| 1:D:411:GLU:H    | 4:9:333:PRO:CB   | 2.29                     | 0.45              |
| 1:G:148:ARG:HE   | 1:G:764:MLY:CH2  | 2.28                     | 0.45              |
| 1:D:835:PHE:O    | 1:D:839:MLY:N    | 2.49                     | 0.45              |
| 1:A:629:GLU:HG2  | 1:A:643:GLY:C    | 2.35                     | 0.45              |
| 1:J:830:PRO:HB3  | 2:K:67:MET:CE    | 2.47                     | 0.45              |
| 4:7:288:ASP:CA   | 4:9:204:ALA:HB2  | 2.31                     | 0.45              |
| 1:A:723:ARG:CG   | 1:A:723:ARG:NH1  | 2.80                     | 0.45              |
| 1:A:667:THR:O    | 1:A:669:PRO:HD3  | 2.16                     | 0.45              |
| 1:M:418:THR:CG2  | 1:M:419:VAL:N    | 2.79                     | 0.45              |
| 4:8:253:GLU:HA   | 4:8:256:ARG:CG   | 2.42                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:476:GLU:OE2  | 1:A:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:M:326:ASP:O    | 1:M:330:GLU:HG2  | 2.16                     | 0.45              |
| 4:X:32:PRO:HB2   | 4:X:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:P:330:GLU:O    | 1:P:333:ALA:HB3  | 2.16                     | 0.45              |
| 1:D:724:TYR:HE1  | 1:D:779:ARG:N    | 2.12                     | 0.45              |
| 1:D:732:ILE:CD1  | 1:D:782:MLY:CH2  | 2.94                     | 0.45              |
| 1:A:97:LEU:HD12  | 1:A:97:LEU:HA    | 1.67                     | 0.45              |
| 2:Q:88:LEU:HB3   | 2:Q:91:ALA:HB2   | 1.98                     | 0.45              |
| 1:P:642:LYS:NZ   | 4:O:340:TRP:O    | 2.50                     | 0.45              |
| 1:A:725:ARG:CG   | 1:A:733:PRO:HA   | 2.43                     | 0.45              |
| 1:J:642:LYS:CB   | 4:W:24:ASP:O     | 2.60                     | 0.45              |
| 1:M:835:PHE:O    | 1:M:839:MLY:N    | 2.49                     | 0.45              |
| 1:M:794:CYS:O    | 1:M:797:PHE:HB3  | 2.17                     | 0.45              |
| 1:M:782:MLY:CD   | 3:O:86:ASP:OD1   | 2.49                     | 0.45              |
| 1:G:93:MET:CE    | 1:G:764:MLY:HD2  | 2.01                     | 0.45              |
| 1:D:712:PRO:CG   | 1:D:771:LEU:HD13 | 2.47                     | 0.45              |
| 1:A:214:MET:HA   | 1:A:340:ILE:CD1  | 2.42                     | 0.45              |
| 1:J:94:MET:C     | 1:J:713:SER:CB   | 2.65                     | 0.45              |
| 1:G:55:MLY:HH23  | 1:G:60:VAL:HG22  | 1.99                     | 0.45              |
| 4:X:6:THR:HG22   | 4:X:101:HIS:HA   | 1.98                     | 0.45              |
| 1:A:55:MLY:HH23  | 1:A:60:VAL:HG22  | 1.99                     | 0.45              |
| 1:M:55:MLY:HH23  | 1:M:60:VAL:HG22  | 1.99                     | 0.45              |
| 4:Z:6:THR:HG22   | 4:Z:101:HIS:HA   | 1.98                     | 0.45              |
| 1:M:278:GLN:HE21 | 1:M:278:GLN:HB3  | 1.42                     | 0.45              |
| 1:A:278:GLN:HB3  | 1:A:278:GLN:HE21 | 1.42                     | 0.45              |
| 1:G:418:THR:CG2  | 1:G:419:VAL:N    | 2.79                     | 0.45              |
| 4:9:223:PHE:CD2  | 4:9:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:4:223:PHE:CD2  | 4:4:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:P:695:LEU:HB3  | 1:P:701:LEU:HD22 | 1.97                     | 0.45              |
| 1:J:89:GLU:CD    | 1:J:153:PRO:HD2  | 2.37                     | 0.45              |
| 1:P:186:THR:O    | 1:P:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:G:186:THR:O    | 1:G:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:M:335:ASP:OD1  | 1:M:348:MLY:NZ   | 2.49                     | 0.45              |
| 4:3:366:GLY:O    | 4:3:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:1:366:GLY:O    | 4:1:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:D:464:ILE:CG2  | 1:D:465:ALA:N    | 2.79                     | 0.45              |
| 1:A:106:LEU:HD12 | 1:A:106:LEU:HA   | 1.79                     | 0.45              |
| 1:M:400:ALA:HB1  | 1:M:606:THR:CG2  | 2.45                     | 0.45              |
| 4:7:324:THR:N    | 4:9:245:GLY:CA   | 2.69                     | 0.45              |
| 1:J:476:GLU:OE2  | 1:J:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:M:448:GLN:C    | 1:M:450:ASP:H    | 2.19                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:299:MET:HE2  | 4:Y:331:ALA:HB2  | 1.98                     | 0.45              |
| 1:G:783:LEU:CD1  | 1:G:783:LEU:N    | 2.78                     | 0.45              |
| 1:G:529:PRO:HB2  | 4:V:354:GLN:HB3  | 1.98                     | 0.45              |
| 2:H:112:ILE:O    | 2:H:148:VAL:HA   | 2.16                     | 0.45              |
| 1:P:786:ILE:CG2  | 1:P:787:ILE:N    | 2.78                     | 0.45              |
| 1:P:789:ALA:HB2  | 3:R:81:GLN:CD    | 2.35                     | 0.45              |
| 1:A:529:PRO:HB2  | 4:8:354:GLN:HB3  | 1.98                     | 0.45              |
| 1:M:793:ARG:O    | 1:M:797:PHE:N    | 2.39                     | 0.45              |
| 1:P:839:MLY:HD2  | 2:Q:159:HIS:HB3  | 1.99                     | 0.45              |
| 1:M:725:ARG:CG   | 1:M:733:PRO:CA   | 2.95                     | 0.45              |
| 4:0:110:LEU:O    | 4:1:195:GLU:CB   | 2.64                     | 0.45              |
| 1:D:632:GLY:HA3  | 1:D:643:GLY:N    | 2.17                     | 0.45              |
| 1:A:632:GLY:HA3  | 1:A:643:GLY:N    | 2.17                     | 0.45              |
| 1:D:332:MET:HG2  | 1:D:332:MET:H    | 1.52                     | 0.45              |
| 1:G:332:MET:O    | 1:G:336:SER:OG   | 2.27                     | 0.45              |
| 4:3:6:THR:HG22   | 4:3:101:HIS:HA   | 1.98                     | 0.45              |
| 1:M:829:TRP:CH2  | 2:N:84:PHE:CE1   | 3.04                     | 0.45              |
| 1:G:173:GLN:HG3  | 1:G:670:HIS:HD2  | 1.82                     | 0.45              |
| 1:M:753:VAL:HG13 | 1:M:775:LEU:HD21 | 1.96                     | 0.45              |
| 1:A:701:LEU:HA   | 1:A:701:LEU:HD12 | 1.55                     | 0.45              |
| 1:G:496:PHE:CE2  | 1:G:514:ASP:HA   | 2.50                     | 0.45              |
| 1:P:89:GLU:CD    | 1:P:153:PRO:HD2  | 2.36                     | 0.45              |
| 1:J:292:MET:HE1  | 1:J:309:PRO:CG   | 2.47                     | 0.45              |
| 1:A:296:MLY:O    | 1:A:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:M:322:VAL:HB   | 1:M:325:ILE:HG13 | 1.98                     | 0.45              |
| 1:P:524:GLU:HB3  | 1:P:528:MLY:HG2  | 1.97                     | 0.45              |
| 1:P:265:ILE:CG2  | 1:P:266:GLU:N    | 2.79                     | 0.45              |
| 1:D:106:LEU:HD12 | 1:D:106:LEU:HA   | 1.79                     | 0.45              |
| 1:J:326:ASP:O    | 1:J:330:GLU:HG2  | 2.16                     | 0.45              |
| 1:D:326:ASP:O    | 1:D:330:GLU:HG2  | 2.16                     | 0.45              |
| 1:J:194:GLN:HE21 | 1:J:194:GLN:HB3  | 1.43                     | 0.45              |
| 1:P:673:ARG:HD2  | 1:P:673:ARG:HA   | 1.79                     | 0.45              |
| 1:J:595:TRP:N    | 1:J:595:TRP:CD1  | 2.80                     | 0.45              |
| 1:D:179:GLY:O    | 1:D:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:P:476:GLU:OE2  | 1:P:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:A:448:GLN:C    | 1:A:450:ASP:H    | 2.19                     | 0.45              |
| 1:G:795:ARG:HA   | 3:I:118:MET:SD   | 2.57                     | 0.45              |
| 1:G:629:GLU:CB   | 1:G:645:SER:N    | 2.74                     | 0.45              |
| 2:Q:117:LEU:CG   | 2:Q:147:ASN:OD1  | 2.52                     | 0.45              |
| 1:P:725:ARG:HH21 | 1:P:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:J:747:LEU:C    | 1:J:749:GLY:H    | 2.20                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:715:VAL:CG1  | 1:J:720:PHE:HB2  | 2.45                     | 0.45              |
| 1:M:408:VAL:CG1  | 4:Z:332:PRO:HB3  | 2.40                     | 0.45              |
| 1:J:640:LYS:HB3  | 1:J:645:SER:CB   | 2.41                     | 0.45              |
| 1:P:795:ARG:CD   | 3:R:118:MET:HE2  | 2.46                     | 0.45              |
| 1:G:725:ARG:CG   | 1:G:733:PRO:HA   | 2.43                     | 0.45              |
| 2:E:88:LEU:HB3   | 2:E:91:ALA:HB2   | 1.98                     | 0.45              |
| 1:M:84:MLY:CB    | 1:M:723:ARG:CZ   | 2.94                     | 0.45              |
| 1:D:642:LYS:NZ   | 4:9:340:TRP:O    | 2.50                     | 0.45              |
| 1:D:642:LYS:HB3  | 4:9:24:ASP:HB2   | 1.37                     | 0.45              |
| 1:D:640:LYS:C    | 1:D:645:SER:HG   | 2.09                     | 0.45              |
| 1:M:646:PHE:HE2  | 1:M:652:LEU:CG   | 2.25                     | 0.45              |
| 1:D:295:MLY:CG   | 1:D:332:MET:HE1  | 2.46                     | 0.45              |
| 1:M:214:MET:CA   | 1:M:340:ILE:HD11 | 2.45                     | 0.45              |
| 1:D:41:VAL:CG1   | 1:D:42:HIS:N     | 2.75                     | 0.45              |
| 1:M:103:LEU:HD22 | 1:M:692:LEU:HG   | 1.98                     | 0.45              |
| 1:J:173:GLN:HG3  | 1:J:670:HIS:HD2  | 1.82                     | 0.45              |
| 1:P:99:GLU:N     | 1:P:100:PRO:CD   | 2.80                     | 0.45              |
| 1:D:103:LEU:HD22 | 1:D:692:LEU:HG   | 1.98                     | 0.45              |
| 4:X:190:MET:O    | 4:X:194:THR:HG23 | 2.16                     | 0.45              |
| 4:7:190:MET:O    | 4:7:194:THR:HG23 | 2.16                     | 0.45              |
| 4:4:366:GLY:O    | 4:4:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:5:366:GLY:O    | 4:5:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:M:488:GLN:O    | 1:M:491:PHE:HB3  | 2.17                     | 0.45              |
| 1:P:326:ASP:O    | 1:P:330:GLU:HG2  | 2.16                     | 0.45              |
| 1:D:330:GLU:O    | 1:D:333:ALA:HB3  | 2.17                     | 0.45              |
| 4:7:32:PRO:HB2   | 4:7:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:3:32:PRO:HB2   | 4:3:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:9:299:MET:HE2  | 4:9:331:ALA:HB2  | 1.98                     | 0.45              |
| 4:V:32:PRO:HB2   | 4:V:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:179:GLY:O    | 1:A:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:P:30:MLY:HB3   | 1:P:31:PRO:HD2   | 1.97                     | 0.45              |
| 2:N:137:TRP:CZ3  | 2:N:145:ALA:N    | 2.81                     | 0.45              |
| 1:G:642:LYS:NZ   | 4:V:340:TRP:O    | 2.50                     | 0.45              |
| 1:G:639:GLY:CA   | 4:V:344:SER:O    | 2.40                     | 0.45              |
| 1:J:817:GLN:HB3  | 2:K:127:ARG:HD3  | 1.97                     | 0.45              |
| 1:J:816:ILE:HD11 | 2:K:100:ALA:HB1  | 1.99                     | 0.45              |
| 1:J:449:LEU:HA   | 1:J:449:LEU:HD12 | 1.60                     | 0.45              |
| 1:M:578:HIS:HB3  | 1:M:592:ILE:CD1  | 2.38                     | 0.45              |
| 1:A:411:GLU:H    | 4:8:333:PRO:CB   | 2.30                     | 0.45              |
| 1:P:835:PHE:O    | 1:P:839:MLY:N    | 2.49                     | 0.45              |
| 1:P:836:PHE:CD2  | 2:Q:160:GLY:CA   | 3.00                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:714:ARG:HD3  | 1:G:766:PHE:CE2  | 2.50                     | 0.45              |
| 1:A:836:PHE:CE2  | 2:B:160:GLY:N    | 2.81                     | 0.45              |
| 1:P:506:GLU:HG2  | 1:P:759:ALA:CB   | 2.47                     | 0.45              |
| 1:A:642:LYS:NZ   | 4:8:340:TRP:O    | 2.50                     | 0.45              |
| 1:A:642:LYS:HB3  | 4:8:24:ASP:HB2   | 1.37                     | 0.45              |
| 1:P:84:MLY:HH13  | 1:P:724:TYR:OH   | 2.15                     | 0.45              |
| 1:A:332:MET:HG2  | 1:A:332:MET:H    | 1.52                     | 0.45              |
| 1:M:769:ALA:C    | 1:M:770:GLY:C    | 2.76                     | 0.45              |
| 4:8:6:THR:HG22   | 4:8:101:HIS:HA   | 1.97                     | 0.45              |
| 1:P:664:LEU:HA   | 1:P:664:LEU:HD12 | 1.52                     | 0.45              |
| 1:P:418:THR:CG2  | 1:P:419:VAL:N    | 2.79                     | 0.45              |
| 4:X:223:PHE:CD2  | 4:X:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:D:296:MLY:O    | 1:D:299:LEU:HB2  | 2.17                     | 0.45              |
| 4:Y:190:MET:O    | 4:Y:194:THR:HG23 | 2.16                     | 0.45              |
| 4:8:366:GLY:O    | 4:8:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:P:17:LEU:HD12  | 1:P:17:LEU:HA    | 1.67                     | 0.45              |
| 1:J:179:GLY:O    | 1:J:185:LYS:HE2  | 2.17                     | 0.45              |
| 1:G:597:GLU:O    | 1:G:600:MLY:N    | 2.50                     | 0.45              |
| 4:5:32:PRO:HB2   | 4:5:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:G:476:GLU:OE2  | 1:G:598:MLY:HH13 | 2.17                     | 0.45              |
| 1:A:501:GLU:HB3  | 1:A:762:HIS:CG   | 2.52                     | 0.45              |
| 1:A:711:PHE:HB3  | 1:A:766:PHE:HB3  | 1.99                     | 0.45              |
| 1:P:530:MET:HE3  | 4:0:354:GLN:CG   | 2.38                     | 0.45              |
| 1:D:226:ASN:N    | 1:D:227:PRO:HD2  | 2.32                     | 0.45              |
| 1:M:800:ARG:CB   | 3:O:149:VAL:HG22 | 2.35                     | 0.45              |
| 1:M:795:ARG:HB2  | 3:O:35:ARG:CZ    | 2.47                     | 0.45              |
| 1:M:642:LYS:NZ   | 4:Z:340:TRP:O    | 2.50                     | 0.45              |
| 1:J:332:MET:O    | 1:J:336:SER:OG   | 2.27                     | 0.45              |
| 4:V:6:THR:HG22   | 4:V:101:HIS:HA   | 1.98                     | 0.45              |
| 4:1:322:PRO:CA   | 4:3:244:ASP:HB2  | 2.47                     | 0.45              |
| 1:P:173:GLN:HG3  | 1:P:670:HIS:HD2  | 1.82                     | 0.45              |
| 1:G:99:GLU:N     | 1:G:100:PRO:CD   | 2.80                     | 0.45              |
| 1:D:612:GLN:NE2  | 1:D:627:GLY:H    | 2.14                     | 0.45              |
| 4:5:223:PHE:CD2  | 4:5:259:GLU:HG3  | 2.52                     | 0.45              |
| 4:V:223:PHE:CD2  | 4:V:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:Z:223:PHE:CD2  | 4:Z:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:D:486:MLY:HH22 | 1:D:527:GLU:CD   | 2.37                     | 0.45              |
| 1:D:186:THR:O    | 1:D:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:A:163:TYR:O    | 1:A:166:MET:HB3  | 2.16                     | 0.45              |
| 1:D:14:ALA:N     | 1:D:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:P:292:MET:HE1  | 1:P:309:PRO:CG   | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:322:VAL:HA   | 1:P:323:PRO:HD3  | 1.87                     | 0.45              |
| 1:G:296:MLY:O    | 1:G:299:LEU:HB2  | 2.17                     | 0.45              |
| 1:M:296:MLY:O    | 1:M:299:LEU:HB2  | 2.17                     | 0.45              |
| 4:0:190:MET:O    | 4:0:194:THR:HG23 | 2.16                     | 0.45              |
| 4:8:190:MET:O    | 4:8:194:THR:HG23 | 2.16                     | 0.45              |
| 4:1:190:MET:O    | 4:1:194:THR:HG23 | 2.16                     | 0.45              |
| 1:D:361:TYR:O    | 1:D:364:LEU:HB2  | 2.16                     | 0.45              |
| 4:5:171:LEU:HA   | 4:5:172:PRO:HD2  | 1.84                     | 0.45              |
| 1:J:793:ARG:O    | 1:J:797:PHE:N    | 2.39                     | 0.45              |
| 1:D:725:ARG:HH21 | 1:D:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:G:757:GLN:CB   | 1:G:776:GLU:CG   | 2.89                     | 0.45              |
| 1:P:817:GLN:HG3  | 2:Q:128:PHE:CE1  | 2.52                     | 0.45              |
| 1:P:725:ARG:HA   | 1:P:732:ILE:HG22 | 1.99                     | 0.45              |
| 1:A:206:LYS:HD2  | 1:A:217:THR:CG2  | 2.17                     | 0.45              |
| 2:H:139:ALA:C    | 2:H:141:PRO:HD3  | 2.33                     | 0.45              |
| 2:B:137:TRP:CZ3  | 2:B:145:ALA:N    | 2.81                     | 0.45              |
| 1:A:725:ARG:CG   | 1:A:733:PRO:CA   | 2.95                     | 0.45              |
| 1:A:725:ARG:HH21 | 1:A:733:PRO:HB2  | 1.81                     | 0.45              |
| 1:P:794:CYS:O    | 1:P:797:PHE:HB3  | 2.17                     | 0.45              |
| 1:A:794:CYS:O    | 1:A:797:PHE:HB3  | 2.17                     | 0.45              |
| 1:A:795:ARG:NH2  | 3:C:116:GLU:CB   | 2.60                     | 0.45              |
| 1:P:568:PRO:CG   | 1:P:578:HIS:H    | 2.30                     | 0.45              |
| 1:A:637:LYS:HD2  | 4:8:144:ALA:HB3  | 1.21                     | 0.45              |
| 1:A:540:CYS:N    | 4:8:349:LEU:HD11 | 2.31                     | 0.45              |
| 1:M:759:ALA:O    | 1:M:766:PHE:N    | 2.32                     | 0.45              |
| 1:M:829:TRP:HZ3  | 2:N:84:PHE:CE1   | 2.31                     | 0.45              |
| 1:M:829:TRP:HZ3  | 2:N:84:PHE:CE2   | 2.34                     | 0.45              |
| 4:8:223:PHE:CD2  | 4:8:259:GLU:HG3  | 2.52                     | 0.45              |
| 1:A:89:GLU:CD    | 1:A:153:PRO:HD2  | 2.37                     | 0.45              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:HD12 | 2.52                     | 0.45              |
| 1:A:346:ASP:O    | 1:A:350:ALA:N    | 2.46                     | 0.45              |
| 1:P:436:MLY:HE3  | 1:P:626:TYR:HE1  | 1.77                     | 0.45              |
| 1:D:37:SER:O     | 1:D:38:VAL:HG23  | 2.17                     | 0.45              |
| 1:P:87:MLY:HH12  | 1:P:87:MLY:HD3   | 1.61                     | 0.45              |
| 1:G:14:ALA:N     | 1:G:15:PRO:HD2   | 2.32                     | 0.45              |
| 1:M:322:VAL:CG1  | 1:M:325:ILE:HD11 | 2.47                     | 0.45              |
| 1:J:136:ASN:HA   | 1:J:137:PRO:HD3  | 1.50                     | 0.45              |
| 1:G:136:ASN:O    | 1:G:139:VAL:N    | 2.47                     | 0.45              |
| 4:X:366:GLY:O    | 4:X:369:ILE:HG22 | 2.16                     | 0.45              |
| 4:Z:366:GLY:O    | 4:Z:369:ILE:HG22 | 2.16                     | 0.45              |
| 1:D:675:ILE:HG23 | 1:D:676:ILE:N    | 2.32                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:2:32:PRO:HB2   | 4:2:34:ILE:HD11  | 1.98                     | 0.45              |
| 1:M:476:GLU:OE2  | 1:M:598:MLY:HH13 | 2.16                     | 0.45              |
| 1:J:597:GLU:O    | 1:J:600:MLY:N    | 2.50                     | 0.45              |
| 1:D:795:ARG:HE   | 3:F:116:GLU:CB   | 2.28                     | 0.45              |
| 1:G:795:ARG:HG3  | 3:I:116:GLU:OE2  | 2.17                     | 0.45              |
| 1:A:93:MET:HG2   | 1:A:715:VAL:HG23 | 1.91                     | 0.45              |
| 1:M:821:ARG:HH22 | 2:N:127:ARG:NE   | 2.14                     | 0.45              |
| 1:G:640:LYS:C    | 4:V:23:GLY:C     | 2.75                     | 0.45              |
| 1:P:817:GLN:CG   | 2:Q:127:ARG:CG   | 2.77                     | 0.45              |
| 2:Q:121:LEU:O    | 2:Q:128:PHE:CG   | 2.61                     | 0.45              |
| 2:Q:137:TRP:CA   | 2:Q:145:ALA:CB   | 2.82                     | 0.45              |
| 4:X:324:THR:HG22 | 4:Z:247:VAL:CB   | 2.46                     | 0.45              |
| 1:A:224:SER:O    | 1:A:227:PRO:HD2  | 2.17                     | 0.45              |
| 1:J:725:ARG:CG   | 1:J:733:PRO:CA   | 2.95                     | 0.45              |
| 1:G:819:ASN:HD21 | 2:H:91:ALA:C     | 2.21                     | 0.45              |
| 2:K:140:PHE:HA   | 2:K:141:PRO:HD2  | 1.57                     | 0.45              |
| 1:J:93:MET:HE1   | 1:J:716:LEU:HD12 | 1.97                     | 0.45              |
| 1:M:636:LYS:O    | 4:Z:144:ALA:HB1  | 2.14                     | 0.45              |
| 1:M:411:GLU:H    | 4:Z:333:PRO:HB2  | 1.81                     | 0.45              |
| 1:J:543:PRO:CD   | 4:W:143:TYR:O    | 2.64                     | 0.45              |
| 1:D:568:PRO:CG   | 1:D:578:HIS:H    | 2.30                     | 0.45              |
| 1:G:725:ARG:CG   | 1:G:733:PRO:CA   | 2.95                     | 0.45              |
| 1:M:725:ARG:HA   | 1:M:732:ILE:HG22 | 1.99                     | 0.45              |
| 1:G:92:ALA:O     | 1:G:714:ARG:HG3  | 2.16                     | 0.45              |
| 1:D:838:ILE:CD1  | 2:E:54:MET:HE1   | 2.45                     | 0.45              |
| 1:P:711:PHE:HB3  | 1:P:766:PHE:HB3  | 1.99                     | 0.45              |
| 1:M:810:ARG:NH1  | 1:M:810:ARG:HG2  | 2.29                     | 0.45              |
| 1:A:642:LYS:HB2  | 4:8:24:ASP:O     | 1.88                     | 0.45              |
| 1:P:829:TRP:O    | 1:P:832:MET:N    | 2.50                     | 0.45              |
| 1:J:667:THR:O    | 1:J:669:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:99:GLU:N     | 1:A:100:PRO:CD   | 2.80                     | 0.45              |
| 4:7:223:PHE:CD2  | 4:7:259:GLU:HG3  | 2.51                     | 0.45              |
| 4:2:223:PHE:CD2  | 4:2:259:GLU:HG3  | 2.51                     | 0.45              |
| 1:G:64:THR:HB    | 1:G:68:GLU:N     | 2.32                     | 0.45              |
| 1:D:64:THR:HB    | 1:D:68:GLU:N     | 2.33                     | 0.45              |
| 4:0:253:GLU:HA   | 4:0:256:ARG:CG   | 2.42                     | 0.45              |
| 1:P:346:ASP:O    | 1:P:350:ALA:N    | 2.45                     | 0.45              |
| 4:Y:253:GLU:HA   | 4:Y:256:ARG:CG   | 2.42                     | 0.45              |
| 1:A:37:SER:O     | 1:A:38:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:186:THR:O    | 1:A:190:MLY:HG2  | 2.17                     | 0.45              |
| 1:A:322:VAL:CG1  | 1:A:325:ILE:HD11 | 2.47                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:9:190:MET:O    | 4:9:194:THR:HG23 | 2.16                     | 0.45              |
| 1:A:292:MET:HE1  | 1:A:309:PRO:HD3  | 1.99                     | 0.45              |
| 1:G:17:LEU:HA    | 1:G:17:LEU:HD12  | 1.67                     | 0.45              |
| 4:0:246:GLN:HG2  | 4:Y:325:MET:HE2  | 1.98                     | 0.45              |
| 1:G:485:GLU:OE1  | 1:G:583:HIS:ND1  | 2.49                     | 0.45              |
| 1:A:488:GLN:O    | 1:A:491:PHE:HB3  | 2.17                     | 0.45              |
| 1:G:488:GLN:O    | 1:G:491:PHE:HB3  | 2.17                     | 0.45              |
| 1:J:443:ILE:HG22 | 1:J:444:ARG:N    | 2.29                     | 0.45              |
| 4:8:32:PRO:HB2   | 4:8:34:ILE:HD11  | 1.98                     | 0.45              |
| 4:0:299:MET:HE2  | 4:0:331:ALA:HB2  | 1.99                     | 0.45              |
| 1:D:597:GLU:O    | 1:D:600:MLY:N    | 2.50                     | 0.45              |
| 1:D:723:ARG:NH2  | 1:D:779:ARG:CZ   | 2.79                     | 0.44              |
| 1:G:794:CYS:O    | 1:G:797:PHE:HB3  | 2.17                     | 0.44              |
| 1:A:754:ASP:OD2  | 1:A:774:LEU:HD23 | 2.16                     | 0.44              |
| 1:M:821:ARG:NH2  | 2:N:127:ARG:CD   | 2.80                     | 0.44              |
| 1:G:629:GLU:HG2  | 1:G:643:GLY:C    | 2.35                     | 0.44              |
| 1:G:408:VAL:CG1  | 4:V:332:PRO:HB3  | 2.41                     | 0.44              |
| 2:E:112:ILE:O    | 2:E:148:VAL:HA   | 2.16                     | 0.44              |
| 2:E:129:THR:HG23 | 2:E:132:GLU:OE1  | 2.17                     | 0.44              |
| 2:E:139:ALA:C    | 2:E:141:PRO:HD3  | 2.33                     | 0.44              |
| 1:J:226:ASN:N    | 1:J:227:PRO:HD2  | 2.32                     | 0.44              |
| 1:D:818:TYR:CD2  | 2:E:90:GLY:HA3   | 2.52                     | 0.44              |
| 4:3:288:ASP:OD2  | 4:5:203:THR:OG1  | 2.33                     | 0.44              |
| 1:G:214:MET:CA   | 1:G:340:ILE:HD11 | 2.45                     | 0.44              |
| 1:G:95:THR:HA    | 1:G:713:SER:OG   | 2.16                     | 0.44              |
| 1:J:689:GLU:HA   | 1:J:692:LEU:HB2  | 2.00                     | 0.44              |
| 1:M:99:GLU:N     | 1:M:100:PRO:CD   | 2.80                     | 0.44              |
| 1:G:612:GLN:NE2  | 1:G:627:GLY:H    | 2.14                     | 0.44              |
| 1:P:278:GLN:HB3  | 1:P:278:GLN:HE21 | 1.42                     | 0.44              |
| 1:M:556:ASP:CB   | 4:1:49:GLN:CD    | 2.03                     | 0.44              |
| 4:9:223:PHE:HB3  | 4:9:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:7:223:PHE:HB3  | 4:7:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:G:519:LEU:CD1  | 1:G:519:LEU:N    | 2.77                     | 0.44              |
| 1:J:14:ALA:N     | 1:J:15:PRO:HD2   | 2.32                     | 0.44              |
| 1:G:292:MET:HE1  | 1:G:309:PRO:CG   | 2.46                     | 0.44              |
| 1:J:308:ASN:HA   | 1:J:309:PRO:HD2  | 1.88                     | 0.44              |
| 1:A:48:VAL:HA    | 1:A:104:TYR:OH   | 2.17                     | 0.44              |
| 3:F:69:LEU:HB3   | 3:F:70:PRO:HD3   | 1.99                     | 0.44              |
| 4:W:32:PRO:HB2   | 4:W:34:ILE:HD11  | 1.98                     | 0.44              |
| 4:9:32:PRO:HB2   | 4:9:34:ILE:HD11  | 1.98                     | 0.44              |
| 1:M:179:GLY:O    | 1:M:185:LYS:HE2  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:597:GLU:O    | 1:P:600:MLY:N    | 2.50                     | 0.44              |
| 1:D:795:ARG:HB3  | 3:F:35:ARG:HH22  | 1.74                     | 0.44              |
| 2:N:112:ILE:O    | 2:N:148:VAL:HA   | 2.16                     | 0.44              |
| 2:Q:129:THR:HG23 | 2:Q:132:GLU:OE1  | 2.18                     | 0.44              |
| 1:P:411:GLU:H    | 4:0:333:PRO:CB   | 2.30                     | 0.44              |
| 1:P:640:LYS:HB3  | 1:P:645:SER:CB   | 2.42                     | 0.44              |
| 1:J:715:VAL:HG11 | 1:J:720:PHE:CD1  | 2.50                     | 0.44              |
| 1:P:795:ARG:NE   | 3:R:118:MET:HE2  | 2.31                     | 0.44              |
| 1:A:530:MET:HE3  | 4:8:354:GLN:CB   | 2.47                     | 0.44              |
| 1:A:835:PHE:O    | 1:A:839:MLY:N    | 2.49                     | 0.44              |
| 1:G:829:TRP:CE3  | 2:H:87:LYS:NZ    | 2.78                     | 0.44              |
| 1:P:829:TRP:CE2  | 2:Q:87:LYS:HE2   | 2.48                     | 0.44              |
| 1:J:99:GLU:N     | 1:J:100:PRO:CD   | 2.80                     | 0.44              |
| 1:D:689:GLU:HA   | 1:D:692:LEU:HB2  | 1.99                     | 0.44              |
| 1:G:667:THR:O    | 1:G:669:PRO:HD3  | 2.16                     | 0.44              |
| 1:D:278:GLN:HB3  | 1:D:278:GLN:HE21 | 1.42                     | 0.44              |
| 4:W:223:PHE:HB3  | 4:W:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:2:223:PHE:HB3  | 4:2:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:0:223:PHE:CD2  | 4:0:259:GLU:HG3  | 2.51                     | 0.44              |
| 1:J:64:THR:HB    | 1:J:68:GLU:N     | 2.33                     | 0.44              |
| 4:X:253:GLU:HA   | 4:X:256:ARG:CG   | 2.42                     | 0.44              |
| 1:J:486:MLY:HH22 | 1:J:527:GLU:CD   | 2.37                     | 0.44              |
| 4:4:253:GLU:HA   | 4:4:256:ARG:CG   | 2.42                     | 0.44              |
| 1:J:37:SER:O     | 1:J:38:VAL:HG23  | 2.17                     | 0.44              |
| 1:P:14:ALA:N     | 1:P:15:PRO:HD2   | 2.32                     | 0.44              |
| 1:J:322:VAL:CG1  | 1:J:325:ILE:HD11 | 2.47                     | 0.44              |
| 1:G:485:GLU:HA   | 1:G:584:TYR:HE2  | 1.83                     | 0.44              |
| 1:P:488:GLN:O    | 1:P:491:PHE:HB3  | 2.16                     | 0.44              |
| 4:Y:32:PRO:HB2   | 4:Y:34:ILE:HD11  | 1.98                     | 0.44              |
| 1:M:30:MLY:HB3   | 1:M:31:PRO:HD2   | 1.97                     | 0.44              |
| 1:D:724:TYR:HD1  | 1:D:727:LEU:CD1  | 2.27                     | 0.44              |
| 1:D:711:PHE:HB3  | 1:D:766:PHE:HB3  | 1.99                     | 0.44              |
| 1:G:411:GLU:H    | 4:V:333:PRO:CB   | 2.29                     | 0.44              |
| 1:J:725:ARG:NE   | 1:J:733:PRO:CB   | 1.95                     | 0.44              |
| 1:G:822:SER:OG   | 2:H:88:LEU:HA    | 2.17                     | 0.44              |
| 1:P:409:GLY:N    | 1:P:636:LYS:CD   | 2.70                     | 0.44              |
| 1:A:725:ARG:HA   | 1:A:732:ILE:HG22 | 1.99                     | 0.44              |
| 1:A:725:ARG:CZ   | 1:A:733:PRO:CB   | 2.83                     | 0.44              |
| 1:A:747:LEU:C    | 1:A:749:GLY:H    | 2.20                     | 0.44              |
| 1:J:639:GLY:H    | 4:W:344:SER:HB3  | 1.82                     | 0.44              |
| 1:D:530:MET:CE   | 4:9:354:GLN:HG3  | 2.35                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:747:LEU:C    | 1:G:749:GLY:H    | 2.20                     | 0.44              |
| 3:O:122:GLU:HA   | 3:O:125:GLU:OE1  | 2.18                     | 0.44              |
| 1:P:226:ASN:N    | 1:P:227:PRO:HD2  | 2.32                     | 0.44              |
| 1:M:725:ARG:HH21 | 1:M:733:PRO:HB2  | 1.81                     | 0.44              |
| 1:D:85:TYR:HH    | 1:D:772:LEU:HD22 | 1.55                     | 0.44              |
| 1:M:84:MLY:HD3   | 1:M:724:TYR:CE2  | 2.52                     | 0.44              |
| 1:M:803:TYR:CE1  | 1:M:807:VAL:HG21 | 2.52                     | 0.44              |
| 1:J:599:ASN:CG   | 1:J:649:VAL:CB   | 2.80                     | 0.44              |
| 1:D:799:MET:SD   | 3:F:32:ASP:OD2   | 2.75                     | 0.44              |
| 4:9:290:ARG:HH22 | 4:W:202:THR:CG2  | 2.17                     | 0.44              |
| 1:J:692:LEU:O    | 1:J:696:ARG:HG3  | 2.18                     | 0.44              |
| 2:E:162:ASP:O    | 2:K:21:GLU:HB3   | 2.12                     | 0.44              |
| 1:P:129:TYR:HD1  | 1:P:129:TYR:HA   | 1.65                     | 0.44              |
| 4:5:223:PHE:HB3  | 4:5:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:Y:223:PHE:HB3  | 4:Y:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:Y:223:PHE:CD2  | 4:Y:259:GLU:HG3  | 2.52                     | 0.44              |
| 4:0:223:PHE:HB3  | 4:0:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:A:64:THR:HB    | 1:A:68:GLU:N     | 2.33                     | 0.44              |
| 1:M:64:THR:HB    | 1:M:68:GLU:N     | 2.33                     | 0.44              |
| 1:P:64:THR:HB    | 1:P:68:GLU:N     | 2.32                     | 0.44              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:M:195:TYR:CE2  | 1:M:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:P:296:MLY:O    | 1:P:299:LEU:HB2  | 2.17                     | 0.44              |
| 1:J:17:LEU:HA    | 1:J:17:LEU:HD12  | 1.68                     | 0.44              |
| 4:0:32:PRO:HB2   | 4:0:34:ILE:HD11  | 1.98                     | 0.44              |
| 1:D:229:LEU:HD12 | 1:D:229:LEU:HA   | 1.75                     | 0.44              |
| 1:A:597:GLU:O    | 1:A:600:MLY:N    | 2.50                     | 0.44              |
| 3:C:69:LEU:HB3   | 3:C:70:PRO:HD3   | 2.00                     | 0.44              |
| 4:1:32:PRO:HB2   | 4:1:34:ILE:HD11  | 1.98                     | 0.44              |
| 1:A:715:VAL:HG11 | 1:A:720:PHE:CD1  | 2.50                     | 0.44              |
| 2:N:129:THR:HG23 | 2:N:132:GLU:OE1  | 2.18                     | 0.44              |
| 1:G:530:MET:CB   | 4:V:354:GLN:CB   | 2.96                     | 0.44              |
| 1:P:732:ILE:CG2  | 1:P:747:LEU:HD12 | 0.35                     | 0.44              |
| 1:G:817:GLN:HB3  | 2:H:127:ARG:HH11 | 1.82                     | 0.44              |
| 2:K:129:THR:HG23 | 2:K:132:GLU:OE1  | 2.17                     | 0.44              |
| 2:B:129:THR:HG23 | 2:B:132:GLU:OE1  | 2.18                     | 0.44              |
| 1:P:643:GLY:CA   | 4:0:24:ASP:OD1   | 2.62                     | 0.44              |
| 1:J:711:PHE:HB3  | 1:J:766:PHE:HB3  | 1.99                     | 0.44              |
| 1:D:449:LEU:HA   | 1:D:449:LEU:HD12 | 1.60                     | 0.44              |
| 1:M:711:PHE:HB3  | 1:M:766:PHE:HB3  | 2.00                     | 0.44              |
| 1:D:838:ILE:CD1  | 2:E:54:MET:HE3   | 2.45                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:287:ILE:CB   | 4:9:204:ALA:H    | 2.13                     | 0.44              |
| 1:G:829:TRP:O    | 1:G:832:MET:N    | 2.50                     | 0.44              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:CG1  | 2.47                     | 0.44              |
| 4:3:324:THR:HG23 | 4:5:244:ASP:O    | 2.17                     | 0.44              |
| 4:1:6:THR:HG22   | 4:1:101:HIS:HA   | 1.97                     | 0.44              |
| 1:G:103:LEU:HD22 | 1:G:692:LEU:HG   | 1.98                     | 0.44              |
| 1:G:176:LEU:N    | 1:G:176:LEU:CD1  | 2.75                     | 0.44              |
| 1:D:418:THR:CG2  | 1:D:419:VAL:N    | 2.79                     | 0.44              |
| 4:8:223:PHE:HB3  | 4:8:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:P:195:TYR:CE2  | 1:P:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:J:155:ILE:HG22 | 1:J:156:PHE:N    | 2.32                     | 0.44              |
| 1:D:163:TYR:O    | 1:D:166:MET:HB3  | 2.17                     | 0.44              |
| 1:G:163:TYR:O    | 1:G:166:MET:HB3  | 2.17                     | 0.44              |
| 1:A:14:ALA:N     | 1:A:15:PRO:HD2   | 2.32                     | 0.44              |
| 1:A:519:LEU:CD1  | 1:A:519:LEU:N    | 2.77                     | 0.44              |
| 1:G:810:ARG:HG2  | 1:G:810:ARG:NH1  | 2.28                     | 0.44              |
| 1:A:675:ILE:HG23 | 1:A:676:ILE:N    | 2.32                     | 0.44              |
| 4:0:290:ARG:HH21 | 4:2:202:THR:HG22 | 1.82                     | 0.44              |
| 1:M:597:GLU:O    | 1:M:600:MLY:N    | 2.50                     | 0.44              |
| 1:M:516:GLY:O    | 1:M:518:ASP:N    | 2.51                     | 0.44              |
| 4:4:32:PRO:HB2   | 4:4:34:ILE:HD11  | 1.98                     | 0.44              |
| 1:G:179:GLY:O    | 1:G:185:LYS:HE2  | 2.17                     | 0.44              |
| 1:J:794:CYS:O    | 1:J:797:PHE:HB3  | 2.17                     | 0.44              |
| 1:P:747:LEU:C    | 1:P:749:GLY:H    | 2.21                     | 0.44              |
| 2:H:112:ILE:O    | 2:H:148:VAL:N    | 2.50                     | 0.44              |
| 1:P:538:GLU:OE1  | 4:0:355:MET:HE3  | 2.17                     | 0.44              |
| 1:J:540:CYS:C    | 4:W:349:LEU:HD21 | 2.36                     | 0.44              |
| 1:M:839:MLY:HH11 | 2:N:158:THR:CG2  | 2.48                     | 0.44              |
| 1:M:782:MLY:O    | 1:M:786:ILE:HD11 | 2.18                     | 0.44              |
| 1:M:783:LEU:O    | 1:M:786:ILE:N    | 2.50                     | 0.44              |
| 1:P:224:SER:O    | 1:P:227:PRO:HD2  | 2.17                     | 0.44              |
| 1:G:641:LYS:CD   | 1:G:647:GLN:CG   | 2.72                     | 0.44              |
| 1:M:715:VAL:HG12 | 1:M:720:PHE:HB2  | 2.00                     | 0.44              |
| 1:P:148:ARG:NE   | 1:P:764:MLY:HH21 | 2.32                     | 0.44              |
| 1:M:642:LYS:HB2  | 4:Z:24:ASP:O     | 1.89                     | 0.44              |
| 1:P:332:MET:O    | 1:P:336:SER:OG   | 2.27                     | 0.44              |
| 3:I:48:LYS:HD3   | 3:I:48:LYS:HA    | 1.17                     | 0.44              |
| 1:P:667:THR:O    | 1:P:669:PRO:HD3  | 2.17                     | 0.44              |
| 1:P:689:GLU:HA   | 1:P:692:LEU:HB2  | 2.00                     | 0.44              |
| 1:A:103:LEU:HD22 | 1:A:692:LEU:HG   | 1.98                     | 0.44              |
| 1:A:173:GLN:HG3  | 1:A:670:HIS:HD2  | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:V:287:ILE:HG13 | 4:X:202:THR:HG23 | 1.65                     | 0.44              |
| 4:V:223:PHE:HB3  | 4:V:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:P:493:HIS:O    | 1:P:496:PHE:HB3  | 2.18                     | 0.44              |
| 1:G:493:HIS:O    | 1:G:496:PHE:HB3  | 2.18                     | 0.44              |
| 1:G:155:ILE:HG22 | 1:G:156:PHE:N    | 2.33                     | 0.44              |
| 1:P:37:SER:O     | 1:P:38:VAL:HG23  | 2.17                     | 0.44              |
| 1:J:163:TYR:O    | 1:J:166:MET:HB3  | 2.17                     | 0.44              |
| 1:A:123:CYS:CB   | 1:A:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:D:322:VAL:CG1  | 1:D:325:ILE:HD11 | 2.47                     | 0.44              |
| 1:J:139:VAL:HG12 | 1:J:143:TYR:HD2  | 1.81                     | 0.44              |
| 1:D:134:VAL:C    | 1:D:136:ASN:H    | 2.16                     | 0.44              |
| 1:D:139:VAL:HG12 | 1:D:143:TYR:HD2  | 1.81                     | 0.44              |
| 4:V:190:MET:O    | 4:V:194:THR:HG23 | 2.16                     | 0.44              |
| 4:V:366:GLY:O    | 4:V:369:ILE:HG22 | 2.16                     | 0.44              |
| 1:D:91:MET:CE    | 1:D:119:SER:HB2  | 2.48                     | 0.44              |
| 1:J:485:GLU:OE1  | 1:J:583:HIS:ND1  | 2.49                     | 0.44              |
| 1:D:488:GLN:O    | 1:D:491:PHE:HB3  | 2.17                     | 0.44              |
| 1:M:330:GLU:O    | 1:M:333:ALA:HB3  | 2.16                     | 0.44              |
| 3:R:122:GLU:HA   | 3:R:125:GLU:OE1  | 2.18                     | 0.44              |
| 1:J:775:LEU:HD12 | 1:J:775:LEU:HA   | 1.71                     | 0.44              |
| 3:L:69:LEU:HB3   | 3:L:70:PRO:HD3   | 1.99                     | 0.44              |
| 1:P:516:GLY:O    | 1:P:518:ASP:N    | 2.51                     | 0.44              |
| 1:J:516:GLY:O    | 1:J:518:ASP:N    | 2.51                     | 0.44              |
| 1:J:792:ALA:HA   | 3:L:42:THR:HA    | 2.00                     | 0.44              |
| 1:D:725:ARG:HA   | 1:D:732:ILE:HG22 | 1.99                     | 0.44              |
| 1:G:796:GLY:CA   | 3:I:35:ARG:NH2   | 2.79                     | 0.44              |
| 1:M:818:TYR:CD1  | 2:N:127:ARG:NH1  | 2.86                     | 0.44              |
| 2:E:112:ILE:O    | 2:E:148:VAL:N    | 2.50                     | 0.44              |
| 1:P:725:ARG:CG   | 1:P:733:PRO:CA   | 2.95                     | 0.44              |
| 1:J:732:ILE:HG23 | 1:J:747:LEU:HD12 | 0.95                     | 0.44              |
| 2:H:129:THR:HG23 | 2:H:132:GLU:OE1  | 2.17                     | 0.44              |
| 2:B:117:LEU:CG   | 2:B:147:ASN:OD1  | 2.52                     | 0.44              |
| 2:B:112:ILE:O    | 2:B:148:VAL:HA   | 2.17                     | 0.44              |
| 1:P:540:CYS:C    | 4:O:349:LEU:HD21 | 2.36                     | 0.44              |
| 1:P:797:PHE:CD1  | 3:R:149:VAL:HG12 | 2.44                     | 0.44              |
| 1:M:783:LEU:HA   | 1:M:786:ILE:HG12 | 1.67                     | 0.44              |
| 1:M:747:LEU:C    | 1:M:749:GLY:H    | 2.21                     | 0.44              |
| 4:8:324:THR:N    | 4:V:245:GLY:CA   | 2.69                     | 0.44              |
| 1:M:692:LEU:HA   | 1:M:692:LEU:HD23 | 1.85                     | 0.44              |
| 1:G:692:LEU:O    | 1:G:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:M:320:ILE:HG22 | 1:M:320:ILE:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:155:ILE:HG22 | 1:P:156:PHE:N    | 2.33                     | 0.44              |
| 1:P:486:MLY:HH22 | 1:P:527:GLU:CD   | 2.37                     | 0.44              |
| 4:8:193:LEU:O    | 4:8:198:TYR:HD2  | 2.01                     | 0.44              |
| 1:M:519:LEU:N    | 1:M:519:LEU:CD1  | 2.77                     | 0.44              |
| 1:J:296:MLY:O    | 1:J:299:LEU:HB2  | 2.17                     | 0.44              |
| 1:G:675:ILE:HG23 | 1:G:676:ILE:N    | 2.32                     | 0.44              |
| 1:G:659:MLY:HH22 | 1:G:659:MLY:HD2  | 1.42                     | 0.44              |
| 1:A:485:GLU:OE2  | 1:A:584:TYR:N    | 2.50                     | 0.44              |
| 3:C:101:THR:HA   | 3:C:137:ILE:O    | 2.18                     | 0.44              |
| 1:J:488:GLN:O    | 1:J:491:PHE:HB3  | 2.17                     | 0.44              |
| 4:W:299:MET:HE2  | 4:W:331:ALA:HB2  | 2.00                     | 0.44              |
| 1:J:789:ALA:HA   | 3:L:81:GLN:NE2   | 2.33                     | 0.44              |
| 3:R:69:LEU:HB3   | 3:R:70:PRO:HD3   | 1.99                     | 0.44              |
| 1:D:747:LEU:C    | 1:D:749:GLY:H    | 2.21                     | 0.44              |
| 2:N:139:ALA:O    | 2:N:141:PRO:CD   | 2.51                     | 0.44              |
| 1:G:642:LYS:HG3  | 4:V:23:GLY:CA    | 2.31                     | 0.44              |
| 1:A:449:LEU:HD12 | 1:A:449:LEU:HA   | 1.60                     | 0.44              |
| 1:J:725:ARG:CZ   | 1:J:737:PHE:CZ   | 3.01                     | 0.44              |
| 2:K:114:LYS:CG   | 2:K:146:GLY:HA2  | 2.46                     | 0.44              |
| 1:A:732:ILE:HG21 | 1:A:747:LEU:CD1  | 0.64                     | 0.44              |
| 1:M:548:THR:O    | 4:1:46:GLY:O     | 2.04                     | 0.44              |
| 1:J:408:VAL:HA   | 1:J:636:LYS:HG3  | 1.03                     | 0.44              |
| 1:J:408:VAL:HG22 | 1:J:636:LYS:HG2  | 1.52                     | 0.44              |
| 1:D:541:MET:HB3  | 4:9:345:ILE:HG22 | 2.00                     | 0.44              |
| 1:M:787:ILE:HG23 | 1:M:791:GLN:HG3  | 2.00                     | 0.44              |
| 1:M:641:LYS:CD   | 1:M:647:GLN:CG   | 2.72                     | 0.44              |
| 1:J:835:PHE:O    | 1:J:839:MLY:N    | 2.49                     | 0.44              |
| 4:3:287:ILE:HB   | 4:5:204:ALA:H    | 1.83                     | 0.44              |
| 1:M:629:GLU:HG2  | 1:M:643:GLY:C    | 2.35                     | 0.44              |
| 1:M:332:MET:O    | 1:M:336:SER:OG   | 2.27                     | 0.44              |
| 4:2:324:THR:HG23 | 4:4:244:ASP:O    | 1.63                     | 0.44              |
| 3:L:50:LEU:O     | 3:L:53:PRO:HG2   | 2.18                     | 0.44              |
| 1:J:576:GLU:CG   | 1:J:577:ALA:N    | 2.44                     | 0.44              |
| 1:M:173:GLN:HG3  | 1:M:670:HIS:HD2  | 1.82                     | 0.44              |
| 1:G:320:ILE:O    | 1:G:320:ILE:HG22 | 2.18                     | 0.44              |
| 4:X:220:ALA:HB3  | 4:X:223:PHE:CD1  | 2.53                     | 0.44              |
| 1:G:701:LEU:HD12 | 1:G:701:LEU:HA   | 1.55                     | 0.44              |
| 4:1:220:ALA:HB3  | 4:1:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:Z:220:ALA:HB3  | 4:Z:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:Z:223:PHE:HB3  | 4:Z:259:GLU:OE2  | 2.18                     | 0.44              |
| 1:J:493:HIS:O    | 1:J:496:PHE:HB3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:346:ASP:O    | 1:D:350:ALA:N    | 2.46                     | 0.44              |
| 4:7:193:LEU:O    | 4:7:198:TYR:HD2  | 2.01                     | 0.44              |
| 1:M:486:MLY:HH22 | 1:M:527:GLU:CD   | 2.37                     | 0.44              |
| 1:M:123:CYS:CB   | 1:M:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:M:136:ASN:HA   | 1:M:137:PRO:HD3  | 1.49                     | 0.44              |
| 4:Z:190:MET:O    | 4:Z:194:THR:HG23 | 2.16                     | 0.44              |
| 1:D:266:GLU:OE1  | 1:D:659:MLY:NZ   | 2.51                     | 0.44              |
| 1:A:17:LEU:HA    | 1:A:17:LEU:HD12  | 1.67                     | 0.44              |
| 1:A:485:GLU:HA   | 1:A:584:TYR:HE2  | 1.83                     | 0.44              |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:CD1  | 2.48                     | 0.44              |
| 1:J:476:GLU:CD   | 1:J:476:GLU:H    | 2.21                     | 0.44              |
| 1:A:439:LEU:CD1  | 1:A:439:LEU:N    | 2.81                     | 0.44              |
| 1:J:439:LEU:CD1  | 1:J:439:LEU:N    | 2.81                     | 0.44              |
| 1:D:439:LEU:CD1  | 1:D:439:LEU:N    | 2.81                     | 0.44              |
| 1:A:516:GLY:O    | 1:A:518:ASP:N    | 2.51                     | 0.44              |
| 1:J:783:LEU:HA   | 1:J:786:ILE:HB   | 2.00                     | 0.44              |
| 3:F:122:GLU:HA   | 3:F:125:GLU:OE1  | 2.18                     | 0.44              |
| 1:A:501:GLU:CA   | 1:A:762:HIS:ND1  | 2.68                     | 0.44              |
| 1:G:643:GLY:CA   | 4:V:24:ASP:OD1   | 2.62                     | 0.44              |
| 1:A:226:ASN:N    | 1:A:227:PRO:HD2  | 2.32                     | 0.44              |
| 1:P:529:PRO:HB3  | 4:0:354:GLN:HA   | 1.99                     | 0.44              |
| 1:P:541:MET:CE   | 4:0:346:LEU:HD12 | 2.47                     | 0.44              |
| 1:J:206:LYS:CE   | 1:J:217:THR:HG23 | 2.29                     | 0.44              |
| 1:M:543:PRO:CD   | 4:Z:143:TYR:O    | 2.64                     | 0.44              |
| 1:P:792:ALA:HB2  | 3:R:42:THR:HA    | 1.98                     | 0.44              |
| 1:D:206:LYS:CE   | 1:D:217:THR:HG23 | 2.30                     | 0.44              |
| 1:A:795:ARG:CG   | 3:C:118:MET:HE1  | 2.44                     | 0.44              |
| 4:0:202:THR:CB   | 4:Y:287:ILE:H    | 2.30                     | 0.44              |
| 1:A:530:MET:CE   | 4:8:354:GLN:CB   | 2.96                     | 0.44              |
| 1:M:795:ARG:CD   | 3:O:118:MET:CE   | 2.75                     | 0.44              |
| 1:M:28:GLN:HB3   | 1:M:723:ARG:NH2  | 2.32                     | 0.44              |
| 1:A:837:MLY:HH22 | 2:H:21:GLU:H     | 1.82                     | 0.44              |
| 1:G:834:LEU:HD22 | 2:H:34:ILE:CD1   | 2.48                     | 0.44              |
| 1:G:829:TRP:CZ3  | 2:H:87:LYS:CE    | 2.99                     | 0.44              |
| 1:P:55:MLY:HH23  | 1:P:60:VAL:HG22  | 1.99                     | 0.44              |
| 1:J:568:PRO:CG   | 1:J:578:HIS:H    | 2.30                     | 0.44              |
| 1:J:55:MLY:HH23  | 1:J:60:VAL:HG22  | 1.99                     | 0.44              |
| 1:M:692:LEU:O    | 1:M:696:ARG:HG3  | 2.18                     | 0.44              |
| 1:D:667:THR:O    | 1:D:669:PRO:HD3  | 2.16                     | 0.44              |
| 1:D:692:LEU:O    | 1:D:696:ARG:HG3  | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:175:ILE:C    | 1:G:176:LEU:HD12 | 2.38                     | 0.44              |
| 1:M:775:LEU:HD12 | 1:M:775:LEU:HA   | 1.71                     | 0.44              |
| 4:X:223:PHE:HB3  | 4:X:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:V:220:ALA:HB3  | 4:V:223:PHE:CD1  | 2.53                     | 0.44              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:HD12 | 2.52                     | 0.44              |
| 1:M:155:ILE:HG22 | 1:M:156:PHE:N    | 2.33                     | 0.44              |
| 1:A:436:MLY:HE3  | 1:A:626:TYR:HE1  | 1.77                     | 0.44              |
| 1:P:163:TYR:O    | 1:P:166:MET:HB3  | 2.17                     | 0.44              |
| 1:M:186:THR:O    | 1:M:190:MLY:HG2  | 2.17                     | 0.44              |
| 1:M:37:SER:O     | 1:M:38:VAL:HG23  | 2.17                     | 0.44              |
| 1:G:37:SER:O     | 1:G:38:VAL:HG23  | 2.17                     | 0.44              |
| 1:M:14:ALA:N     | 1:M:15:PRO:HD2   | 2.32                     | 0.44              |
| 1:P:123:CYS:CB   | 1:P:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:J:91:MET:CE    | 1:J:119:SER:HB2  | 2.48                     | 0.44              |
| 1:P:139:VAL:HG12 | 1:P:143:TYR:HD2  | 1.81                     | 0.44              |
| 1:M:48:VAL:HA    | 1:M:104:TYR:OH   | 2.18                     | 0.44              |
| 3:O:119:THR:O    | 3:O:123:VAL:HG23 | 2.18                     | 0.44              |
| 3:L:119:THR:O    | 3:L:123:VAL:HG23 | 2.18                     | 0.44              |
| 1:D:485:GLU:OE2  | 1:D:584:TYR:N    | 2.50                     | 0.44              |
| 1:D:747:LEU:C    | 1:D:749:GLY:N    | 2.71                     | 0.44              |
| 1:D:795:ARG:CA   | 3:F:118:MET:HE3  | 2.47                     | 0.44              |
| 1:G:754:ASP:O    | 1:G:776:GLU:OE2  | 2.34                     | 0.44              |
| 1:P:725:ARG:CZ   | 1:P:737:PHE:CZ   | 3.01                     | 0.44              |
| 1:A:725:ARG:CZ   | 1:A:737:PHE:CZ   | 3.01                     | 0.44              |
| 1:A:747:LEU:C    | 1:A:749:GLY:N    | 2.71                     | 0.44              |
| 1:G:224:SER:O    | 1:G:227:PRO:HD2  | 2.17                     | 0.44              |
| 1:M:541:MET:HG2  | 4:Z:345:ILE:HG22 | 2.00                     | 0.44              |
| 1:M:411:GLU:H    | 4:Z:333:PRO:CB   | 2.30                     | 0.44              |
| 1:J:541:MET:HB3  | 4:W:345:ILE:HG22 | 2.00                     | 0.44              |
| 1:D:218:LEU:HD22 | 1:D:222:ILE:HG13 | 1.95                     | 0.44              |
| 1:A:530:MET:CB   | 4:8:354:GLN:CB   | 2.95                     | 0.44              |
| 4:2:290:ARG:NH1  | 4:4:202:THR:CG2  | 2.75                     | 0.44              |
| 1:P:715:VAL:HG11 | 1:P:720:PHE:CD1  | 2.50                     | 0.44              |
| 3:I:50:LEU:O     | 3:I:53:PRO:HG2   | 2.18                     | 0.44              |
| 3:R:48:LYS:HD3   | 3:R:48:LYS:HA    | 1.17                     | 0.44              |
| 3:R:50:LEU:O     | 3:R:53:PRO:HG2   | 2.18                     | 0.44              |
| 3:C:52:ASN:CB    | 3:C:53:PRO:CD    | 2.92                     | 0.44              |
| 1:J:103:LEU:HD22 | 1:J:692:LEU:HG   | 1.98                     | 0.44              |
| 4:1:324:THR:OG1  | 4:3:244:ASP:HB3  | 2.16                     | 0.44              |
| 1:J:174:SER:OG   | 1:J:669:PRO:HA   | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:103:LEU:HD22 | 1:P:692:LEU:HG   | 1.98                     | 0.44              |
| 1:A:692:LEU:O    | 1:A:696:ARG:HG3  | 2.18                     | 0.44              |
| 4:8:220:ALA:HB3  | 4:8:223:PHE:CD1  | 2.53                     | 0.44              |
| 4:4:223:PHE:HB3  | 4:4:259:GLU:OE2  | 2.18                     | 0.44              |
| 4:3:220:ALA:HB3  | 4:3:223:PHE:CD1  | 2.53                     | 0.44              |
| 1:D:64:THR:CG2   | 1:D:65:GLU:H     | 2.31                     | 0.44              |
| 4:5:193:LEU:O    | 4:5:198:TYR:HD2  | 2.01                     | 0.44              |
| 4:3:193:LEU:O    | 4:3:198:TYR:HD2  | 2.01                     | 0.44              |
| 1:G:486:MLY:HH22 | 1:G:527:GLU:CD   | 2.37                     | 0.44              |
| 1:D:292:MET:HE1  | 1:D:309:PRO:CG   | 2.48                     | 0.44              |
| 4:4:193:LEU:O    | 4:4:198:TYR:HD2  | 2.01                     | 0.44              |
| 1:G:14:ALA:N     | 1:G:15:PRO:CD    | 2.81                     | 0.44              |
| 1:J:123:CYS:CB   | 1:J:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:D:123:CYS:CB   | 1:D:158:ILE:HD13 | 2.48                     | 0.44              |
| 1:J:675:ILE:HG23 | 1:J:676:ILE:N    | 2.33                     | 0.44              |
| 1:M:91:MET:CE    | 1:M:119:SER:HB2  | 2.48                     | 0.44              |
| 1:D:17:LEU:HA    | 1:D:17:LEU:HD12  | 1.68                     | 0.44              |
| 1:P:485:GLU:OE1  | 1:P:583:HIS:ND1  | 2.49                     | 0.44              |
| 1:P:485:GLU:HA   | 1:P:584:TYR:HE2  | 1.83                     | 0.44              |
| 3:R:101:THR:HA   | 3:R:137:ILE:O    | 2.18                     | 0.44              |
| 3:F:101:THR:HA   | 3:F:137:ILE:O    | 2.18                     | 0.44              |
| 1:D:400:ALA:CB   | 1:D:606:THR:HG22 | 2.48                     | 0.44              |
| 1:G:330:GLU:O    | 1:G:333:ALA:HB3  | 2.17                     | 0.44              |
| 1:D:476:GLU:H    | 1:D:476:GLU:CD   | 2.22                     | 0.44              |
| 1:P:476:GLU:H    | 1:P:476:GLU:CD   | 2.22                     | 0.44              |
| 1:P:439:LEU:N    | 1:P:439:LEU:CD1  | 2.81                     | 0.44              |
| 4:2:299:MET:HE2  | 4:2:331:ALA:HB2  | 2.00                     | 0.44              |
| 4:2:205:GLU:O    | 4:2:208:ILE:HG22 | 2.18                     | 0.44              |
| 1:D:791:GLN:OE1  | 3:F:116:GLU:CG   | 2.48                     | 0.43              |
| 3:I:122:GLU:HA   | 3:I:125:GLU:OE1  | 2.18                     | 0.43              |
| 1:G:639:GLY:H    | 4:V:344:SER:HB3  | 1.83                     | 0.43              |
| 1:P:725:ARG:CG   | 1:P:733:PRO:HA   | 2.43                     | 0.43              |
| 1:J:821:ARG:CZ   | 2:K:127:ARG:NE   | 2.81                     | 0.43              |
| 1:M:529:PRO:HB3  | 4:Z:354:GLN:HA   | 1.99                     | 0.43              |
| 1:J:411:GLU:H    | 4:W:333:PRO:CB   | 2.30                     | 0.43              |
| 1:D:540:CYS:C    | 4:9:349:LEU:HD21 | 2.36                     | 0.43              |
| 1:D:530:MET:CB   | 4:9:354:GLN:CB   | 2.95                     | 0.43              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:M:224:SER:O    | 1:M:227:PRO:HD2  | 2.17                     | 0.43              |
| 1:A:787:ILE:HG23 | 1:A:791:GLN:HG3  | 2.00                     | 0.43              |
| 1:A:798:LEU:HD21 | 3:C:122:GLU:HB3  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:122:GLU:HA   | 3:C:125:GLU:OE1  | 2.18                     | 0.43              |
| 1:A:639:GLY:H    | 4:8:344:SER:HB3  | 1.83                     | 0.43              |
| 1:D:836:PHE:CE1  | 2:E:159:HIS:CB   | 2.98                     | 0.43              |
| 1:A:836:PHE:CZ   | 2:B:159:HIS:HA   | 2.53                     | 0.43              |
| 4:X:286:ASP:OD1  | 4:Z:202:THR:C    | 2.57                     | 0.43              |
| 1:J:129:TYR:HD1  | 1:J:129:TYR:HA   | 1.65                     | 0.43              |
| 1:A:129:TYR:HD1  | 1:A:129:TYR:HA   | 1.65                     | 0.43              |
| 4:3:223:PHE:HB3  | 4:3:259:GLU:OE2  | 2.18                     | 0.43              |
| 1:D:155:ILE:HG22 | 1:D:156:PHE:N    | 2.33                     | 0.43              |
| 1:M:163:TYR:O    | 1:M:166:MET:HB3  | 2.17                     | 0.43              |
| 1:A:123:CYS:HB2  | 1:A:158:ILE:HD13 | 2.00                     | 0.43              |
| 1:G:123:CYS:CB   | 1:G:158:ILE:HD13 | 2.48                     | 0.43              |
| 1:G:309:PRO:C    | 1:G:311:ASP:H    | 2.22                     | 0.43              |
| 1:J:322:VAL:HA   | 1:J:323:PRO:HD3  | 1.87                     | 0.43              |
| 1:P:91:MET:CE    | 1:P:119:SER:HB2  | 2.47                     | 0.43              |
| 1:M:675:ILE:HG23 | 1:M:676:ILE:N    | 2.32                     | 0.43              |
| 1:G:48:VAL:HA    | 1:G:104:TYR:OH   | 2.18                     | 0.43              |
| 3:R:119:THR:O    | 3:R:123:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:485:GLU:OE1  | 1:D:583:HIS:ND1  | 2.49                     | 0.43              |
| 3:L:101:THR:HA   | 3:L:137:ILE:O    | 2.18                     | 0.43              |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:CD1  | 2.48                     | 0.43              |
| 3:L:122:GLU:HA   | 3:L:125:GLU:OE1  | 2.18                     | 0.43              |
| 1:P:179:GLY:O    | 1:P:185:LYS:HE2  | 2.17                     | 0.43              |
| 1:A:229:LEU:HA   | 1:A:229:LEU:HD12 | 1.75                     | 0.43              |
| 1:G:439:LEU:N    | 1:G:439:LEU:CD1  | 2.81                     | 0.43              |
| 1:A:554:LEU:HD12 | 1:A:554:LEU:HA   | 1.76                     | 0.43              |
| 1:J:791:GLN:NE2  | 3:L:116:GLU:N    | 2.66                     | 0.43              |
| 1:G:818:TYR:CD1  | 2:H:127:ARG:NH1  | 2.86                     | 0.43              |
| 1:P:530:MET:CB   | 4:0:354:GLN:CB   | 2.95                     | 0.43              |
| 1:G:226:ASN:HB2  | 1:G:227:PRO:CD   | 2.48                     | 0.43              |
| 1:J:529:PRO:HB3  | 4:W:354:GLN:HA   | 1.99                     | 0.43              |
| 1:P:786:ILE:HG22 | 1:P:787:ILE:N    | 2.31                     | 0.43              |
| 1:P:793:ARG:HH11 | 3:R:40:ASN:HD22  | 0.54                     | 0.43              |
| 4:0:205:GLU:O    | 4:0:208:ILE:HG22 | 2.18                     | 0.43              |
| 1:M:795:ARG:NH2  | 3:O:116:GLU:OE2  | 2.48                     | 0.43              |
| 1:M:725:ARG:CZ   | 1:M:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:M:747:LEU:C    | 1:M:749:GLY:N    | 2.71                     | 0.43              |
| 1:G:503:TYR:OH   | 1:G:711:PHE:CE2  | 2.56                     | 0.43              |
| 1:A:201:ALA:O    | 1:A:202:SER:OG   | 2.36                     | 0.43              |
| 1:A:295:MLY:CE   | 1:A:332:MET:CE   | 2.96                     | 0.43              |
| 4:W:205:GLU:O    | 4:W:208:ILE:HG22 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:55:MLY:HH23  | 1:D:60:VAL:HG22  | 1.99                     | 0.43              |
| 1:A:175:ILE:C    | 1:A:176:LEU:HD12 | 2.39                     | 0.43              |
| 1:M:175:ILE:C    | 1:M:176:LEU:HD12 | 2.39                     | 0.43              |
| 1:J:799:MET:CE   | 3:L:32:ASP:HB3   | 2.48                     | 0.43              |
| 1:D:166:MET:CE   | 1:D:254:PHE:CD2  | 3.01                     | 0.43              |
| 4:1:193:LEU:O    | 4:1:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:P:166:MET:CE   | 1:P:254:PHE:CD2  | 3.01                     | 0.43              |
| 1:A:486:MLY:HH22 | 1:A:527:GLU:CD   | 2.37                     | 0.43              |
| 4:V:193:LEU:O    | 4:V:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:A:348:MLY:HH12 | 1:A:348:MLY:HD2  | 1.82                     | 0.43              |
| 1:M:296:MLY:HH11 | 1:M:348:MLY:CH2  | 2.48                     | 0.43              |
| 1:A:322:VAL:CG1  | 1:A:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:G:322:VAL:CG1  | 1:G:325:ILE:HD11 | 2.47                     | 0.43              |
| 1:G:322:VAL:CG1  | 1:G:325:ILE:HG13 | 2.48                     | 0.43              |
| 1:D:48:VAL:HA    | 1:D:104:TYR:OH   | 2.18                     | 0.43              |
| 1:J:266:GLU:OE1  | 1:J:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:G:266:GLU:OE1  | 1:G:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:D:485:GLU:HA   | 1:D:584:TYR:HE2  | 1.83                     | 0.43              |
| 3:I:101:THR:HA   | 3:I:137:ILE:O    | 2.18                     | 0.43              |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:CD1  | 2.48                     | 0.43              |
| 1:D:516:GLY:O    | 1:D:518:ASP:N    | 2.51                     | 0.43              |
| 4:4:205:GLU:O    | 4:4:208:ILE:HG22 | 2.18                     | 0.43              |
| 4:Y:205:GLU:O    | 4:Y:208:ILE:HG22 | 2.18                     | 0.43              |
| 1:J:673:ARG:HD2  | 1:J:673:ARG:HA   | 1.79                     | 0.43              |
| 1:A:505:MLY:CE   | 1:A:762:HIS:CG   | 2.76                     | 0.43              |
| 1:A:504:MLY:HB2  | 1:A:762:HIS:NE2  | 2.33                     | 0.43              |
| 1:A:217:THR:HG22 | 1:A:218:LEU:N    | 2.34                     | 0.43              |
| 2:K:137:TRP:CA   | 2:K:145:ALA:HB2  | 2.37                     | 0.43              |
| 1:J:149:GLN:HB3  | 1:J:716:LEU:HD21 | 1.99                     | 0.43              |
| 1:M:545:ALA:HB2  | 4:1:45:VAL:HG13  | 1.99                     | 0.43              |
| 1:J:409:GLY:N    | 1:J:636:LYS:CD   | 2.70                     | 0.43              |
| 1:D:639:GLY:H    | 4:9:344:SER:HB3  | 1.83                     | 0.43              |
| 1:G:725:ARG:HA   | 1:G:732:ILE:HG22 | 1.99                     | 0.43              |
| 1:D:226:ASN:HB2  | 1:D:227:PRO:CD   | 2.47                     | 0.43              |
| 1:M:218:LEU:HD22 | 1:M:222:ILE:HG13 | 1.95                     | 0.43              |
| 1:M:226:ASN:N    | 1:M:227:PRO:HD2  | 2.32                     | 0.43              |
| 1:A:540:CYS:C    | 4:8:349:LEU:HD21 | 2.36                     | 0.43              |
| 1:A:537:GLU:OE1  | 4:8:350:SER:HA   | 2.19                     | 0.43              |
| 1:G:715:VAL:HG11 | 1:G:720:PHE:CD1  | 2.50                     | 0.43              |
| 1:G:723:ARG:CG   | 1:G:723:ARG:NH1  | 2.80                     | 0.43              |
| 4:0:243:PRO:C    | 4:Y:291:LYS:HZ1  | 2.20                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:84:MLY:CH1   | 1:M:715:VAL:HG21 | 2.48                     | 0.43              |
| 1:D:599:ASN:CG   | 1:D:649:VAL:CB   | 2.80                     | 0.43              |
| 1:J:756:THR:CG2  | 1:J:779:ARG:HB3  | 2.48                     | 0.43              |
| 1:P:724:TYR:HD1  | 1:P:727:LEU:CD1  | 2.27                     | 0.43              |
| 1:J:712:PRO:HB2  | 1:J:713:SER:H    | 1.61                     | 0.43              |
| 1:D:800:ARG:HD2  | 3:F:149:VAL:O    | 2.16                     | 0.43              |
| 1:D:40:VAL:HG23  | 1:D:76:GLN:O     | 2.19                     | 0.43              |
| 1:G:578:HIS:HB3  | 1:G:592:ILE:CD1  | 2.38                     | 0.43              |
| 1:G:568:PRO:CG   | 1:G:578:HIS:H    | 2.30                     | 0.43              |
| 1:D:173:GLN:HG3  | 1:D:670:HIS:HD2  | 1.82                     | 0.43              |
| 1:P:174:SER:OG   | 1:P:669:PRO:HA   | 2.18                     | 0.43              |
| 1:A:174:SER:OG   | 1:A:669:PRO:HA   | 2.18                     | 0.43              |
| 1:A:320:ILE:O    | 1:A:320:ILE:HG22 | 2.18                     | 0.43              |
| 1:J:496:PHE:HB2  | 1:J:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:D:292:MET:CE   | 1:D:309:PRO:CA   | 2.97                     | 0.43              |
| 1:D:322:VAL:CG1  | 1:D:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:J:144:ARG:HA   | 1:J:144:ARG:HD2  | 1.78                     | 0.43              |
| 1:M:144:ARG:HD2  | 1:M:144:ARG:HA   | 1.78                     | 0.43              |
| 1:G:91:MET:CE    | 1:G:119:SER:HB2  | 2.48                     | 0.43              |
| 1:P:675:ILE:HG23 | 1:P:676:ILE:N    | 2.33                     | 0.43              |
| 1:J:48:VAL:HA    | 1:J:104:TYR:OH   | 2.18                     | 0.43              |
| 1:A:109:ARG:CD   | 1:A:117:THR:HB   | 2.48                     | 0.43              |
| 1:M:193:ILE:HD11 | 1:M:250:ILE:CD1  | 2.48                     | 0.43              |
| 1:M:391:GLY:HA3  | 1:M:616:VAL:HG23 | 2.01                     | 0.43              |
| 1:P:391:GLY:HA3  | 1:P:616:VAL:HG23 | 2.01                     | 0.43              |
| 4:2:149:THR:HA   | 4:2:165:ILE:O    | 2.19                     | 0.43              |
| 4:7:149:THR:HA   | 4:7:165:ILE:O    | 2.19                     | 0.43              |
| 1:J:246:PHE:HB3  | 1:J:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:A:768:MLY:CB   | 1:A:771:LEU:CD1  | 2.83                     | 0.43              |
| 1:A:733:PRO:O    | 1:A:737:PHE:CE1  | 2.53                     | 0.43              |
| 1:G:218:LEU:HD22 | 1:G:222:ILE:HG13 | 1.95                     | 0.43              |
| 1:J:93:MET:CE    | 1:J:716:LEU:HB2  | 2.48                     | 0.43              |
| 1:J:410:ASN:HA   | 4:W:334:GLU:HB3  | 1.29                     | 0.43              |
| 1:J:541:MET:CE   | 4:W:346:LEU:HD12 | 2.47                     | 0.43              |
| 1:D:224:SER:O    | 1:D:227:PRO:HD2  | 2.17                     | 0.43              |
| 1:A:534:SER:CB   | 4:8:351:THR:HA   | 2.48                     | 0.43              |
| 1:D:642:LYS:HG3  | 4:9:23:GLY:CA    | 2.31                     | 0.43              |
| 1:J:829:TRP:HA   | 1:J:830:PRO:HD2  | 1.86                     | 0.43              |
| 1:J:97:LEU:HD12  | 1:J:97:LEU:HA    | 1.67                     | 0.43              |
| 4:8:287:ILE:HA   | 4:V:202:THR:HG21 | 1.59                     | 0.43              |
| 1:A:40:VAL:HG23  | 1:A:76:GLN:O     | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:612:GLN:NE2  | 1:A:627:GLY:H    | 2.14                     | 0.43              |
| 4:V:290:ARG:NH1  | 4:X:202:THR:CG2  | 2.81                     | 0.43              |
| 1:A:496:PHE:HB2  | 1:A:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:G:496:PHE:HB2  | 1:G:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:P:64:THR:CG2   | 1:P:65:GLU:H     | 2.31                     | 0.43              |
| 1:A:155:ILE:HG22 | 1:A:156:PHE:N    | 2.33                     | 0.43              |
| 4:9:253:GLU:HA   | 4:9:256:ARG:CG   | 2.42                     | 0.43              |
| 1:D:123:CYS:HB2  | 1:D:158:ILE:HD13 | 2.00                     | 0.43              |
| 3:C:119:THR:O    | 3:C:123:VAL:HG23 | 2.18                     | 0.43              |
| 1:M:485:GLU:HA   | 1:M:584:TYR:HE2  | 1.83                     | 0.43              |
| 1:P:193:ILE:HD11 | 1:P:250:ILE:CD1  | 2.48                     | 0.43              |
| 1:P:443:ILE:HG22 | 1:P:444:ARG:N    | 2.29                     | 0.43              |
| 1:M:439:LEU:CD1  | 1:M:439:LEU:N    | 2.81                     | 0.43              |
| 4:4:149:THR:HA   | 4:4:165:ILE:O    | 2.19                     | 0.43              |
| 4:W:149:THR:HA   | 4:W:165:ILE:O    | 2.19                     | 0.43              |
| 3:I:69:LEU:HB3   | 3:I:70:PRO:HD3   | 1.99                     | 0.43              |
| 1:G:516:GLY:O    | 1:G:518:ASP:N    | 2.51                     | 0.43              |
| 4:7:205:GLU:O    | 4:7:208:ILE:HG22 | 2.18                     | 0.43              |
| 1:A:391:GLY:HA3  | 1:A:616:VAL:HG23 | 2.00                     | 0.43              |
| 4:V:149:THR:HA   | 4:V:165:ILE:O    | 2.19                     | 0.43              |
| 1:J:792:ALA:H    | 3:L:42:THR:CG2   | 2.20                     | 0.43              |
| 1:D:725:ARG:CG   | 1:D:733:PRO:CA   | 2.95                     | 0.43              |
| 1:D:793:ARG:CZ   | 3:F:87:PHE:CE1   | 3.01                     | 0.43              |
| 1:M:817:GLN:HB3  | 2:N:127:ARG:NE   | 2.33                     | 0.43              |
| 1:A:442:VAL:O    | 1:A:445:ILE:HB   | 2.19                     | 0.43              |
| 1:G:818:TYR:CE2  | 2:H:127:ARG:NH1  | 2.74                     | 0.43              |
| 1:G:821:ARG:HH22 | 2:H:127:ARG:CG   | 2.03                     | 0.43              |
| 1:A:813:ILE:HG12 | 2:B:128:PHE:CE1  | 2.51                     | 0.43              |
| 1:P:639:GLY:H    | 4:0:344:SER:HB3  | 1.83                     | 0.43              |
| 1:G:217:THR:HG22 | 1:G:218:LEU:N    | 2.34                     | 0.43              |
| 1:J:224:SER:O    | 1:J:227:PRO:HD2  | 2.17                     | 0.43              |
| 1:M:639:GLY:H    | 4:Z:344:SER:HB3  | 1.83                     | 0.43              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:G:747:LEU:C    | 1:G:749:GLY:N    | 2.71                     | 0.43              |
| 1:A:568:PRO:CG   | 1:A:578:HIS:H    | 2.30                     | 0.43              |
| 1:A:549:SER:C    | 4:V:45:VAL:O     | 2.56                     | 0.43              |
| 1:J:710:GLY:CA   | 1:J:772:LEU:HD23 | 2.26                     | 0.43              |
| 4:2:287:ILE:HG13 | 4:4:202:THR:HG22 | 1.89                     | 0.43              |
| 1:M:732:ILE:HG23 | 1:M:747:LEU:HD12 | 0.95                     | 0.43              |
| 1:G:715:VAL:HG12 | 1:G:720:PHE:HB2  | 2.00                     | 0.43              |
| 1:G:201:ALA:O    | 1:G:202:SER:OG   | 2.36                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:214:MET:CA   | 1:P:340:ILE:HD11 | 2.45                     | 0.43              |
| 1:G:295:MLY:CE   | 1:G:332:MET:CE   | 2.97                     | 0.43              |
| 1:J:94:MET:O     | 1:J:713:SER:HA   | 2.16                     | 0.43              |
| 3:O:50:LEU:O     | 3:O:53:PRO:HG2   | 2.18                     | 0.43              |
| 1:D:174:SER:OG   | 1:D:669:PRO:HA   | 2.18                     | 0.43              |
| 1:G:689:GLU:HA   | 1:G:692:LEU:HB2  | 1.99                     | 0.43              |
| 1:P:612:GLN:NE2  | 1:P:627:GLY:H    | 2.14                     | 0.43              |
| 1:J:64:THR:CG2   | 1:J:65:GLU:H     | 2.31                     | 0.43              |
| 1:M:496:PHE:HB2  | 1:M:515:PHE:CD2  | 2.53                     | 0.43              |
| 1:G:354:LEU:HD12 | 1:G:354:LEU:HA   | 1.56                     | 0.43              |
| 4:Y:193:LEU:O    | 4:Y:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:G:86:ASP:OD2   | 1:G:87:MLY:HH22  | 2.19                     | 0.43              |
| 1:D:810:ARG:HG2  | 1:D:810:ARG:NH1  | 2.29                     | 0.43              |
| 1:G:292:MET:CE   | 1:G:309:PRO:CA   | 2.97                     | 0.43              |
| 1:P:292:MET:CE   | 1:P:309:PRO:CA   | 2.97                     | 0.43              |
| 1:J:322:VAL:CG1  | 1:J:325:ILE:HG13 | 2.49                     | 0.43              |
| 1:M:109:ARG:CD   | 1:M:117:THR:HB   | 2.49                     | 0.43              |
| 3:O:101:THR:HA   | 3:O:137:ILE:O    | 2.18                     | 0.43              |
| 1:J:400:ALA:CB   | 1:J:606:THR:HG22 | 2.49                     | 0.43              |
| 1:G:391:GLY:HA3  | 1:G:616:VAL:HG23 | 2.01                     | 0.43              |
| 1:D:246:PHE:HB3  | 1:D:270:LEU:HD12 | 2.01                     | 0.43              |
| 3:O:69:LEU:HB3   | 3:O:70:PRO:HD3   | 1.99                     | 0.43              |
| 4:5:149:THR:HA   | 4:5:165:ILE:O    | 2.19                     | 0.43              |
| 1:A:151:ALA:HB1  | 1:A:152:PRO:HD2  | 2.01                     | 0.43              |
| 1:P:246:PHE:HB3  | 1:P:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:725:ARG:CZ   | 1:D:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:D:508:ILE:CG1  | 1:D:766:PHE:HE1  | 2.21                     | 0.43              |
| 1:J:725:ARG:CZ   | 1:J:737:PHE:CE1  | 3.02                     | 0.43              |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:HD13 | 1.92                     | 0.43              |
| 2:H:114:LYS:CG   | 2:H:146:GLY:HA2  | 2.46                     | 0.43              |
| 1:P:541:MET:HG2  | 4:0:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:P:537:GLU:OE1  | 4:0:350:SER:HA   | 2.19                     | 0.43              |
| 1:P:530:MET:CE   | 4:0:354:GLN:CB   | 2.95                     | 0.43              |
| 1:A:725:ARG:CZ   | 1:A:737:PHE:CE1  | 3.02                     | 0.43              |
| 1:J:217:THR:HG22 | 1:J:218:LEU:N    | 2.34                     | 0.43              |
| 1:D:541:MET:CE   | 4:9:346:LEU:HD12 | 2.47                     | 0.43              |
| 1:D:530:MET:HA   | 4:9:354:GLN:CD   | 2.11                     | 0.43              |
| 1:G:725:ARG:CZ   | 1:G:737:PHE:CZ   | 3.01                     | 0.43              |
| 1:M:217:THR:HG22 | 1:M:218:LEU:N    | 2.34                     | 0.43              |
| 1:A:529:PRO:HB3  | 4:8:354:GLN:HA   | 2.00                     | 0.43              |
| 1:A:530:MET:CE   | 4:8:354:GLN:HG3  | 2.35                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:442:VAL:O    | 1:P:445:ILE:HB   | 2.19                     | 0.43              |
| 1:J:829:TRP:O    | 1:J:832:MET:N    | 2.50                     | 0.43              |
| 1:P:829:TRP:HA   | 1:P:830:PRO:HD2  | 1.86                     | 0.43              |
| 1:G:40:VAL:HG23  | 1:G:76:GLN:O     | 2.19                     | 0.43              |
| 1:M:40:VAL:HG23  | 1:M:76:GLN:O     | 2.19                     | 0.43              |
| 1:M:689:GLU:HA   | 1:M:692:LEU:HB2  | 2.00                     | 0.43              |
| 1:G:692:LEU:HD23 | 1:G:692:LEU:HA   | 1.84                     | 0.43              |
| 1:P:692:LEU:HA   | 1:P:692:LEU:HD23 | 1.84                     | 0.43              |
| 1:P:692:LEU:O    | 1:P:696:ARG:HG3  | 2.18                     | 0.43              |
| 1:M:493:HIS:O    | 1:M:496:PHE:HB3  | 2.18                     | 0.43              |
| 1:M:64:THR:CG2   | 1:M:65:GLU:H     | 2.32                     | 0.43              |
| 1:M:354:LEU:HA   | 1:M:354:LEU:HD12 | 1.56                     | 0.43              |
| 1:A:14:ALA:N     | 1:A:15:PRO:CD    | 2.81                     | 0.43              |
| 1:G:505:MLY:HD2  | 1:G:762:HIS:NE2  | 2.34                     | 0.43              |
| 1:M:292:MET:CE   | 1:M:309:PRO:CA   | 2.97                     | 0.43              |
| 1:P:464:ILE:CG2  | 1:P:465:ALA:N    | 2.80                     | 0.43              |
| 3:I:119:THR:O    | 3:I:123:VAL:HG23 | 2.18                     | 0.43              |
| 3:F:119:THR:O    | 3:F:123:VAL:HG23 | 2.18                     | 0.43              |
| 1:J:485:GLU:OE2  | 1:J:584:TYR:N    | 2.50                     | 0.43              |
| 1:A:330:GLU:O    | 1:A:333:ALA:HB3  | 2.17                     | 0.43              |
| 1:A:476:GLU:H    | 1:A:476:GLU:CD   | 2.21                     | 0.43              |
| 4:8:149:THR:HA   | 4:8:165:ILE:O    | 2.19                     | 0.43              |
| 4:Y:149:THR:HA   | 4:Y:165:ILE:O    | 2.19                     | 0.43              |
| 1:M:500:GLN:HB2  | 1:M:512:PHE:CZ   | 2.54                     | 0.43              |
| 1:M:151:ALA:HB1  | 1:M:152:PRO:HD2  | 2.01                     | 0.43              |
| 1:J:391:GLY:HA3  | 1:J:616:VAL:HG23 | 2.01                     | 0.43              |
| 1:J:384:ASP:OD1  | 1:J:394:SER:OG   | 2.28                     | 0.43              |
| 1:D:391:GLY:HA3  | 1:D:616:VAL:HG23 | 2.00                     | 0.43              |
| 4:4:171:LEU:HA   | 4:4:172:PRO:HD2  | 1.84                     | 0.43              |
| 1:D:724:TYR:HB3  | 1:D:727:LEU:CD1  | 2.48                     | 0.43              |
| 1:G:787:ILE:HG23 | 1:G:791:GLN:HG3  | 2.00                     | 0.43              |
| 1:G:797:PHE:HE1  | 3:I:146:ILE:HA   | 1.82                     | 0.43              |
| 1:G:793:ARG:HD3  | 3:I:40:ASN:ND2   | 2.32                     | 0.43              |
| 1:G:642:LYS:HB2  | 4:V:24:ASP:O     | 1.89                     | 0.43              |
| 2:E:137:TRP:CA   | 2:E:145:ALA:HB2  | 2.37                     | 0.43              |
| 1:P:408:VAL:HG22 | 1:P:636:LYS:HG2  | 1.51                     | 0.43              |
| 1:G:206:LYS:CE   | 1:G:217:THR:HG23 | 2.30                     | 0.43              |
| 1:G:226:ASN:N    | 1:G:227:PRO:HD2  | 2.32                     | 0.43              |
| 1:M:537:GLU:OE1  | 4:Z:350:SER:HA   | 2.19                     | 0.43              |
| 1:M:541:MET:HB3  | 4:Z:345:ILE:HG22 | 2.00                     | 0.43              |
| 1:M:568:PRO:CG   | 1:M:578:HIS:H    | 2.30                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:553:MLY:HE2  | 4:Y:45:VAL:HB    | 2.01                     | 0.43              |
| 1:G:725:ARG:NE   | 1:G:733:PRO:CB   | 1.95                     | 0.43              |
| 1:D:217:THR:HG22 | 1:D:218:LEU:N    | 2.33                     | 0.43              |
| 1:M:723:ARG:NH1  | 1:M:723:ARG:CG   | 2.79                     | 0.43              |
| 1:M:506:GLU:HG3  | 1:M:760:PHE:O    | 2.09                     | 0.43              |
| 1:M:84:MLY:HG2   | 1:M:723:ARG:CG   | 2.48                     | 0.43              |
| 1:P:715:VAL:HG12 | 1:P:720:PHE:HB2  | 2.00                     | 0.43              |
| 1:P:803:TYR:O    | 1:P:807:VAL:HB   | 2.19                     | 0.43              |
| 1:D:295:MLY:HG3  | 1:D:332:MET:HE2  | 2.00                     | 0.43              |
| 1:G:174:SER:OG   | 1:G:669:PRO:HA   | 2.18                     | 0.43              |
| 4:5:220:ALA:HB3  | 4:5:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:J:406:VAL:O    | 1:J:412:ALA:HA   | 2.19                     | 0.43              |
| 4:1:223:PHE:HB3  | 4:1:259:GLU:OE2  | 2.18                     | 0.43              |
| 1:P:195:TYR:CD2  | 1:P:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:D:493:HIS:O    | 1:D:496:PHE:HB3  | 2.18                     | 0.43              |
| 4:0:193:LEU:O    | 4:0:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:J:14:ALA:N     | 1:J:15:PRO:CD    | 2.82                     | 0.43              |
| 1:D:14:ALA:N     | 1:D:15:PRO:CD    | 2.81                     | 0.43              |
| 1:J:292:MET:CE   | 1:J:309:PRO:CA   | 2.97                     | 0.43              |
| 1:P:48:VAL:HA    | 1:P:104:TYR:OH   | 2.18                     | 0.43              |
| 1:A:266:GLU:OE1  | 1:A:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:P:400:ALA:CB   | 1:P:606:THR:HG22 | 2.49                     | 0.43              |
| 1:A:369:MLY:HD3  | 1:A:369:MLY:HH22 | 1.79                     | 0.43              |
| 1:G:443:ILE:HG22 | 1:G:444:ARG:N    | 2.29                     | 0.43              |
| 1:M:246:PHE:HB3  | 1:M:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:G:793:ARG:HA   | 3:I:40:ASN:HB3   | 2.01                     | 0.43              |
| 1:D:506:GLU:O    | 1:D:762:HIS:CB   | 2.67                     | 0.43              |
| 2:N:114:LYS:CG   | 2:N:146:GLY:HA2  | 2.46                     | 0.43              |
| 2:Q:139:ALA:C    | 2:Q:141:PRO:HD3  | 2.33                     | 0.43              |
| 1:P:747:LEU:C    | 1:P:749:GLY:N    | 2.71                     | 0.43              |
| 1:J:642:LYS:HB2  | 4:W:24:ASP:O     | 1.88                     | 0.43              |
| 1:P:787:ILE:HG23 | 1:P:791:GLN:HG3  | 2.00                     | 0.43              |
| 1:A:831:TRP:HH2  | 2:B:50:THR:HB    | 1.34                     | 0.43              |
| 1:G:747:LEU:O    | 1:G:749:GLY:N    | 2.52                     | 0.43              |
| 1:M:786:ILE:C    | 1:M:787:ILE:C    | 2.78                     | 0.43              |
| 4:2:290:ARG:CZ   | 4:4:202:THR:HG22 | 2.37                     | 0.43              |
| 1:A:641:LYS:CE   | 1:A:647:GLN:CB   | 2.74                     | 0.43              |
| 1:J:201:ALA:O    | 1:J:202:SER:OG   | 2.36                     | 0.43              |
| 4:3:287:ILE:HG13 | 4:5:202:THR:HA   | 1.40                     | 0.43              |
| 3:F:63:ILE:CG2   | 3:F:64:THR:H     | 2.32                     | 0.43              |
| 4:1:244:ASP:HB2  | 4:Z:322:PRO:CA   | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:220:ALA:HB3  | 4:Y:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:0:220:ALA:HB3  | 4:0:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:493:HIS:O    | 1:A:496:PHE:HB3  | 2.18                     | 0.43              |
| 1:D:195:TYR:CD2  | 1:D:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:A:86:ASP:OD2   | 1:A:87:MLY:HH22  | 2.19                     | 0.43              |
| 1:J:123:CYS:HB2  | 1:J:158:ILE:HD13 | 2.00                     | 0.43              |
| 1:J:309:PRO:C    | 1:J:311:ASP:H    | 2.22                     | 0.43              |
| 1:M:141:LEU:HD12 | 1:M:141:LEU:N    | 2.32                     | 0.43              |
| 1:M:266:GLU:OE1  | 1:M:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:J:464:ILE:CG2  | 1:J:465:ALA:N    | 2.80                     | 0.43              |
| 1:P:266:GLU:OE1  | 1:P:659:MLY:NZ   | 2.51                     | 0.43              |
| 1:G:109:ARG:CD   | 1:G:117:THR:HB   | 2.49                     | 0.43              |
| 1:J:169:ASP:O    | 1:J:170:ARG:HB2  | 2.19                     | 0.43              |
| 4:0:149:THR:HA   | 4:0:165:ILE:O    | 2.19                     | 0.43              |
| 1:G:442:VAL:O    | 1:G:445:ILE:HB   | 2.19                     | 0.43              |
| 1:J:715:VAL:HG12 | 1:J:720:PHE:HB2  | 2.00                     | 0.43              |
| 1:M:546:THR:H    | 4:1:46:GLY:HA3   | 1.83                     | 0.43              |
| 1:J:537:GLU:OE1  | 4:W:350:SER:HA   | 2.19                     | 0.43              |
| 1:D:541:MET:HG2  | 4:9:345:ILE:HG23 | 2.01                     | 0.43              |
| 1:A:639:GLY:CA   | 4:8:344:SER:O    | 2.40                     | 0.43              |
| 1:A:408:VAL:HG22 | 1:A:636:LYS:HG2  | 1.51                     | 0.43              |
| 1:P:217:THR:HG22 | 1:P:218:LEU:N    | 2.34                     | 0.43              |
| 1:M:201:ALA:O    | 1:M:202:SER:OG   | 2.36                     | 0.43              |
| 1:A:819:ASN:N    | 2:B:90:GLY:C     | 2.72                     | 0.43              |
| 1:J:831:TRP:HZ3  | 2:K:34:ILE:HG21  | 1.81                     | 0.43              |
| 1:P:40:VAL:HG23  | 1:P:76:GLN:O     | 2.19                     | 0.43              |
| 1:D:692:LEU:HD23 | 1:D:692:LEU:HA   | 1.84                     | 0.43              |
| 1:J:278:GLN:HE21 | 1:J:278:GLN:HB3  | 1.42                     | 0.43              |
| 4:4:220:ALA:HB3  | 4:4:223:PHE:CD1  | 2.53                     | 0.43              |
| 4:Z:193:LEU:O    | 4:Z:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:D:144:ARG:HD2  | 1:D:144:ARG:HA   | 1.78                     | 0.43              |
| 1:M:322:VAL:CG1  | 1:M:325:ILE:HG13 | 2.49                     | 0.43              |
| 4:7:180:LEU:HD11 | 4:7:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:7:217:CYS:C    | 4:7:218:TYR:HD1  | 2.22                     | 0.43              |
| 4:2:217:CYS:C    | 4:2:218:TYR:HD1  | 2.22                     | 0.43              |
| 4:5:205:GLU:O    | 4:5:208:ILE:HG22 | 2.18                     | 0.43              |
| 1:G:294:ASN:OD1  | 1:G:307:THR:HG21 | 2.19                     | 0.43              |
| 1:G:500:GLN:HB2  | 1:G:512:PHE:CZ   | 2.54                     | 0.43              |
| 1:G:246:PHE:HB3  | 1:G:270:LEU:HD12 | 2.01                     | 0.43              |
| 1:G:151:ALA:HB1  | 1:G:152:PRO:HD2  | 2.01                     | 0.43              |
| 1:A:500:GLN:HB2  | 1:A:512:PHE:CZ   | 2.54                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:294:ASN:OD1  | 1:P:307:THR:HG21 | 2.19                     | 0.43              |
| 1:A:715:VAL:HG12 | 1:A:720:PHE:HB2  | 2.00                     | 0.43              |
| 1:A:501:GLU:C    | 1:A:762:HIS:CG   | 2.88                     | 0.43              |
| 1:D:715:VAL:HG12 | 1:D:720:PHE:HB2  | 2.00                     | 0.43              |
| 2:Q:140:PHE:CD2  | 2:Q:144:VAL:HG11 | 2.54                     | 0.43              |
| 2:Q:144:VAL:HG12 | 2:Q:153:ILE:HD11 | 1.75                     | 0.43              |
| 1:G:817:GLN:CG   | 2:H:127:ARG:CG   | 2.97                     | 0.43              |
| 1:G:213:LYS:HA   | 1:G:220:ASP:OD2  | 2.19                     | 0.43              |
| 1:M:553:MLY:CH2  | 4:1:43:VAL:HG23  | 2.49                     | 0.43              |
| 1:J:533:PHE:HD1  | 1:J:533:PHE:HA   | 1.79                     | 0.43              |
| 1:P:792:ALA:CB   | 3:R:42:THR:N     | 2.82                     | 0.43              |
| 1:M:445:ILE:HG22 | 1:M:449:LEU:HD22 | 2.01                     | 0.43              |
| 4:O:202:THR:O    | 4:Y:287:ILE:HD13 | 2.19                     | 0.43              |
| 1:M:798:LEU:HA   | 1:M:798:LEU:HD12 | 1.37                     | 0.43              |
| 2:B:54:MET:SD    | 2:H:21:GLU:OE1   | 2.76                     | 0.43              |
| 1:G:835:PHE:CD1  | 2:H:30:ALA:HB2   | 2.54                     | 0.43              |
| 1:P:93:MET:CE    | 1:P:764:MLY:CD   | 2.96                     | 0.43              |
| 1:M:295:MLY:CE   | 1:M:332:MET:CE   | 2.97                     | 0.43              |
| 1:A:214:MET:CA   | 1:A:340:ILE:HD11 | 2.46                     | 0.43              |
| 3:I:63:ILE:CG2   | 3:I:64:THR:H     | 2.32                     | 0.43              |
| 1:J:568:PRO:O    | 1:J:570:PRO:HD3  | 2.19                     | 0.43              |
| 1:J:320:ILE:HG22 | 1:J:320:ILE:O    | 2.18                     | 0.43              |
| 1:G:129:TYR:HD1  | 1:G:129:TYR:HA   | 1.65                     | 0.43              |
| 4:W:220:ALA:HB3  | 4:W:223:PHE:CD1  | 2.53                     | 0.43              |
| 1:A:62:VAL:O     | 1:A:69:THR:HA    | 2.19                     | 0.43              |
| 1:J:195:TYR:CD2  | 1:J:199:ILE:HD13 | 2.54                     | 0.43              |
| 1:G:195:TYR:CD2  | 1:G:199:ILE:HD13 | 2.54                     | 0.43              |
| 4:2:193:LEU:O    | 4:2:198:TYR:HD2  | 2.01                     | 0.43              |
| 1:P:322:VAL:CG1  | 1:P:325:ILE:HD11 | 2.47                     | 0.43              |
| 1:A:292:MET:CE   | 1:A:309:PRO:CA   | 2.97                     | 0.43              |
| 1:J:109:ARG:CD   | 1:J:117:THR:HB   | 2.49                     | 0.43              |
| 4:8:180:LEU:HD11 | 4:8:261:LEU:HD23 | 2.01                     | 0.43              |
| 4:9:180:LEU:HD11 | 4:9:261:LEU:HD23 | 2.01                     | 0.43              |
| 1:A:400:ALA:CB   | 1:A:606:THR:HG22 | 2.49                     | 0.43              |
| 1:D:169:ASP:O    | 1:D:170:ARG:HB2  | 2.19                     | 0.43              |
| 1:P:169:ASP:O    | 1:P:170:ARG:HB2  | 2.19                     | 0.43              |
| 3:I:11:LYS:HE2   | 3:I:11:LYS:HB3   | 1.83                     | 0.43              |
| 4:Z:149:THR:HA   | 4:Z:165:ILE:O    | 2.19                     | 0.43              |
| 1:J:294:ASN:OD1  | 1:J:307:THR:HG21 | 2.19                     | 0.43              |
| 1:A:294:ASN:OD1  | 1:A:307:THR:HG21 | 2.19                     | 0.43              |
| 1:D:787:ILE:HG23 | 1:D:791:GLN:HG3  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:791:GLN:HE22 | 3:I:115:GLY:C    | 2.15                     | 0.42              |
| 2:N:140:PHE:O    | 2:N:141:PRO:C    | 2.33                     | 0.42              |
| 1:P:818:TYR:CD1  | 2:Q:127:ARG:CZ   | 3.02                     | 0.42              |
| 1:J:747:LEU:C    | 1:J:749:GLY:N    | 2.71                     | 0.42              |
| 1:P:406:VAL:O    | 1:P:412:ALA:HA   | 2.19                     | 0.42              |
| 1:M:534:SER:CB   | 4:Z:351:THR:HA   | 2.49                     | 0.42              |
| 1:J:530:MET:CB   | 4:W:354:GLN:CB   | 2.95                     | 0.42              |
| 1:D:549:SER:C    | 4:W:45:VAL:O     | 2.57                     | 0.42              |
| 1:A:636:LYS:CB   | 4:8:334:GLU:OE1  | 2.67                     | 0.42              |
| 1:A:541:MET:HB3  | 4:8:345:ILE:HG22 | 2.00                     | 0.42              |
| 1:A:578:HIS:HB3  | 1:A:592:ILE:CD1  | 2.38                     | 0.42              |
| 1:P:836:PHE:CD1  | 2:Q:159:HIS:HA   | 2.36                     | 0.42              |
| 1:M:92:ALA:O     | 1:M:714:ARG:HG3  | 2.19                     | 0.42              |
| 3:R:63:ILE:CG2   | 3:R:64:THR:H     | 2.32                     | 0.42              |
| 1:J:175:ILE:C    | 1:J:176:LEU:HD12 | 2.38                     | 0.42              |
| 1:M:174:SER:OG   | 1:M:669:PRO:HA   | 2.18                     | 0.42              |
| 4:2:220:ALA:HB3  | 4:2:223:PHE:CD1  | 2.53                     | 0.42              |
| 1:D:496:PHE:HB2  | 1:D:515:PHE:CD2  | 2.54                     | 0.42              |
| 4:X:193:LEU:O    | 4:X:198:TYR:HD2  | 2.01                     | 0.42              |
| 1:P:485:GLU:OE2  | 1:P:584:TYR:N    | 2.50                     | 0.42              |
| 1:G:185:LYS:H    | 1:G:185:LYS:HG3  | 1.62                     | 0.42              |
| 4:8:205:GLU:O    | 4:8:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:A:246:PHE:HB3  | 1:A:270:LEU:HD12 | 2.00                     | 0.42              |
| 4:1:149:THR:HA   | 4:1:165:ILE:O    | 2.19                     | 0.42              |
| 1:A:768:MLY:H    | 1:A:771:LEU:HD22 | 1.84                     | 0.42              |
| 1:M:817:GLN:CG   | 2:N:127:ARG:CG   | 2.77                     | 0.42              |
| 1:G:529:PRO:HB3  | 4:V:354:GLN:HA   | 2.00                     | 0.42              |
| 1:A:445:ILE:HG22 | 1:A:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:P:541:MET:HB3  | 4:0:345:ILE:HG22 | 2.00                     | 0.42              |
| 1:P:541:MET:HG2  | 4:0:345:ILE:HG23 | 2.01                     | 0.42              |
| 1:G:445:ILE:HG22 | 1:G:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:J:442:VAL:O    | 1:J:445:ILE:HB   | 2.19                     | 0.42              |
| 1:M:408:VAL:HG22 | 1:M:636:LYS:HG2  | 1.52                     | 0.42              |
| 1:D:537:GLU:OE1  | 4:9:350:SER:HA   | 2.19                     | 0.42              |
| 1:D:819:ASN:HA   | 2:E:91:ALA:HA    | 2.00                     | 0.42              |
| 4:0:205:GLU:CB   | 4:Y:287:ILE:HD13 | 2.48                     | 0.42              |
| 1:M:836:PHE:CD2  | 2:N:160:GLY:HA3  | 2.53                     | 0.42              |
| 1:P:226:ASN:HB2  | 1:P:227:PRO:CD   | 2.47                     | 0.42              |
| 1:M:725:ARG:CZ   | 1:M:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:G:97:LEU:HD12  | 1:G:97:LEU:HA    | 1.67                     | 0.42              |
| 1:P:201:ALA:O    | 1:P:202:SER:OG   | 2.36                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:642:LYS:HG3  | 4:8:23:GLY:CA    | 2.32                     | 0.42              |
| 1:P:806:MET:CA   | 1:P:809:ARG:HD2  | 2.45                     | 0.42              |
| 1:J:556:ASP:HB3  | 4:Y:47:MET:HB2   | 1.00                     | 0.42              |
| 1:A:295:MLY:CD   | 1:A:332:MET:HE2  | 2.50                     | 0.42              |
| 3:F:50:LEU:O     | 3:F:53:PRO:HG2   | 2.18                     | 0.42              |
| 3:C:50:LEU:O     | 3:C:53:PRO:HG2   | 2.18                     | 0.42              |
| 4:3:322:PRO:CA   | 4:5:244:ASP:HB2  | 2.49                     | 0.42              |
| 1:G:568:PRO:O    | 1:G:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:P:173:GLN:HG3  | 1:P:670:HIS:CD2  | 2.54                     | 0.42              |
| 1:J:418:THR:CG2  | 1:J:419:VAL:N    | 2.79                     | 0.42              |
| 1:G:64:THR:CG2   | 1:G:65:GLU:H     | 2.32                     | 0.42              |
| 1:M:195:TYR:CD2  | 1:M:199:ILE:HD13 | 2.54                     | 0.42              |
| 1:A:195:TYR:CD2  | 1:A:199:ILE:HD13 | 2.54                     | 0.42              |
| 4:9:193:LEU:O    | 4:9:198:TYR:HD2  | 2.01                     | 0.42              |
| 1:G:346:ASP:O    | 1:G:350:ALA:N    | 2.46                     | 0.42              |
| 1:P:14:ALA:N     | 1:P:15:PRO:CD    | 2.82                     | 0.42              |
| 1:G:762:HIS:N    | 1:G:762:HIS:CD2  | 2.78                     | 0.42              |
| 1:P:309:PRO:C    | 1:P:311:ASP:H    | 2.22                     | 0.42              |
| 4:4:180:LEU:HD11 | 4:4:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:1:217:CYS:C    | 4:1:218:TYR:HD1  | 2.22                     | 0.42              |
| 1:G:476:GLU:H    | 1:G:476:GLU:CD   | 2.21                     | 0.42              |
| 1:D:673:ARG:HA   | 1:D:673:ARG:HD2  | 1.79                     | 0.42              |
| 1:D:829:TRP:O    | 1:D:832:MET:N    | 2.50                     | 0.42              |
| 4:X:149:THR:HA   | 4:X:165:ILE:O    | 2.19                     | 0.42              |
| 1:D:724:TYR:HB3  | 1:D:782:MLY:CE   | 2.48                     | 0.42              |
| 1:D:727:LEU:CG   | 1:D:782:MLY:HG2  | 2.40                     | 0.42              |
| 1:P:826:VAL:O    | 1:P:828:HIS:N    | 2.53                     | 0.42              |
| 2:E:140:PHE:CD2  | 2:E:144:VAL:HG11 | 2.54                     | 0.42              |
| 2:H:140:PHE:CD2  | 2:H:144:VAL:HG11 | 2.55                     | 0.42              |
| 1:P:534:SER:CB   | 4:0:351:THR:HA   | 2.49                     | 0.42              |
| 1:J:445:ILE:HG22 | 1:J:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:D:529:PRO:HB3  | 4:9:354:GLN:HA   | 2.00                     | 0.42              |
| 1:D:550:PHE:C    | 4:W:46:GLY:CA    | 2.88                     | 0.42              |
| 1:G:725:ARG:CZ   | 1:G:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:G:732:ILE:CG2  | 1:G:747:LEU:CD1  | 0.65                     | 0.42              |
| 1:D:449:LEU:N    | 1:D:449:LEU:CD1  | 2.82                     | 0.42              |
| 1:M:221:GLN:H    | 1:M:221:GLN:HG2  | 1.47                     | 0.42              |
| 4:0:201:VAL:HG21 | 4:Y:290:ARG:NH2  | 2.34                     | 0.42              |
| 1:P:445:ILE:HG22 | 1:P:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:G:711:PHE:HB3  | 1:G:766:PHE:HB3  | 1.99                     | 0.42              |
| 4:1:204:ALA:H    | 4:Z:287:ILE:HB   | 1.83                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:8:324:THR:HG23 | 4:V:245:GLY:HA2  | 1.09                     | 0.42              |
| 4:V:205:GLU:O    | 4:V:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:G:741:LYS:HG2  | 1:G:742:LYS:N    | 2.35                     | 0.42              |
| 1:A:60:VAL:O     | 1:A:72:VAL:N     | 2.51                     | 0.42              |
| 1:D:175:ILE:C    | 1:D:176:LEU:HD12 | 2.39                     | 0.42              |
| 1:A:689:GLU:HA   | 1:A:692:LEU:HB2  | 2.00                     | 0.42              |
| 1:A:692:LEU:HA   | 1:A:692:LEU:HD23 | 1.84                     | 0.42              |
| 2:E:163:ALA:C    | 2:K:22:THR:OG1   | 2.57                     | 0.42              |
| 1:P:496:PHE:HB2  | 1:P:515:PHE:CD2  | 2.53                     | 0.42              |
| 1:G:62:VAL:O     | 1:G:69:THR:HA    | 2.19                     | 0.42              |
| 1:P:62:VAL:O     | 1:P:69:THR:HA    | 2.20                     | 0.42              |
| 1:D:62:VAL:HG12  | 1:D:63:MLY:N     | 2.35                     | 0.42              |
| 1:M:14:ALA:N     | 1:M:15:PRO:CD    | 2.82                     | 0.42              |
| 1:J:86:ASP:OD2   | 1:J:87:MLY:HH22  | 2.19                     | 0.42              |
| 1:G:141:LEU:N    | 1:G:141:LEU:HD12 | 2.32                     | 0.42              |
| 1:A:91:MET:CE    | 1:A:119:SER:HB2  | 2.48                     | 0.42              |
| 4:8:206:ARG:O    | 4:8:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:5:180:LEU:HD11 | 4:5:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:W:180:LEU:HD11 | 4:W:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:2:180:LEU:HD11 | 4:2:261:LEU:HD23 | 2.02                     | 0.42              |
| 1:M:169:ASP:O    | 1:M:170:ARG:HB2  | 2.19                     | 0.42              |
| 4:Y:217:CYS:C    | 4:Y:218:TYR:HD1  | 2.22                     | 0.42              |
| 1:M:443:ILE:HG22 | 1:M:444:ARG:N    | 2.29                     | 0.42              |
| 1:D:725:ARG:CZ   | 1:D:737:PHE:CE1  | 3.02                     | 0.42              |
| 2:K:112:ILE:O    | 2:K:148:VAL:N    | 2.50                     | 0.42              |
| 2:B:140:PHE:CD2  | 2:B:144:VAL:HG11 | 2.54                     | 0.42              |
| 1:M:568:PRO:O    | 1:M:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:D:442:VAL:O    | 1:D:445:ILE:HB   | 2.19                     | 0.42              |
| 1:D:445:ILE:HG22 | 1:D:449:LEU:HD22 | 2.01                     | 0.42              |
| 1:M:442:VAL:O    | 1:M:445:ILE:HB   | 2.19                     | 0.42              |
| 1:P:641:LYS:CD   | 1:P:647:GLN:CG   | 2.72                     | 0.42              |
| 4:1:196:ARG:HH21 | 4:1:249:THR:HG23 | 1.85                     | 0.42              |
| 1:J:295:MLY:CE   | 1:J:332:MET:CE   | 2.97                     | 0.42              |
| 1:J:214:MET:CA   | 1:J:340:ILE:HD11 | 2.45                     | 0.42              |
| 1:G:332:MET:HG2  | 1:G:332:MET:H    | 1.52                     | 0.42              |
| 1:J:173:GLN:HG3  | 1:J:670:HIS:CD2  | 2.54                     | 0.42              |
| 1:P:175:ILE:C    | 1:P:176:LEU:HD12 | 2.38                     | 0.42              |
| 1:G:173:GLN:HG3  | 1:G:670:HIS:CD2  | 2.55                     | 0.42              |
| 1:M:107:MLY:CB   | 1:M:686:MET:HE2  | 2.38                     | 0.42              |
| 4:9:220:ALA:HB3  | 4:9:223:PHE:CD1  | 2.53                     | 0.42              |
| 1:A:64:THR:CG2   | 1:A:65:GLU:H     | 2.32                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:62:VAL:O     | 1:J:69:THR:HA    | 2.20                     | 0.42              |
| 1:M:38:VAL:HG13  | 1:M:39:PHE:N     | 2.35                     | 0.42              |
| 1:P:86:ASP:OD2   | 1:P:87:MLY:HH22  | 2.18                     | 0.42              |
| 1:G:123:CYS:HB2  | 1:G:158:ILE:HD13 | 2.00                     | 0.42              |
| 4:2:206:ARG:O    | 4:2:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:X:206:ARG:O    | 4:X:209:VAL:HG12 | 2.20                     | 0.42              |
| 1:D:659:MLY:HH22 | 1:D:659:MLY:HD2  | 1.42                     | 0.42              |
| 1:A:485:GLU:OE1  | 1:A:583:HIS:ND1  | 2.49                     | 0.42              |
| 1:D:402:CYS:C    | 1:D:404:PRO:HD3  | 2.40                     | 0.42              |
| 1:J:485:GLU:HA   | 1:J:584:TYR:HE2  | 1.83                     | 0.42              |
| 4:V:180:LEU:HD11 | 4:V:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:0:180:LEU:HD11 | 4:0:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:X:180:LEU:HD11 | 4:X:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:4:217:CYS:C    | 4:4:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:0:217:CYS:C    | 4:0:218:TYR:HD1  | 2.23                     | 0.42              |
| 4:X:217:CYS:C    | 4:X:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:X:222:ASP:OD1  | 4:X:224:GLU:HB3  | 2.19                     | 0.42              |
| 3:L:11:LYS:HE2   | 3:L:11:LYS:HB3   | 1.83                     | 0.42              |
| 1:M:294:ASN:OD1  | 1:M:307:THR:HG21 | 2.19                     | 0.42              |
| 1:D:724:TYR:CB   | 1:D:782:MLY:CE   | 2.94                     | 0.42              |
| 1:G:406:VAL:O    | 1:G:412:ALA:HA   | 2.19                     | 0.42              |
| 1:G:534:SER:CB   | 4:V:351:THR:HA   | 2.49                     | 0.42              |
| 1:P:725:ARG:CZ   | 1:P:737:PHE:CE1  | 3.02                     | 0.42              |
| 1:J:819:ASN:ND2  | 2:K:92:ASP:CA    | 2.80                     | 0.42              |
| 1:P:642:LYS:HB2  | 4:0:24:ASP:O     | 1.88                     | 0.42              |
| 1:J:449:LEU:N    | 1:J:449:LEU:CD1  | 2.81                     | 0.42              |
| 1:J:530:MET:HA   | 4:W:354:GLN:CD   | 2.11                     | 0.42              |
| 1:J:541:MET:HG2  | 4:W:345:ILE:HG23 | 2.02                     | 0.42              |
| 1:J:534:SER:CB   | 4:W:351:THR:HA   | 2.49                     | 0.42              |
| 1:P:795:ARG:CG   | 3:R:35:ARG:HH12  | 2.31                     | 0.42              |
| 1:D:534:SER:CB   | 4:9:351:THR:HA   | 2.49                     | 0.42              |
| 1:D:406:VAL:O    | 1:D:412:ALA:HA   | 2.20                     | 0.42              |
| 1:P:552:ASN:HB3  | 4:2:41:GLN:HE22  | 1.84                     | 0.42              |
| 1:P:568:PRO:O    | 1:P:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:A:541:MET:CE   | 4:8:346:LEU:HD12 | 2.48                     | 0.42              |
| 1:A:568:PRO:O    | 1:A:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:D:768:MLY:C    | 1:D:771:LEU:HA   | 2.50                     | 0.42              |
| 1:G:839:MLY:N    | 1:G:840:PRO:HD2  | 2.35                     | 0.42              |
| 1:D:295:MLY:CE   | 1:D:332:MET:CE   | 2.97                     | 0.42              |
| 1:D:741:LYS:HG2  | 1:D:742:LYS:N    | 2.35                     | 0.42              |
| 1:J:40:VAL:HG23  | 1:J:76:GLN:O     | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:174:SER:HA   | 1:J:460:GLY:O    | 2.20                     | 0.42              |
| 1:P:271:GLU:OE1  | 1:P:274:ARG:NH1  | 2.53                     | 0.42              |
| 1:P:62:VAL:HG12  | 1:P:63:MLY:N     | 2.35                     | 0.42              |
| 1:M:826:VAL:O    | 1:M:828:HIS:N    | 2.53                     | 0.42              |
| 4:W:193:LEU:O    | 4:W:198:TYR:HD2  | 2.01                     | 0.42              |
| 1:M:25:ILE:HG23  | 1:M:29:ASN:HD22  | 1.85                     | 0.42              |
| 1:A:38:VAL:HG13  | 1:A:39:PHE:N     | 2.35                     | 0.42              |
| 1:A:166:MET:CE   | 1:A:254:PHE:HB2  | 2.46                     | 0.42              |
| 1:M:86:ASP:OD2   | 1:M:87:MLY:HH22  | 2.18                     | 0.42              |
| 1:P:109:ARG:CD   | 1:P:117:THR:HB   | 2.49                     | 0.42              |
| 4:3:180:LEU:HD11 | 4:3:261:LEU:HD23 | 2.01                     | 0.42              |
| 4:Y:180:LEU:HD11 | 4:Y:261:LEU:HD23 | 2.01                     | 0.42              |
| 1:M:400:ALA:CB   | 1:M:606:THR:HG22 | 2.49                     | 0.42              |
| 4:W:217:CYS:C    | 4:W:218:TYR:HD1  | 2.22                     | 0.42              |
| 4:5:217:CYS:C    | 4:5:218:TYR:HD1  | 2.23                     | 0.42              |
| 4:9:217:CYS:C    | 4:9:218:TYR:HD1  | 2.23                     | 0.42              |
| 4:8:217:CYS:C    | 4:8:218:TYR:HD1  | 2.23                     | 0.42              |
| 4:3:217:CYS:C    | 4:3:218:TYR:HD1  | 2.22                     | 0.42              |
| 1:A:330:GLU:H    | 1:A:330:GLU:HG2  | 1.55                     | 0.42              |
| 1:P:330:GLU:H    | 1:P:330:GLU:HG2  | 1.54                     | 0.42              |
| 4:8:196:ARG:HH21 | 4:8:249:THR:HG23 | 1.85                     | 0.42              |
| 3:R:96:LYS:HG3   | 3:R:96:LYS:H     | 1.67                     | 0.42              |
| 4:0:222:ASP:OD1  | 4:0:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:8:222:ASP:OD1  | 4:8:224:GLU:HB3  | 2.20                     | 0.42              |
| 4:W:222:ASP:OD1  | 4:W:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:D:798:LEU:HA   | 1:D:798:LEU:HD12 | 1.37                     | 0.42              |
| 1:D:795:ARG:NH1  | 3:F:116:GLU:OE2  | 2.39                     | 0.42              |
| 1:G:510:TRP:CH2  | 1:G:768:MLY:HH11 | 2.55                     | 0.42              |
| 1:A:744:SER:O    | 1:A:748:LEU:HD12 | 2.20                     | 0.42              |
| 1:P:819:ASN:OD1  | 2:Q:91:ALA:CA    | 2.67                     | 0.42              |
| 1:A:213:LYS:HA   | 1:A:220:ASP:OD2  | 2.18                     | 0.42              |
| 2:B:112:ILE:O    | 2:B:148:VAL:N    | 2.50                     | 0.42              |
| 1:J:84:MLY:CH2   | 1:J:719:ASP:C    | 2.88                     | 0.42              |
| 1:M:578:HIS:CD2  | 1:M:592:ILE:H    | 2.38                     | 0.42              |
| 1:M:541:MET:CE   | 4:Z:346:LEU:HD12 | 2.47                     | 0.42              |
| 1:P:797:PHE:CE2  | 3:R:126:LEU:HD22 | 2.49                     | 0.42              |
| 1:M:213:LYS:HA   | 1:M:220:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:798:LEU:HA   | 1:A:798:LEU:HD12 | 1.37                     | 0.42              |
| 1:P:449:LEU:CD1  | 1:P:449:LEU:N    | 2.82                     | 0.42              |
| 1:D:204:GLU:N    | 1:D:207:LYS:HE3  | 2.23                     | 0.42              |
| 4:7:287:ILE:HA   | 4:9:202:THR:HG21 | 1.59                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:9:205:GLU:O    | 4:9:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:J:578:HIS:CD2  | 1:J:592:ILE:H    | 2.38                     | 0.42              |
| 1:G:578:HIS:CD2  | 1:G:592:ILE:H    | 2.38                     | 0.42              |
| 4:V:286:ASP:HA   | 4:X:202:THR:HG22 | 1.63                     | 0.42              |
| 1:P:320:ILE:HG22 | 1:P:320:ILE:O    | 2.18                     | 0.42              |
| 1:D:279:LEU:CB   | 1:D:280:PRO:HD2  | 2.49                     | 0.42              |
| 1:J:271:GLU:OE1  | 1:J:274:ARG:NH1  | 2.53                     | 0.42              |
| 4:7:220:ALA:HB3  | 4:7:223:PHE:CD1  | 2.53                     | 0.42              |
| 4:1:180:LEU:HD11 | 4:1:261:LEU:HD23 | 2.02                     | 0.42              |
| 1:M:62:VAL:O     | 1:M:69:THR:HA    | 2.20                     | 0.42              |
| 1:G:166:MET:CE   | 1:G:254:PHE:HB2  | 2.46                     | 0.42              |
| 1:D:519:LEU:H    | 1:D:519:LEU:HD12 | 1.83                     | 0.42              |
| 1:P:464:ILE:HG21 | 1:P:464:ILE:HD13 | 1.69                     | 0.42              |
| 1:J:462:LEU:HD11 | 1:J:464:ILE:CD1  | 2.50                     | 0.42              |
| 1:D:109:ARG:CD   | 1:D:117:THR:HB   | 2.49                     | 0.42              |
| 4:V:217:CYS:C    | 4:V:218:TYR:HD1  | 2.22                     | 0.42              |
| 1:J:789:ALA:HB1  | 3:L:81:GLN:CG    | 2.49                     | 0.42              |
| 1:A:842:LEU:N    | 1:A:842:LEU:CD1  | 2.82                     | 0.42              |
| 4:Z:205:GLU:O    | 4:Z:208:ILE:HG22 | 2.19                     | 0.42              |
| 4:Y:222:ASP:OD1  | 4:Y:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:D:294:ASN:OD1  | 1:D:307:THR:HG21 | 2.19                     | 0.42              |
| 1:P:690:LEU:O    | 1:P:694:GLN:HG3  | 2.20                     | 0.42              |
| 1:D:725:ARG:HA   | 1:D:732:ILE:CG2  | 2.50                     | 0.42              |
| 2:Q:113:LYS:O    | 2:Q:147:ASN:HB2  | 2.20                     | 0.42              |
| 1:P:747:LEU:O    | 1:P:749:GLY:N    | 2.53                     | 0.42              |
| 1:P:797:PHE:CD1  | 3:R:146:ILE:HG23 | 2.55                     | 0.42              |
| 1:D:636:LYS:CB   | 4:9:334:GLU:OE1  | 2.68                     | 0.42              |
| 1:D:409:GLY:N    | 1:D:636:LYS:CD   | 2.71                     | 0.42              |
| 1:D:206:LYS:HD2  | 1:D:217:THR:CG2  | 2.17                     | 0.42              |
| 1:M:791:GLN:HE22 | 3:O:115:GLY:HA3  | 1.84                     | 0.42              |
| 1:M:788:THR:HG22 | 3:O:42:THR:HG21  | 2.01                     | 0.42              |
| 1:D:215:GLN:H    | 1:D:340:ILE:CD1  | 2.20                     | 0.42              |
| 2:K:149:ASP:CG   | 2:K:150:TYR:N    | 2.49                     | 0.42              |
| 1:M:756:THR:HB   | 1:M:757:GLN:H    | 1.64                     | 0.42              |
| 4:4:193:LEU:HD11 | 4:4:250:ILE:HG13 | 2.02                     | 0.42              |
| 1:P:322:VAL:CG1  | 1:P:325:ILE:HG13 | 2.49                     | 0.42              |
| 1:M:309:PRO:C    | 1:M:311:ASP:H    | 2.22                     | 0.42              |
| 4:Z:369:ILE:HG23 | 4:Z:370:VAL:N    | 2.35                     | 0.42              |
| 4:3:206:ARG:O    | 4:3:209:VAL:HG12 | 2.20                     | 0.42              |
| 1:A:309:PRO:C    | 1:A:311:ASP:H    | 2.22                     | 0.42              |
| 1:A:402:CYS:C    | 1:A:404:PRO:HD3  | 2.40                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:402:CYS:C    | 1:J:404:PRO:HD3  | 2.40                     | 0.42              |
| 1:A:169:ASP:O    | 1:A:170:ARG:HB2  | 2.20                     | 0.42              |
| 4:Z:217:CYS:C    | 4:Z:218:TYR:HD1  | 2.23                     | 0.42              |
| 4:3:149:THR:HA   | 4:3:165:ILE:O    | 2.19                     | 0.42              |
| 1:A:625:THR:HG22 | 1:A:625:THR:H    | 1.48                     | 0.42              |
| 4:8:315:LYS:HA   | 4:8:315:LYS:HD2  | 1.92                     | 0.42              |
| 1:M:690:LEU:O    | 1:M:694:GLN:HG3  | 2.20                     | 0.42              |
| 4:9:149:THR:HA   | 4:9:165:ILE:O    | 2.19                     | 0.42              |
| 1:D:826:VAL:O    | 1:D:828:HIS:N    | 2.53                     | 0.42              |
| 4:5:196:ARG:HH21 | 4:5:249:THR:HG23 | 1.85                     | 0.42              |
| 4:2:222:ASP:OD1  | 4:2:224:GLU:HB3  | 2.20                     | 0.42              |
| 1:P:151:ALA:HB1  | 1:P:152:PRO:HD2  | 2.01                     | 0.42              |
| 1:J:151:ALA:HB1  | 1:J:152:PRO:HD2  | 2.01                     | 0.42              |
| 1:A:499:GLU:CD   | 1:A:766:PHE:CE2  | 2.92                     | 0.42              |
| 2:Q:112:ILE:O    | 2:Q:148:VAL:N    | 2.50                     | 0.42              |
| 1:D:827:MLY:HH21 | 2:E:139:ALA:HB3  | 2.00                     | 0.42              |
| 2:E:144:VAL:HG12 | 2:E:153:ILE:HD13 | 1.92                     | 0.42              |
| 1:J:747:LEU:O    | 1:J:749:GLY:N    | 2.52                     | 0.42              |
| 2:B:113:LYS:O    | 2:B:147:ASN:HB2  | 2.20                     | 0.42              |
| 1:P:408:VAL:HA   | 1:P:636:LYS:HG3  | 1.03                     | 0.42              |
| 1:J:226:ASN:HB2  | 1:J:227:PRO:CD   | 2.47                     | 0.42              |
| 1:D:534:SER:HB2  | 4:9:354:GLN:HE22 | 1.56                     | 0.42              |
| 1:M:725:ARG:HA   | 1:M:732:ILE:CG2  | 2.50                     | 0.42              |
| 1:J:839:MLY:N    | 1:J:840:PRO:HD2  | 2.35                     | 0.42              |
| 1:M:28:GLN:CB    | 1:M:723:ARG:NH2  | 2.83                     | 0.42              |
| 1:M:744:SER:O    | 1:M:748:LEU:HD12 | 2.20                     | 0.42              |
| 1:P:295:MLY:CE   | 1:P:332:MET:CE   | 2.97                     | 0.42              |
| 4:9:287:ILE:CB   | 4:W:204:ALA:H    | 2.13                     | 0.42              |
| 1:A:800:ARG:CB   | 3:C:149:VAL:CG2  | 2.62                     | 0.42              |
| 3:L:63:ILE:CG2   | 3:L:64:THR:H     | 2.33                     | 0.42              |
| 3:O:25:ILE:O     | 3:O:63:ILE:CB    | 2.66                     | 0.42              |
| 1:M:829:TRP:HA   | 1:M:830:PRO:HD2  | 1.86                     | 0.42              |
| 1:D:320:ILE:O    | 1:D:320:ILE:HG22 | 2.18                     | 0.42              |
| 1:M:556:ASP:CB   | 4:1:49:GLN:OE1   | 2.62                     | 0.42              |
| 1:A:406:VAL:O    | 1:A:412:ALA:HA   | 2.19                     | 0.42              |
| 1:M:62:VAL:HG12  | 1:M:63:MLY:N     | 2.35                     | 0.42              |
| 4:5:193:LEU:HD11 | 4:5:250:ILE:HG13 | 2.02                     | 0.42              |
| 1:A:240:ASN:OD1  | 1:A:241:ASP:N    | 2.52                     | 0.42              |
| 1:M:11:GLY:O     | 1:M:14:ALA:HB3   | 2.20                     | 0.42              |
| 1:J:11:GLY:O     | 1:J:14:ALA:HB3   | 2.20                     | 0.42              |
| 1:A:141:LEU:HD12 | 1:A:141:LEU:N    | 2.32                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:322:VAL:HA   | 1:A:323:PRO:HD3  | 1.87                     | 0.42              |
| 1:A:134:VAL:C    | 1:A:136:ASN:H    | 2.16                     | 0.42              |
| 4:5:206:ARG:O    | 4:5:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:9:222:ASP:OD1  | 4:9:224:GLU:HB3  | 2.19                     | 0.42              |
| 4:Z:222:ASP:OD1  | 4:Z:224:GLU:HB3  | 2.20                     | 0.42              |
| 4:1:205:GLU:O    | 4:1:208:ILE:HG22 | 2.18                     | 0.42              |
| 4:V:222:ASP:OD1  | 4:V:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:J:500:GLN:HB2  | 1:J:512:PHE:CZ   | 2.54                     | 0.42              |
| 4:X:205:GLU:O    | 4:X:208:ILE:HG22 | 2.18                     | 0.42              |
| 1:J:787:ILE:HG23 | 1:J:791:GLN:HG3  | 2.00                     | 0.42              |
| 1:A:741:LYS:HG2  | 1:A:742:LYS:N    | 2.35                     | 0.42              |
| 4:1:45:VAL:CG2   | 4:Z:148:THR:HG21 | 2.50                     | 0.42              |
| 1:J:632:GLY:HA3  | 1:J:643:GLY:N    | 2.17                     | 0.42              |
| 1:D:541:MET:CG   | 4:9:345:ILE:C    | 2.87                     | 0.42              |
| 1:A:578:HIS:CD2  | 1:A:592:ILE:H    | 2.38                     | 0.42              |
| 1:P:724:TYR:HB3  | 1:P:727:LEU:CD1  | 2.48                     | 0.42              |
| 1:J:97:LEU:CD2   | 1:J:712:PRO:HB2  | 2.41                     | 0.42              |
| 1:A:800:ARG:O    | 3:C:149:VAL:HG23 | 2.11                     | 0.42              |
| 3:F:48:LYS:HA    | 3:F:48:LYS:HD3   | 1.17                     | 0.42              |
| 1:M:741:LYS:HG2  | 1:M:742:LYS:N    | 2.35                     | 0.42              |
| 1:M:829:TRP:O    | 1:M:832:MET:N    | 2.50                     | 0.42              |
| 1:A:173:GLN:HG3  | 1:A:670:HIS:CD2  | 2.54                     | 0.42              |
| 1:G:62:VAL:HG12  | 1:G:63:MLY:N     | 2.35                     | 0.42              |
| 1:A:195:TYR:CE2  | 1:A:199:ILE:HD13 | 2.55                     | 0.42              |
| 4:3:193:LEU:HD11 | 4:3:250:ILE:HG13 | 2.02                     | 0.42              |
| 1:P:354:LEU:HA   | 1:P:354:LEU:HD12 | 1.56                     | 0.42              |
| 4:2:193:LEU:HD11 | 4:2:250:ILE:HG13 | 2.02                     | 0.42              |
| 1:G:38:VAL:HG13  | 1:G:39:PHE:N     | 2.35                     | 0.42              |
| 1:P:11:GLY:O     | 1:P:14:ALA:HB3   | 2.20                     | 0.42              |
| 1:D:86:ASP:OD2   | 1:D:87:MLY:HH22  | 2.19                     | 0.42              |
| 1:J:166:MET:CE   | 1:J:254:PHE:HB2  | 2.47                     | 0.42              |
| 4:W:206:ARG:O    | 4:W:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:Z:206:ARG:O    | 4:Z:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:V:206:ARG:O    | 4:V:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:0:369:ILE:HG23 | 4:0:370:VAL:N    | 2.35                     | 0.42              |
| 4:7:369:ILE:HG23 | 4:7:370:VAL:N    | 2.35                     | 0.42              |
| 1:D:462:LEU:HD11 | 1:D:464:ILE:CD1  | 2.50                     | 0.42              |
| 1:P:106:LEU:HD12 | 1:P:106:LEU:HA   | 1.79                     | 0.42              |
| 4:Z:180:LEU:HD11 | 4:Z:261:LEU:HD23 | 2.01                     | 0.42              |
| 1:G:633:GLY:HA2  | 4:V:25:ASP:HA    | 1.26                     | 0.42              |
| 1:G:400:ALA:CB   | 1:G:606:THR:HG22 | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:476:GLU:CD   | 1:M:476:GLU:H    | 2.22                     | 0.42              |
| 1:A:110:TYR:O    | 1:A:113:TRP:N    | 2.42                     | 0.42              |
| 4:4:315:LYS:HA   | 4:4:315:LYS:HD2  | 1.92                     | 0.42              |
| 4:4:196:ARG:HH21 | 4:4:249:THR:HG23 | 1.85                     | 0.42              |
| 4:1:222:ASP:OD1  | 4:1:224:GLU:HB3  | 2.19                     | 0.42              |
| 1:D:690:LEU:O    | 1:D:694:GLN:HG3  | 2.19                     | 0.42              |
| 4:V:196:ARG:HH21 | 4:V:249:THR:HG23 | 1.85                     | 0.42              |
| 1:J:795:ARG:HD2  | 3:L:43:ASN:N     | 2.34                     | 0.42              |
| 1:G:787:ILE:HD13 | 1:G:787:ILE:HG21 | 1.67                     | 0.42              |
| 1:A:508:ILE:HD11 | 1:A:759:ALA:C    | 2.40                     | 0.42              |
| 1:A:498:LEU:HD21 | 1:A:764:MLY:HH22 | 1.98                     | 0.42              |
| 2:H:140:PHE:HA   | 2:H:141:PRO:HD2  | 1.57                     | 0.42              |
| 1:P:408:VAL:HA   | 1:P:636:LYS:HG2  | 1.14                     | 0.42              |
| 1:M:406:VAL:O    | 1:M:412:ALA:HA   | 2.19                     | 0.42              |
| 1:M:541:MET:HG2  | 4:Z:345:ILE:HG23 | 2.01                     | 0.42              |
| 1:M:636:LYS:CB   | 4:Z:334:GLU:OE1  | 2.68                     | 0.42              |
| 1:D:568:PRO:O    | 1:D:570:PRO:HD3  | 2.19                     | 0.42              |
| 1:D:578:HIS:CD2  | 1:D:592:ILE:H    | 2.38                     | 0.42              |
| 1:A:797:PHE:CD2  | 1:A:798:LEU:HD12 | 2.55                     | 0.42              |
| 1:M:797:PHE:CD2  | 1:M:798:LEU:HD12 | 2.55                     | 0.42              |
| 1:D:838:ILE:HD13 | 2:E:54:MET:HE1   | 2.02                     | 0.42              |
| 1:P:744:SER:O    | 1:P:748:LEU:HD12 | 2.20                     | 0.42              |
| 4:X:291:LYS:HG3  | 4:Z:243:PRO:O    | 2.19                     | 0.42              |
| 1:P:803:TYR:CE1  | 1:P:807:VAL:HG21 | 2.55                     | 0.42              |
| 1:P:295:MLY:CD   | 1:P:332:MET:HE2  | 2.50                     | 0.42              |
| 3:F:49:ILE:CA    | 3:F:52:ASN:ND2   | 2.53                     | 0.42              |
| 3:F:62:ALA:O     | 3:F:63:ILE:HG13  | 2.14                     | 0.42              |
| 1:P:741:LYS:HG2  | 1:P:742:LYS:N    | 2.35                     | 0.42              |
| 3:O:63:ILE:CG2   | 3:O:64:THR:H     | 2.33                     | 0.42              |
| 1:P:174:SER:HA   | 1:P:460:GLY:O    | 2.20                     | 0.42              |
| 4:9:221:LEU:HA   | 4:9:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:W:221:LEU:HA   | 4:W:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:7:221:LEU:HA   | 4:7:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:Y:221:LEU:HA   | 4:Y:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:0:221:LEU:HA   | 4:0:312:ARG:HG2  | 2.02                     | 0.42              |
| 4:Z:193:LEU:HD11 | 4:Z:250:ILE:HG13 | 2.02                     | 0.42              |
| 4:V:193:LEU:HD11 | 4:V:250:ILE:HG13 | 2.02                     | 0.42              |
| 1:D:308:ASN:HA   | 1:D:309:PRO:HD2  | 1.88                     | 0.42              |
| 1:D:14:ALA:HB3   | 1:D:15:PRO:CD    | 2.46                     | 0.42              |
| 4:1:206:ARG:O    | 4:1:209:VAL:HG12 | 2.20                     | 0.42              |
| 4:X:369:ILE:HG23 | 4:X:370:VAL:N    | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:Y:369:ILE:HG23 | 4:Y:370:VAL:N    | 2.35                     | 0.42              |
| 4:9:369:ILE:HG23 | 4:9:370:VAL:N    | 2.35                     | 0.42              |
| 1:M:402:CYS:C    | 1:M:404:PRO:HD3  | 2.40                     | 0.42              |
| 1:D:471:ASP:CB   | 1:D:573:GLY:O    | 2.68                     | 0.42              |
| 1:G:169:ASP:O    | 1:G:170:ARG:HB2  | 2.19                     | 0.42              |
| 4:9:324:THR:N    | 4:W:245:GLY:CA   | 2.69                     | 0.42              |
| 4:V:315:LYS:HD2  | 4:V:315:LYS:HA   | 1.92                     | 0.42              |
| 1:M:673:ARG:HA   | 1:M:673:ARG:HD2  | 1.79                     | 0.42              |
| 1:J:690:LEU:O    | 1:J:694:GLN:HG3  | 2.20                     | 0.42              |
| 1:D:747:LEU:O    | 1:D:749:GLY:N    | 2.52                     | 0.41              |
| 1:D:787:ILE:HG21 | 1:D:787:ILE:HD13 | 1.67                     | 0.41              |
| 1:D:797:PHE:CD2  | 1:D:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:G:539:GLU:OE2  | 1:G:553:MLY:HD3  | 2.20                     | 0.41              |
| 1:J:725:ARG:HA   | 1:J:732:ILE:CG2  | 2.50                     | 0.41              |
| 1:G:817:GLN:HG3  | 2:H:128:PHE:CZ   | 2.55                     | 0.41              |
| 2:H:141:PRO:CB   | 2:H:142:PRO:HD3  | 2.48                     | 0.41              |
| 1:P:642:LYS:HE2  | 4:0:344:SER:HA   | 1.57                     | 0.41              |
| 1:J:84:MLY:HH12  | 1:J:715:VAL:HG21 | 2.01                     | 0.41              |
| 1:J:636:LYS:CB   | 4:W:334:GLU:OE1  | 2.68                     | 0.41              |
| 1:J:541:MET:CG   | 4:W:345:ILE:C    | 2.87                     | 0.41              |
| 1:M:217:THR:CA   | 1:M:221:GLN:HE21 | 2.33                     | 0.41              |
| 1:P:578:HIS:CD2  | 1:P:592:ILE:H    | 2.38                     | 0.41              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:HG23 | 2.01                     | 0.41              |
| 1:M:839:MLY:HD2  | 2:N:159:HIS:HB3  | 2.01                     | 0.41              |
| 1:M:747:LEU:O    | 1:M:749:GLY:N    | 2.52                     | 0.41              |
| 1:D:712:PRO:HB2  | 1:D:771:LEU:HD22 | 1.99                     | 0.41              |
| 1:D:839:MLY:N    | 1:D:840:PRO:HD2  | 2.35                     | 0.41              |
| 1:G:829:TRP:HE1  | 2:H:70:GLU:CD    | 2.24                     | 0.41              |
| 1:J:741:LYS:HG2  | 1:J:742:LYS:N    | 2.35                     | 0.41              |
| 3:O:48:LYS:HA    | 3:O:48:LYS:HD3   | 1.17                     | 0.41              |
| 1:A:800:ARG:CA   | 3:C:149:VAL:HG22 | 2.46                     | 0.41              |
| 4:3:324:THR:CG2  | 4:5:244:ASP:O    | 2.68                     | 0.41              |
| 1:G:56:GLU:HB2   | 1:G:59:MLY:CB    | 2.30                     | 0.41              |
| 2:N:149:ASP:OD2  | 2:N:150:TYR:CA   | 2.64                     | 0.41              |
| 1:G:568:PRO:CG   | 1:G:578:HIS:N    | 2.83                     | 0.41              |
| 1:D:174:SER:HA   | 1:D:460:GLY:O    | 2.20                     | 0.41              |
| 1:D:129:TYR:HD1  | 1:D:129:TYR:HA   | 1.65                     | 0.41              |
| 1:D:701:LEU:HA   | 1:D:701:LEU:HD12 | 1.55                     | 0.41              |
| 4:Z:226:GLU:HG3  | 4:Z:255:PHE:CE2  | 2.56                     | 0.41              |
| 1:J:195:TYR:CE2  | 1:J:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:J:346:ASP:O    | 1:J:350:ALA:N    | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:193:LEU:HD11 | 4:7:250:ILE:HG13 | 2.02                     | 0.41              |
| 1:G:166:MET:CE   | 1:G:254:PHE:CD2  | 3.01                     | 0.41              |
| 1:G:11:GLY:O     | 1:G:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:P:296:MLY:HH11 | 1:P:348:MLY:CH2  | 2.48                     | 0.41              |
| 1:P:335:ASP:O    | 1:P:338:ILE:HB   | 2.20                     | 0.41              |
| 1:D:296:MLY:HH11 | 1:D:348:MLY:CH2  | 2.48                     | 0.41              |
| 4:0:206:ARG:O    | 4:0:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:Y:206:ARG:O    | 4:Y:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:V:369:ILE:HG23 | 4:V:370:VAL:N    | 2.35                     | 0.41              |
| 4:W:369:ILE:HG23 | 4:W:370:VAL:N    | 2.35                     | 0.41              |
| 4:3:369:ILE:HG23 | 4:3:370:VAL:N    | 2.35                     | 0.41              |
| 1:P:135:TYR:HD2  | 1:P:191:ARG:CG   | 2.33                     | 0.41              |
| 1:A:659:MLY:HH22 | 1:A:659:MLY:HD2  | 1.42                     | 0.41              |
| 1:P:402:CYS:C    | 1:P:404:PRO:HD3  | 2.40                     | 0.41              |
| 1:D:151:ALA:HB1  | 1:D:152:PRO:HD2  | 2.01                     | 0.41              |
| 1:G:369:MLY:HD3  | 1:G:369:MLY:HH22 | 1.79                     | 0.41              |
| 1:M:842:LEU:N    | 1:M:842:LEU:CD1  | 2.83                     | 0.41              |
| 1:A:690:LEU:O    | 1:A:694:GLN:HG3  | 2.20                     | 0.41              |
| 4:2:196:ARG:HH21 | 4:2:249:THR:HG23 | 1.85                     | 0.41              |
| 4:4:222:ASP:OD1  | 4:4:224:GLU:HB3  | 2.19                     | 0.41              |
| 4:7:222:ASP:OD1  | 4:7:224:GLU:HB3  | 2.19                     | 0.41              |
| 1:A:829:TRP:O    | 1:A:832:MET:N    | 2.50                     | 0.41              |
| 1:G:541:MET:HB3  | 4:V:345:ILE:HG22 | 2.01                     | 0.41              |
| 1:P:813:ILE:CG2  | 2:Q:128:PHE:HE1  | 2.32                     | 0.41              |
| 2:Q:137:TRP:CA   | 2:Q:145:ALA:HB2  | 2.37                     | 0.41              |
| 1:P:725:ARG:HA   | 1:P:732:ILE:CG2  | 2.50                     | 0.41              |
| 2:B:137:TRP:CA   | 2:B:145:ALA:HB2  | 2.37                     | 0.41              |
| 1:P:636:LYS:CB   | 4:0:334:GLU:OE1  | 2.68                     | 0.41              |
| 1:J:744:SER:O    | 1:J:748:LEU:HD12 | 2.20                     | 0.41              |
| 1:D:568:PRO:CG   | 1:D:578:HIS:N    | 2.84                     | 0.41              |
| 1:P:568:PRO:CG   | 1:P:578:HIS:N    | 2.83                     | 0.41              |
| 1:A:553:MLY:HE2  | 4:V:45:VAL:CA    | 2.38                     | 0.41              |
| 1:D:769:ALA:N    | 1:D:771:LEU:HA   | 2.25                     | 0.41              |
| 4:7:287:ILE:N    | 4:9:202:THR:CG2  | 2.77                     | 0.41              |
| 1:M:60:VAL:O     | 1:M:72:VAL:N     | 2.51                     | 0.41              |
| 1:D:271:GLU:OE1  | 1:D:274:ARG:NH1  | 2.53                     | 0.41              |
| 4:4:226:GLU:HG3  | 4:4:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:3:221:LEU:HA   | 4:3:312:ARG:HG2  | 2.02                     | 0.41              |
| 1:P:195:TYR:CE2  | 1:P:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:G:195:TYR:CE2  | 1:G:199:ILE:HD13 | 2.55                     | 0.41              |
| 4:1:193:LEU:HD11 | 4:1:250:ILE:HG13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:W:193:LEU:HD11 | 4:W:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:X:193:LEU:HD11 | 4:X:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:Y:193:LEU:HD11 | 4:Y:250:ILE:HG13 | 2.02                     | 0.41              |
| 1:M:166:MET:CE   | 1:M:254:PHE:HB2  | 2.47                     | 0.41              |
| 1:J:166:MET:CE   | 1:J:254:PHE:CD2  | 3.01                     | 0.41              |
| 1:D:466:GLY:CA   | 1:D:484:ASN:HD21 | 2.32                     | 0.41              |
| 4:7:206:ARG:O    | 4:7:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:5:369:ILE:HG23 | 4:5:370:VAL:N    | 2.35                     | 0.41              |
| 1:M:135:TYR:HD2  | 1:M:191:ARG:CG   | 2.33                     | 0.41              |
| 1:A:330:GLU:OE1  | 1:A:330:GLU:HA   | 2.21                     | 0.41              |
| 4:3:222:ASP:OD1  | 4:3:224:GLU:HB3  | 2.19                     | 0.41              |
| 1:D:398:LEU:HA   | 1:D:398:LEU:HD12 | 1.83                     | 0.41              |
| 1:D:356:GLY:HA2  | 1:D:359:MET:HG3  | 2.02                     | 0.41              |
| 4:9:196:ARG:HH21 | 4:9:249:THR:HG23 | 1.85                     | 0.41              |
| 4:3:205:GLU:O    | 4:3:208:ILE:HG22 | 2.18                     | 0.41              |
| 1:J:793:ARG:HH11 | 3:L:40:ASN:HD22  | 1.67                     | 0.41              |
| 1:J:797:PHE:CD2  | 1:J:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:D:723:ARG:NH1  | 1:D:723:ARG:CG   | 2.80                     | 0.41              |
| 2:N:140:PHE:CD2  | 2:N:144:VAL:HG11 | 2.54                     | 0.41              |
| 2:N:113:LYS:O    | 2:N:147:ASN:HB2  | 2.20                     | 0.41              |
| 1:G:553:MLY:C    | 4:X:46:GLY:HA3   | 2.50                     | 0.41              |
| 2:K:140:PHE:CD2  | 2:K:144:VAL:HG11 | 2.54                     | 0.41              |
| 2:B:139:ALA:O    | 2:B:141:PRO:CD   | 2.51                     | 0.41              |
| 1:A:732:ILE:CG2  | 1:A:747:LEU:HD12 | 0.35                     | 0.41              |
| 1:A:747:LEU:O    | 1:A:749:GLY:N    | 2.52                     | 0.41              |
| 1:M:539:GLU:OE2  | 1:M:553:MLY:HD3  | 2.20                     | 0.41              |
| 1:M:543:PRO:CG   | 4:Z:146:GLY:O    | 2.66                     | 0.41              |
| 1:P:792:ALA:CA   | 3:R:42:THR:HG22  | 2.41                     | 0.41              |
| 1:D:815:CYS:O    | 2:E:90:GLY:O     | 2.38                     | 0.41              |
| 4:0:205:GLU:HG2  | 4:Y:287:ILE:CD1  | 2.47                     | 0.41              |
| 1:M:725:ARG:CG   | 1:M:733:PRO:HA   | 2.43                     | 0.41              |
| 1:G:744:SER:O    | 1:G:748:LEU:HD12 | 2.20                     | 0.41              |
| 1:A:839:MLY:N    | 1:A:840:PRO:HD2  | 2.35                     | 0.41              |
| 1:M:805:ALA:O    | 1:M:808:GLU:N    | 2.54                     | 0.41              |
| 3:L:25:ILE:O     | 3:L:63:ILE:CB    | 2.66                     | 0.41              |
| 1:A:775:LEU:HD12 | 1:A:775:LEU:HA   | 1.71                     | 0.41              |
| 1:J:568:PRO:CG   | 1:J:578:HIS:N    | 2.84                     | 0.41              |
| 1:M:173:GLN:HG3  | 1:M:670:HIS:CD2  | 2.54                     | 0.41              |
| 1:A:62:VAL:HG12  | 1:A:63:MLY:N     | 2.35                     | 0.41              |
| 4:0:193:LEU:HD11 | 4:0:250:ILE:HG13 | 2.02                     | 0.41              |
| 4:8:193:LEU:HD11 | 4:8:250:ILE:HG13 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:25:ILE:HG23  | 1:A:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:D:11:GLY:O     | 1:D:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:G:136:ASN:O    | 1:G:138:MLY:N    | 2.54                     | 0.41              |
| 1:P:136:ASN:O    | 1:P:138:MLY:N    | 2.54                     | 0.41              |
| 4:8:369:ILE:HG23 | 4:8:370:VAL:N    | 2.35                     | 0.41              |
| 4:2:369:ILE:HG23 | 4:2:370:VAL:N    | 2.35                     | 0.41              |
| 1:A:135:TYR:HD2  | 1:A:191:ARG:CG   | 2.33                     | 0.41              |
| 1:P:471:ASP:CB   | 1:P:573:GLY:O    | 2.68                     | 0.41              |
| 3:I:56:GLU:OE1   | 3:I:59:ASN:ND2   | 2.54                     | 0.41              |
| 1:P:500:GLN:HB2  | 1:P:512:PHE:CZ   | 2.54                     | 0.41              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:HG22 | 2.00                     | 0.41              |
| 1:G:541:MET:HG2  | 4:V:345:ILE:HG23 | 2.01                     | 0.41              |
| 1:G:534:SER:HB2  | 4:V:354:GLN:HE22 | 1.57                     | 0.41              |
| 2:E:113:LYS:O    | 2:E:147:ASN:HB2  | 2.20                     | 0.41              |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:HD13 | 1.37                     | 0.41              |
| 1:G:826:VAL:O    | 1:G:828:HIS:N    | 2.53                     | 0.41              |
| 1:G:813:ILE:CG2  | 2:H:128:PHE:HZ   | 2.09                     | 0.41              |
| 1:G:725:ARG:HA   | 1:G:732:ILE:CG2  | 2.50                     | 0.41              |
| 1:A:568:PRO:CG   | 1:A:578:HIS:N    | 2.84                     | 0.41              |
| 1:P:204:GLU:N    | 1:P:207:LYS:HE3  | 2.23                     | 0.41              |
| 1:J:332:MET:HG2  | 1:J:332:MET:H    | 1.52                     | 0.41              |
| 1:M:215:GLN:H    | 1:M:340:ILE:CD1  | 2.20                     | 0.41              |
| 3:C:63:ILE:CG2   | 3:C:64:THR:H     | 2.33                     | 0.41              |
| 1:D:739:ASP:C    | 1:D:739:ASP:OD1  | 2.58                     | 0.41              |
| 1:G:60:VAL:O     | 1:G:72:VAL:N     | 2.51                     | 0.41              |
| 4:9:226:GLU:HG3  | 4:9:255:PHE:CE2  | 2.55                     | 0.41              |
| 1:A:11:GLY:O     | 1:A:14:ALA:HB3   | 2.20                     | 0.41              |
| 1:D:87:MLY:HD3   | 1:D:87:MLY:HH12  | 1.61                     | 0.41              |
| 1:J:136:ASN:O    | 1:J:138:MLY:N    | 2.54                     | 0.41              |
| 1:A:462:LEU:HD11 | 1:A:464:ILE:CD1  | 2.50                     | 0.41              |
| 1:G:471:ASP:CB   | 1:G:573:GLY:O    | 2.68                     | 0.41              |
| 1:J:471:ASP:CB   | 1:J:573:GLY:O    | 2.68                     | 0.41              |
| 4:1:148:THR:OG1  | 4:3:45:VAL:HG23  | 2.21                     | 0.41              |
| 1:G:330:GLU:HA   | 1:G:330:GLU:OE1  | 2.20                     | 0.41              |
| 4:Z:315:LYS:HD2  | 4:Z:315:LYS:HA   | 1.92                     | 0.41              |
| 3:C:11:LYS:HE2   | 3:C:11:LYS:HB3   | 1.83                     | 0.41              |
| 4:8:227:MET:O    | 4:8:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:Z:196:ARG:HH21 | 4:Z:249:THR:HG23 | 1.85                     | 0.41              |
| 1:D:500:GLN:HB2  | 1:D:512:PHE:CZ   | 2.54                     | 0.41              |
| 1:D:798:LEU:CD2  | 3:F:126:LEU:CD1  | 2.95                     | 0.41              |
| 1:A:505:MLY:CH1  | 1:A:762:HIS:O    | 2.61                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:636:LYS:CB   | 4:V:334:GLU:OE1  | 2.68                     | 0.41              |
| 1:G:541:MET:CE   | 4:V:346:LEU:HD12 | 2.48                     | 0.41              |
| 1:J:732:ILE:HG21 | 1:J:747:LEU:CD1  | 0.63                     | 0.41              |
| 1:G:817:GLN:NE2  | 2:H:127:ARG:CG   | 2.81                     | 0.41              |
| 2:K:144:VAL:HG12 | 2:K:153:ILE:HD13 | 1.92                     | 0.41              |
| 1:P:539:GLU:OE2  | 1:P:553:MLY:HD3  | 2.20                     | 0.41              |
| 1:G:217:THR:CA   | 1:G:221:GLN:HE21 | 2.33                     | 0.41              |
| 1:G:717:TYR:OH   | 1:G:760:PHE:HB3  | 2.21                     | 0.41              |
| 1:M:727:LEU:HD21 | 1:M:776:GLU:OE2  | 2.21                     | 0.41              |
| 4:X:325:MET:HE1  | 4:Z:244:ASP:CG   | 2.39                     | 0.41              |
| 1:D:629:GLU:HB3  | 1:D:643:GLY:C    | 2.41                     | 0.41              |
| 1:M:804:ARG:O    | 1:M:808:GLU:HB2  | 2.20                     | 0.41              |
| 1:J:826:VAL:O    | 1:J:828:HIS:N    | 2.53                     | 0.41              |
| 1:D:173:GLN:HG3  | 1:D:670:HIS:CD2  | 2.55                     | 0.41              |
| 1:P:756:THR:HB   | 1:P:757:GLN:H    | 1.63                     | 0.41              |
| 1:J:320:ILE:O    | 1:J:320:ILE:CG2  | 2.68                     | 0.41              |
| 4:W:226:GLU:HG3  | 4:W:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:7:226:GLU:HG3  | 4:7:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:5:221:LEU:HA   | 4:5:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:0:226:GLU:HG3  | 4:0:255:PHE:CE2  | 2.55                     | 0.41              |
| 1:J:63:MLY:HH23  | 1:J:63:MLY:HD3   | 1.76                     | 0.41              |
| 1:M:195:TYR:CE2  | 1:M:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:J:354:LEU:HA   | 1:J:354:LEU:HD12 | 1.55                     | 0.41              |
| 4:9:193:LEU:HD11 | 4:9:250:ILE:HG13 | 2.02                     | 0.41              |
| 1:D:25:ILE:HG23  | 1:D:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:A:166:MET:CE   | 1:A:254:PHE:CD2  | 3.01                     | 0.41              |
| 1:M:14:ALA:HB3   | 1:M:15:PRO:CD    | 2.46                     | 0.41              |
| 1:M:166:MET:CE   | 1:M:254:PHE:CD2  | 3.01                     | 0.41              |
| 1:A:136:ASN:O    | 1:A:138:MLY:N    | 2.54                     | 0.41              |
| 1:J:659:MLY:HD2  | 1:J:659:MLY:HH22 | 1.42                     | 0.41              |
| 1:D:135:TYR:CD2  | 1:D:191:ARG:HD3  | 2.55                     | 0.41              |
| 1:M:462:LEU:HD11 | 1:M:464:ILE:CD1  | 2.50                     | 0.41              |
| 1:G:135:TYR:HD2  | 1:G:191:ARG:CG   | 2.33                     | 0.41              |
| 1:G:402:CYS:C    | 1:G:404:PRO:HD3  | 2.40                     | 0.41              |
| 4:X:315:LYS:HD2  | 4:X:315:LYS:HA   | 1.92                     | 0.41              |
| 1:A:398:LEU:HD12 | 1:A:398:LEU:HA   | 1.84                     | 0.41              |
| 4:5:222:ASP:OD1  | 4:5:224:GLU:HB3  | 2.19                     | 0.41              |
| 4:3:148:THR:HG21 | 4:5:45:VAL:CG2   | 2.50                     | 0.41              |
| 4:2:227:MET:O    | 4:2:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:712:PRO:HB2  | 1:A:713:SER:H    | 1.61                     | 0.41              |
| 1:D:506:GLU:HG2  | 1:D:764:MLY:HE2  | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:744:SER:O    | 1:D:748:LEU:HD12 | 2.20                     | 0.41              |
| 1:G:553:MLY:CB   | 4:X:46:GLY:HA3   | 2.49                     | 0.41              |
| 1:A:221:GLN:HG2  | 1:A:221:GLN:H    | 1.47                     | 0.41              |
| 1:P:530:MET:HE3  | 4:0:354:GLN:CB   | 2.50                     | 0.41              |
| 1:J:717:TYR:OH   | 1:J:760:PHE:HB3  | 2.21                     | 0.41              |
| 1:M:568:PRO:CG   | 1:M:578:HIS:N    | 2.83                     | 0.41              |
| 1:P:797:PHE:CD2  | 1:P:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:A:798:LEU:HD13 | 3:C:126:LEU:CD1  | 2.41                     | 0.41              |
| 1:M:795:ARG:CZ   | 3:O:116:GLU:CD   | 2.84                     | 0.41              |
| 1:P:839:MLY:N    | 1:P:840:PRO:HD2  | 2.34                     | 0.41              |
| 1:D:838:ILE:HD13 | 2:E:54:MET:HE3   | 2.03                     | 0.41              |
| 4:3:288:ASP:CA   | 4:5:203:THR:CG2  | 2.99                     | 0.41              |
| 1:J:295:MLY:CE   | 1:J:332:MET:HE1  | 2.51                     | 0.41              |
| 4:8:288:ASP:OD1  | 4:V:204:ALA:HA   | 2.20                     | 0.41              |
| 3:I:25:ILE:O     | 3:I:63:ILE:CB    | 2.66                     | 0.41              |
| 4:1:244:ASP:O    | 4:Z:324:THR:CG2  | 2.68                     | 0.41              |
| 1:M:95:THR:CA    | 1:M:713:SER:CB   | 2.79                     | 0.41              |
| 1:M:174:SER:HA   | 1:M:460:GLY:O    | 2.20                     | 0.41              |
| 1:G:174:SER:HA   | 1:G:460:GLY:O    | 2.20                     | 0.41              |
| 1:M:701:LEU:HD12 | 1:M:701:LEU:HA   | 1.55                     | 0.41              |
| 4:2:221:LEU:HA   | 4:2:312:ARG:HG2  | 2.02                     | 0.41              |
| 4:Y:226:GLU:HG3  | 4:Y:255:PHE:CE2  | 2.55                     | 0.41              |
| 1:D:62:VAL:O     | 1:D:69:THR:HA    | 2.20                     | 0.41              |
| 1:D:309:PRO:C    | 1:D:311:ASP:H    | 2.22                     | 0.41              |
| 1:M:240:ASN:OD1  | 1:M:241:ASP:N    | 2.52                     | 0.41              |
| 1:P:14:ALA:HB3   | 1:P:15:PRO:CD    | 2.46                     | 0.41              |
| 1:G:308:ASN:HA   | 1:G:309:PRO:HD2  | 1.88                     | 0.41              |
| 1:A:49:MLY:HH23  | 1:A:80:MET:CE    | 2.51                     | 0.41              |
| 1:G:462:LEU:HD11 | 1:G:464:ILE:CD1  | 2.50                     | 0.41              |
| 1:J:464:ILE:HD13 | 1:J:464:ILE:HG21 | 1.69                     | 0.41              |
| 1:M:330:GLU:OE1  | 1:M:330:GLU:HA   | 2.20                     | 0.41              |
| 1:P:330:GLU:HA   | 1:P:330:GLU:OE1  | 2.21                     | 0.41              |
| 1:D:330:GLU:OE1  | 1:D:330:GLU:HA   | 2.21                     | 0.41              |
| 4:7:32:PRO:HB2   | 4:7:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:X:227:MET:O    | 4:X:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:2:144:ALA:HB2  | 4:2:342:GLY:CA   | 2.51                     | 0.41              |
| 3:O:56:GLU:OE1   | 3:O:59:ASN:ND2   | 2.54                     | 0.41              |
| 3:R:56:GLU:OE1   | 3:R:59:ASN:ND2   | 2.54                     | 0.41              |
| 1:A:826:VAL:O    | 1:A:828:HIS:N    | 2.53                     | 0.41              |
| 1:G:797:PHE:CD2  | 1:G:798:LEU:HD12 | 2.55                     | 0.41              |
| 1:G:792:ALA:CB   | 3:I:42:THR:CB    | 2.41                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:642:LYS:HE2  | 4:V:344:SER:HA   | 1.56                     | 0.41              |
| 1:G:449:LEU:HD12 | 1:G:449:LEU:HA   | 1.60                     | 0.41              |
| 1:M:536:LEU:HA   | 1:M:536:LEU:HD12 | 1.69                     | 0.41              |
| 1:M:530:MET:CB   | 4:Z:354:GLN:CB   | 2.95                     | 0.41              |
| 1:P:783:LEU:C    | 1:P:786:ILE:HG13 | 2.41                     | 0.41              |
| 1:M:226:ASN:HB2  | 1:M:227:PRO:CD   | 2.47                     | 0.41              |
| 1:P:549:SER:HA   | 4:2:49:GLN:CG    | 2.49                     | 0.41              |
| 4:8:144:ALA:HB2  | 4:8:342:GLY:CA   | 2.51                     | 0.41              |
| 1:P:218:LEU:HD22 | 1:P:222:ILE:HG13 | 1.95                     | 0.41              |
| 4:0:204:ALA:HB1  | 4:Y:288:ASP:CB   | 2.48                     | 0.41              |
| 1:J:204:GLU:N    | 1:J:207:LYS:HE3  | 2.23                     | 0.41              |
| 4:1:203:THR:CG2  | 4:Z:288:ASP:CA   | 2.99                     | 0.41              |
| 1:P:148:ARG:NH2  | 1:P:764:MLY:HH11 | 2.36                     | 0.41              |
| 1:M:803:TYR:CE2  | 3:O:17:PHE:CZ    | 3.08                     | 0.41              |
| 1:P:767:PHE:HB3  | 1:P:772:LEU:CD2  | 2.50                     | 0.41              |
| 1:J:829:TRP:CD2  | 2:K:87:LYS:NZ    | 2.76                     | 0.41              |
| 4:2:322:PRO:HB2  | 4:4:244:ASP:CG   | 2.17                     | 0.41              |
| 1:P:60:VAL:O     | 1:P:72:VAL:N     | 2.51                     | 0.41              |
| 2:Q:149:ASP:OD2  | 2:Q:150:TYR:CA   | 2.64                     | 0.41              |
| 2:B:150:TYR:HB3  | 2:B:151:LYS:HG3  | 2.03                     | 0.41              |
| 1:A:174:SER:HA   | 1:A:460:GLY:O    | 2.20                     | 0.41              |
| 1:G:665:ARG:C    | 1:G:667:THR:N    | 2.74                     | 0.41              |
| 1:P:320:ILE:CG2  | 1:P:320:ILE:O    | 2.68                     | 0.41              |
| 4:8:226:GLU:HG3  | 4:8:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:3:226:GLU:HG3  | 4:3:255:PHE:CE2  | 2.56                     | 0.41              |
| 1:J:62:VAL:HG12  | 1:J:63:MLY:N     | 2.34                     | 0.41              |
| 1:D:354:LEU:HA   | 1:D:354:LEU:HD12 | 1.56                     | 0.41              |
| 1:J:14:ALA:HB3   | 1:J:15:PRO:CD    | 2.46                     | 0.41              |
| 1:J:335:ASP:O    | 1:J:338:ILE:HB   | 2.20                     | 0.41              |
| 4:9:206:ARG:O    | 4:9:209:VAL:HG12 | 2.20                     | 0.41              |
| 4:4:206:ARG:O    | 4:4:209:VAL:HG12 | 2.20                     | 0.41              |
| 1:P:193:ILE:CD1  | 1:P:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:M:471:ASP:CB   | 1:M:573:GLY:O    | 2.68                     | 0.41              |
| 4:X:32:PRO:HB2   | 4:X:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:2:32:PRO:HB2   | 4:2:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:9:32:PRO:HB2   | 4:9:34:ILE:CD1   | 2.51                     | 0.41              |
| 1:P:356:GLY:HA2  | 1:P:359:MET:HG3  | 2.02                     | 0.41              |
| 3:C:96:LYS:H     | 3:C:96:LYS:HG3   | 1.66                     | 0.41              |
| 4:0:196:ARG:HH21 | 4:0:249:THR:HG23 | 1.85                     | 0.41              |
| 4:Y:196:ARG:HH21 | 4:Y:249:THR:HG23 | 1.85                     | 0.41              |
| 4:3:196:ARG:HH21 | 4:3:249:THR:HG23 | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:7:196:ARG:HH21 | 4:7:249:THR:HG23 | 1.85                     | 0.41              |
| 4:W:227:MET:O    | 4:W:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:717:TYR:OH   | 1:A:760:PHE:HB3  | 2.21                     | 0.41              |
| 4:V:144:ALA:HB2  | 4:V:342:GLY:CA   | 2.51                     | 0.41              |
| 1:P:725:ARG:CZ   | 1:P:733:PRO:CB   | 2.83                     | 0.41              |
| 1:J:735:GLY:HA3  | 1:J:743:ALA:HA   | 2.01                     | 0.41              |
| 1:A:812:SER:O    | 1:A:816:ILE:HG13 | 2.21                     | 0.41              |
| 1:G:449:LEU:N    | 1:G:449:LEU:CD1  | 2.82                     | 0.41              |
| 1:M:541:MET:SD   | 4:Z:345:ILE:C    | 2.95                     | 0.41              |
| 4:Z:144:ALA:HB2  | 4:Z:342:GLY:CA   | 2.51                     | 0.41              |
| 1:J:539:GLU:OE2  | 1:J:553:MLY:HD3  | 2.20                     | 0.41              |
| 1:J:629:GLU:HB3  | 1:J:643:GLY:C    | 2.41                     | 0.41              |
| 1:M:786:ILE:O    | 1:M:789:ALA:CB   | 2.64                     | 0.41              |
| 1:P:831:TRP:NE1  | 2:Q:67:MET:CG    | 2.83                     | 0.41              |
| 1:P:805:ALA:O    | 1:P:809:ARG:HG3  | 2.20                     | 0.41              |
| 1:J:829:TRP:HZ3  | 2:K:84:PHE:CD1   | 2.26                     | 0.41              |
| 1:A:801:VAL:N    | 3:C:149:VAL:HG21 | 2.32                     | 0.41              |
| 1:P:739:ASP:C    | 1:P:739:ASP:OD1  | 2.58                     | 0.41              |
| 4:1:324:THR:H    | 4:3:244:ASP:HA   | 1.86                     | 0.41              |
| 1:M:612:GLN:NE2  | 1:M:627:GLY:H    | 2.15                     | 0.41              |
| 3:I:95:ASP:OD1   | 3:I:139:TYR:HE1  | 2.04                     | 0.41              |
| 1:M:129:TYR:HD1  | 1:M:129:TYR:HA   | 1.65                     | 0.41              |
| 4:V:226:GLU:HG3  | 4:V:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:X:256:ARG:HD2  | 4:X:256:ARG:HH11 | 1.79                     | 0.41              |
| 1:J:322:VAL:HG12 | 1:J:325:ILE:HG13 | 2.03                     | 0.41              |
| 1:D:322:VAL:HB   | 1:D:325:ILE:HD12 | 2.03                     | 0.41              |
| 1:J:296:MLY:HH11 | 1:J:348:MLY:CH2  | 2.48                     | 0.41              |
| 1:P:135:TYR:CD2  | 1:P:191:ARG:HD3  | 2.55                     | 0.41              |
| 1:P:462:LEU:HD11 | 1:P:464:ILE:CD1  | 2.50                     | 0.41              |
| 1:P:193:ILE:HD11 | 1:P:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:G:193:ILE:CD1  | 1:G:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:M:193:ILE:CD1  | 1:M:250:ILE:HD13 | 2.51                     | 0.41              |
| 4:3:32:PRO:HB2   | 4:3:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:5:32:PRO:HB2   | 4:5:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:1:144:ALA:HB2  | 4:1:342:GLY:CA   | 2.51                     | 0.41              |
| 1:G:384:ASP:HA   | 1:G:394:SER:OG   | 2.21                     | 0.41              |
| 4:7:171:LEU:HA   | 4:7:172:PRO:HD2  | 1.84                     | 0.41              |
| 1:J:657:LEU:HD12 | 1:J:657:LEU:O    | 2.21                     | 0.41              |
| 1:M:369:MLY:HD3  | 1:M:369:MLY:HH22 | 1.79                     | 0.41              |
| 1:J:610:LEU:CD1  | 1:J:610:LEU:N    | 2.84                     | 0.41              |
| 1:G:690:LEU:O    | 1:G:694:GLN:HG3  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:172:ASN:OD1  | 1:G:457:TYR:HA   | 2.21                     | 0.41              |
| 1:G:791:GLN:CD   | 3:I:116:GLU:N    | 2.74                     | 0.41              |
| 1:A:711:PHE:O    | 1:A:714:ARG:NH2  | 2.54                     | 0.41              |
| 1:G:538:GLU:CA   | 4:V:351:THR:N    | 2.68                     | 0.41              |
| 1:G:553:MLY:HA   | 4:X:45:VAL:O     | 2.21                     | 0.41              |
| 1:P:732:ILE:CG2  | 1:P:747:LEU:CD1  | 0.65                     | 0.41              |
| 3:R:95:ASP:OD1   | 3:R:139:TYR:HE1  | 2.04                     | 0.41              |
| 1:P:732:ILE:HG23 | 1:P:747:LEU:HD12 | 0.94                     | 0.41              |
| 1:A:217:THR:CA   | 1:A:221:GLN:HE21 | 2.33                     | 0.41              |
| 2:H:144:VAL:HG12 | 2:H:153:ILE:HD11 | 1.75                     | 0.41              |
| 1:P:642:LYS:HB3  | 4:O:24:ASP:HB2   | 1.37                     | 0.41              |
| 1:A:725:ARG:HA   | 1:A:732:ILE:CG2  | 2.50                     | 0.41              |
| 1:A:735:GLY:HA3  | 1:A:743:ALA:HA   | 2.01                     | 0.41              |
| 1:M:410:ASN:HA   | 4:Z:334:GLU:HB3  | 1.29                     | 0.41              |
| 1:M:553:MLY:CD   | 4:1:43:VAL:CG2   | 2.69                     | 0.41              |
| 1:M:540:CYS:C    | 4:Z:349:LEU:HD21 | 2.36                     | 0.41              |
| 4:W:144:ALA:HB2  | 4:W:342:GLY:CA   | 2.51                     | 0.41              |
| 1:J:642:LYS:HE2  | 4:W:344:SER:HA   | 1.56                     | 0.41              |
| 4:9:144:ALA:HB2  | 4:9:342:GLY:CA   | 2.51                     | 0.41              |
| 1:D:407:GLY:HA2  | 1:D:411:GLU:O    | 2.21                     | 0.41              |
| 1:P:548:THR:HB   | 4:2:48:GLY:CA    | 2.51                     | 0.41              |
| 1:A:551:MLY:C    | 4:V:47:MET:HA    | 2.48                     | 0.41              |
| 1:J:836:PHE:CD2  | 2:K:160:GLY:N    | 2.86                     | 0.41              |
| 1:G:838:ILE:HG13 | 2:H:54:MET:HE1   | 1.99                     | 0.41              |
| 4:3:287:ILE:CB   | 4:5:203:THR:HG22 | 2.44                     | 0.41              |
| 1:J:831:TRP:CH2  | 2:K:34:ILE:HG21  | 2.56                     | 0.41              |
| 1:P:834:LEU:HD12 | 2:Q:51:PHE:CE1   | 2.45                     | 0.41              |
| 1:A:72:VAL:O     | 1:A:73:LYS:O     | 2.39                     | 0.41              |
| 1:M:72:VAL:O     | 1:M:73:LYS:O     | 2.39                     | 0.41              |
| 2:E:150:TYR:HB3  | 2:E:151:LYS:HG3  | 2.03                     | 0.41              |
| 1:D:664:LEU:HD12 | 1:D:664:LEU:HA   | 1.53                     | 0.41              |
| 1:P:176:LEU:N    | 1:P:176:LEU:CD1  | 2.74                     | 0.41              |
| 1:D:47:PHE:HE1   | 1:D:78:PHE:CE1   | 2.39                     | 0.41              |
| 4:W:288:ASP:N    | 4:Y:202:THR:OG1  | 2.23                     | 0.41              |
| 1:M:753:VAL:O    | 1:M:755:HIS:ND1  | 2.54                     | 0.41              |
| 3:C:95:ASP:OD1   | 3:C:139:TYR:HE1  | 2.04                     | 0.41              |
| 4:X:226:GLU:HG3  | 4:X:255:PHE:CE2  | 2.55                     | 0.41              |
| 4:5:226:GLU:HG3  | 4:5:255:PHE:CE2  | 2.55                     | 0.41              |
| 1:G:823:PHE:CE1  | 2:H:160:GLY:HA2  | 2.52                     | 0.41              |
| 4:Z:221:LEU:HA   | 4:Z:312:ARG:HG2  | 2.02                     | 0.41              |
| 1:P:107:MLY:N    | 1:P:686:MET:HE1  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:493:HIS:O    | 1:J:496:PHE:N    | 2.54                     | 0.41              |
| 1:M:51:THR:O     | 1:M:62:VAL:CG1   | 2.64                     | 0.41              |
| 1:D:195:TYR:CE2  | 1:D:199:ILE:HD13 | 2.55                     | 0.41              |
| 1:D:493:HIS:O    | 1:D:496:PHE:N    | 2.54                     | 0.41              |
| 4:V:256:ARG:HH11 | 4:V:256:ARG:HD2  | 1.78                     | 0.41              |
| 1:D:38:VAL:HG13  | 1:D:39:PHE:N     | 2.35                     | 0.41              |
| 1:J:25:ILE:HG23  | 1:J:29:ASN:HD22  | 1.85                     | 0.41              |
| 1:D:335:ASP:O    | 1:D:338:ILE:HB   | 2.20                     | 0.41              |
| 1:D:322:VAL:HG12 | 1:D:325:ILE:HG13 | 2.03                     | 0.41              |
| 1:P:322:VAL:HG12 | 1:P:325:ILE:HG13 | 2.03                     | 0.41              |
| 1:A:335:ASP:O    | 1:A:338:ILE:HB   | 2.20                     | 0.41              |
| 1:G:335:ASP:O    | 1:G:338:ILE:HB   | 2.20                     | 0.41              |
| 1:G:466:GLY:CA   | 1:G:484:ASN:HD21 | 2.32                     | 0.41              |
| 1:G:322:VAL:HA   | 1:G:323:PRO:HD3  | 1.87                     | 0.41              |
| 1:D:136:ASN:O    | 1:D:138:MLY:N    | 2.54                     | 0.41              |
| 1:A:724:TYR:HB3  | 1:A:727:LEU:CD1  | 2.48                     | 0.41              |
| 1:A:303:LEU:O    | 1:A:304:LEU:HB2  | 2.21                     | 0.41              |
| 4:4:369:ILE:HG23 | 4:4:370:VAL:N    | 2.35                     | 0.41              |
| 1:M:49:MLY:HH23  | 1:M:80:MET:CE    | 2.51                     | 0.41              |
| 1:J:135:TYR:CD2  | 1:J:191:ARG:HD3  | 2.55                     | 0.41              |
| 1:J:193:ILE:HD11 | 1:J:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:193:ILE:CD1  | 1:A:250:ILE:HD13 | 2.51                     | 0.41              |
| 1:M:193:ILE:HD11 | 1:M:250:ILE:HD12 | 2.03                     | 0.41              |
| 1:J:330:GLU:OE1  | 1:J:330:GLU:HA   | 2.20                     | 0.41              |
| 4:Z:32:PRO:HB2   | 4:Z:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:W:32:PRO:HB2   | 4:W:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:Y:32:PRO:HB2   | 4:Y:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:0:32:PRO:HB2   | 4:0:34:ILE:CD1   | 2.51                     | 0.41              |
| 4:4:32:PRO:HB2   | 4:4:34:ILE:CD1   | 2.51                     | 0.41              |
| 1:J:384:ASP:HA   | 1:J:394:SER:OG   | 2.20                     | 0.41              |
| 1:J:356:GLY:HA2  | 1:J:359:MET:HG3  | 2.02                     | 0.41              |
| 1:P:657:LEU:HD12 | 1:P:657:LEU:O    | 2.21                     | 0.41              |
| 1:M:657:LEU:HD12 | 1:M:657:LEU:O    | 2.21                     | 0.41              |
| 4:1:227:MET:O    | 4:1:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:V:227:MET:O    | 4:V:230:ALA:HB3  | 2.21                     | 0.41              |
| 4:9:227:MET:O    | 4:9:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:J:229:LEU:HA   | 1:J:229:LEU:HD12 | 1.75                     | 0.41              |
| 1:G:842:LEU:N    | 1:G:842:LEU:CD1  | 2.82                     | 0.41              |
| 4:Y:144:ALA:HB2  | 4:Y:342:GLY:CA   | 2.51                     | 0.41              |
| 4:5:227:MET:O    | 4:5:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:M:356:GLY:HA2  | 1:M:359:MET:HG3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:356:GLY:HA2  | 1:G:359:MET:HG3  | 2.02                     | 0.41              |
| 1:A:356:GLY:HA2  | 1:A:359:MET:HG3  | 2.02                     | 0.41              |
| 4:7:227:MET:O    | 4:7:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:172:ASN:OD1  | 1:A:457:TYR:HA   | 2.21                     | 0.41              |
| 4:X:196:ARG:HH21 | 4:X:249:THR:HG23 | 1.85                     | 0.41              |
| 1:D:747:LEU:HD22 | 1:D:782:MLY:HH11 | 1.96                     | 0.41              |
| 1:G:768:MLY:HB2  | 1:G:772:LEU:HB2  | 1.71                     | 0.41              |
| 2:N:141:PRO:HB3  | 2:N:142:PRO:CD   | 2.49                     | 0.41              |
| 1:G:528:MLY:HB2  | 1:G:529:PRO:HD2  | 2.03                     | 0.41              |
| 1:J:818:TYR:HB3  | 2:K:90:GLY:CA    | 2.51                     | 0.41              |
| 4:0:144:ALA:HB2  | 4:0:342:GLY:CA   | 2.51                     | 0.41              |
| 1:P:544:LYS:HE2  | 4:2:45:VAL:HG22  | 2.03                     | 0.41              |
| 1:P:629:GLU:HB3  | 1:P:643:GLY:C    | 2.41                     | 0.41              |
| 1:M:528:MLY:HB2  | 1:M:529:PRO:HD2  | 2.03                     | 0.41              |
| 1:P:785:GLU:CD   | 3:R:81:GLN:OE1   | 2.58                     | 0.41              |
| 1:D:528:MLY:HB2  | 1:D:529:PRO:HD2  | 2.03                     | 0.41              |
| 1:D:568:PRO:HG3  | 1:D:578:HIS:N    | 2.36                     | 0.41              |
| 1:A:541:MET:HG2  | 4:8:345:ILE:HG22 | 2.00                     | 0.41              |
| 1:M:797:PHE:CE1  | 3:O:146:ILE:CA   | 2.94                     | 0.41              |
| 1:P:449:LEU:HD12 | 1:P:449:LEU:HA   | 1.60                     | 0.41              |
| 1:J:839:MLY:HH13 | 2:K:159:HIS:CD2  | 2.55                     | 0.41              |
| 4:0:110:LEU:HB3  | 4:1:195:GLU:HG3  | 2.03                     | 0.41              |
| 1:P:506:GLU:CG   | 1:P:760:PHE:O    | 2.64                     | 0.41              |
| 1:P:769:ALA:C    | 1:P:770:GLY:N    | 2.75                     | 0.41              |
| 4:9:288:ASP:OD1  | 4:W:204:ALA:HA   | 2.21                     | 0.41              |
| 1:G:769:ALA:HB1  | 1:G:770:GLY:CA   | 2.34                     | 0.41              |
| 3:I:49:ILE:HD13  | 3:I:49:ILE:HG21  | 1.89                     | 0.41              |
| 4:1:244:ASP:O    | 4:Z:324:THR:HG23 | 2.17                     | 0.41              |
| 1:M:97:LEU:HD12  | 1:M:97:LEU:HA    | 1.68                     | 0.41              |
| 3:L:95:ASP:OD1   | 3:L:139:TYR:HE1  | 2.03                     | 0.41              |
| 4:2:226:GLU:HG3  | 4:2:255:PHE:CE2  | 2.56                     | 0.41              |
| 1:D:556:ASP:OD1  | 4:W:50:LYS:CG    | 2.69                     | 0.41              |
| 1:J:322:VAL:HB   | 1:J:325:ILE:HD12 | 2.03                     | 0.41              |
| 1:M:466:GLY:CA   | 1:M:484:ASN:HD21 | 2.32                     | 0.41              |
| 4:8:219:VAL:HG22 | 4:8:258:PRO:CB   | 2.51                     | 0.41              |
| 4:V:219:VAL:HG22 | 4:V:258:PRO:CB   | 2.51                     | 0.41              |
| 4:3:219:VAL:HG22 | 4:3:258:PRO:CB   | 2.51                     | 0.41              |
| 4:X:219:VAL:HG22 | 4:X:258:PRO:CB   | 2.51                     | 0.41              |
| 4:1:369:ILE:HG23 | 4:1:370:VAL:N    | 2.35                     | 0.41              |
| 1:M:676:ILE:HA   | 1:M:677:PRO:HD3  | 1.82                     | 0.41              |
| 1:G:485:GLU:OE2  | 1:G:584:TYR:N    | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:471:ASP:CB   | 1:A:573:GLY:O    | 2.68                     | 0.41              |
| 4:3:227:MET:O    | 4:3:230:ALA:HB3  | 2.21                     | 0.41              |
| 1:G:657:LEU:O    | 1:G:657:LEU:HD12 | 2.21                     | 0.41              |
| 1:D:625:THR:H    | 1:D:625:THR:HG22 | 1.48                     | 0.41              |
| 3:C:56:GLU:OE1   | 3:C:59:ASN:ND2   | 2.54                     | 0.41              |
| 4:X:144:ALA:HB2  | 4:X:342:GLY:CA   | 2.51                     | 0.41              |
| 4:4:144:ALA:HB2  | 4:4:342:GLY:CA   | 2.51                     | 0.41              |
| 4:3:299:MET:HE2  | 4:3:331:ALA:HB2  | 2.02                     | 0.41              |
| 1:G:795:ARG:CZ   | 3:I:116:GLU:CB   | 2.96                     | 0.40              |
| 1:A:499:GLU:OE2  | 1:A:766:PHE:HE2  | 2.00                     | 0.40              |
| 2:H:113:LYS:O    | 2:H:147:ASN:HB2  | 2.20                     | 0.40              |
| 1:P:792:ALA:HB1  | 3:R:42:THR:N     | 2.35                     | 0.40              |
| 1:D:217:THR:CA   | 1:D:221:GLN:HE21 | 2.33                     | 0.40              |
| 4:3:287:ILE:CG2  | 4:5:204:ALA:N    | 2.68                     | 0.40              |
| 1:P:332:MET:HG2  | 1:P:332:MET:H    | 1.52                     | 0.40              |
| 1:J:776:GLU:O    | 1:J:780:ASP:N    | 2.45                     | 0.40              |
| 3:C:48:LYS:HA    | 3:C:48:LYS:HD3   | 1.17                     | 0.40              |
| 3:C:62:ALA:O     | 3:C:63:ILE:HG13  | 2.13                     | 0.40              |
| 1:G:789:ALA:HB1  | 3:I:81:GLN:CG    | 2.49                     | 0.40              |
| 1:D:320:ILE:CG2  | 1:D:320:ILE:O    | 2.68                     | 0.40              |
| 4:X:221:LEU:HA   | 4:X:312:ARG:HG2  | 2.02                     | 0.40              |
| 1:J:107:MLY:N    | 1:J:686:MET:HE1  | 2.35                     | 0.40              |
| 1:P:493:HIS:O    | 1:P:496:PHE:N    | 2.54                     | 0.40              |
| 1:G:25:ILE:HG23  | 1:G:29:ASN:HD22  | 1.85                     | 0.40              |
| 1:P:25:ILE:HG23  | 1:P:29:ASN:HD22  | 1.85                     | 0.40              |
| 1:M:308:ASN:HA   | 1:M:309:PRO:HD2  | 1.88                     | 0.40              |
| 1:G:303:LEU:O    | 1:G:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:D:135:TYR:HD2  | 1:D:191:ARG:CG   | 2.33                     | 0.40              |
| 1:M:485:GLU:OE2  | 1:M:584:TYR:N    | 2.50                     | 0.40              |
| 1:A:193:ILE:HD11 | 1:A:250:ILE:HD12 | 2.03                     | 0.40              |
| 1:G:110:TYR:O    | 1:G:113:TRP:N    | 2.42                     | 0.40              |
| 1:D:657:LEU:HD12 | 1:D:657:LEU:O    | 2.21                     | 0.40              |
| 4:4:227:MET:O    | 4:4:230:ALA:HB3  | 2.21                     | 0.40              |
| 4:3:171:LEU:HA   | 4:3:172:PRO:HD2  | 1.84                     | 0.40              |
| 1:P:384:ASP:HA   | 1:P:394:SER:OG   | 2.20                     | 0.40              |
| 4:7:144:ALA:HB2  | 4:7:342:GLY:CA   | 2.51                     | 0.40              |
| 1:D:723:ARG:HH21 | 1:D:779:ARG:CZ   | 2.34                     | 0.40              |
| 1:G:537:GLU:OE1  | 4:V:350:SER:HA   | 2.20                     | 0.40              |
| 1:P:821:ARG:NH2  | 2:Q:127:ARG:NE   | 2.69                     | 0.40              |
| 2:E:140:PHE:HA   | 2:E:141:PRO:HD2  | 1.57                     | 0.40              |
| 2:K:113:LYS:O    | 2:K:147:ASN:HB2  | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:544:LYS:N    | 4:O:146:GLY:O    | 2.55                     | 0.40              |
| 1:M:544:LYS:N    | 4:Z:146:GLY:O    | 2.54                     | 0.40              |
| 1:P:795:ARG:CD   | 3:R:35:ARG:HH12  | 2.34                     | 0.40              |
| 1:D:408:VAL:HG22 | 1:D:636:LYS:HG2  | 1.52                     | 0.40              |
| 1:D:213:LYS:HA   | 1:D:220:ASP:OD2  | 2.19                     | 0.40              |
| 1:M:786:ILE:C    | 1:M:789:ALA:H    | 2.25                     | 0.40              |
| 1:D:201:ALA:O    | 1:D:202:SER:OG   | 2.36                     | 0.40              |
| 1:J:822:SER:OG   | 2:K:91:ALA:N     | 2.54                     | 0.40              |
| 1:P:772:LEU:HD12 | 1:P:772:LEU:HA   | 1.83                     | 0.40              |
| 1:M:295:MLY:CD   | 1:M:332:MET:HE2  | 2.51                     | 0.40              |
| 1:D:60:VAL:O     | 1:D:72:VAL:N     | 2.51                     | 0.40              |
| 1:J:612:GLN:NE2  | 1:J:627:GLY:H    | 2.14                     | 0.40              |
| 1:M:753:VAL:HG12 | 1:M:775:LEU:HD22 | 2.02                     | 0.40              |
| 3:O:95:ASP:OD1   | 3:O:139:TYR:HE1  | 2.04                     | 0.40              |
| 4:V:221:LEU:HA   | 4:V:312:ARG:HG2  | 2.02                     | 0.40              |
| 1:M:772:LEU:HD12 | 1:M:772:LEU:HA   | 1.83                     | 0.40              |
| 1:G:493:HIS:O    | 1:G:496:PHE:N    | 2.54                     | 0.40              |
| 1:D:237:THR:CG2  | 1:D:238:VAL:N    | 2.85                     | 0.40              |
| 1:M:123:CYS:HB2  | 1:M:158:ILE:HD13 | 2.00                     | 0.40              |
| 1:M:136:ASN:O    | 1:M:138:MLY:N    | 2.54                     | 0.40              |
| 4:4:219:VAL:HG22 | 4:4:258:PRO:CB   | 2.51                     | 0.40              |
| 4:9:120:THR:HG21 | 4:9:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:1:219:VAL:HG22 | 4:1:258:PRO:CB   | 2.52                     | 0.40              |
| 1:P:303:LEU:O    | 1:P:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:D:48:VAL:CG2   | 1:D:49:MLY:N     | 2.84                     | 0.40              |
| 1:P:48:VAL:CG2   | 1:P:49:MLY:N     | 2.84                     | 0.40              |
| 1:D:193:ILE:HD11 | 1:D:250:ILE:HD12 | 2.03                     | 0.40              |
| 1:G:193:ILE:HD11 | 1:G:250:ILE:HD12 | 2.03                     | 0.40              |
| 4:W:196:ARG:HH21 | 4:W:249:THR:HG23 | 1.85                     | 0.40              |
| 4:1:171:LEU:HA   | 4:1:172:PRO:HD2  | 1.84                     | 0.40              |
| 1:M:610:LEU:CD1  | 1:M:610:LEU:N    | 2.84                     | 0.40              |
| 1:P:610:LEU:CD1  | 1:P:610:LEU:N    | 2.84                     | 0.40              |
| 4:3:144:ALA:HB2  | 4:3:342:GLY:CA   | 2.51                     | 0.40              |
| 1:J:88:ILE:HG22  | 1:J:90:ASP:C     | 2.42                     | 0.40              |
| 1:J:172:ASN:OD1  | 1:J:457:TYR:HA   | 2.21                     | 0.40              |
| 2:B:63:GLU:O     | 2:B:67:MET:HG3   | 2.22                     | 0.40              |
| 1:A:508:ILE:HD13 | 1:A:508:ILE:HG21 | 1.88                     | 0.40              |
| 1:M:821:ARG:NH2  | 2:N:127:ARG:NE   | 2.69                     | 0.40              |
| 1:G:407:GLY:HA2  | 1:G:411:GLU:O    | 2.21                     | 0.40              |
| 1:P:817:GLN:CD   | 2:Q:127:ARG:CG   | 2.89                     | 0.40              |
| 2:Q:111:SER:OG   | 2:Q:148:VAL:CA   | 2.69                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:141:PRO:CB   | 2:K:142:PRO:HD3  | 2.48                     | 0.40              |
| 2:B:111:SER:OG   | 2:B:148:VAL:CA   | 2.69                     | 0.40              |
| 1:M:538:GLU:CA   | 4:Z:351:THR:N    | 2.68                     | 0.40              |
| 1:J:528:MLY:HB2  | 1:J:529:PRO:HD2  | 2.03                     | 0.40              |
| 1:M:206:LYS:CE   | 1:M:217:THR:HG23 | 2.29                     | 0.40              |
| 1:G:724:TYR:HB3  | 1:G:727:LEU:CD1  | 2.48                     | 0.40              |
| 1:P:806:MET:O    | 1:P:809:ARG:CB   | 2.67                     | 0.40              |
| 1:M:35:MLY:CH2   | 1:M:778:MET:CA   | 3.00                     | 0.40              |
| 2:H:150:TYR:HB3  | 2:H:151:LYS:HG3  | 2.03                     | 0.40              |
| 4:1:226:GLU:HG3  | 4:1:255:PHE:CE2  | 2.56                     | 0.40              |
| 1:G:63:MLY:HD3   | 1:G:63:MLY:HH23  | 1.76                     | 0.40              |
| 4:V:193:LEU:HA   | 4:V:193:LEU:HD12 | 1.96                     | 0.40              |
| 1:P:38:VAL:HG13  | 1:P:39:PHE:N     | 2.35                     | 0.40              |
| 1:G:14:ALA:HB3   | 1:G:15:PRO:CD    | 2.46                     | 0.40              |
| 1:P:237:THR:CG2  | 1:P:238:VAL:N    | 2.84                     | 0.40              |
| 1:D:348:MLY:HD2  | 1:D:348:MLY:HH12 | 1.82                     | 0.40              |
| 1:M:303:LEU:O    | 1:M:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:J:303:LEU:O    | 1:J:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:A:464:ILE:HG22 | 1:A:465:ALA:H    | 1.87                     | 0.40              |
| 1:M:193:ILE:HD13 | 1:M:252:ILE:HD11 | 2.04                     | 0.40              |
| 1:A:384:ASP:HA   | 1:A:394:SER:OG   | 2.21                     | 0.40              |
| 4:Y:227:MET:O    | 4:Y:230:ALA:HB3  | 2.21                     | 0.40              |
| 3:F:56:GLU:OE1   | 3:F:59:ASN:ND2   | 2.54                     | 0.40              |
| 1:D:717:TYR:OH   | 1:D:760:PHE:HB3  | 2.21                     | 0.40              |
| 1:A:757:GLN:CG   | 1:A:771:LEU:CG   | 2.86                     | 0.40              |
| 1:P:817:GLN:OE1  | 2:Q:127:ARG:CD   | 2.66                     | 0.40              |
| 1:A:226:ASN:HB2  | 1:A:227:PRO:CD   | 2.47                     | 0.40              |
| 1:M:533:PHE:O    | 1:M:537:GLU:N    | 2.49                     | 0.40              |
| 1:P:793:ARG:CD   | 3:R:40:ASN:HD22  | 2.20                     | 0.40              |
| 1:P:580:SER:O    | 1:P:581:LEU:HD12 | 2.22                     | 0.40              |
| 1:M:839:MLY:N    | 1:M:840:PRO:HD2  | 2.35                     | 0.40              |
| 1:P:839:MLY:CH2  | 2:Q:158:THR:HG22 | 2.48                     | 0.40              |
| 4:0:243:PRO:CB   | 4:Y:291:LYS:CE   | 2.91                     | 0.40              |
| 1:M:717:TYR:OH   | 1:M:760:PHE:HB3  | 2.21                     | 0.40              |
| 2:H:63:GLU:O     | 2:H:67:MET:HG3   | 2.22                     | 0.40              |
| 1:J:60:VAL:O     | 1:J:72:VAL:N     | 2.51                     | 0.40              |
| 2:E:149:ASP:O    | 2:E:150:TYR:CD1  | 2.75                     | 0.40              |
| 1:P:279:LEU:CB   | 1:P:280:PRO:HD2  | 2.49                     | 0.40              |
| 4:8:221:LEU:HA   | 4:8:312:ARG:HG2  | 2.02                     | 0.40              |
| 4:1:221:LEU:HA   | 4:1:312:ARG:HG2  | 2.02                     | 0.40              |
| 1:J:89:GLU:HB3   | 1:J:153:PRO:HG3  | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:64:THR:HG22  | 1:D:65:GLU:H     | 1.87                     | 0.40              |
| 1:D:64:THR:OG1   | 1:D:68:GLU:HB3   | 2.22                     | 0.40              |
| 1:M:519:LEU:H    | 1:M:519:LEU:HD12 | 1.83                     | 0.40              |
| 1:G:87:MLY:HH12  | 1:G:87:MLY:HD3   | 1.62                     | 0.40              |
| 4:7:219:VAL:HG22 | 4:7:258:PRO:CB   | 2.51                     | 0.40              |
| 4:X:120:THR:HG21 | 4:X:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:Z:219:VAL:HG22 | 4:Z:258:PRO:CB   | 2.52                     | 0.40              |
| 1:J:193:ILE:CD1  | 1:J:250:ILE:HD13 | 2.51                     | 0.40              |
| 1:D:193:ILE:CD1  | 1:D:250:ILE:HD13 | 2.51                     | 0.40              |
| 1:G:193:ILE:HD13 | 1:G:252:ILE:HD11 | 2.04                     | 0.40              |
| 1:D:400:ALA:CB   | 1:D:606:THR:CG2  | 3.00                     | 0.40              |
| 4:V:32:PRO:HB2   | 4:V:34:ILE:CD1   | 2.51                     | 0.40              |
| 4:1:32:PRO:HB2   | 4:1:34:ILE:CD1   | 2.51                     | 0.40              |
| 1:P:172:ASN:OD1  | 1:P:457:TYR:HA   | 2.21                     | 0.40              |
| 1:D:610:LEU:CD1  | 1:D:610:LEU:N    | 2.84                     | 0.40              |
| 1:D:261:ALA:O    | 1:D:451:THR:OG1  | 2.40                     | 0.40              |
| 1:P:110:TYR:O    | 1:P:113:TRP:N    | 2.42                     | 0.40              |
| 4:0:227:MET:O    | 4:0:230:ALA:HB3  | 2.21                     | 0.40              |
| 1:P:88:ILE:HG22  | 1:P:90:ASP:C     | 2.42                     | 0.40              |
| 3:L:56:GLU:OE1   | 3:L:59:ASN:ND2   | 2.54                     | 0.40              |
| 1:A:93:MET:C     | 1:A:713:SER:CB   | 2.87                     | 0.40              |
| 1:P:821:ARG:HH22 | 2:Q:127:ARG:CG   | 2.30                     | 0.40              |
| 1:D:812:SER:O    | 1:D:816:ILE:HG13 | 2.21                     | 0.40              |
| 1:P:407:GLY:HA2  | 1:P:411:GLU:O    | 2.21                     | 0.40              |
| 1:J:93:MET:HE1   | 1:J:764:MLY:HD2  | 2.04                     | 0.40              |
| 1:M:407:GLY:HA2  | 1:M:411:GLU:O    | 2.22                     | 0.40              |
| 1:M:580:SER:O    | 1:M:581:LEU:HD12 | 2.22                     | 0.40              |
| 1:J:553:MLY:HH12 | 4:Y:45:VAL:HG11  | 2.00                     | 0.40              |
| 1:A:553:MLY:NZ   | 4:V:45:VAL:CA    | 2.58                     | 0.40              |
| 1:M:836:PHE:CE1  | 2:N:159:HIS:C    | 2.92                     | 0.40              |
| 1:M:92:ALA:O     | 1:M:714:ARG:HG2  | 2.22                     | 0.40              |
| 4:0:287:ILE:HB   | 4:2:203:THR:HG21 | 2.03                     | 0.40              |
| 1:M:803:TYR:O    | 1:M:807:VAL:HB   | 2.22                     | 0.40              |
| 4:X:285:CYS:O    | 4:Z:202:THR:HG22 | 2.17                     | 0.40              |
| 1:P:776:GLU:O    | 1:P:780:ASP:N    | 2.45                     | 0.40              |
| 4:7:290:ARG:HH22 | 4:9:202:THR:CG2  | 2.17                     | 0.40              |
| 1:A:800:ARG:HB3  | 3:C:149:VAL:CB   | 2.49                     | 0.40              |
| 2:K:149:ASP:OD2  | 2:K:150:TYR:CA   | 2.65                     | 0.40              |
| 1:G:580:SER:O    | 1:G:581:LEU:HD12 | 2.22                     | 0.40              |
| 1:J:47:PHE:HE1   | 1:J:78:PHE:CE1   | 2.40                     | 0.40              |
| 3:F:95:ASP:OD1   | 3:F:139:TYR:HE1  | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:709:LYS:C    | 1:D:710:GLY:CA   | 2.89                     | 0.40              |
| 1:A:556:ASP:OD1  | 4:V:50:LYS:CG    | 2.69                     | 0.40              |
| 1:J:64:THR:HG22  | 1:J:65:GLU:H     | 1.87                     | 0.40              |
| 4:9:250:ILE:HG22 | 4:9:254:ARG:HB2  | 2.04                     | 0.40              |
| 1:M:435:GLU:O    | 1:M:438:PHE:N    | 2.55                     | 0.40              |
| 1:J:38:VAL:HG13  | 1:J:39:PHE:N     | 2.35                     | 0.40              |
| 1:J:519:LEU:H    | 1:J:519:LEU:HD12 | 1.83                     | 0.40              |
| 1:P:240:ASN:OD1  | 1:P:241:ASP:N    | 2.52                     | 0.40              |
| 1:G:305:ILE:HG22 | 1:G:312:TYR:OH   | 2.22                     | 0.40              |
| 1:D:322:VAL:HA   | 1:D:323:PRO:HD3  | 1.87                     | 0.40              |
| 1:M:305:ILE:HG22 | 1:M:312:TYR:OH   | 2.21                     | 0.40              |
| 4:Y:219:VAL:HG22 | 4:Y:258:PRO:CB   | 2.51                     | 0.40              |
| 4:0:219:VAL:HG22 | 4:0:258:PRO:CB   | 2.51                     | 0.40              |
| 4:V:120:THR:HG21 | 4:V:370:VAL:CG1  | 2.52                     | 0.40              |
| 4:7:120:THR:HG21 | 4:7:370:VAL:CG1  | 2.52                     | 0.40              |
| 1:D:303:LEU:O    | 1:D:304:LEU:HB2  | 2.21                     | 0.40              |
| 1:A:308:ASN:HA   | 1:A:309:PRO:HD2  | 1.88                     | 0.40              |
| 1:G:464:ILE:HG22 | 1:G:465:ALA:H    | 1.87                     | 0.40              |
| 1:P:485:GLU:OE1  | 1:P:583:HIS:HB3  | 2.21                     | 0.40              |
| 1:M:384:ASP:HA   | 1:M:394:SER:OG   | 2.21                     | 0.40              |
| 1:G:229:LEU:HA   | 1:G:229:LEU:HD12 | 1.75                     | 0.40              |
| 1:A:194:GLN:HE21 | 1:A:194:GLN:HB3  | 1.43                     | 0.40              |
| 4:Z:227:MET:O    | 4:Z:230:ALA:HB3  | 2.21                     | 0.40              |
| 1:M:172:ASN:OD1  | 1:M:457:TYR:HA   | 2.21                     | 0.40              |
| 1:D:88:ILE:HG22  | 1:D:90:ASP:C     | 2.42                     | 0.40              |

All (10396) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:196:ARG:O   | 4:9:212:ILE:CG1[1_554] | 0.16                     | 2.04              |
| 4:5:191:LYS:CA  | 4:9:186:THR:C[1_554]   | 0.19                     | 2.01              |
| 4:5:194:THR:C   | 4:9:209:VAL:CG2[1_554] | 0.21                     | 1.99              |
| 4:3:26:ALA:CB   | 4:7:122:ILE:C[1_554]   | 0.22                     | 1.98              |
| 4:3:305:MET:C   | 4:7:11:ASP:OD1[1_554]  | 0.22                     | 1.98              |
| 4:4:214:GLU:CD  | 4:8:33:SER:OG[1_554]   | 0.22                     | 1.98              |
| 4:3:243:PRO:CB  | 4:7:61:LYS:N[1_554]    | 0.22                     | 1.98              |
| 4:3:186:THR:OG1 | 4:7:183:ARG:NH2[1_554] | 0.23                     | 1.97              |
| 4:4:304:THR:CA  | 4:8:137:GLN:CD[1_554]  | 0.23                     | 1.97              |
| 4:3:243:PRO:N   | 4:7:60:SER:CA[1_554]   | 0.24                     | 1.96              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:340:TRP:CB  | 4:7:118:LYS:CA[1_554]  | 0.24                     | 1.96              |
| 4:3:281:SER:OG  | 4:7:173:HIS:N[1_554]   | 0.25                     | 1.95              |
| 4:3:333:PRO:CA  | 4:7:105:LEU:N[1_554]   | 0.25                     | 1.95              |
| 4:3:340:TRP:CH2 | 4:7:121:GLN:CG[1_554]  | 0.26                     | 1.94              |
| 4:5:112:PRO:C   | 4:V:253:GLU:CD[1_554]  | 0.26                     | 1.94              |
| 4:2:372:ARG:CG  | 4:7:227:MET:CA[1_554]  | 0.27                     | 1.93              |
| 4:4:277:THR:CG2 | 4:8:175:ILE:C[1_554]   | 0.27                     | 1.93              |
| 4:5:188:TYR:CZ  | 4:9:185:LEU:CD2[1_554] | 0.27                     | 1.93              |
| 4:5:304:THR:N   | 4:9:137:GLN:OE1[1_554] | 0.27                     | 1.93              |
| 4:3:277:THR:CG2 | 4:7:175:ILE:C[1_554]   | 0.28                     | 1.92              |
| 4:4:339:VAL:N   | 4:8:116:ARG:CA[1_554]  | 0.28                     | 1.92              |
| 4:4:255:PHE:CG  | 4:8:305:MET:CG[1_554]  | 0.28                     | 1.92              |
| 4:4:281:SER:OG  | 4:8:173:HIS:N[1_554]   | 0.29                     | 1.91              |
| 4:4:315:LYS:CD  | 4:8:147:ARG:NE[1_554]  | 0.29                     | 1.91              |
| 4:5:221:LEU:CB  | 4:9:332:PRO:CD[1_554]  | 0.29                     | 1.91              |
| 4:4:273:GLY:CA  | 4:8:162:ASN:OD1[1_554] | 0.29                     | 1.91              |
| 4:2:75:ILE:CD1  | 4:7:193:LEU:O[1_554]   | 0.30                     | 1.90              |
| 4:3:192:ILE:CG1 | 4:7:213:LYS:NZ[1_554]  | 0.30                     | 1.90              |
| 4:3:262:PHE:CG  | 4:7:153:LEU:C[1_554]   | 0.30                     | 1.90              |
| 4:4:114:ALA:CA  | 4:9:250:ILE:C[1_554]   | 0.30                     | 1.90              |
| 4:4:300:SER:CA  | 4:8:107:GLU:CG[1_554]  | 0.31                     | 1.89              |
| 4:5:141:SER:O   | 4:9:116:ARG:NH1[1_554] | 0.31                     | 1.89              |
| 4:4:154:ASP:OD2 | 4:8:111:ASN:C[1_554]   | 0.31                     | 1.89              |
| 4:3:24:ASP:CA   | 4:7:125:GLU:CG[1_554]  | 0.31                     | 1.89              |
| 4:4:161:HIS:C   | 4:8:110:LEU:CG[1_554]  | 0.31                     | 1.89              |
| 4:4:215:LYS:CD  | 4:8:31:PHE:CB[1_554]   | 0.31                     | 1.89              |
| 4:4:227:MET:CE  | 4:8:306:TYR:CA[1_554]  | 0.31                     | 1.89              |
| 4:3:287:ILE:O   | 4:9:63:GLY:CA[1_554]   | 0.31                     | 1.89              |
| 4:5:346:LEU:CG  | 4:9:368:SER:CB[1_554]  | 0.32                     | 1.88              |
| 4:3:213:LYS:CE  | 4:7:14:SER:C[1_554]    | 0.32                     | 1.88              |
| 4:3:369:ILE:O   | 4:8:229:THR:C[1_554]   | 0.32                     | 1.88              |
| 4:2:75:ILE:N    | 4:7:198:TYR:N[1_554]   | 0.32                     | 1.88              |
| 4:5:193:LEU:O   | 4:9:209:VAL:C[1_554]   | 0.33                     | 1.87              |
| 4:5:166:TYR:CD1 | 4:W:40:HIS:ND1[1_554]  | 0.33                     | 1.87              |
| 4:4:367:PRO:N   | 4:9:234:SER:C[1_554]   | 0.34                     | 1.86              |
| 4:3:274:ILE:N   | 4:7:162:ASN:N[1_554]   | 0.34                     | 1.86              |
| 4:5:335:ARG:N   | 4:9:105:LEU:C[1_554]   | 0.34                     | 1.86              |
| 4:4:18:LYS:CG   | 4:8:79:TRP:CE3[1_554]  | 0.34                     | 1.86              |
| 4:4:305:MET:O   | 4:8:11:ASP:CG[1_554]   | 0.35                     | 1.85              |
| 4:4:162:ASN:N   | 4:8:110:LEU:CD2[1_554] | 0.36                     | 1.84              |
| 4:4:299:MET:CB  | 4:8:136:ILE:CA[1_554]  | 0.36                     | 1.84              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:200:PHE:CA  | 4:9:206:ARG:CG[1_554]  | 0.36                     | 1.84              |
| 4:5:267:ILE:CG1 | 4:9:180:LEU:CG[1_554]  | 0.36                     | 1.84              |
| 4:3:30:VAL:CB   | 4:7:79:TRP:O[1_554]    | 0.37                     | 1.83              |
| 4:3:223:PHE:O   | 4:7:335:ARG:NH2[1_554] | 0.37                     | 1.83              |
| 4:5:286:ASP:CB  | 4:V:270:GLU:OE1[1_554] | 0.38                     | 1.82              |
| 4:5:189:LEU:O   | 4:9:186:THR:OG1[1_554] | 0.38                     | 1.82              |
| 4:5:284:LYS:O   | 4:V:268:GLY:O[1_554]   | 0.38                     | 1.82              |
| 4:3:367:PRO:CD  | 4:8:235:SER:CA[1_554]  | 0.38                     | 1.82              |
| 4:3:286:ASP:CA  | 4:8:270:GLU:CD[1_554]  | 0.38                     | 1.82              |
| 4:2:284:LYS:O   | 4:7:268:GLY:C[1_554]   | 0.38                     | 1.82              |
| 4:4:186:THR:OG1 | 4:8:183:ARG:NH2[1_554] | 0.38                     | 1.82              |
| 4:4:144:ALA:CA  | 4:8:370:VAL:C[1_554]   | 0.38                     | 1.82              |
| 1:D:637:LYS:NZ  | 4:5:311:ASP:CA[1_556]  | 0.38                     | 1.82              |
| 4:3:273:GLY:CA  | 4:7:162:ASN:OD1[1_554] | 0.38                     | 1.82              |
| 4:3:161:HIS:C   | 4:7:110:LEU:CG[1_554]  | 0.39                     | 1.81              |
| 4:5:340:TRP:CD1 | 4:9:118:LYS:C[1_554]   | 0.39                     | 1.81              |
| 4:2:357:ILE:CB  | 4:7:232:SER:C[1_554]   | 0.39                     | 1.81              |
| 4:4:273:GLY:O   | 4:8:162:ASN:CB[1_554]  | 0.39                     | 1.81              |
| 4:5:369:ILE:CG2 | 4:V:232:SER:CA[1_554]  | 0.40                     | 1.80              |
| 4:3:116:ARG:CG  | 4:8:252:ASN:OD1[1_554] | 0.40                     | 1.80              |
| 4:4:274:ILE:N   | 4:8:162:ASN:N[1_554]   | 0.40                     | 1.80              |
| 4:3:345:ILE:CA  | 4:7:366:GLY:C[1_554]   | 0.40                     | 1.80              |
| 4:4:192:ILE:CB  | 4:8:213:LYS:CD[1_554]  | 0.40                     | 1.80              |
| 4:5:188:TYR:CE1 | 4:9:185:LEU:CG[1_554]  | 0.41                     | 1.79              |
| 4:4:274:ILE:C   | 4:8:162:ASN:C[1_554]   | 0.41                     | 1.79              |
| 4:3:75:ILE:N    | 4:8:198:TYR:N[1_554]   | 0.41                     | 1.79              |
| 4:4:298:VAL:O   | 4:8:136:ILE:CD1[1_554] | 0.41                     | 1.79              |
| 4:3:200:PHE:N   | 4:7:206:ARG:CG[1_554]  | 0.41                     | 1.79              |
| 4:4:194:THR:CA  | 4:8:209:VAL:CG1[1_554] | 0.41                     | 1.79              |
| 4:3:314:GLN:C   | 4:7:142:LEU:CG[1_554]  | 0.41                     | 1.79              |
| 4:4:300:SER:CB  | 4:8:107:GLU:CD[1_554]  | 0.41                     | 1.79              |
| 4:5:257:CYS:CA  | 4:9:303:THR:OG1[1_554] | 0.42                     | 1.78              |
| 4:5:185:LEU:C   | 4:9:157:ASP:O[1_554]   | 0.42                     | 1.78              |
| 4:3:74:GLY:O    | 4:8:197:GLY:CA[1_554]  | 0.42                     | 1.78              |
| 4:2:108:ALA:CB  | 4:7:195:GLU:C[1_554]   | 0.42                     | 1.78              |
| 4:5:162:ASN:ND2 | 4:9:175:ILE:CG1[1_554] | 0.42                     | 1.78              |
| 4:3:115:ASN:C   | 4:8:196:ARG:NH2[1_554] | 0.43                     | 1.77              |
| 4:3:299:MET:CE  | 4:7:136:ILE:O[1_554]   | 0.43                     | 1.77              |
| 4:4:262:PHE:CG  | 4:8:153:LEU:C[1_554]   | 0.43                     | 1.77              |
| 4:5:151:ILE:CD1 | 4:9:171:LEU:CA[1_554]  | 0.43                     | 1.77              |
| 4:5:25:ASP:OD2  | 4:9:129:VAL:O[1_554]   | 0.43                     | 1.77              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:27:PRO:CG   | 4:7:122:ILE:CD1[1_554] | 0.44                     | 1.76              |
| 4:3:137:GLN:O   | 4:7:113:LYS:CA[1_554]  | 0.44                     | 1.76              |
| 4:5:337:TYR:CE1 | 4:9:86:TRP:CZ2[1_554]  | 0.44                     | 1.76              |
| 4:5:223:PHE:CZ  | 4:9:304:THR:OG1[1_554] | 0.44                     | 1.76              |
| 4:3:109:PRO:CA  | 4:8:195:GLU:CD[1_554]  | 0.44                     | 1.76              |
| 4:5:113:LYS:CB  | 4:V:252:ASN:C[1_554]   | 0.45                     | 1.75              |
| 4:5:204:ALA:C   | 4:9:62:ARG:CD[1_554]   | 0.45                     | 1.75              |
| 4:4:200:PHE:N   | 4:8:206:ARG:CG[1_554]  | 0.45                     | 1.75              |
| 4:4:312:ARG:NE  | 4:8:299:MET:CA[1_554]  | 0.45                     | 1.75              |
| 4:5:211:ASP:CB  | 4:9:32:PRO:CB[1_554]   | 0.46                     | 1.74              |
| 4:5:210:ARG:CZ  | 4:9:33:SER:O[1_554]    | 0.46                     | 1.74              |
| 4:3:340:TRP:CA  | 4:7:118:LYS:N[1_554]   | 0.46                     | 1.74              |
| 4:3:367:PRO:O   | 4:8:236:LEU:CD2[1_554] | 0.46                     | 1.74              |
| 4:4:25:ASP:OD1  | 4:8:124:PHE:CD1[1_554] | 0.46                     | 1.74              |
| 4:5:255:PHE:CG  | 4:9:305:MET:CB[1_554]  | 0.46                     | 1.74              |
| 4:4:311:ASP:CG  | 4:8:144:ALA:CB[1_554]  | 0.46                     | 1.74              |
| 4:5:283:MET:CB  | 4:9:285:CYS:C[1_554]   | 0.46                     | 1.74              |
| 4:5:343:GLY:O   | 4:9:367:PRO:CA[1_554]  | 0.46                     | 1.74              |
| 4:2:169:TYR:OH  | 4:7:266:PHE:CE1[1_554] | 0.46                     | 1.74              |
| 4:5:258:PRO:CA  | 4:9:155:SER:O[1_554]   | 0.47                     | 1.73              |
| 4:3:30:VAL:C    | 4:7:80:ASP:N[1_554]    | 0.47                     | 1.73              |
| 4:5:325:MET:SD  | 4:9:166:TYR:OH[1_554]  | 0.47                     | 1.73              |
| 4:5:167:GLU:OE2 | 4:W:41:GLN:N[1_554]    | 0.47                     | 1.73              |
| 4:4:287:ILE:O   | 4:V:63:GLY:CA[1_554]   | 0.47                     | 1.73              |
| 4:4:26:ALA:C    | 4:8:122:ILE:CA[1_554]  | 0.48                     | 1.72              |
| 4:5:221:LEU:C   | 4:9:331:ALA:C[1_554]   | 0.48                     | 1.72              |
| 4:4:326:LYS:CA  | 4:8:167:GLU:CD[1_554]  | 0.48                     | 1.72              |
| 4:5:368:SER:O   | 4:V:230:ALA:N[1_554]   | 0.48                     | 1.72              |
| 4:5:273:GLY:C   | 4:9:162:ASN:CG[1_554]  | 0.48                     | 1.72              |
| 4:4:196:ARG:CG  | 4:8:211:ASP:C[1_554]   | 0.48                     | 1.72              |
| 4:3:154:ASP:OD2 | 4:7:111:ASN:C[1_554]   | 0.48                     | 1.72              |
| 4:5:109:PRO:C   | 4:V:195:GLU:CD[1_554]  | 0.48                     | 1.72              |
| 4:3:283:MET:CG  | 4:7:286:ASP:N[1_554]   | 0.48                     | 1.72              |
| 4:2:115:ASN:CB  | 4:7:249:THR:O[1_554]   | 0.48                     | 1.72              |
| 4:3:25:ASP:CB   | 4:7:124:PHE:CA[1_554]  | 0.49                     | 1.71              |
| 4:4:284:LYS:O   | 4:9:268:GLY:O[1_554]   | 0.49                     | 1.71              |
| 4:2:77:THR:C    | 4:7:246:GLN:NE2[1_554] | 0.49                     | 1.71              |
| 4:4:208:ILE:CG2 | 4:8:59:GLN:CD[1_554]   | 0.49                     | 1.71              |
| 4:5:315:LYS:CD  | 4:9:147:ARG:NH1[1_554] | 0.49                     | 1.71              |
| 4:4:286:ASP:CA  | 4:9:270:GLU:CD[1_554]  | 0.49                     | 1.71              |
| 4:3:30:VAL:O    | 4:7:80:ASP:CA[1_554]   | 0.49                     | 1.71              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:114:ALA:CB  | 4:V:250:ILE:C[1_554]   | 0.49                     | 1.71              |
| 4:2:113:LYS:CG  | 4:7:254:ARG:CA[1_554]  | 0.49                     | 1.71              |
| 4:4:218:TYR:CE1 | 4:8:337:TYR:CE1[1_554] | 0.50                     | 1.70              |
| 4:4:24:ASP:CB   | 4:8:125:GLU:CB[1_554]  | 0.50                     | 1.70              |
| 4:4:30:VAL:C    | 4:8:80:ASP:N[1_554]    | 0.50                     | 1.70              |
| 4:5:23:GLY:N    | 4:9:362:TYR:CE2[1_554] | 0.50                     | 1.70              |
| 4:4:333:PRO:CG  | 4:8:104:LEU:CA[1_554]  | 0.50                     | 1.70              |
| 4:3:332:PRO:O   | 4:7:105:LEU:O[1_554]   | 0.50                     | 1.70              |
| 4:3:329:ILE:CG2 | 4:7:139:VAL:CB[1_554]  | 0.50                     | 1.70              |
| 4:4:154:ASP:CG  | 4:8:111:ASN:CA[1_554]  | 0.50                     | 1.70              |
| 4:3:341:ILE:CG2 | 4:7:120:THR:CG2[1_554] | 0.50                     | 1.70              |
| 4:4:222:ASP:CA  | 4:8:331:ALA:C[1_554]   | 0.51                     | 1.69              |
| 4:4:340:TRP:CZ3 | 4:8:121:GLN:CA[1_554]  | 0.51                     | 1.69              |
| 4:5:211:ASP:OD1 | 4:9:32:PRO:CD[1_554]   | 0.51                     | 1.69              |
| 4:5:299:MET:C   | 4:9:136:ILE:CA[1_554]  | 0.51                     | 1.69              |
| 4:5:333:PRO:N   | 4:9:104:LEU:CD2[1_554] | 0.51                     | 1.69              |
| 4:5:270:GLU:O   | 4:9:272:ALA:CB[1_554]  | 0.51                     | 1.69              |
| 4:4:109:PRO:CA  | 4:9:195:GLU:CD[1_554]  | 0.52                     | 1.68              |
| 4:3:15:GLY:CA   | 4:7:77:THR:CG2[1_554]  | 0.52                     | 1.68              |
| 4:4:310:ALA:CB  | 4:8:140:LEU:CA[1_554]  | 0.52                     | 1.68              |
| 4:5:272:ALA:C   | 4:9:277:THR:CG2[1_554] | 0.52                     | 1.68              |
| 4:5:222:ASP:N   | 4:9:331:ALA:CA[1_554]  | 0.52                     | 1.68              |
| 4:3:345:ILE:N   | 4:7:367:PRO:N[1_554]   | 0.52                     | 1.68              |
| 4:4:154:ASP:CB  | 4:8:111:ASN:N[1_554]   | 0.53                     | 1.67              |
| 4:4:320:LEU:CB  | 4:8:293:LEU:CB[1_554]  | 0.53                     | 1.67              |
| 4:3:256:ARG:O   | 4:7:303:THR:CB[1_554]  | 0.53                     | 1.67              |
| 4:5:262:PHE:CD1 | 4:9:153:LEU:CA[1_554]  | 0.53                     | 1.67              |
| 4:2:177:ARG:NH1 | 4:7:194:THR:CG2[1_554] | 0.53                     | 1.67              |
| 4:5:18:LYS:N    | 4:9:79:TRP:CD2[1_554]  | 0.53                     | 1.67              |
| 4:4:139:VAL:C   | 4:8:371:HIS:NE2[1_554] | 0.53                     | 1.67              |
| 4:3:260:THR:CA  | 4:7:155:SER:OG[1_554]  | 0.53                     | 1.67              |
| 4:3:196:ARG:N   | 4:7:209:VAL:O[1_554]   | 0.53                     | 1.67              |
| 4:3:340:TRP:CZ3 | 4:7:121:GLN:CB[1_554]  | 0.53                     | 1.67              |
| 4:5:263:GLN:CA  | 4:9:274:ILE:CG1[1_554] | 0.54                     | 1.66              |
| 4:5:289:ILE:N   | 4:W:63:GLY:C[1_554]    | 0.54                     | 1.66              |
| 4:5:276:GLU:CG  | 4:9:278:THR:O[1_554]   | 0.54                     | 1.66              |
| 4:2:291:LYS:CG  | 4:8:64:ILE:CD1[1_554]  | 0.54                     | 1.66              |
| 4:4:193:LEU:O   | 4:8:210:ARG:N[1_554]   | 0.54                     | 1.66              |
| 4:3:213:LYS:C   | 4:7:16:LEU:N[1_554]    | 0.54                     | 1.66              |
| 4:3:227:MET:CE  | 4:7:306:TYR:CA[1_554]  | 0.54                     | 1.66              |
| 4:3:185:LEU:CB  | 4:7:158:GLY:N[1_554]   | 0.54                     | 1.66              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:24:ASP:OD2  | 4:9:125:GLU:CA[1_554]  | 0.54                     | 1.66              |
| 4:5:266:PHE:CG  | 4:9:261:LEU:CG[1_554]  | 0.54                     | 1.66              |
| 4:5:326:LYS:CA  | 4:9:167:GLU:OE2[1_554] | 0.54                     | 1.66              |
| 4:4:335:ARG:CG  | 4:8:106:THR:CA[1_554]  | 0.54                     | 1.66              |
| 4:5:279:TYR:O   | 4:9:285:CYS:SG[1_554]  | 0.54                     | 1.66              |
| 4:4:223:PHE:O   | 4:8:335:ARG:NH2[1_554] | 0.55                     | 1.65              |
| 4:4:308:GLY:CA  | 4:8:338:SER:C[1_554]   | 0.55                     | 1.65              |
| 4:2:74:GLY:O    | 4:7:197:GLY:CA[1_554]  | 0.55                     | 1.65              |
| 4:3:169:TYR:OH  | 4:8:266:PHE:CE1[1_554] | 0.55                     | 1.65              |
| 4:5:278:THR:CB  | 4:9:164:PRO:N[1_554]   | 0.55                     | 1.65              |
| 4:5:205:GLU:OE2 | 4:7:288:ASP:OD2[1_554] | 0.55                     | 1.65              |
| 4:4:243:PRO:CB  | 4:8:60:SER:C[1_554]    | 0.55                     | 1.65              |
| 4:4:312:ARG:NH2 | 4:8:299:MET:CG[1_554]  | 0.55                     | 1.65              |
| 4:5:15:GLY:N    | 4:9:77:THR:OG1[1_554]  | 0.55                     | 1.65              |
| 4:4:143:TYR:CA  | 4:8:372:ARG:N[1_554]   | 0.55                     | 1.65              |
| 4:5:313:MET:CB  | 4:9:152:VAL:CG2[1_554] | 0.56                     | 1.64              |
| 4:2:286:ASP:N   | 4:7:270:GLU:OE2[1_554] | 0.56                     | 1.64              |
| 4:3:162:ASN:N   | 4:7:110:LEU:CD2[1_554] | 0.56                     | 1.64              |
| 4:5:28:ARG:CB   | 4:9:126:THR:CG2[1_554] | 0.56                     | 1.64              |
| 4:3:154:ASP:CB  | 4:7:111:ASN:N[1_554]   | 0.56                     | 1.64              |
| 4:5:277:THR:N   | 4:9:281:SER:OG[1_554]  | 0.56                     | 1.64              |
| 4:4:31:PHE:C    | 4:8:78:ASN:CG[1_554]   | 0.56                     | 1.64              |
| 4:4:207:GLU:OE2 | 4:8:67:LEU:C[1_554]    | 0.56                     | 1.64              |
| 4:5:314:GLN:NE2 | 4:9:147:ARG:O[1_554]   | 0.56                     | 1.64              |
| 4:4:185:LEU:CB  | 4:8:158:GLY:N[1_554]   | 0.57                     | 1.63              |
| 4:4:344:SER:OG  | 4:8:362:TYR:OH[1_554]  | 0.57                     | 1.63              |
| 4:3:154:ASP:CG  | 4:7:111:ASN:CA[1_554]  | 0.57                     | 1.63              |
| 4:5:145:SER:N   | 4:9:372:ARG:NH2[1_554] | 0.57                     | 1.63              |
| 4:5:255:PHE:CD1 | 4:9:305:MET:CA[1_554]  | 0.57                     | 1.63              |
| 4:4:256:ARG:N   | 4:8:302:GLY:O[1_554]   | 0.57                     | 1.63              |
| 4:4:145:SER:OG  | 4:8:372:ARG:CZ[1_554]  | 0.57                     | 1.63              |
| 4:4:215:LYS:CB  | 4:8:31:PHE:N[1_554]    | 0.57                     | 1.63              |
| 4:5:173:HIS:CE1 | 4:V:265:SER:C[1_554]   | 0.57                     | 1.63              |
| 4:4:314:GLN:OE1 | 4:8:147:ARG:O[1_554]   | 0.57                     | 1.63              |
| 4:4:218:TYR:CE2 | 4:8:337:TYR:CD2[1_554] | 0.58                     | 1.62              |
| 4:4:337:TYR:CZ  | 4:8:86:TRP:CZ3[1_554]  | 0.58                     | 1.62              |
| 4:5:270:GLU:CA  | 4:9:272:ALA:CA[1_554]  | 0.58                     | 1.62              |
| 4:5:312:ARG:NE  | 4:9:299:MET:CB[1_554]  | 0.58                     | 1.62              |
| 4:3:114:ALA:CA  | 4:8:250:ILE:O[1_554]   | 0.58                     | 1.62              |
| 4:5:310:ALA:C   | 4:9:141:SER:C[1_554]   | 0.58                     | 1.62              |
| 4:5:210:ARG:NH2 | 4:9:33:SER:C[1_554]    | 0.58                     | 1.62              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:259:GLU:OE1 | 4:7:304:THR:C[1_554]   | 0.58                     | 1.62              |
| 4:3:341:ILE:CG1 | 4:7:120:THR:CA[1_554]  | 0.58                     | 1.62              |
| 4:5:157:ASP:CG  | 4:9:72:GLU:CA[1_554]   | 0.58                     | 1.62              |
| 4:5:172:PRO:C   | 4:V:266:PHE:O[1_554]   | 0.58                     | 1.62              |
| 4:3:369:ILE:C   | 4:8:229:THR:O[1_554]   | 0.58                     | 1.62              |
| 4:5:198:TYR:CD1 | 4:9:208:ILE:CB[1_554]  | 0.58                     | 1.62              |
| 4:5:157:ASP:OD2 | 4:9:72:GLU:CB[1_554]   | 0.58                     | 1.62              |
| 4:5:367:PRO:N   | 4:V:234:SER:N[1_554]   | 0.58                     | 1.62              |
| 4:3:145:SER:OG  | 4:7:372:ARG:NE[1_554]  | 0.59                     | 1.61              |
| 4:3:305:MET:O   | 4:7:11:ASP:CG[1_554]   | 0.59                     | 1.61              |
| 4:5:339:VAL:CG1 | 4:9:116:ARG:N[1_554]   | 0.59                     | 1.61              |
| 4:5:305:MET:CB  | 4:9:11:ASP:OD1[1_554]  | 0.60                     | 1.60              |
| 4:4:340:TRP:CA  | 4:8:118:LYS:N[1_554]   | 0.60                     | 1.60              |
| 4:3:207:GLU:CD  | 4:7:67:LEU:CA[1_554]   | 0.60                     | 1.60              |
| 4:3:204:ALA:CB  | 4:7:62:ARG:C[1_554]    | 0.60                     | 1.60              |
| 4:3:117:GLU:C   | 4:8:237:GLU:CG[1_554]  | 0.60                     | 1.60              |
| 4:3:339:VAL:N   | 4:7:116:ARG:CA[1_554]  | 0.60                     | 1.60              |
| 4:3:194:THR:O   | 4:7:209:VAL:CB[1_554]  | 0.60                     | 1.60              |
| 4:4:262:PHE:O   | 4:8:153:LEU:CD1[1_554] | 0.60                     | 1.60              |
| 4:3:109:PRO:N   | 4:8:195:GLU:CG[1_554]  | 0.60                     | 1.60              |
| 4:5:295:ALA:CA  | 4:9:167:GLU:C[1_554]   | 0.60                     | 1.60              |
| 4:5:24:ASP:CB   | 4:9:124:PHE:C[1_554]   | 0.61                     | 1.59              |
| 4:3:299:MET:CB  | 4:7:136:ILE:CA[1_554]  | 0.61                     | 1.59              |
| 4:4:326:LYS:O   | 4:8:167:GLU:CB[1_554]  | 0.61                     | 1.59              |
| 4:5:337:TYR:CZ  | 4:9:86:TRP:CE2[1_554]  | 0.61                     | 1.59              |
| 4:5:115:ASN:CA  | 4:V:196:ARG:CZ[1_554]  | 0.61                     | 1.59              |
| 4:2:116:ARG:CD  | 4:7:252:ASN:CG[1_554]  | 0.61                     | 1.59              |
| 4:3:31:PHE:C    | 4:7:78:ASN:OD1[1_554]  | 0.61                     | 1.59              |
| 4:5:219:VAL:CG1 | 4:9:300:SER:CA[1_554]  | 0.61                     | 1.59              |
| 4:3:255:PHE:CD1 | 4:7:305:MET:CG[1_554]  | 0.61                     | 1.59              |
| 4:4:311:ASP:CA  | 4:8:141:SER:O[1_554]   | 0.61                     | 1.59              |
| 4:5:371:HIS:CB  | 4:V:230:ALA:CB[1_554]  | 0.61                     | 1.59              |
| 4:5:114:ALA:CA  | 4:V:251:GLY:N[1_554]   | 0.61                     | 1.59              |
| 4:5:335:ARG:CG  | 4:9:106:THR:CB[1_554]  | 0.61                     | 1.59              |
| 4:3:273:GLY:O   | 4:7:162:ASN:CB[1_554]  | 0.61                     | 1.59              |
| 4:3:291:LYS:CG  | 4:9:64:ILE:CD1[1_554]  | 0.61                     | 1.59              |
| 4:5:262:PHE:CB  | 4:9:153:LEU:CG[1_554]  | 0.61                     | 1.59              |
| 4:4:154:ASP:OD1 | 4:8:111:ASN:CB[1_554]  | 0.62                     | 1.58              |
| 4:4:191:LYS:C   | 4:8:186:THR:CA[1_554]  | 0.62                     | 1.58              |
| 4:4:205:GLU:CA  | 4:8:62:ARG:NE[1_554]   | 0.62                     | 1.58              |
| 4:4:19:ALA:N    | 4:8:118:LYS:NZ[1_554]  | 0.62                     | 1.58              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:227:MET:CB  | 4:9:307:PRO:CA[1_554]  | 0.62                     | 1.58              |
| 4:5:255:PHE:CE1 | 4:9:305:MET:C[1_554]   | 0.62                     | 1.58              |
| 4:4:293:LEU:O   | 4:8:169:TYR:CB[1_554]  | 0.62                     | 1.58              |
| 4:4:157:ASP:CA  | 4:8:72:GLU:O[1_554]    | 0.62                     | 1.58              |
| 4:4:162:ASN:ND2 | 4:8:175:ILE:CG1[1_554] | 0.62                     | 1.58              |
| 4:5:193:LEU:CG  | 4:9:210:ARG:CB[1_554]  | 0.62                     | 1.58              |
| 4:4:336:LYS:NZ  | 4:8:86:TRP:CD1[1_554]  | 0.63                     | 1.57              |
| 4:5:338:SER:CB  | 4:9:134:VAL:CG1[1_554] | 0.63                     | 1.57              |
| 4:3:220:ALA:N   | 4:7:335:ARG:O[1_554]   | 0.63                     | 1.57              |
| 4:5:137:GLN:CB  | 4:9:112:PRO:C[1_554]   | 0.63                     | 1.57              |
| 4:4:276:GLU:OE2 | 4:8:278:THR:C[1_554]   | 0.63                     | 1.57              |
| 4:5:173:HIS:CA  | 4:V:267:ILE:CA[1_554]  | 0.63                     | 1.57              |
| 4:4:140:LEU:CD2 | 4:8:117:GLU:OE2[1_554] | 0.64                     | 1.56              |
| 4:5:332:PRO:CD  | 4:9:135:ALA:CB[1_554]  | 0.64                     | 1.56              |
| 4:4:212:ILE:O   | 4:8:16:LEU:CD1[1_554]  | 0.64                     | 1.56              |
| 4:4:336:LYS:CE  | 4:8:86:TRP:NE1[1_554]  | 0.64                     | 1.56              |
| 4:3:310:ALA:CB  | 4:7:140:LEU:CA[1_554]  | 0.64                     | 1.56              |
| 4:4:199:SER:CA  | 4:8:206:ARG:CA[1_554]  | 0.64                     | 1.56              |
| 4:5:255:PHE:CE1 | 4:9:305:MET:O[1_554]   | 0.64                     | 1.56              |
| 4:3:326:LYS:O   | 4:7:167:GLU:CB[1_554]  | 0.64                     | 1.56              |
| 4:3:284:LYS:O   | 4:8:268:GLY:C[1_554]   | 0.64                     | 1.56              |
| 4:5:218:TYR:CG  | 4:9:336:LYS:CG[1_554]  | 0.64                     | 1.56              |
| 4:2:77:THR:CG2  | 4:7:246:GLN:OE1[1_554] | 0.64                     | 1.56              |
| 4:5:337:TYR:CA  | 4:9:119:MET:CE[1_554]  | 0.64                     | 1.56              |
| 4:3:212:ILE:O   | 4:7:16:LEU:CD1[1_554]  | 0.64                     | 1.56              |
| 4:3:318:THR:N   | 4:7:150:GLY:N[1_554]   | 0.64                     | 1.56              |
| 4:5:162:ASN:OD1 | 4:9:175:ILE:CB[1_554]  | 0.64                     | 1.56              |
| 4:4:315:LYS:CE  | 4:8:147:ARG:NH1[1_554] | 0.65                     | 1.55              |
| 4:3:284:LYS:O   | 4:8:268:GLY:O[1_554]   | 0.65                     | 1.55              |
| 4:3:286:ASP:N   | 4:8:270:GLU:OE2[1_554] | 0.65                     | 1.55              |
| 4:3:317:ILE:CA  | 4:7:150:GLY:O[1_554]   | 0.65                     | 1.55              |
| 4:3:255:PHE:CE1 | 4:7:305:MET:CB[1_554]  | 0.65                     | 1.55              |
| 4:3:344:SER:C   | 4:7:367:PRO:CD[1_554]  | 0.65                     | 1.55              |
| 4:1:289:ILE:N   | 4:7:39:ARG:CZ[1_554]   | 0.65                     | 1.55              |
| 4:3:341:ILE:CB  | 4:7:120:THR:CB[1_554]  | 0.65                     | 1.55              |
| 4:3:262:PHE:O   | 4:7:153:LEU:CD1[1_554] | 0.66                     | 1.54              |
| 4:5:278:THR:CA  | 4:9:164:PRO:CD[1_554]  | 0.66                     | 1.54              |
| 4:3:340:TRP:C   | 4:7:117:GLU:C[1_554]   | 0.66                     | 1.54              |
| 4:4:157:ASP:OD2 | 4:8:72:GLU:CB[1_554]   | 0.66                     | 1.54              |
| 4:2:117:GLU:CB  | 4:7:237:GLU:CA[1_554]  | 0.66                     | 1.54              |
| 4:5:334:GLU:CA  | 4:9:105:LEU:N[1_554]   | 0.66                     | 1.54              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:336:LYS:CE  | 4:7:86:TRP:CE2[1_554]  | 0.66                     | 1.54              |
| 4:4:369:ILE:C   | 4:9:229:THR:O[1_554]   | 0.66                     | 1.54              |
| 4:5:195:GLU:CB  | 4:9:189:LEU:CG[1_554]  | 0.66                     | 1.54              |
| 4:3:314:GLN:OE1 | 4:7:147:ARG:O[1_554]   | 0.66                     | 1.54              |
| 4:3:256:ARG:N   | 4:7:302:GLY:O[1_554]   | 0.67                     | 1.53              |
| 1:D:637:LYS:CD  | 4:5:311:ASP:OD1[1_556] | 0.67                     | 1.53              |
| 4:3:215:LYS:CD  | 4:7:31:PHE:CB[1_554]   | 0.67                     | 1.53              |
| 4:1:292:ASP:CG  | 4:7:40:HIS:CB[1_554]   | 0.67                     | 1.53              |
| 4:2:113:LYS:CB  | 4:7:254:ARG:CB[1_554]  | 0.67                     | 1.53              |
| 4:3:211:ASP:C   | 4:7:32:PRO:CA[1_554]   | 0.67                     | 1.53              |
| 4:1:292:ASP:OD1 | 4:7:40:HIS:CA[1_554]   | 0.67                     | 1.53              |
| 4:3:207:GLU:OE2 | 4:7:67:LEU:C[1_554]    | 0.67                     | 1.53              |
| 4:5:334:GLU:C   | 4:9:105:LEU:CA[1_554]  | 0.67                     | 1.53              |
| 4:4:320:LEU:CA  | 4:8:293:LEU:CA[1_554]  | 0.67                     | 1.53              |
| 4:5:340:TRP:NE1 | 4:9:118:LYS:O[1_554]   | 0.67                     | 1.53              |
| 4:3:186:THR:CB  | 4:7:183:ARG:CZ[1_554]  | 0.67                     | 1.53              |
| 4:3:108:ALA:CB  | 4:8:195:GLU:C[1_554]   | 0.67                     | 1.53              |
| 4:4:192:ILE:CG1 | 4:8:213:LYS:NZ[1_554]  | 0.67                     | 1.53              |
| 4:4:311:ASP:OD1 | 4:8:144:ALA:CA[1_554]  | 0.67                     | 1.53              |
| 4:3:226:GLU:CD  | 4:7:333:PRO:O[1_554]   | 0.67                     | 1.53              |
| 4:5:177:ARG:NH1 | 4:V:194:THR:OG1[1_554] | 0.68                     | 1.52              |
| 4:2:115:ASN:N   | 4:7:250:ILE:N[1_554]   | 0.68                     | 1.52              |
| 4:5:294:TYR:C   | 4:9:166:TYR:C[1_554]   | 0.68                     | 1.52              |
| 4:4:305:MET:C   | 4:8:11:ASP:OD1[1_554]  | 0.68                     | 1.52              |
| 4:4:142:LEU:O   | 4:8:372:ARG:CB[1_554]  | 0.68                     | 1.52              |
| 4:3:194:THR:CA  | 4:7:209:VAL:CG1[1_554] | 0.68                     | 1.52              |
| 4:2:367:PRO:N   | 4:7:235:SER:C[1_554]   | 0.68                     | 1.52              |
| 4:5:311:ASP:N   | 4:9:141:SER:O[1_554]   | 0.68                     | 1.52              |
| 4:3:308:GLY:CA  | 4:7:339:VAL:N[1_554]   | 0.68                     | 1.52              |
| 4:4:294:TYR:CD1 | 4:8:166:TYR:CB[1_554]  | 0.68                     | 1.52              |
| 4:2:116:ARG:O   | 4:7:237:GLU:OE2[1_554] | 0.68                     | 1.52              |
| 4:4:344:SER:CA  | 4:8:367:PRO:CG[1_554]  | 0.68                     | 1.52              |
| 4:4:282:ILE:CD1 | 4:8:171:LEU:CG[1_554]  | 0.68                     | 1.52              |
| 4:4:208:ILE:CD1 | 4:8:59:GLN:CB[1_554]   | 0.69                     | 1.51              |
| 4:4:75:ILE:C    | 4:9:197:GLY:O[1_554]   | 0.69                     | 1.51              |
| 4:5:308:GLY:N   | 4:9:338:SER:CA[1_554]  | 0.69                     | 1.51              |
| 4:4:110:LEU:CD1 | 4:9:191:LYS:CG[1_554]  | 0.69                     | 1.51              |
| 4:5:322:PRO:CA  | 4:9:291:LYS:NZ[1_554]  | 0.69                     | 1.51              |
| 4:3:366:GLY:O   | 4:8:234:SER:CB[1_554]  | 0.69                     | 1.51              |
| 4:3:77:THR:O    | 4:8:246:GLN:NE2[1_554] | 0.69                     | 1.51              |
| 4:5:199:SER:CA  | 4:9:206:ARG:CA[1_554]  | 0.69                     | 1.51              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:266:PHE:CB  | 4:8:261:LEU:CD2[1_554] | 0.69                     | 1.51              |
| 4:3:24:ASP:N    | 4:7:125:GLU:OE2[1_554] | 0.69                     | 1.51              |
| 4:4:111:ASN:OD1 | 4:9:196:ARG:CB[1_554]  | 0.69                     | 1.51              |
| 4:4:159:VAL:C   | 4:8:177:ARG:NH1[1_554] | 0.69                     | 1.51              |
| 4:3:274:ILE:C   | 4:7:162:ASN:C[1_554]   | 0.70                     | 1.50              |
| 4:5:255:PHE:CB  | 4:9:305:MET:CG[1_554]  | 0.70                     | 1.50              |
| 4:5:30:VAL:CG1  | 4:9:82:MET:CB[1_554]   | 0.70                     | 1.50              |
| 4:3:111:ASN:N   | 4:8:192:ILE:O[1_554]   | 0.70                     | 1.50              |
| 4:3:318:THR:CA  | 4:7:149:THR:C[1_554]   | 0.70                     | 1.50              |
| 4:5:291:LYS:NZ  | 4:W:64:ILE:CG1[1_554]  | 0.70                     | 1.50              |
| 4:4:371:HIS:N   | 4:9:230:ALA:CA[1_554]  | 0.70                     | 1.50              |
| 4:5:312:ARG:O   | 4:9:298:VAL:CB[1_554]  | 0.70                     | 1.50              |
| 4:5:198:TYR:CE1 | 4:9:208:ILE:CG1[1_554] | 0.70                     | 1.50              |
| 4:3:214:GLU:CD  | 4:7:33:SER:OG[1_554]   | 0.70                     | 1.50              |
| 4:5:166:TYR:CG  | 4:W:40:HIS:CE1[1_554]  | 0.70                     | 1.50              |
| 4:3:208:ILE:CG2 | 4:7:59:GLN:CD[1_554]   | 0.70                     | 1.50              |
| 4:5:309:ILE:C   | 4:9:141:SER:CB[1_554]  | 0.70                     | 1.50              |
| 4:4:283:MET:CG  | 4:8:286:ASP:N[1_554]   | 0.71                     | 1.49              |
| 4:4:15:GLY:CA   | 4:8:77:THR:CB[1_554]   | 0.71                     | 1.49              |
| 4:3:317:ILE:C   | 4:7:150:GLY:N[1_554]   | 0.71                     | 1.49              |
| 4:3:293:LEU:O   | 4:7:169:TYR:CB[1_554]  | 0.71                     | 1.49              |
| 4:3:266:PHE:CB  | 4:7:261:LEU:CD2[1_554] | 0.71                     | 1.49              |
| 4:2:112:PRO:CD  | 4:7:193:LEU:CD1[1_554] | 0.71                     | 1.49              |
| 4:3:211:ASP:O   | 4:7:32:PRO:CA[1_554]   | 0.71                     | 1.49              |
| 4:4:314:GLN:N   | 4:8:142:LEU:CB[1_554]  | 0.71                     | 1.49              |
| 4:4:333:PRO:C   | 4:8:105:LEU:N[1_554]   | 0.71                     | 1.49              |
| 4:4:109:PRO:N   | 4:9:195:GLU:CG[1_554]  | 0.71                     | 1.49              |
| 4:5:308:GLY:CA  | 4:9:338:SER:CB[1_554]  | 0.71                     | 1.49              |
| 4:3:282:ILE:CD1 | 4:7:171:LEU:CG[1_554]  | 0.71                     | 1.49              |
| 4:5:289:ILE:N   | 4:W:63:GLY:O[1_554]    | 0.71                     | 1.49              |
| 4:4:260:THR:CA  | 4:8:155:SER:OG[1_554]  | 0.71                     | 1.49              |
| 4:4:256:ARG:C   | 4:8:303:THR:CA[1_554]  | 0.71                     | 1.49              |
| 4:5:327:ILE:O   | 4:9:148:THR:CB[1_554]  | 0.72                     | 1.48              |
| 4:2:367:PRO:C   | 4:7:236:LEU:N[1_554]   | 0.72                     | 1.48              |
| 4:5:334:GLU:O   | 4:9:105:LEU:CB[1_554]  | 0.72                     | 1.48              |
| 4:5:349:LEU:CA  | 4:9:365:ALA:CA[1_554]  | 0.72                     | 1.48              |
| 4:5:151:ILE:CB  | 4:9:170:ALA:O[1_554]   | 0.72                     | 1.48              |
| 4:5:141:SER:CA  | 4:9:116:ARG:NE[1_554]  | 0.72                     | 1.48              |
| 4:3:166:TYR:CD1 | 4:9:40:HIS:NE2[1_554]  | 0.72                     | 1.48              |
| 4:5:274:ILE:CA  | 4:9:162:ASN:N[1_554]   | 0.72                     | 1.48              |
| 4:5:314:GLN:NE2 | 4:9:147:ARG:C[1_554]   | 0.72                     | 1.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:20:GLY:C    | 4:9:121:GLN:NE2[1_554] | 0.72                     | 1.48              |
| 4:5:161:HIS:CB  | 4:9:110:LEU:CB[1_554]  | 0.72                     | 1.48              |
| 4:4:115:ASN:OD1 | 4:9:249:THR:O[1_554]   | 0.73                     | 1.47              |
| 4:4:31:PHE:C    | 4:8:78:ASN:OD1[1_554]  | 0.73                     | 1.47              |
| 4:4:331:ALA:C   | 4:8:135:ALA:CB[1_554]  | 0.73                     | 1.47              |
| 4:5:341:ILE:N   | 4:9:120:THR:OG1[1_554] | 0.73                     | 1.47              |
| 4:3:291:LYS:CD  | 4:9:64:ILE:CG1[1_554]  | 0.73                     | 1.47              |
| 4:4:341:ILE:CB  | 4:8:120:THR:CB[1_554]  | 0.73                     | 1.47              |
| 4:4:219:VAL:C   | 4:8:335:ARG:O[1_554]   | 0.73                     | 1.47              |
| 4:5:221:LEU:CG  | 4:9:332:PRO:CG[1_554]  | 0.73                     | 1.47              |
| 4:4:154:ASP:N   | 4:8:109:PRO:C[1_554]   | 0.73                     | 1.47              |
| 4:3:191:LYS:C   | 4:7:186:THR:CA[1_554]  | 0.73                     | 1.47              |
| 4:5:159:VAL:C   | 4:9:177:ARG:NH1[1_554] | 0.73                     | 1.47              |
| 4:4:264:PRO:N   | 4:8:274:ILE:CD1[1_554] | 0.73                     | 1.47              |
| 4:5:110:LEU:CD1 | 4:V:191:LYS:CG[1_554]  | 0.73                     | 1.47              |
| 4:3:304:THR:CA  | 4:7:137:GLN:CD[1_554]  | 0.74                     | 1.46              |
| 4:3:337:TYR:CB  | 4:7:119:MET:CB[1_554]  | 0.74                     | 1.46              |
| 4:5:188:TYR:N   | 4:9:184:ASP:N[1_554]   | 0.74                     | 1.46              |
| 4:5:261:LEU:CB  | 4:9:154:ASP:O[1_554]   | 0.74                     | 1.46              |
| 4:4:317:ILE:CA  | 4:8:150:GLY:C[1_554]   | 0.74                     | 1.46              |
| 4:4:30:VAL:O    | 4:8:80:ASP:CA[1_554]   | 0.74                     | 1.46              |
| 4:5:304:THR:OG1 | 4:9:137:GLN:CG[1_554]  | 0.74                     | 1.46              |
| 4:3:110:LEU:CA  | 4:8:192:ILE:CA[1_554]  | 0.74                     | 1.46              |
| 4:3:276:GLU:OE2 | 4:7:278:THR:C[1_554]   | 0.74                     | 1.46              |
| 4:4:109:PRO:C   | 4:9:195:GLU:OE1[1_554] | 0.74                     | 1.46              |
| 4:5:300:SER:CB  | 4:9:107:GLU:CG[1_554]  | 0.74                     | 1.46              |
| 4:4:310:ALA:CA  | 4:8:141:SER:N[1_554]   | 0.74                     | 1.46              |
| 4:3:319:ALA:CB  | 4:7:296:ASN:CB[1_554]  | 0.74                     | 1.46              |
| 4:5:346:LEU:O   | 4:9:365:ALA:O[1_554]   | 0.74                     | 1.46              |
| 4:4:243:PRO:N   | 4:8:60:SER:CA[1_554]   | 0.74                     | 1.46              |
| 4:4:156:GLY:C   | 4:8:75:ILE:N[1_554]    | 0.74                     | 1.46              |
| 4:4:332:PRO:O   | 4:8:105:LEU:O[1_554]   | 0.74                     | 1.46              |
| 4:5:214:GLU:CA  | 4:9:16:LEU:CB[1_554]   | 0.74                     | 1.46              |
| 4:2:75:ILE:CB   | 4:7:198:TYR:CB[1_554]  | 0.75                     | 1.45              |
| 4:5:367:PRO:O   | 4:V:230:ALA:O[1_554]   | 0.75                     | 1.45              |
| 4:3:308:GLY:CA  | 4:7:338:SER:C[1_554]   | 0.75                     | 1.45              |
| 4:3:370:VAL:C   | 4:8:230:ALA:CA[1_554]  | 0.75                     | 1.45              |
| 4:5:205:GLU:N   | 4:9:62:ARG:NE[1_554]   | 0.75                     | 1.45              |
| 4:3:300:SER:CB  | 4:7:107:GLU:OE1[1_554] | 0.75                     | 1.45              |
| 4:3:326:LYS:CE  | 4:9:45:VAL:N[1_554]    | 0.75                     | 1.45              |
| 4:4:344:SER:N   | 4:8:367:PRO:CB[1_554]  | 0.75                     | 1.45              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:357:ILE:CG2 | 4:8:232:SER:C[1_554]   | 0.75                     | 1.45              |
| 4:4:213:LYS:CE  | 4:8:14:SER:C[1_554]    | 0.75                     | 1.45              |
| 4:4:333:PRO:CA  | 4:8:104:LEU:C[1_554]   | 0.75                     | 1.45              |
| 4:3:311:ASP:C   | 4:7:141:SER:O[1_554]   | 0.75                     | 1.45              |
| 4:5:262:PHE:CE2 | 4:9:153:LEU:O[1_554]   | 0.75                     | 1.45              |
| 4:3:18:LYS:CG   | 4:7:79:TRP:CD2[1_554]  | 0.75                     | 1.45              |
| 4:4:281:SER:O   | 4:8:173:HIS:CD2[1_554] | 0.75                     | 1.45              |
| 4:4:253:GLU:CG  | 4:8:214:GLU:CG[1_554]  | 0.75                     | 1.45              |
| 4:4:345:ILE:CA  | 4:8:366:GLY:O[1_554]   | 0.75                     | 1.45              |
| 4:5:150:GLY:O   | 4:9:169:TYR:CE1[1_554] | 0.75                     | 1.45              |
| 4:4:27:PRO:CB   | 4:8:122:ILE:CG1[1_554] | 0.75                     | 1.45              |
| 4:5:274:ILE:O   | 4:9:162:ASN:C[1_554]   | 0.75                     | 1.45              |
| 4:3:154:ASP:OD1 | 4:7:111:ASN:CA[1_554]  | 0.75                     | 1.45              |
| 4:3:75:ILE:CG2  | 4:8:198:TYR:CD2[1_554] | 0.75                     | 1.45              |
| 4:3:24:ASP:N    | 4:7:125:GLU:CD[1_554]  | 0.75                     | 1.45              |
| 4:5:143:TYR:CB  | 4:9:372:ARG:N[1_554]   | 0.76                     | 1.44              |
| 4:3:157:ASP:CA  | 4:7:72:GLU:O[1_554]    | 0.76                     | 1.44              |
| 4:2:286:ASP:CA  | 4:7:270:GLU:CD[1_554]  | 0.76                     | 1.44              |
| 4:3:300:SER:CA  | 4:7:107:GLU:CG[1_554]  | 0.76                     | 1.44              |
| 4:5:276:GLU:OE2 | 4:9:279:TYR:N[1_554]   | 0.76                     | 1.44              |
| 4:4:337:TYR:C   | 4:8:119:MET:CG[1_554]  | 0.76                     | 1.44              |
| 4:5:266:PHE:CD2 | 4:9:261:LEU:CD1[1_554] | 0.76                     | 1.44              |
| 4:3:345:ILE:CB  | 4:7:366:GLY:O[1_554]   | 0.76                     | 1.44              |
| 1:A:411:GLU:OE1 | 4:4:226:GLU:OE1[1_556] | 0.76                     | 1.44              |
| 4:5:327:ILE:CG1 | 4:9:149:THR:CB[1_554]  | 0.76                     | 1.44              |
| 4:4:321:ALA:O   | 4:8:292:ASP:CB[1_554]  | 0.76                     | 1.44              |
| 4:5:263:GLN:C   | 4:9:274:ILE:CD1[1_554] | 0.76                     | 1.44              |
| 4:4:340:TRP:C   | 4:8:117:GLU:O[1_554]   | 0.76                     | 1.44              |
| 4:5:334:GLU:OE1 | 4:9:133:TYR:O[1_554]   | 0.77                     | 1.43              |
| 4:3:77:THR:CG2  | 4:8:246:GLN:OE1[1_554] | 0.77                     | 1.43              |
| 4:2:372:ARG:O   | 4:7:255:PHE:CZ[1_554]  | 0.77                     | 1.43              |
| 4:3:335:ARG:CZ  | 4:7:106:THR:CG2[1_554] | 0.77                     | 1.43              |
| 4:5:367:PRO:CA  | 4:V:233:SER:CA[1_554]  | 0.77                     | 1.43              |
| 4:5:282:ILE:CD1 | 4:9:171:LEU:CD1[1_554] | 0.77                     | 1.43              |
| 4:3:144:ALA:N   | 4:7:371:HIS:N[1_554]   | 0.77                     | 1.43              |
| 4:4:327:ILE:CG2 | 4:8:148:THR:C[1_554]   | 0.77                     | 1.43              |
| 4:5:214:GLU:CB  | 4:9:16:LEU:CA[1_554]   | 0.77                     | 1.43              |
| 4:5:310:ALA:N   | 4:9:141:SER:CB[1_554]  | 0.77                     | 1.43              |
| 4:2:110:LEU:CA  | 4:7:192:ILE:CA[1_554]  | 0.77                     | 1.43              |
| 4:2:111:ASN:O   | 4:7:253:GLU:CG[1_554]  | 0.77                     | 1.43              |
| 4:4:143:TYR:CD2 | 4:8:368:SER:O[1_554]   | 0.77                     | 1.43              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:368:SER:C   | 4:V:229:THR:C[1_554]   | 0.77                     | 1.43              |
| 4:3:338:SER:C   | 4:7:116:ARG:C[1_554]   | 0.77                     | 1.43              |
| 4:3:280:ASN:ND2 | 4:7:281:SER:O[1_554]   | 0.77                     | 1.43              |
| 4:5:341:ILE:CG1 | 4:9:132:MET:CE[1_554]  | 0.77                     | 1.43              |
| 4:4:30:VAL:CB   | 4:8:79:TRP:O[1_554]    | 0.77                     | 1.43              |
| 4:3:144:ALA:C   | 4:7:370:VAL:C[1_554]   | 0.78                     | 1.42              |
| 4:4:294:TYR:CG  | 4:8:166:TYR:CB[1_554]  | 0.78                     | 1.42              |
| 4:4:183:ARG:NE  | 4:8:72:GLU:OE1[1_554]  | 0.78                     | 1.42              |
| 4:3:144:ALA:CA  | 4:7:371:HIS:N[1_554]   | 0.78                     | 1.42              |
| 4:3:270:GLU:CB  | 4:7:272:ALA:CA[1_554]  | 0.78                     | 1.42              |
| 4:5:301:GLY:N   | 4:9:107:GLU:C[1_554]   | 0.78                     | 1.42              |
| 4:4:30:VAL:CA   | 4:8:79:TRP:O[1_554]    | 0.78                     | 1.42              |
| 4:4:276:GLU:CD  | 4:8:278:THR:O[1_554]   | 0.78                     | 1.42              |
| 4:5:367:PRO:N   | 4:V:233:SER:C[1_554]   | 0.78                     | 1.42              |
| 4:3:255:PHE:C   | 4:7:302:GLY:C[1_554]   | 0.78                     | 1.42              |
| 4:4:26:ALA:CA   | 4:8:123:MET:N[1_554]   | 0.78                     | 1.42              |
| 4:5:106:THR:CB  | 4:9:114:ALA:CB[1_554]  | 0.78                     | 1.42              |
| 4:4:178:LEU:CG  | 4:8:177:ARG:CA[1_554]  | 0.78                     | 1.42              |
| 4:3:16:LEU:N    | 4:7:77:THR:C[1_554]    | 0.78                     | 1.42              |
| 4:4:253:GLU:CD  | 4:8:214:GLU:CB[1_554]  | 0.78                     | 1.42              |
| 4:4:177:ARG:NH1 | 4:9:194:THR:CB[1_554]  | 0.78                     | 1.42              |
| 4:4:140:LEU:C   | 4:8:371:HIS:ND1[1_554] | 0.78                     | 1.42              |
| 4:3:142:LEU:O   | 4:7:372:ARG:CB[1_554]  | 0.78                     | 1.42              |
| 4:4:76:ILE:O    | 4:9:198:TYR:CE1[1_554] | 0.79                     | 1.41              |
| 4:4:27:PRO:CA   | 4:8:122:ILE:CG1[1_554] | 0.79                     | 1.41              |
| 4:3:191:LYS:CB  | 4:7:187:ASP:N[1_554]   | 0.79                     | 1.41              |
| 4:3:298:VAL:C   | 4:7:136:ILE:CD1[1_554] | 0.79                     | 1.41              |
| 4:5:274:ILE:CA  | 4:9:162:ASN:CA[1_554]  | 0.79                     | 1.41              |
| 4:3:188:TYR:CD2 | 4:7:182:GLY:N[1_554]   | 0.79                     | 1.41              |
| 4:5:297:ASN:N   | 4:9:168:GLY:O[1_554]   | 0.79                     | 1.41              |
| 4:4:314:GLN:CA  | 4:8:142:LEU:CG[1_554]  | 0.79                     | 1.41              |
| 4:1:326:LYS:CG  | 4:7:43:VAL:O[1_554]    | 0.79                     | 1.41              |
| 4:4:341:ILE:CB  | 4:8:120:THR:OG1[1_554] | 0.79                     | 1.41              |
| 4:4:16:LEU:N    | 4:8:77:THR:C[1_554]    | 0.79                     | 1.41              |
| 4:3:294:TYR:CD1 | 4:7:166:TYR:CB[1_554]  | 0.79                     | 1.41              |
| 4:3:275:HIS:N   | 4:7:163:VAL:N[1_554]   | 0.79                     | 1.41              |
| 4:3:314:GLN:N   | 4:7:142:LEU:CB[1_554]  | 0.79                     | 1.41              |
| 4:5:200:PHE:N   | 4:9:206:ARG:CB[1_554]  | 0.79                     | 1.41              |
| 4:3:222:ASP:N   | 4:7:332:PRO:CD[1_554]  | 0.79                     | 1.41              |
| 4:3:331:ALA:CA  | 4:7:135:ALA:CB[1_554]  | 0.79                     | 1.41              |
| 4:5:372:ARG:O   | 4:V:227:MET:CG[1_554]  | 0.79                     | 1.41              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:198:TYR:CG  | 4:9:208:ILE:CA[1_554]  | 0.79                     | 1.41              |
| 4:4:214:GLU:N   | 4:8:16:LEU:N[1_554]    | 0.79                     | 1.41              |
| 4:5:205:GLU:CA  | 4:9:62:ARG:NE[1_554]   | 0.79                     | 1.41              |
| 4:4:191:LYS:CB  | 4:8:187:ASP:N[1_554]   | 0.80                     | 1.40              |
| 4:5:218:TYR:OH  | 4:9:337:TYR:CE2[1_554] | 0.80                     | 1.40              |
| 4:3:372:ARG:CG  | 4:8:227:MET:CB[1_554]  | 0.80                     | 1.40              |
| 4:4:339:VAL:C   | 4:8:117:GLU:N[1_554]   | 0.80                     | 1.40              |
| 4:3:315:LYS:CD  | 4:7:147:ARG:NE[1_554]  | 0.80                     | 1.40              |
| 4:5:276:GLU:CD  | 4:9:278:THR:C[1_554]   | 0.80                     | 1.40              |
| 4:4:339:VAL:CB  | 4:8:116:ARG:N[1_554]   | 0.80                     | 1.40              |
| 4:4:340:TRP:O   | 4:8:117:GLU:O[1_554]   | 0.80                     | 1.40              |
| 4:3:187:ASP:N   | 4:7:183:ARG:CD[1_554]  | 0.80                     | 1.40              |
| 4:3:139:VAL:O   | 4:7:371:HIS:NE2[1_554] | 0.80                     | 1.40              |
| 4:3:316:GLU:O   | 4:7:151:ILE:N[1_554]   | 0.80                     | 1.40              |
| 4:4:255:PHE:C   | 4:8:302:GLY:O[1_554]   | 0.80                     | 1.40              |
| 4:5:300:SER:C   | 4:9:107:GLU:C[1_554]   | 0.80                     | 1.40              |
| 4:3:75:ILE:CD1  | 4:8:193:LEU:O[1_554]   | 0.80                     | 1.40              |
| 4:4:30:VAL:CA   | 4:8:79:TRP:C[1_554]    | 0.80                     | 1.40              |
| 4:3:214:GLU:C   | 4:7:17:VAL:N[1_554]    | 0.80                     | 1.40              |
| 4:4:27:PRO:N    | 4:8:122:ILE:CB[1_554]  | 0.80                     | 1.40              |
| 4:4:335:ARG:CZ  | 4:8:106:THR:CG2[1_554] | 0.81                     | 1.39              |
| 4:3:367:PRO:N   | 4:8:235:SER:N[1_554]   | 0.81                     | 1.39              |
| 4:4:243:PRO:CB  | 4:8:61:LYS:N[1_554]    | 0.81                     | 1.39              |
| 4:3:116:ARG:C   | 4:8:237:GLU:OE2[1_554] | 0.81                     | 1.39              |
| 4:4:321:ALA:O   | 4:8:292:ASP:CG[1_554]  | 0.81                     | 1.39              |
| 4:3:339:VAL:CG1 | 4:7:115:ASN:N[1_554]   | 0.81                     | 1.39              |
| 4:5:372:ARG:C   | 4:V:227:MET:CA[1_554]  | 0.81                     | 1.39              |
| 4:3:111:ASN:CG  | 4:8:196:ARG:CG[1_554]  | 0.81                     | 1.39              |
| 4:5:255:PHE:CZ  | 4:9:305:MET:O[1_554]   | 0.81                     | 1.39              |
| 4:4:366:GLY:C   | 4:9:234:SER:CA[1_554]  | 0.81                     | 1.39              |
| 4:3:16:LEU:CA   | 4:7:77:THR:C[1_554]    | 0.81                     | 1.39              |
| 4:4:207:GLU:CD  | 4:8:67:LEU:CA[1_554]   | 0.81                     | 1.39              |
| 4:5:253:GLU:CD  | 4:9:214:GLU:N[1_554]   | 0.81                     | 1.39              |
| 4:3:183:ARG:NE  | 4:7:72:GLU:OE1[1_554]  | 0.81                     | 1.39              |
| 4:3:312:ARG:NE  | 4:7:299:MET:C[1_554]   | 0.81                     | 1.39              |
| 4:5:198:TYR:CG  | 4:9:208:ILE:C[1_554]   | 0.81                     | 1.39              |
| 4:4:115:ASN:C   | 4:9:196:ARG:NH2[1_554] | 0.81                     | 1.39              |
| 4:5:24:ASP:C    | 4:9:124:PHE:CA[1_554]  | 0.81                     | 1.39              |
| 4:5:372:ARG:C   | 4:V:227:MET:CB[1_554]  | 0.81                     | 1.39              |
| 4:4:366:GLY:O   | 4:9:234:SER:CB[1_554]  | 0.81                     | 1.39              |
| 4:5:156:GLY:O   | 4:9:74:GLY:N[1_554]    | 0.81                     | 1.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:325:MET:CG  | 4:7:166:TYR:CE2[1_554] | 0.81                     | 1.39              |
| 4:5:218:TYR:CB  | 4:9:336:LYS:CB[1_554]  | 0.81                     | 1.39              |
| 4:5:24:ASP:CG   | 4:9:125:GLU:CA[1_554]  | 0.82                     | 1.38              |
| 4:5:254:ARG:CZ  | 4:9:336:LYS:NZ[1_554]  | 0.82                     | 1.38              |
| 4:3:337:TYR:CB  | 4:7:119:MET:CA[1_554]  | 0.82                     | 1.38              |
| 4:3:192:ILE:CB  | 4:7:213:LYS:CD[1_554]  | 0.82                     | 1.38              |
| 4:5:137:GLN:CA  | 4:9:113:LYS:N[1_554]   | 0.82                     | 1.38              |
| 4:4:339:VAL:O   | 4:8:117:GLU:N[1_554]   | 0.82                     | 1.38              |
| 4:3:157:ASP:CG  | 4:7:72:GLU:CB[1_554]   | 0.82                     | 1.38              |
| 4:4:16:LEU:N    | 4:8:77:THR:CA[1_554]   | 0.82                     | 1.38              |
| 4:4:196:ARG:N   | 4:8:209:VAL:O[1_554]   | 0.82                     | 1.38              |
| 4:4:112:PRO:O   | 4:9:253:GLU:OE2[1_554] | 0.82                     | 1.38              |
| 4:4:118:LYS:N   | 4:9:237:GLU:OE1[1_554] | 0.82                     | 1.38              |
| 4:3:327:ILE:CG2 | 4:7:148:THR:O[1_554]   | 0.82                     | 1.38              |
| 4:5:288:ASP:O   | 4:W:64:ILE:N[1_554]    | 0.82                     | 1.38              |
| 4:3:218:TYR:CE2 | 4:7:337:TYR:CG[1_554]  | 0.82                     | 1.38              |
| 4:5:310:ALA:CA  | 4:9:141:SER:CA[1_554]  | 0.82                     | 1.38              |
| 4:5:137:GLN:CD  | 4:9:112:PRO:CB[1_554]  | 0.82                     | 1.38              |
| 4:5:161:HIS:CA  | 4:9:110:LEU:CD1[1_554] | 0.82                     | 1.38              |
| 4:3:320:LEU:CB  | 4:7:293:LEU:CB[1_554]  | 0.82                     | 1.38              |
| 4:5:337:TYR:OH  | 4:9:86:TRP:CE2[1_554]  | 0.82                     | 1.38              |
| 4:5:369:ILE:N   | 4:V:229:THR:O[1_554]   | 0.82                     | 1.38              |
| 4:5:336:LYS:CG  | 4:9:12:ASN:ND2[1_554]  | 0.82                     | 1.38              |
| 4:5:301:GLY:O   | 4:9:137:GLN:NE2[1_554] | 0.83                     | 1.37              |
| 4:3:177:ARG:NH1 | 4:8:194:THR:CG2[1_554] | 0.83                     | 1.37              |
| 4:4:115:ASN:CB  | 4:9:196:ARG:NE[1_554]  | 0.83                     | 1.37              |
| 4:5:75:ILE:C    | 4:V:197:GLY:C[1_554]   | 0.83                     | 1.37              |
| 4:5:14:SER:C    | 4:9:77:THR:OG1[1_554]  | 0.83                     | 1.37              |
| 4:5:301:GLY:N   | 4:9:107:GLU:CA[1_554]  | 0.83                     | 1.37              |
| 4:3:335:ARG:CG  | 4:7:106:THR:C[1_554]   | 0.83                     | 1.37              |
| 4:3:311:ASP:C   | 4:7:141:SER:C[1_554]   | 0.83                     | 1.37              |
| 4:4:320:LEU:CA  | 4:8:293:LEU:N[1_554]   | 0.83                     | 1.37              |
| 4:2:369:ILE:CG2 | 4:7:234:SER:CB[1_554]  | 0.83                     | 1.37              |
| 4:3:304:THR:CA  | 4:7:137:GLN:NE2[1_554] | 0.83                     | 1.37              |
| 4:3:297:ASN:OD1 | 4:7:170:ALA:CA[1_554]  | 0.83                     | 1.37              |
| 4:3:332:PRO:CD  | 4:7:134:VAL:C[1_554]   | 0.83                     | 1.37              |
| 4:3:318:THR:N   | 4:7:149:THR:C[1_554]   | 0.83                     | 1.37              |
| 4:5:339:VAL:O   | 4:9:116:ARG:C[1_554]   | 0.83                     | 1.37              |
| 4:2:370:VAL:CG2 | 4:7:230:ALA:O[1_554]   | 0.83                     | 1.37              |
| 4:4:345:ILE:N   | 4:8:367:PRO:N[1_554]   | 0.83                     | 1.37              |
| 4:3:293:LEU:O   | 4:7:169:TYR:CG[1_554]  | 0.84                     | 1.36              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:270:GLU:CA  | 4:8:272:ALA:CA[1_554]  | 0.84                     | 1.36              |
| 4:4:340:TRP:C   | 4:8:117:GLU:C[1_554]   | 0.84                     | 1.36              |
| 4:3:357:ILE:CG1 | 4:8:232:SER:N[1_554]   | 0.84                     | 1.36              |
| 4:3:281:SER:C   | 4:7:173:HIS:CD2[1_554] | 0.84                     | 1.36              |
| 4:4:166:TYR:CD1 | 4:V:40:HIS:CE1[1_554]  | 0.84                     | 1.36              |
| 4:5:307:PRO:CB  | 4:9:337:TYR:CA[1_554]  | 0.84                     | 1.36              |
| 4:4:115:ASN:CA  | 4:9:196:ARG:NH2[1_554] | 0.84                     | 1.36              |
| 4:2:115:ASN:N   | 4:7:250:ILE:CA[1_554]  | 0.84                     | 1.36              |
| 4:3:193:LEU:O   | 4:7:210:ARG:N[1_554]   | 0.84                     | 1.36              |
| 4:5:317:ILE:CB  | 4:9:150:GLY:O[1_554]   | 0.84                     | 1.36              |
| 4:5:207:GLU:CB  | 4:9:67:LEU:CD1[1_554]  | 0.84                     | 1.36              |
| 4:4:166:TYR:CG  | 4:V:40:HIS:NE2[1_554]  | 0.84                     | 1.36              |
| 4:3:188:TYR:CG  | 4:7:181:ALA:O[1_554]   | 0.84                     | 1.36              |
| 4:5:159:VAL:CA  | 4:9:177:ARG:NH1[1_554] | 0.84                     | 1.36              |
| 4:5:310:ALA:N   | 4:9:141:SER:CA[1_554]  | 0.84                     | 1.36              |
| 4:4:329:ILE:CG2 | 4:8:139:VAL:CA[1_554]  | 0.84                     | 1.36              |
| 4:3:311:ASP:CG  | 4:7:144:ALA:CB[1_554]  | 0.84                     | 1.36              |
| 4:4:266:PHE:CG  | 4:8:261:LEU:CD1[1_554] | 0.84                     | 1.36              |
| 4:5:312:ARG:CZ  | 4:9:299:MET:CG[1_554]  | 0.84                     | 1.36              |
| 4:5:150:GLY:C   | 4:9:169:TYR:CD1[1_554] | 0.84                     | 1.36              |
| 4:5:174:ALA:O   | 4:9:173:HIS:CB[1_554]  | 0.84                     | 1.36              |
| 4:5:24:ASP:CB   | 4:9:125:GLU:N[1_554]   | 0.85                     | 1.35              |
| 4:3:144:ALA:CA  | 4:7:370:VAL:C[1_554]   | 0.85                     | 1.35              |
| 4:2:284:LYS:C   | 4:7:268:GLY:O[1_554]   | 0.85                     | 1.35              |
| 4:3:266:PHE:CD1 | 4:7:261:LEU:CD1[1_554] | 0.85                     | 1.35              |
| 4:5:331:ALA:CB  | 4:9:140:LEU:CG[1_554]  | 0.85                     | 1.35              |
| 4:4:193:LEU:CD2 | 4:8:210:ARG:CD[1_554]  | 0.85                     | 1.35              |
| 4:5:322:PRO:CG  | 4:9:288:ASP:O[1_554]   | 0.85                     | 1.35              |
| 4:2:287:ILE:O   | 4:8:63:GLY:CA[1_554]   | 0.85                     | 1.35              |
| 4:3:173:HIS:C   | 4:8:267:ILE:CA[1_554]  | 0.85                     | 1.35              |
| 4:5:142:LEU:O   | 4:9:372:ARG:NE[1_554]  | 0.85                     | 1.35              |
| 4:3:276:GLU:CD  | 4:7:278:THR:O[1_554]   | 0.85                     | 1.35              |
| 4:5:21:PHE:CA   | 4:9:125:GLU:OE1[1_554] | 0.85                     | 1.35              |
| 4:5:307:PRO:C   | 4:9:338:SER:N[1_554]   | 0.85                     | 1.35              |
| 4:4:314:GLN:CD  | 4:8:147:ARG:O[1_554]   | 0.85                     | 1.35              |
| 4:5:75:ILE:C    | 4:V:197:GLY:O[1_554]   | 0.85                     | 1.35              |
| 4:4:27:PRO:CB   | 4:8:122:ILE:CD1[1_554] | 0.85                     | 1.35              |
| 4:5:136:ILE:C   | 4:9:113:LYS:CB[1_554]  | 0.85                     | 1.35              |
| 4:5:327:ILE:CG2 | 4:9:149:THR:N[1_554]   | 0.85                     | 1.35              |
| 4:3:213:LYS:CB  | 4:7:15:GLY:CA[1_554]   | 0.85                     | 1.35              |
| 4:4:370:VAL:C   | 4:9:230:ALA:C[1_554]   | 0.85                     | 1.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:289:ILE:N   | 4:V:63:GLY:O[1_554]    | 0.85                     | 1.35              |
| 4:4:298:VAL:C   | 4:8:136:ILE:CD1[1_554] | 0.85                     | 1.35              |
| 4:5:319:ALA:CB  | 4:9:295:ALA:C[1_554]   | 0.85                     | 1.35              |
| 4:5:162:ASN:CG  | 4:9:175:ILE:CB[1_554]  | 0.86                     | 1.34              |
| 4:4:118:LYS:N   | 4:9:237:GLU:CD[1_554]  | 0.86                     | 1.34              |
| 4:3:197:GLY:O   | 4:7:208:ILE:CG2[1_554] | 0.86                     | 1.34              |
| 4:3:196:ARG:CG  | 4:7:211:ASP:C[1_554]   | 0.86                     | 1.34              |
| 4:4:111:ASN:OD1 | 4:9:196:ARG:CG[1_554]  | 0.86                     | 1.34              |
| 4:4:337:TYR:CB  | 4:8:119:MET:CB[1_554]  | 0.86                     | 1.34              |
| 4:4:250:ILE:CD1 | 4:8:210:ARG:NH2[1_554] | 0.86                     | 1.34              |
| 4:3:281:SER:O   | 4:7:173:HIS:CD2[1_554] | 0.86                     | 1.34              |
| 4:5:277:THR:CG2 | 4:9:175:ILE:C[1_554]   | 0.86                     | 1.34              |
| 4:2:110:LEU:CA  | 4:7:192:ILE:CB[1_554]  | 0.86                     | 1.34              |
| 4:3:325:MET:O   | 4:7:167:GLU:OE2[1_554] | 0.86                     | 1.34              |
| 4:3:270:GLU:CA  | 4:7:272:ALA:C[1_554]   | 0.86                     | 1.34              |
| 4:5:370:VAL:CA  | 4:V:231:ALA:CB[1_554]  | 0.86                     | 1.34              |
| 4:3:336:LYS:CE  | 4:7:86:TRP:NE1[1_554]  | 0.86                     | 1.34              |
| 4:2:117:GLU:C   | 4:7:237:GLU:CB[1_554]  | 0.86                     | 1.34              |
| 4:5:346:LEU:CB  | 4:9:368:SER:CA[1_554]  | 0.86                     | 1.34              |
| 4:5:281:SER:O   | 4:9:173:HIS:CD2[1_554] | 0.86                     | 1.34              |
| 4:4:21:PHE:O    | 4:8:125:GLU:OE1[1_554] | 0.86                     | 1.34              |
| 4:5:106:THR:CB  | 4:9:114:ALA:CA[1_554]  | 0.86                     | 1.34              |
| 4:4:198:TYR:CG  | 4:8:208:ILE:CA[1_554]  | 0.86                     | 1.34              |
| 4:3:298:VAL:O   | 4:7:136:ILE:CD1[1_554] | 0.86                     | 1.34              |
| 4:4:188:TYR:CG  | 4:8:181:ALA:O[1_554]   | 0.86                     | 1.34              |
| 4:4:326:LYS:CE  | 4:V:45:VAL:N[1_554]    | 0.86                     | 1.34              |
| 4:5:311:ASP:OD1 | 4:9:144:ALA:C[1_554]   | 0.87                     | 1.33              |
| 4:3:173:HIS:CE1 | 4:8:266:PHE:N[1_554]   | 0.87                     | 1.33              |
| 4:4:166:TYR:OH  | 4:V:39:ARG:C[1_554]    | 0.87                     | 1.33              |
| 4:4:262:PHE:CD2 | 4:8:153:LEU:O[1_554]   | 0.87                     | 1.33              |
| 4:5:313:MET:CG  | 4:9:152:VAL:CB[1_554]  | 0.87                     | 1.33              |
| 4:3:328:LYS:N   | 4:7:168:GLY:CA[1_554]  | 0.87                     | 1.33              |
| 4:4:25:ASP:CB   | 4:8:124:PHE:CA[1_554]  | 0.87                     | 1.33              |
| 4:5:173:HIS:N   | 4:V:266:PHE:C[1_554]   | 0.87                     | 1.33              |
| 4:2:108:ALA:CA  | 4:7:195:GLU:O[1_554]   | 0.87                     | 1.33              |
| 4:5:281:SER:O   | 4:9:173:HIS:NE2[1_554] | 0.87                     | 1.33              |
| 4:4:345:ILE:CA  | 4:8:366:GLY:C[1_554]   | 0.87                     | 1.33              |
| 4:5:340:TRP:CD1 | 4:9:118:LYS:O[1_554]   | 0.87                     | 1.33              |
| 4:5:211:ASP:CG  | 4:9:32:PRO:CD[1_554]   | 0.87                     | 1.33              |
| 4:3:207:GLU:CB  | 4:7:67:LEU:CB[1_554]   | 0.87                     | 1.33              |
| 4:3:166:TYR:OH  | 4:9:39:ARG:O[1_554]    | 0.87                     | 1.33              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:188:TYR:CB  | 4:9:181:ALA:O[1_554]   | 0.87                     | 1.33              |
| 4:3:178:LEU:CG  | 4:7:177:ARG:CA[1_554]  | 0.87                     | 1.33              |
| 4:5:312:ARG:CD  | 4:9:299:MET:CA[1_554]  | 0.87                     | 1.33              |
| 4:5:157:ASP:CG  | 4:9:72:GLU:N[1_554]    | 0.87                     | 1.33              |
| 4:3:315:LYS:CE  | 4:7:147:ARG:NE[1_554]  | 0.87                     | 1.33              |
| 4:5:106:THR:CA  | 4:9:114:ALA:CB[1_554]  | 0.87                     | 1.33              |
| 4:3:370:VAL:CB  | 4:8:230:ALA:O[1_554]   | 0.87                     | 1.33              |
| 4:3:145:SER:N   | 4:7:370:VAL:O[1_554]   | 0.87                     | 1.33              |
| 4:5:142:LEU:O   | 4:9:372:ARG:CD[1_554]  | 0.87                     | 1.33              |
| 4:4:255:PHE:CD1 | 4:8:305:MET:CB[1_554]  | 0.87                     | 1.33              |
| 4:5:154:ASP:N   | 4:9:109:PRO:C[1_554]   | 0.87                     | 1.33              |
| 4:4:370:VAL:CA  | 4:9:231:ALA:N[1_554]   | 0.87                     | 1.33              |
| 4:4:367:PRO:CD  | 4:9:235:SER:N[1_554]   | 0.87                     | 1.33              |
| 4:4:262:PHE:C   | 4:8:153:LEU:CD1[1_554] | 0.88                     | 1.32              |
| 4:5:243:PRO:CB  | 4:9:60:SER:CA[1_554]   | 0.88                     | 1.32              |
| 4:5:368:SER:C   | 4:V:229:THR:O[1_554]   | 0.88                     | 1.32              |
| 4:4:362:TYR:CD1 | 4:9:233:SER:O[1_554]   | 0.88                     | 1.32              |
| 4:2:173:HIS:C   | 4:7:267:ILE:CA[1_554]  | 0.88                     | 1.32              |
| 4:4:32:PRO:N    | 4:8:78:ASN:CG[1_554]   | 0.88                     | 1.32              |
| 4:4:336:LYS:NZ  | 4:8:86:TRP:NE1[1_554]  | 0.88                     | 1.32              |
| 4:3:320:LEU:CA  | 4:7:293:LEU:CA[1_554]  | 0.88                     | 1.32              |
| 4:4:194:THR:C   | 4:8:209:VAL:CB[1_554]  | 0.88                     | 1.32              |
| 4:4:220:ALA:CA  | 4:8:335:ARG:CB[1_554]  | 0.88                     | 1.32              |
| 4:5:190:MET:SD  | 4:9:206:ARG:NH2[1_554] | 0.88                     | 1.32              |
| 4:4:284:LYS:O   | 4:9:268:GLY:C[1_554]   | 0.88                     | 1.32              |
| 4:3:178:LEU:CD2 | 4:7:177:ARG:CA[1_554]  | 0.88                     | 1.32              |
| 4:4:317:ILE:C   | 4:8:150:GLY:N[1_554]   | 0.88                     | 1.32              |
| 4:3:115:ASN:CG  | 4:8:249:THR:O[1_554]   | 0.88                     | 1.32              |
| 4:5:347:ALA:C   | 4:9:366:GLY:CA[1_554]  | 0.88                     | 1.32              |
| 4:4:337:TYR:CA  | 4:8:119:MET:CG[1_554]  | 0.88                     | 1.32              |
| 4:5:339:VAL:C   | 4:9:116:ARG:C[1_554]   | 0.88                     | 1.32              |
| 4:5:288:ASP:C   | 4:W:63:GLY:C[1_554]    | 0.88                     | 1.32              |
| 4:4:274:ILE:O   | 4:8:162:ASN:O[1_554]   | 0.89                     | 1.31              |
| 4:3:186:THR:CA  | 4:7:183:ARG:NE[1_554]  | 0.89                     | 1.31              |
| 4:2:109:PRO:CD  | 4:7:195:GLU:CG[1_554]  | 0.89                     | 1.31              |
| 4:4:281:SER:O   | 4:8:173:HIS:NE2[1_554] | 0.89                     | 1.31              |
| 4:4:186:THR:CB  | 4:8:183:ARG:CZ[1_554]  | 0.89                     | 1.31              |
| 4:2:77:THR:O    | 4:7:246:GLN:NE2[1_554] | 0.89                     | 1.31              |
| 4:3:344:SER:CA  | 4:7:367:PRO:CG[1_554]  | 0.89                     | 1.31              |
| 4:5:242:LEU:CD2 | 4:9:207:GLU:OE1[1_554] | 0.89                     | 1.31              |
| 4:5:187:ASP:O   | 4:9:183:ARG:O[1_554]   | 0.89                     | 1.31              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:267:ILE:N   | 4:7:180:LEU:CD1[1_554] | 0.89                     | 1.31              |
| 4:5:268:GLY:C   | 4:9:264:PRO:CB[1_554]  | 0.89                     | 1.31              |
| 4:4:27:PRO:N    | 4:8:122:ILE:CA[1_554]  | 0.89                     | 1.31              |
| 4:4:214:GLU:CA  | 4:8:16:LEU:C[1_554]    | 0.89                     | 1.31              |
| 4:4:194:THR:O   | 4:8:209:VAL:CB[1_554]  | 0.89                     | 1.31              |
| 4:2:173:HIS:CA  | 4:7:267:ILE:CG2[1_554] | 0.89                     | 1.31              |
| 4:4:337:TYR:CZ  | 4:8:86:TRP:CH2[1_554]  | 0.89                     | 1.31              |
| 4:4:109:PRO:O   | 4:9:195:GLU:OE1[1_554] | 0.89                     | 1.31              |
| 4:4:283:MET:CB  | 4:8:285:CYS:C[1_554]   | 0.89                     | 1.31              |
| 4:4:317:ILE:CA  | 4:8:150:GLY:O[1_554]   | 0.89                     | 1.31              |
| 4:5:274:ILE:CD1 | 4:9:161:HIS:CA[1_554]  | 0.89                     | 1.31              |
| 4:4:280:ASN:ND2 | 4:8:281:SER:O[1_554]   | 0.89                     | 1.31              |
| 4:3:108:ALA:CA  | 4:8:195:GLU:O[1_554]   | 0.89                     | 1.31              |
| 4:3:30:VAL:CB   | 4:7:79:TRP:C[1_554]    | 0.89                     | 1.31              |
| 4:3:194:THR:C   | 4:7:209:VAL:CB[1_554]  | 0.90                     | 1.30              |
| 4:3:337:TYR:CZ  | 4:7:86:TRP:CZ3[1_554]  | 0.90                     | 1.30              |
| 4:5:274:ILE:C   | 4:9:162:ASN:C[1_554]   | 0.90                     | 1.30              |
| 4:3:162:ASN:ND2 | 4:7:175:ILE:CD1[1_554] | 0.90                     | 1.30              |
| 4:5:327:ILE:CB  | 4:9:149:THR:N[1_554]   | 0.90                     | 1.30              |
| 4:5:327:ILE:CD1 | 4:9:149:THR:CG2[1_554] | 0.90                     | 1.30              |
| 4:5:110:LEU:O   | 4:V:192:ILE:C[1_554]   | 0.90                     | 1.30              |
| 4:4:335:ARG:NH1 | 4:8:106:THR:CG2[1_554] | 0.90                     | 1.30              |
| 4:3:199:SER:CA  | 4:7:206:ARG:CA[1_554]  | 0.90                     | 1.30              |
| 4:4:318:THR:N   | 4:8:150:GLY:N[1_554]   | 0.90                     | 1.30              |
| 4:4:255:PHE:C   | 4:8:302:GLY:C[1_554]   | 0.90                     | 1.30              |
| 4:4:218:TYR:CA  | 4:8:336:LYS:O[1_554]   | 0.90                     | 1.30              |
| 4:3:222:ASP:CA  | 4:7:331:ALA:C[1_554]   | 0.90                     | 1.30              |
| 4:4:213:LYS:CE  | 4:8:15:GLY:N[1_554]    | 0.90                     | 1.30              |
| 4:4:112:PRO:CG  | 4:9:193:LEU:CD1[1_554] | 0.90                     | 1.30              |
| 4:3:151:ILE:CD1 | 4:7:172:PRO:N[1_554]   | 0.90                     | 1.30              |
| 4:5:194:THR:CA  | 4:9:209:VAL:CG1[1_554] | 0.90                     | 1.30              |
| 4:3:214:GLU:CG  | 4:7:33:SER:OG[1_554]   | 0.90                     | 1.30              |
| 4:5:334:GLU:OE1 | 4:9:133:TYR:C[1_554]   | 0.90                     | 1.30              |
| 4:3:333:PRO:CB  | 4:7:104:LEU:C[1_554]   | 0.90                     | 1.30              |
| 4:5:316:GLU:OE1 | 4:9:297:ASN:CG[1_554]  | 0.90                     | 1.30              |
| 4:5:221:LEU:O   | 4:9:331:ALA:O[1_554]   | 0.90                     | 1.30              |
| 4:3:276:GLU:OE2 | 4:7:278:THR:CA[1_554]  | 0.90                     | 1.30              |
| 4:4:367:PRO:CA  | 4:9:234:SER:O[1_554]   | 0.90                     | 1.30              |
| 4:5:264:PRO:N   | 4:9:274:ILE:CD1[1_554] | 0.91                     | 1.29              |
| 4:5:279:TYR:CD1 | 4:9:293:LEU:CD2[1_554] | 0.91                     | 1.29              |
| 4:3:198:TYR:CB  | 4:7:208:ILE:N[1_554]   | 0.91                     | 1.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:327:ILE:CB  | 4:7:148:THR:O[1_554]   | 0.91                     | 1.29              |
| 4:5:370:VAL:CA  | 4:V:231:ALA:CA[1_554]  | 0.91                     | 1.29              |
| 4:4:185:LEU:C   | 4:8:157:ASP:O[1_554]   | 0.91                     | 1.29              |
| 4:5:27:PRO:C    | 4:9:122:ILE:CG2[1_554] | 0.91                     | 1.29              |
| 4:4:261:LEU:CB  | 4:8:154:ASP:O[1_554]   | 0.91                     | 1.29              |
| 4:5:214:GLU:C   | 4:9:16:LEU:CB[1_554]   | 0.91                     | 1.29              |
| 4:5:221:LEU:CG  | 4:9:332:PRO:CB[1_554]  | 0.91                     | 1.29              |
| 4:3:139:VAL:C   | 4:7:371:HIS:NE2[1_554] | 0.91                     | 1.29              |
| 4:5:28:ARG:NE   | 4:9:126:THR:CA[1_554]  | 0.91                     | 1.29              |
| 4:4:371:HIS:CA  | 4:9:230:ALA:CB[1_554]  | 0.91                     | 1.29              |
| 4:4:254:ARG:NH2 | 4:8:337:TYR:OH[1_554]  | 0.91                     | 1.29              |
| 4:4:220:ALA:CA  | 4:8:335:ARG:CA[1_554]  | 0.91                     | 1.29              |
| 4:3:284:LYS:C   | 4:8:268:GLY:O[1_554]   | 0.91                     | 1.29              |
| 4:5:190:MET:O   | 4:9:186:THR:CG2[1_554] | 0.91                     | 1.29              |
| 4:5:173:HIS:N   | 4:V:266:PHE:O[1_554]   | 0.91                     | 1.29              |
| 4:3:25:ASP:O    | 4:7:120:THR:O[1_554]   | 0.91                     | 1.29              |
| 4:4:372:ARG:CA  | 4:9:227:MET:CA[1_554]  | 0.91                     | 1.29              |
| 4:5:288:ASP:CB  | 4:W:62:ARG:O[1_554]    | 0.91                     | 1.29              |
| 4:4:340:TRP:CB  | 4:8:118:LYS:C[1_554]   | 0.91                     | 1.29              |
| 4:5:26:ALA:CA   | 4:9:123:MET:CA[1_554]  | 0.91                     | 1.29              |
| 4:5:304:THR:CB  | 4:9:137:GLN:CB[1_554]  | 0.91                     | 1.29              |
| 4:2:110:LEU:N   | 4:7:192:ILE:CA[1_554]  | 0.91                     | 1.29              |
| 4:3:253:GLU:CD  | 4:7:214:GLU:CG[1_554]  | 0.91                     | 1.29              |
| 4:4:116:ARG:CB  | 4:9:252:ASN:OD1[1_554] | 0.91                     | 1.29              |
| 4:3:256:ARG:C   | 4:7:303:THR:CA[1_554]  | 0.91                     | 1.29              |
| 4:5:336:LYS:CB  | 4:9:12:ASN:ND2[1_554]  | 0.91                     | 1.29              |
| 4:5:110:LEU:CD2 | 4:V:191:LYS:CE[1_554]  | 0.91                     | 1.29              |
| 4:5:210:ARG:NH2 | 4:9:34:ILE:N[1_554]    | 0.91                     | 1.29              |
| 4:5:161:HIS:CA  | 4:9:110:LEU:CG[1_554]  | 0.91                     | 1.29              |
| 4:5:249:THR:C   | 4:9:211:ASP:OD2[1_554] | 0.91                     | 1.29              |
| 4:4:198:TYR:CB  | 4:8:208:ILE:N[1_554]   | 0.91                     | 1.29              |
| 4:4:266:PHE:CD1 | 4:8:261:LEU:CD1[1_554] | 0.91                     | 1.29              |
| 4:3:300:SER:CB  | 4:7:107:GLU:CD[1_554]  | 0.91                     | 1.29              |
| 4:4:41:GLN:CG   | 4:7:224:GLU:CD[1_554]  | 0.91                     | 1.29              |
| 4:2:116:ARG:CG  | 4:7:252:ASN:OD1[1_554] | 0.91                     | 1.29              |
| 4:4:17:VAL:O    | 4:8:79:TRP:CB[1_554]   | 0.92                     | 1.28              |
| 4:5:143:TYR:CB  | 4:9:372:ARG:CA[1_554]  | 0.92                     | 1.28              |
| 4:4:17:VAL:C    | 4:8:79:TRP:CD1[1_554]  | 0.92                     | 1.28              |
| 4:2:286:ASP:CA  | 4:7:270:GLU:OE2[1_554] | 0.92                     | 1.28              |
| 4:5:145:SER:CA  | 4:9:372:ARG:NH2[1_554] | 0.92                     | 1.28              |
| 4:4:137:GLN:O   | 4:8:113:LYS:CA[1_554]  | 0.92                     | 1.28              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:259:GLU:OE2 | 4:9:309:ILE:CB[1_554]  | 0.92                     | 1.28              |
| 4:5:341:ILE:CA  | 4:9:120:THR:OG1[1_554] | 0.92                     | 1.28              |
| 4:3:370:VAL:CA  | 4:8:230:ALA:C[1_554]   | 0.92                     | 1.28              |
| 4:4:305:MET:CA  | 4:8:11:ASP:OD1[1_554]  | 0.92                     | 1.28              |
| 4:4:256:ARG:O   | 4:8:303:THR:CB[1_554]  | 0.92                     | 1.28              |
| 4:5:335:ARG:N   | 4:9:105:LEU:O[1_554]   | 0.92                     | 1.28              |
| 4:5:316:GLU:CB  | 4:9:151:ILE:O[1_554]   | 0.92                     | 1.28              |
| 4:3:332:PRO:N   | 4:7:135:ALA:N[1_554]   | 0.92                     | 1.28              |
| 4:5:186:THR:CB  | 4:9:183:ARG:NE[1_554]  | 0.92                     | 1.28              |
| 4:3:140:LEU:C   | 4:7:371:HIS:ND1[1_554] | 0.92                     | 1.28              |
| 4:4:26:ALA:CA   | 4:8:122:ILE:C[1_554]   | 0.92                     | 1.28              |
| 4:4:110:LEU:O   | 4:9:192:ILE:C[1_554]   | 0.92                     | 1.28              |
| 4:4:299:MET:CE  | 4:8:136:ILE:O[1_554]   | 0.92                     | 1.28              |
| 4:5:259:GLU:OE2 | 4:9:309:ILE:CG1[1_554] | 0.92                     | 1.28              |
| 4:3:193:LEU:CA  | 4:7:210:ARG:CB[1_554]  | 0.92                     | 1.28              |
| 4:5:249:THR:O   | 4:9:211:ASP:CG[1_554]  | 0.92                     | 1.28              |
| 4:5:204:ALA:CA  | 4:9:62:ARG:CB[1_554]   | 0.92                     | 1.28              |
| 4:4:59:GLN:CG   | 4:8:68:LYS:CG[1_554]   | 0.92                     | 1.28              |
| 4:3:214:GLU:C   | 4:7:16:LEU:C[1_554]    | 0.92                     | 1.28              |
| 4:4:145:SER:OG  | 4:8:372:ARG:NE[1_554]  | 0.93                     | 1.27              |
| 4:4:286:ASP:N   | 4:9:270:GLU:OE2[1_554] | 0.93                     | 1.27              |
| 4:5:370:VAL:N   | 4:V:231:ALA:CA[1_554]  | 0.93                     | 1.27              |
| 4:4:341:ILE:CG1 | 4:8:120:THR:CA[1_554]  | 0.93                     | 1.27              |
| 4:4:193:LEU:C   | 4:8:210:ARG:N[1_554]   | 0.93                     | 1.27              |
| 4:5:140:LEU:N   | 4:9:371:HIS:CE1[1_554] | 0.93                     | 1.27              |
| 4:4:173:HIS:C   | 4:9:267:ILE:CA[1_554]  | 0.93                     | 1.27              |
| 4:3:337:TYR:CE2 | 4:7:86:TRP:CZ3[1_554]  | 0.93                     | 1.27              |
| 4:5:308:GLY:N   | 4:9:338:SER:N[1_554]   | 0.93                     | 1.27              |
| 4:4:41:GLN:CB   | 4:7:224:GLU:CD[1_554]  | 0.93                     | 1.27              |
| 4:4:331:ALA:CA  | 4:8:135:ALA:CB[1_554]  | 0.93                     | 1.27              |
| 4:5:208:ILE:CB  | 4:9:59:GLN:CG[1_554]   | 0.93                     | 1.27              |
| 4:4:151:ILE:CG2 | 4:8:170:ALA:O[1_554]   | 0.93                     | 1.27              |
| 4:3:227:MET:CE  | 4:7:306:TYR:N[1_554]   | 0.93                     | 1.27              |
| 4:3:318:THR:CB  | 4:7:149:THR:O[1_554]   | 0.93                     | 1.27              |
| 4:4:276:GLU:CD  | 4:8:278:THR:C[1_554]   | 0.93                     | 1.27              |
| 4:5:337:TYR:CZ  | 4:9:86:TRP:CZ2[1_554]  | 0.93                     | 1.27              |
| 4:4:326:LYS:CA  | 4:8:167:GLU:OE1[1_554] | 0.93                     | 1.27              |
| 4:5:75:ILE:CA   | 4:V:197:GLY:CA[1_554]  | 0.93                     | 1.27              |
| 4:5:274:ILE:C   | 4:9:162:ASN:CA[1_554]  | 0.93                     | 1.27              |
| 4:3:218:TYR:CE2 | 4:7:337:TYR:CD2[1_554] | 0.93                     | 1.27              |
| 4:3:215:LYS:CB  | 4:7:31:PHE:N[1_554]    | 0.93                     | 1.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:262:PHE:CA  | 4:9:153:LEU:CD1[1_554] | 0.93                     | 1.27              |
| 4:5:273:GLY:C   | 4:9:162:ASN:OD1[1_554] | 0.93                     | 1.27              |
| 4:5:110:LEU:CD1 | 4:V:191:LYS:CD[1_554]  | 0.93                     | 1.27              |
| 4:3:314:GLN:CA  | 4:7:142:LEU:CB[1_554]  | 0.93                     | 1.27              |
| 4:4:199:SER:CB  | 4:8:206:ARG:N[1_554]   | 0.93                     | 1.27              |
| 4:3:110:LEU:CB  | 4:8:192:ILE:N[1_554]   | 0.93                     | 1.27              |
| 4:5:143:TYR:N   | 4:9:372:ARG:CB[1_554]  | 0.93                     | 1.27              |
| 4:5:17:VAL:C    | 4:9:79:TRP:CG[1_554]   | 0.93                     | 1.27              |
| 4:4:315:LYS:CE  | 4:8:147:ARG:CZ[1_554]  | 0.93                     | 1.27              |
| 4:3:312:ARG:NE  | 4:7:299:MET:CA[1_554]  | 0.93                     | 1.27              |
| 4:5:192:ILE:CG1 | 4:9:213:LYS:CD[1_554]  | 0.93                     | 1.27              |
| 4:3:18:LYS:CD   | 4:7:79:TRP:CE2[1_554]  | 0.93                     | 1.27              |
| 4:4:173:HIS:CE1 | 4:9:266:PHE:N[1_554]   | 0.94                     | 1.26              |
| 4:3:153:LEU:C   | 4:7:109:PRO:O[1_554]   | 0.94                     | 1.26              |
| 4:5:59:GLN:CG   | 4:9:68:LYS:CG[1_554]   | 0.94                     | 1.26              |
| 4:3:339:VAL:CG1 | 4:7:114:ALA:C[1_554]   | 0.94                     | 1.26              |
| 4:5:340:TRP:CH2 | 4:9:121:GLN:C[1_554]   | 0.94                     | 1.26              |
| 4:5:253:GLU:CD  | 4:9:214:GLU:CA[1_554]  | 0.94                     | 1.26              |
| 4:4:75:ILE:CA   | 4:9:197:GLY:C[1_554]   | 0.94                     | 1.26              |
| 4:5:279:TYR:C   | 4:9:285:CYS:SG[1_554]  | 0.94                     | 1.26              |
| 4:4:319:ALA:C   | 4:8:292:ASP:O[1_554]   | 0.94                     | 1.26              |
| 4:4:265:SER:CA  | 4:8:261:LEU:O[1_554]   | 0.94                     | 1.26              |
| 4:5:299:MET:CA  | 4:9:136:ILE:CB[1_554]  | 0.94                     | 1.26              |
| 4:2:284:LYS:O   | 4:7:268:GLY:O[1_554]   | 0.94                     | 1.26              |
| 4:5:227:MET:SD  | 4:9:306:TYR:C[1_554]   | 0.94                     | 1.26              |
| 4:3:367:PRO:CA  | 4:8:234:SER:O[1_554]   | 0.94                     | 1.26              |
| 4:4:314:GLN:C   | 4:8:142:LEU:CG[1_554]  | 0.94                     | 1.26              |
| 4:4:18:LYS:CE   | 4:8:79:TRP:CZ2[1_554]  | 0.94                     | 1.26              |
| 4:4:75:ILE:CG2  | 4:9:198:TYR:CD2[1_554] | 0.94                     | 1.26              |
| 4:3:110:LEU:CD1 | 4:8:191:LYS:CG[1_554]  | 0.94                     | 1.26              |
| 4:4:340:TRP:CZ2 | 4:8:121:GLN:CG[1_554]  | 0.94                     | 1.26              |
| 4:4:193:LEU:CA  | 4:8:210:ARG:CA[1_554]  | 0.94                     | 1.26              |
| 4:5:180:LEU:CG  | 4:9:178:LEU:O[1_554]   | 0.94                     | 1.26              |
| 4:3:196:ARG:CG  | 4:7:211:ASP:CA[1_554]  | 0.94                     | 1.26              |
| 4:5:253:GLU:OE1 | 4:9:214:GLU:N[1_554]   | 0.94                     | 1.26              |
| 4:2:74:GLY:C    | 4:7:197:GLY:C[1_554]   | 0.94                     | 1.26              |
| 4:4:137:GLN:CA  | 4:8:113:LYS:N[1_554]   | 0.94                     | 1.26              |
| 4:3:198:TYR:CB  | 4:7:207:GLU:C[1_554]   | 0.94                     | 1.26              |
| 4:3:255:PHE:CG  | 4:7:305:MET:CG[1_554]  | 0.94                     | 1.26              |
| 4:4:208:ILE:CA  | 4:8:59:GLN:NE2[1_554]  | 0.94                     | 1.26              |
| 4:3:340:TRP:C   | 4:7:117:GLU:O[1_554]   | 0.94                     | 1.26              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:282:ILE:CG1 | 4:8:171:LEU:CD2[1_554] | 0.94                     | 1.26              |
| 4:2:175:ILE:CD1 | 4:7:191:LYS:NZ[1_554]  | 0.94                     | 1.26              |
| 4:5:321:ALA:N   | 4:9:293:LEU:N[1_554]   | 0.94                     | 1.26              |
| 4:5:208:ILE:CB  | 4:9:59:GLN:CD[1_554]   | 0.94                     | 1.26              |
| 4:4:191:LYS:CA  | 4:8:186:THR:C[1_554]   | 0.94                     | 1.26              |
| 4:5:219:VAL:CG2 | 4:9:301:GLY:N[1_554]   | 0.95                     | 1.25              |
| 4:5:254:ARG:NH2 | 4:9:336:LYS:NZ[1_554]  | 0.95                     | 1.25              |
| 4:3:345:ILE:N   | 4:7:367:PRO:CD[1_554]  | 0.95                     | 1.25              |
| 4:5:273:GLY:CA  | 4:9:162:ASN:OD1[1_554] | 0.95                     | 1.25              |
| 4:3:18:LYS:CE   | 4:7:79:TRP:CE2[1_554]  | 0.95                     | 1.25              |
| 4:4:204:ALA:CB  | 4:8:62:ARG:C[1_554]    | 0.95                     | 1.25              |
| 4:3:154:ASP:OD2 | 4:7:112:PRO:N[1_554]   | 0.95                     | 1.25              |
| 4:4:117:GLU:C   | 4:9:237:GLU:CG[1_554]  | 0.95                     | 1.25              |
| 4:3:223:PHE:CA  | 4:7:335:ARG:NE[1_554]  | 0.95                     | 1.25              |
| 4:3:110:LEU:C   | 4:8:192:ILE:C[1_554]   | 0.95                     | 1.25              |
| 4:3:137:GLN:C   | 4:7:113:LYS:N[1_554]   | 0.95                     | 1.25              |
| 4:5:56:ASP:CB   | 4:9:37:ARG:NH1[1_554]  | 0.95                     | 1.25              |
| 4:3:264:PRO:N   | 4:7:274:ILE:CD1[1_554] | 0.95                     | 1.25              |
| 4:5:26:ALA:C    | 4:9:123:MET:N[1_554]   | 0.95                     | 1.25              |
| 4:5:334:GLU:N   | 4:9:104:LEU:C[1_554]   | 0.95                     | 1.25              |
| 4:2:111:ASN:N   | 4:7:192:ILE:O[1_554]   | 0.95                     | 1.25              |
| 4:5:187:ASP:C   | 4:9:183:ARG:C[1_554]   | 0.95                     | 1.25              |
| 4:3:260:THR:N   | 4:7:155:SER:OG[1_554]  | 0.95                     | 1.25              |
| 4:4:166:TYR:OH  | 4:V:39:ARG:O[1_554]    | 0.95                     | 1.25              |
| 4:4:193:LEU:CB  | 4:8:210:ARG:CB[1_554]  | 0.95                     | 1.25              |
| 4:4:157:ASP:OD1 | 4:8:72:GLU:N[1_554]    | 0.95                     | 1.25              |
| 4:4:270:GLU:CB  | 4:8:272:ALA:CA[1_554]  | 0.95                     | 1.25              |
| 4:5:327:ILE:CD1 | 4:9:149:THR:CB[1_554]  | 0.95                     | 1.25              |
| 4:4:263:GLN:C   | 4:8:274:ILE:CD1[1_554] | 0.95                     | 1.25              |
| 4:3:310:ALA:CB  | 4:7:140:LEU:CB[1_554]  | 0.95                     | 1.25              |
| 4:5:137:GLN:CG  | 4:9:112:PRO:C[1_554]   | 0.95                     | 1.25              |
| 4:5:41:GLN:CG   | 4:8:224:GLU:OE2[1_554] | 0.95                     | 1.25              |
| 4:4:339:VAL:CG1 | 4:8:115:ASN:N[1_554]   | 0.95                     | 1.25              |
| 4:3:315:LYS:CE  | 4:7:147:ARG:CZ[1_554]  | 0.95                     | 1.25              |
| 4:4:294:TYR:OH  | 4:8:289:ILE:CD1[1_554] | 0.96                     | 1.24              |
| 4:3:161:HIS:O   | 4:7:110:LEU:CG[1_554]  | 0.96                     | 1.24              |
| 4:3:118:LYS:N   | 4:8:237:GLU:OE1[1_554] | 0.96                     | 1.24              |
| 4:4:258:PRO:CA  | 4:8:155:SER:O[1_554]   | 0.96                     | 1.24              |
| 4:3:259:GLU:CG  | 4:7:304:THR:CB[1_554]  | 0.96                     | 1.24              |
| 4:4:173:HIS:CE1 | 4:9:265:SER:C[1_554]   | 0.96                     | 1.24              |
| 4:5:157:ASP:C   | 4:9:72:GLU:O[1_554]    | 0.96                     | 1.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:159:VAL:C   | 4:7:177:ARG:NH1[1_554] | 0.96                     | 1.24              |
| 4:5:186:THR:C   | 4:9:183:ARG:CB[1_554]  | 0.96                     | 1.24              |
| 4:4:311:ASP:OD2 | 4:8:144:ALA:CB[1_554]  | 0.96                     | 1.24              |
| 4:5:294:TYR:C   | 4:9:166:TYR:O[1_554]   | 0.96                     | 1.24              |
| 4:4:30:VAL:O    | 4:8:80:ASP:C[1_554]    | 0.96                     | 1.24              |
| 4:4:286:ASP:CA  | 4:9:270:GLU:OE1[1_554] | 0.96                     | 1.24              |
| 4:5:174:ALA:O   | 4:9:173:HIS:CA[1_554]  | 0.96                     | 1.24              |
| 4:5:110:LEU:O   | 4:V:192:ILE:CA[1_554]  | 0.96                     | 1.24              |
| 4:4:327:ILE:CG2 | 4:8:148:THR:O[1_554]   | 0.96                     | 1.24              |
| 4:5:196:ARG:CA  | 4:9:212:ILE:CB[1_554]  | 0.96                     | 1.24              |
| 4:4:278:THR:CG2 | 4:8:164:PRO:O[1_554]   | 0.96                     | 1.24              |
| 4:5:282:ILE:CG1 | 4:9:171:LEU:CG[1_554]  | 0.97                     | 1.23              |
| 4:5:154:ASP:N   | 4:9:109:PRO:CA[1_554]  | 0.97                     | 1.23              |
| 4:1:291:LYS:N   | 4:7:64:ILE:CG2[1_554]  | 0.97                     | 1.23              |
| 4:3:16:LEU:CA   | 4:7:77:THR:O[1_554]    | 0.97                     | 1.23              |
| 4:5:262:PHE:CA  | 4:9:153:LEU:CG[1_554]  | 0.97                     | 1.23              |
| 4:3:274:ILE:O   | 4:7:162:ASN:O[1_554]   | 0.97                     | 1.23              |
| 4:3:270:GLU:CA  | 4:7:272:ALA:CA[1_554]  | 0.97                     | 1.23              |
| 4:4:255:PHE:CE1 | 4:8:305:MET:CB[1_554]  | 0.97                     | 1.23              |
| 4:5:196:ARG:CG  | 4:9:212:ILE:CA[1_554]  | 0.97                     | 1.23              |
| 4:4:314:GLN:OE1 | 4:8:147:ARG:C[1_554]   | 0.97                     | 1.23              |
| 4:5:340:TRP:CZ2 | 4:9:121:GLN:C[1_554]   | 0.97                     | 1.23              |
| 4:2:372:ARG:CA  | 4:7:226:GLU:O[1_554]   | 0.97                     | 1.23              |
| 4:5:141:SER:C   | 4:9:116:ARG:NH1[1_554] | 0.97                     | 1.23              |
| 4:4:41:GLN:CB   | 4:7:224:GLU:OE2[1_554] | 0.97                     | 1.23              |
| 4:3:337:TYR:CA  | 4:7:119:MET:CB[1_554]  | 0.97                     | 1.23              |
| 4:4:288:ASP:O   | 4:V:64:ILE:CA[1_554]   | 0.97                     | 1.23              |
| 4:3:372:ARG:CB  | 4:8:227:MET:CA[1_554]  | 0.97                     | 1.23              |
| 4:5:154:ASP:OD2 | 4:9:111:ASN:CA[1_554]  | 0.97                     | 1.23              |
| 4:4:341:ILE:CG2 | 4:8:120:THR:CG2[1_554] | 0.97                     | 1.23              |
| 4:5:28:ARG:NH2  | 4:9:125:GLU:O[1_554]   | 0.97                     | 1.23              |
| 4:4:270:GLU:CA  | 4:8:272:ALA:C[1_554]   | 0.97                     | 1.23              |
| 4:4:317:ILE:N   | 4:8:150:GLY:C[1_554]   | 0.97                     | 1.23              |
| 4:4:214:GLU:N   | 4:8:16:LEU:CA[1_554]   | 0.97                     | 1.23              |
| 4:3:109:PRO:CB  | 4:8:195:GLU:OE2[1_554] | 0.97                     | 1.23              |
| 4:5:214:GLU:CA  | 4:9:16:LEU:CA[1_554]   | 0.97                     | 1.23              |
| 4:5:29:ALA:CA   | 4:9:83:GLU:OE1[1_554]  | 0.97                     | 1.23              |
| 4:5:266:PHE:N   | 4:9:261:LEU:CA[1_554]  | 0.97                     | 1.23              |
| 4:4:16:LEU:CA   | 4:8:77:THR:C[1_554]    | 0.97                     | 1.23              |
| 4:5:299:MET:CB  | 4:9:136:ILE:C[1_554]   | 0.97                     | 1.23              |
| 4:4:161:HIS:CA  | 4:8:110:LEU:CD1[1_554] | 0.97                     | 1.23              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:227:MET:CA  | 4:9:307:PRO:CB[1_554]  | 0.97                     | 1.23              |
| 4:5:207:GLU:OE1 | 4:9:67:LEU:CD2[1_554]  | 0.97                     | 1.23              |
| 4:3:256:ARG:NH1 | 4:7:306:TYR:CE1[1_554] | 0.97                     | 1.23              |
| 4:3:220:ALA:CB  | 4:7:335:ARG:CA[1_554]  | 0.97                     | 1.23              |
| 4:4:137:GLN:C   | 4:8:113:LYS:N[1_554]   | 0.98                     | 1.22              |
| 4:5:183:ARG:NE  | 4:9:72:GLU:CD[1_554]   | 0.98                     | 1.22              |
| 4:4:276:GLU:OE2 | 4:8:278:THR:CA[1_554]  | 0.98                     | 1.22              |
| 4:4:172:PRO:C   | 4:9:266:PHE:O[1_554]   | 0.98                     | 1.22              |
| 4:4:310:ALA:O   | 4:8:142:LEU:N[1_554]   | 0.98                     | 1.22              |
| 4:4:214:GLU:CA  | 4:8:16:LEU:CA[1_554]   | 0.98                     | 1.22              |
| 4:3:172:PRO:CG  | 4:8:266:PHE:CG[1_554]  | 0.98                     | 1.22              |
| 4:3:318:THR:CA  | 4:7:149:THR:O[1_554]   | 0.98                     | 1.22              |
| 4:3:258:PRO:O   | 4:7:155:SER:N[1_554]   | 0.98                     | 1.22              |
| 4:5:204:ALA:CA  | 4:9:62:ARG:CG[1_554]   | 0.98                     | 1.22              |
| 4:2:72:GLU:O    | 4:7:199:SER:N[1_554]   | 0.98                     | 1.22              |
| 4:5:220:ALA:CA  | 4:9:335:ARG:CG[1_554]  | 0.98                     | 1.22              |
| 4:5:283:MET:CB  | 4:9:285:CYS:O[1_554]   | 0.98                     | 1.22              |
| 4:5:115:ASN:CB  | 4:V:196:ARG:NE[1_554]  | 0.98                     | 1.22              |
| 4:5:288:ASP:CA  | 4:W:62:ARG:O[1_554]    | 0.98                     | 1.22              |
| 4:5:255:PHE:CD1 | 4:9:305:MET:C[1_554]   | 0.98                     | 1.22              |
| 4:5:223:PHE:CD1 | 4:9:304:THR:O[1_554]   | 0.98                     | 1.22              |
| 4:3:253:GLU:CG  | 4:7:214:GLU:CG[1_554]  | 0.98                     | 1.22              |
| 4:4:337:TYR:N   | 4:8:119:MET:CE[1_554]  | 0.98                     | 1.22              |
| 4:5:299:MET:O   | 4:9:136:ILE:N[1_554]   | 0.98                     | 1.22              |
| 4:4:15:GLY:N    | 4:8:77:THR:OG1[1_554]  | 0.98                     | 1.22              |
| 4:4:74:GLY:O    | 4:9:197:GLY:CA[1_554]  | 0.98                     | 1.22              |
| 4:4:31:PHE:N    | 4:8:80:ASP:N[1_554]    | 0.98                     | 1.22              |
| 4:4:271:SER:O   | 4:8:277:THR:OG1[1_554] | 0.98                     | 1.22              |
| 4:5:278:THR:CG2 | 4:9:164:PRO:C[1_554]   | 0.98                     | 1.22              |
| 4:5:319:ALA:CB  | 4:9:296:ASN:N[1_554]   | 0.98                     | 1.22              |
| 4:4:191:LYS:CD  | 4:8:185:LEU:O[1_554]   | 0.98                     | 1.22              |
| 4:3:340:TRP:CD1 | 4:7:118:LYS:CD[1_554]  | 0.98                     | 1.22              |
| 4:4:75:ILE:N    | 4:9:198:TYR:N[1_554]   | 0.98                     | 1.22              |
| 4:2:115:ASN:CA  | 4:7:249:THR:C[1_554]   | 0.98                     | 1.22              |
| 4:3:154:ASP:OD1 | 4:7:111:ASN:CB[1_554]  | 0.98                     | 1.22              |
| 4:5:348:SER:CB  | 4:9:362:TYR:O[1_554]   | 0.98                     | 1.22              |
| 4:5:158:GLY:O   | 4:9:177:ARG:NH2[1_554] | 0.99                     | 1.21              |
| 4:5:214:GLU:OE2 | 4:9:33:SER:OG[1_554]   | 0.99                     | 1.21              |
| 4:2:173:HIS:CE1 | 4:7:266:PHE:N[1_554]   | 0.99                     | 1.21              |
| 4:4:145:SER:CB  | 4:8:372:ARG:NH2[1_554] | 0.99                     | 1.21              |
| 4:3:250:ILE:CD1 | 4:7:210:ARG:NH2[1_554] | 0.99                     | 1.21              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:18:LYS:CD   | 4:7:79:TRP:CD2[1_554]  | 0.99                     | 1.21              |
| 4:5:312:ARG:CD  | 4:9:299:MET:N[1_554]   | 0.99                     | 1.21              |
| 4:5:115:ASN:N   | 4:V:196:ARG:NH2[1_554] | 0.99                     | 1.21              |
| 4:5:210:ARG:O   | 4:9:15:GLY:O[1_554]    | 0.99                     | 1.21              |
| 4:3:341:ILE:N   | 4:7:117:GLU:O[1_554]   | 0.99                     | 1.21              |
| 4:4:162:ASN:ND2 | 4:8:175:ILE:CD1[1_554] | 0.99                     | 1.21              |
| 4:3:222:ASP:CA  | 4:7:332:PRO:N[1_554]   | 0.99                     | 1.21              |
| 4:4:281:SER:C   | 4:8:173:HIS:NE2[1_554] | 0.99                     | 1.21              |
| 4:4:15:GLY:CA   | 4:8:77:THR:CG2[1_554]  | 0.99                     | 1.21              |
| 4:4:157:ASP:C   | 4:8:72:GLU:O[1_554]    | 0.99                     | 1.21              |
| 4:4:31:PHE:O    | 4:8:78:ASN:OD1[1_554]  | 0.99                     | 1.21              |
| 4:3:177:ARG:NH1 | 4:8:194:THR:CB[1_554]  | 0.99                     | 1.21              |
| 4:4:211:ASP:C   | 4:8:32:PRO:CA[1_554]   | 0.99                     | 1.21              |
| 4:5:256:ARG:CD  | 4:9:306:TYR:CD1[1_554] | 0.99                     | 1.21              |
| 4:4:282:ILE:CG1 | 4:8:171:LEU:CG[1_554]  | 0.99                     | 1.21              |
| 4:4:283:MET:CB  | 4:8:286:ASP:N[1_554]   | 0.99                     | 1.21              |
| 4:5:31:PHE:O    | 4:9:78:ASN:C[1_554]    | 0.99                     | 1.21              |
| 4:5:312:ARG:CA  | 4:9:298:VAL:CG1[1_554] | 0.99                     | 1.21              |
| 4:2:111:ASN:ND2 | 4:7:196:ARG:CG[1_554]  | 0.99                     | 1.21              |
| 4:5:218:TYR:CA  | 4:9:336:LYS:CA[1_554]  | 0.99                     | 1.21              |
| 4:3:191:LYS:CD  | 4:7:185:LEU:C[1_554]   | 0.99                     | 1.21              |
| 4:5:308:GLY:C   | 4:9:338:SER:CB[1_554]  | 0.99                     | 1.21              |
| 4:4:137:GLN:OE1 | 4:8:112:PRO:CB[1_554]  | 0.99                     | 1.21              |
| 4:2:368:SER:N   | 4:7:236:LEU:CA[1_554]  | 0.99                     | 1.21              |
| 4:4:25:ASP:C    | 4:8:124:PHE:N[1_554]   | 0.99                     | 1.21              |
| 4:3:180:LEU:CA  | 4:7:179:ASP:OD1[1_554] | 0.99                     | 1.21              |
| 4:5:166:TYR:CB  | 4:W:40:HIS:NE2[1_554]  | 0.99                     | 1.21              |
| 4:4:262:PHE:CG  | 4:8:153:LEU:O[1_554]   | 0.99                     | 1.21              |
| 4:5:196:ARG:NE  | 4:9:211:ASP:O[1_554]   | 0.99                     | 1.21              |
| 4:4:111:ASN:N   | 4:9:192:ILE:O[1_554]   | 0.99                     | 1.21              |
| 4:3:198:TYR:CG  | 4:7:208:ILE:N[1_554]   | 0.99                     | 1.21              |
| 4:5:180:LEU:CB  | 4:9:178:LEU:C[1_554]   | 1.00                     | 1.20              |
| 4:3:371:HIS:ND1 | 4:8:252:ASN:CA[1_554]  | 1.00                     | 1.20              |
| 4:4:157:ASP:OD1 | 4:8:72:GLU:CA[1_554]   | 1.00                     | 1.20              |
| 4:3:326:LYS:C   | 4:7:167:GLU:CB[1_554]  | 1.00                     | 1.20              |
| 4:2:109:PRO:CA  | 4:7:195:GLU:CD[1_554]  | 1.00                     | 1.20              |
| 4:5:271:SER:O   | 4:9:277:THR:OG1[1_554] | 1.00                     | 1.20              |
| 4:5:294:TYR:CG  | 4:9:166:TYR:CG[1_554]  | 1.00                     | 1.20              |
| 4:4:345:ILE:C   | 4:8:366:GLY:C[1_554]   | 1.00                     | 1.20              |
| 4:3:191:LYS:CD  | 4:7:185:LEU:O[1_554]   | 1.00                     | 1.20              |
| 4:5:210:ARG:CZ  | 4:9:33:SER:C[1_554]    | 1.00                     | 1.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:260:THR:N   | 4:7:155:SER:CB[1_554]  | 1.00                     | 1.20              |
| 4:3:220:ALA:CA  | 4:7:335:ARG:CA[1_554]  | 1.00                     | 1.20              |
| 4:4:18:LYS:CE   | 4:8:79:TRP:CE2[1_554]  | 1.00                     | 1.20              |
| 4:5:59:GLN:CB   | 4:9:68:LYS:CD[1_554]   | 1.00                     | 1.20              |
| 4:5:348:SER:N   | 4:9:366:GLY:CA[1_554]  | 1.00                     | 1.20              |
| 4:5:268:GLY:CA  | 4:9:264:PRO:CA[1_554]  | 1.00                     | 1.20              |
| 4:5:140:LEU:CA  | 4:9:371:HIS:ND1[1_554] | 1.00                     | 1.20              |
| 4:5:115:ASN:N   | 4:V:196:ARG:CZ[1_554]  | 1.00                     | 1.20              |
| 4:5:24:ASP:C    | 4:9:124:PHE:CB[1_554]  | 1.00                     | 1.20              |
| 4:3:320:LEU:CA  | 4:7:293:LEU:N[1_554]   | 1.00                     | 1.20              |
| 4:4:193:LEU:CB  | 4:8:210:ARG:CG[1_554]  | 1.00                     | 1.20              |
| 4:4:258:PRO:C   | 4:8:155:SER:O[1_554]   | 1.00                     | 1.20              |
| 4:4:314:GLN:CA  | 4:8:142:LEU:CB[1_554]  | 1.00                     | 1.20              |
| 4:5:348:SER:OG  | 4:9:362:TYR:O[1_554]   | 1.00                     | 1.20              |
| 4:4:267:ILE:CG1 | 4:8:180:LEU:CG[1_554]  | 1.00                     | 1.20              |
| 4:5:156:GLY:O   | 4:9:74:GLY:CA[1_554]   | 1.00                     | 1.20              |
| 4:5:334:GLU:CA  | 4:9:105:LEU:CA[1_554]  | 1.00                     | 1.20              |
| 4:3:288:ASP:O   | 4:9:64:ILE:CA[1_554]   | 1.00                     | 1.20              |
| 4:4:344:SER:N   | 4:8:367:PRO:CG[1_554]  | 1.01                     | 1.19              |
| 4:5:336:LYS:CD  | 4:9:12:ASN:OD1[1_554]  | 1.01                     | 1.19              |
| 4:5:199:SER:C   | 4:9:206:ARG:CA[1_554]  | 1.01                     | 1.19              |
| 4:5:221:LEU:O   | 4:9:331:ALA:C[1_554]   | 1.01                     | 1.19              |
| 4:4:188:TYR:O   | 4:8:182:GLY:O[1_554]   | 1.01                     | 1.19              |
| 4:3:218:TYR:CB  | 4:7:336:LYS:O[1_554]   | 1.01                     | 1.19              |
| 4:3:281:SER:C   | 4:7:173:HIS:NE2[1_554] | 1.01                     | 1.19              |
| 4:3:370:VAL:C   | 4:8:230:ALA:C[1_554]   | 1.01                     | 1.19              |
| 4:4:25:ASP:CA   | 4:8:124:PHE:CA[1_554]  | 1.01                     | 1.19              |
| 4:5:223:PHE:CE2 | 4:9:304:THR:OG1[1_554] | 1.01                     | 1.19              |
| 4:2:357:ILE:CG1 | 4:7:232:SER:N[1_554]   | 1.01                     | 1.19              |
| 4:3:195:GLU:CG  | 4:7:189:LEU:CD2[1_554] | 1.01                     | 1.19              |
| 4:4:333:PRO:CB  | 4:8:104:LEU:C[1_554]   | 1.01                     | 1.19              |
| 4:5:273:GLY:O   | 4:9:162:ASN:CB[1_554]  | 1.01                     | 1.19              |
| 4:3:114:ALA:CA  | 4:8:250:ILE:C[1_554]   | 1.01                     | 1.19              |
| 4:5:340:TRP:CZ3 | 4:9:120:THR:O[1_554]   | 1.01                     | 1.19              |
| 4:5:157:ASP:OD2 | 4:9:72:GLU:CA[1_554]   | 1.01                     | 1.19              |
| 4:4:114:ALA:CA  | 4:9:250:ILE:O[1_554]   | 1.01                     | 1.19              |
| 4:4:318:THR:CA  | 4:8:149:THR:O[1_554]   | 1.01                     | 1.19              |
| 4:3:180:LEU:CD2 | 4:7:178:LEU:O[1_554]   | 1.01                     | 1.19              |
| 4:4:211:ASP:O   | 4:8:32:PRO:N[1_554]    | 1.01                     | 1.19              |
| 4:3:326:LYS:N   | 4:7:167:GLU:CG[1_554]  | 1.01                     | 1.19              |
| 4:3:332:PRO:CD  | 4:7:134:VAL:O[1_554]   | 1.01                     | 1.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:281:SER:C   | 4:8:173:HIS:CD2[1_554] | 1.01                     | 1.19              |
| 4:5:113:LYS:CD  | 4:V:252:ASN:O[1_554]   | 1.01                     | 1.19              |
| 4:5:220:ALA:N   | 4:9:335:ARG:CG[1_554]  | 1.01                     | 1.19              |
| 4:5:178:LEU:CB  | 4:9:177:ARG:N[1_554]   | 1.01                     | 1.19              |
| 4:5:22:ALA:CA   | 4:9:362:TYR:OH[1_554]  | 1.01                     | 1.19              |
| 4:5:196:ARG:NH2 | 4:9:215:LYS:CG[1_554]  | 1.01                     | 1.19              |
| 4:4:198:TYR:CG  | 4:8:208:ILE:N[1_554]   | 1.01                     | 1.19              |
| 4:5:187:ASP:N   | 4:9:183:ARG:CB[1_554]  | 1.01                     | 1.19              |
| 4:5:75:ILE:CA   | 4:V:197:GLY:C[1_554]   | 1.01                     | 1.19              |
| 4:4:221:LEU:C   | 4:8:332:PRO:CD[1_554]  | 1.01                     | 1.19              |
| 4:5:215:LYS:CG  | 4:9:31:PHE:N[1_554]    | 1.01                     | 1.19              |
| 4:3:162:ASN:ND2 | 4:7:175:ILE:CG1[1_554] | 1.01                     | 1.19              |
| 4:5:20:GLY:O    | 4:9:121:GLN:NE2[1_554] | 1.01                     | 1.19              |
| 4:5:189:LEU:N   | 4:9:182:GLY:C[1_554]   | 1.01                     | 1.19              |
| 4:3:108:ALA:CB  | 4:8:195:GLU:O[1_554]   | 1.01                     | 1.19              |
| 4:2:291:LYS:N   | 4:8:64:ILE:CG2[1_554]  | 1.02                     | 1.18              |
| 4:4:272:ALA:C   | 4:8:277:THR:CG2[1_554] | 1.02                     | 1.18              |
| 4:3:258:PRO:C   | 4:7:155:SER:O[1_554]   | 1.02                     | 1.18              |
| 4:5:198:TYR:CD2 | 4:9:208:ILE:C[1_554]   | 1.02                     | 1.18              |
| 4:5:339:VAL:CA  | 4:9:116:ARG:CA[1_554]  | 1.02                     | 1.18              |
| 4:5:257:CYS:C   | 4:9:303:THR:CB[1_554]  | 1.02                     | 1.18              |
| 4:3:76:ILE:O    | 4:8:198:TYR:CE1[1_554] | 1.02                     | 1.18              |
| 4:5:262:PHE:C   | 4:9:153:LEU:CD1[1_554] | 1.02                     | 1.18              |
| 4:3:26:ALA:C    | 4:7:122:ILE:CA[1_554]  | 1.02                     | 1.18              |
| 4:4:262:PHE:CD1 | 4:8:153:LEU:C[1_554]   | 1.02                     | 1.18              |
| 4:4:305:MET:C   | 4:8:11:ASP:CG[1_554]   | 1.02                     | 1.18              |
| 4:3:75:ILE:CB   | 4:8:198:TYR:CB[1_554]  | 1.02                     | 1.18              |
| 4:5:181:ALA:O   | 4:9:158:GLY:C[1_554]   | 1.02                     | 1.18              |
| 4:4:32:PRO:CD   | 4:8:78:ASN:ND2[1_554]  | 1.02                     | 1.18              |
| 4:3:117:GLU:CB  | 4:8:237:GLU:CA[1_554]  | 1.02                     | 1.18              |
| 4:5:112:PRO:C   | 4:V:253:GLU:OE1[1_554] | 1.02                     | 1.18              |
| 4:3:265:SER:CA  | 4:7:261:LEU:O[1_554]   | 1.02                     | 1.18              |
| 4:4:187:ASP:N   | 4:8:183:ARG:CD[1_554]  | 1.02                     | 1.18              |
| 4:4:157:ASP:CG  | 4:8:72:GLU:CB[1_554]   | 1.02                     | 1.18              |
| 4:5:314:GLN:OE1 | 4:9:147:ARG:CG[1_554]  | 1.02                     | 1.18              |
| 4:3:175:ILE:CD1 | 4:8:191:LYS:NZ[1_554]  | 1.02                     | 1.18              |
| 4:4:183:ARG:CG  | 4:8:72:GLU:OE2[1_554]  | 1.02                     | 1.18              |
| 4:3:191:LYS:C   | 4:7:186:THR:CB[1_554]  | 1.02                     | 1.18              |
| 4:4:166:TYR:CD1 | 4:V:40:HIS:NE2[1_554]  | 1.02                     | 1.18              |
| 4:4:317:ILE:CB  | 4:8:150:GLY:O[1_554]   | 1.02                     | 1.18              |
| 4:4:208:ILE:CB  | 4:8:59:GLN:NE2[1_554]  | 1.02                     | 1.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:136:ILE:O   | 4:9:113:LYS:CB[1_554]  | 1.02                     | 1.18              |
| 4:5:60:SER:CB   | 4:9:37:ARG:CB[1_554]   | 1.02                     | 1.18              |
| 4:5:109:PRO:C   | 4:V:195:GLU:OE2[1_554] | 1.02                     | 1.18              |
| 4:5:310:ALA:CB  | 4:9:140:LEU:C[1_554]   | 1.02                     | 1.18              |
| 4:3:183:ARG:CG  | 4:7:72:GLU:OE2[1_554]  | 1.02                     | 1.18              |
| 4:4:276:GLU:C   | 4:8:281:SER:OG[1_554]  | 1.02                     | 1.18              |
| 4:3:297:ASN:ND2 | 4:7:170:ALA:CB[1_554]  | 1.02                     | 1.18              |
| 4:4:215:LYS:CG  | 4:8:31:PHE:CA[1_554]   | 1.02                     | 1.18              |
| 4:2:367:PRO:CA  | 4:7:236:LEU:N[1_554]   | 1.02                     | 1.18              |
| 4:4:304:THR:N   | 4:8:137:GLN:NE2[1_554] | 1.03                     | 1.17              |
| 4:4:274:ILE:CG1 | 4:8:161:HIS:CB[1_554]  | 1.03                     | 1.17              |
| 4:4:210:ARG:CB  | 4:8:69:TYR:CE2[1_554]  | 1.03                     | 1.17              |
| 4:5:276:GLU:C   | 4:9:281:SER:CB[1_554]  | 1.03                     | 1.17              |
| 4:5:208:ILE:N   | 4:9:59:GLN:NE2[1_554]  | 1.03                     | 1.17              |
| 4:1:326:LYS:CE  | 4:7:43:VAL:CG2[1_554]  | 1.03                     | 1.17              |
| 4:3:227:MET:SD  | 4:7:305:MET:O[1_554]   | 1.03                     | 1.17              |
| 4:5:24:ASP:O    | 4:9:124:PHE:CB[1_554]  | 1.03                     | 1.17              |
| 4:3:259:GLU:C   | 4:7:155:SER:CB[1_554]  | 1.03                     | 1.17              |
| 4:3:321:ALA:O   | 4:7:292:ASP:CG[1_554]  | 1.03                     | 1.17              |
| 4:5:327:ILE:CG1 | 4:9:149:THR:CA[1_554]  | 1.03                     | 1.17              |
| 4:5:162:ASN:CG  | 4:9:175:ILE:CG1[1_554] | 1.03                     | 1.17              |
| 4:4:370:VAL:CA  | 4:9:230:ALA:C[1_554]   | 1.03                     | 1.17              |
| 4:2:286:ASP:C   | 4:7:270:GLU:OE1[1_554] | 1.03                     | 1.17              |
| 4:4:108:ALA:CB  | 4:9:195:GLU:O[1_554]   | 1.03                     | 1.17              |
| 4:3:333:PRO:O   | 4:7:105:LEU:CB[1_554]  | 1.03                     | 1.17              |
| 4:5:16:LEU:N    | 4:9:77:THR:N[1_554]    | 1.03                     | 1.17              |
| 4:5:199:SER:CA  | 4:9:206:ARG:N[1_554]   | 1.03                     | 1.17              |
| 4:4:339:VAL:CA  | 4:8:116:ARG:N[1_554]   | 1.03                     | 1.17              |
| 4:5:177:ARG:NH1 | 4:V:194:THR:CB[1_554]  | 1.03                     | 1.17              |
| 4:3:267:ILE:CA  | 4:7:180:LEU:CD1[1_554] | 1.03                     | 1.17              |
| 4:3:265:SER:CB  | 4:7:261:LEU:O[1_554]   | 1.03                     | 1.17              |
| 4:2:109:PRO:CB  | 4:7:195:GLU:CD[1_554]  | 1.03                     | 1.17              |
| 4:5:264:PRO:CB  | 4:9:178:LEU:CD2[1_554] | 1.03                     | 1.17              |
| 4:2:116:ARG:O   | 4:7:237:GLU:CD[1_554]  | 1.03                     | 1.17              |
| 4:4:166:TYR:CZ  | 4:V:39:ARG:O[1_554]    | 1.03                     | 1.17              |
| 4:5:295:ALA:CA  | 4:9:167:GLU:O[1_554]   | 1.03                     | 1.17              |
| 4:3:218:TYR:CA  | 4:7:336:LYS:O[1_554]   | 1.03                     | 1.17              |
| 4:3:188:TYR:O   | 4:7:182:GLY:O[1_554]   | 1.04                     | 1.16              |
| 4:4:340:TRP:CB  | 4:8:118:LYS:CA[1_554]  | 1.04                     | 1.16              |
| 4:4:204:ALA:CB  | 4:8:62:ARG:CA[1_554]   | 1.04                     | 1.16              |
| 4:4:327:ILE:CD1 | 4:8:149:THR:OG1[1_554] | 1.04                     | 1.16              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:215:LYS:O   | 4:8:30:VAL:CG1[1_554]  | 1.04                     | 1.16              |
| 4:4:222:ASP:CA  | 4:8:331:ALA:CA[1_554]  | 1.04                     | 1.16              |
| 4:3:304:THR:OG1 | 4:7:107:GLU:O[1_554]   | 1.04                     | 1.16              |
| 4:5:137:GLN:N   | 4:9:113:LYS:N[1_554]   | 1.04                     | 1.16              |
| 4:2:370:VAL:O   | 4:7:230:ALA:CA[1_554]  | 1.04                     | 1.16              |
| 4:3:151:ILE:CD1 | 4:7:172:PRO:CD[1_554]  | 1.04                     | 1.16              |
| 4:3:332:PRO:CB  | 4:7:134:VAL:N[1_554]   | 1.04                     | 1.16              |
| 4:5:345:ILE:CA  | 4:9:369:ILE:CG2[1_554] | 1.04                     | 1.16              |
| 4:2:110:LEU:CB  | 4:7:192:ILE:N[1_554]   | 1.04                     | 1.16              |
| 4:3:154:ASP:CG  | 4:7:111:ASN:C[1_554]   | 1.04                     | 1.16              |
| 4:3:331:ALA:CA  | 4:7:135:ALA:CA[1_554]  | 1.04                     | 1.16              |
| 4:3:267:ILE:C   | 4:7:180:LEU:CD2[1_554] | 1.04                     | 1.16              |
| 4:5:342:GLY:O   | 4:9:367:PRO:O[1_554]   | 1.04                     | 1.16              |
| 4:3:205:GLU:CA  | 4:7:62:ARG:NE[1_554]   | 1.04                     | 1.16              |
| 4:5:266:PHE:CB  | 4:9:261:LEU:CG[1_554]  | 1.04                     | 1.16              |
| 4:4:316:GLU:C   | 4:8:151:ILE:N[1_554]   | 1.04                     | 1.16              |
| 4:5:319:ALA:O   | 4:9:294:TYR:C[1_554]   | 1.04                     | 1.16              |
| 4:3:112:PRO:CG  | 4:8:193:LEU:CD1[1_554] | 1.04                     | 1.16              |
| 4:5:156:GLY:CA  | 4:9:74:GLY:C[1_554]    | 1.04                     | 1.16              |
| 4:4:109:PRO:CB  | 4:9:195:GLU:OE2[1_554] | 1.04                     | 1.16              |
| 4:3:299:MET:CA  | 4:7:136:ILE:CG1[1_554] | 1.04                     | 1.16              |
| 4:5:164:PRO:N   | 4:9:172:PRO:CG[1_554]  | 1.04                     | 1.16              |
| 4:5:106:THR:CG2 | 4:9:114:ALA:CA[1_554]  | 1.04                     | 1.16              |
| 4:3:156:GLY:C   | 4:7:75:ILE:N[1_554]    | 1.04                     | 1.16              |
| 4:5:166:TYR:CG  | 4:W:40:HIS:NE2[1_554]  | 1.04                     | 1.16              |
| 4:3:339:VAL:N   | 4:7:116:ARG:N[1_554]   | 1.04                     | 1.16              |
| 4:3:154:ASP:CB  | 4:7:110:LEU:C[1_554]   | 1.05                     | 1.15              |
| 4:4:253:GLU:OE2 | 4:8:214:GLU:CB[1_554]  | 1.05                     | 1.15              |
| 4:4:335:ARG:CG  | 4:8:106:THR:C[1_554]   | 1.05                     | 1.15              |
| 4:4:333:PRO:C   | 4:8:105:LEU:CA[1_554]  | 1.05                     | 1.15              |
| 4:4:318:THR:CB  | 4:8:149:THR:O[1_554]   | 1.05                     | 1.15              |
| 4:4:145:SER:CB  | 4:8:372:ARG:CZ[1_554]  | 1.05                     | 1.15              |
| 4:4:205:GLU:N   | 4:8:62:ARG:CD[1_554]   | 1.05                     | 1.15              |
| 4:3:153:LEU:CA  | 4:7:109:PRO:O[1_554]   | 1.05                     | 1.15              |
| 4:3:310:ALA:C   | 4:7:141:SER:N[1_554]   | 1.05                     | 1.15              |
| 4:5:26:ALA:CA   | 4:9:123:MET:CB[1_554]  | 1.05                     | 1.15              |
| 4:5:278:THR:CG2 | 4:9:164:PRO:O[1_554]   | 1.05                     | 1.15              |
| 4:5:310:ALA:O   | 4:9:142:LEU:N[1_554]   | 1.05                     | 1.15              |
| 4:3:16:LEU:N    | 4:7:77:THR:CA[1_554]   | 1.05                     | 1.15              |
| 4:3:256:ARG:N   | 4:7:302:GLY:C[1_554]   | 1.05                     | 1.15              |
| 4:5:263:GLN:C   | 4:9:274:ILE:CG1[1_554] | 1.05                     | 1.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:192:ILE:CB  | 4:9:213:LYS:CD[1_554]  | 1.05                     | 1.15              |
| 4:5:193:LEU:CD2 | 4:9:210:ARG:CD[1_554]  | 1.05                     | 1.15              |
| 4:5:114:ALA:CB  | 4:V:251:GLY:N[1_554]   | 1.05                     | 1.15              |
| 4:4:283:MET:CG  | 4:8:286:ASP:CA[1_554]  | 1.05                     | 1.15              |
| 4:4:16:LEU:CA   | 4:8:78:ASN:N[1_554]    | 1.05                     | 1.15              |
| 4:4:318:THR:N   | 4:8:149:THR:C[1_554]   | 1.05                     | 1.15              |
| 4:4:113:LYS:O   | 4:9:252:ASN:N[1_554]   | 1.05                     | 1.15              |
| 4:4:327:ILE:CB  | 4:8:148:THR:C[1_554]   | 1.05                     | 1.15              |
| 4:3:329:ILE:CB  | 4:7:139:VAL:CG1[1_554] | 1.05                     | 1.15              |
| 4:4:172:PRO:CG  | 4:9:266:PHE:CG[1_554]  | 1.05                     | 1.15              |
| 4:2:370:VAL:O   | 4:7:230:ALA:CB[1_554]  | 1.05                     | 1.15              |
| 4:5:187:ASP:N   | 4:9:183:ARG:CG[1_554]  | 1.05                     | 1.15              |
| 4:5:339:VAL:C   | 4:9:116:ARG:CA[1_554]  | 1.05                     | 1.15              |
| 4:4:186:THR:CB  | 4:8:183:ARG:NE[1_554]  | 1.05                     | 1.15              |
| 4:2:169:TYR:CZ  | 4:7:266:PHE:CE1[1_554] | 1.06                     | 1.14              |
| 4:3:303:THR:OG1 | 4:7:74:GLY:CA[1_554]   | 1.06                     | 1.14              |
| 4:3:276:GLU:C   | 4:7:281:SER:OG[1_554]  | 1.06                     | 1.14              |
| 4:5:115:ASN:CG  | 4:V:196:ARG:NE[1_554]  | 1.06                     | 1.14              |
| 4:4:173:HIS:N   | 4:9:266:PHE:C[1_554]   | 1.06                     | 1.14              |
| 4:3:267:ILE:CD1 | 4:7:180:LEU:N[1_554]   | 1.06                     | 1.14              |
| 4:3:113:LYS:O   | 4:8:251:GLY:C[1_554]   | 1.06                     | 1.14              |
| 4:5:140:LEU:N   | 4:9:371:HIS:ND1[1_554] | 1.06                     | 1.14              |
| 4:5:252:ASN:OD1 | 4:9:215:LYS:O[1_554]   | 1.06                     | 1.14              |
| 4:5:299:MET:CB  | 4:9:136:ILE:O[1_554]   | 1.06                     | 1.14              |
| 4:5:115:ASN:CB  | 4:V:196:ARG:CD[1_554]  | 1.06                     | 1.14              |
| 4:5:195:GLU:CB  | 4:9:189:LEU:CB[1_554]  | 1.06                     | 1.14              |
| 4:4:340:TRP:CA  | 4:8:117:GLU:C[1_554]   | 1.06                     | 1.14              |
| 4:3:208:ILE:CD1 | 4:7:59:GLN:CB[1_554]   | 1.06                     | 1.14              |
| 4:5:317:ILE:CB  | 4:9:150:GLY:C[1_554]   | 1.06                     | 1.14              |
| 4:2:111:ASN:CG  | 4:7:196:ARG:CG[1_554]  | 1.06                     | 1.14              |
| 4:3:283:MET:CG  | 4:7:286:ASP:CA[1_554]  | 1.06                     | 1.14              |
| 4:4:369:ILE:C   | 4:9:229:THR:C[1_554]   | 1.06                     | 1.14              |
| 4:4:333:PRO:O   | 4:8:105:LEU:CA[1_554]  | 1.06                     | 1.14              |
| 4:5:26:ALA:O    | 4:9:122:ILE:O[1_554]   | 1.06                     | 1.14              |
| 4:4:260:THR:N   | 4:8:155:SER:OG[1_554]  | 1.06                     | 1.14              |
| 4:5:344:SER:O   | 4:9:362:TYR:CD1[1_554] | 1.06                     | 1.14              |
| 4:2:367:PRO:N   | 4:7:235:SER:CA[1_554]  | 1.06                     | 1.14              |
| 4:3:214:GLU:O   | 4:7:17:VAL:N[1_554]    | 1.06                     | 1.14              |
| 4:3:196:ARG:NE  | 4:7:211:ASP:CG[1_554]  | 1.06                     | 1.14              |
| 4:4:326:LYS:O   | 4:8:167:GLU:CA[1_554]  | 1.06                     | 1.14              |
| 4:3:271:SER:O   | 4:7:277:THR:OG1[1_554] | 1.06                     | 1.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:185:LEU:CD1 | 4:7:159:VAL:N[1_554]   | 1.06                     | 1.14              |
| 4:5:294:TYR:CA  | 4:9:166:TYR:C[1_554]   | 1.06                     | 1.14              |
| 4:5:178:LEU:CG  | 4:9:177:ARG:CA[1_554]  | 1.06                     | 1.14              |
| 4:5:213:LYS:CD  | 4:9:157:ASP:CB[1_554]  | 1.07                     | 1.13              |
| 4:1:292:ASP:CB  | 4:7:40:HIS:CG[1_554]   | 1.07                     | 1.13              |
| 4:5:346:LEU:CD2 | 4:9:368:SER:OG[1_554]  | 1.07                     | 1.13              |
| 4:5:193:LEU:CD1 | 4:9:210:ARG:C[1_554]   | 1.07                     | 1.13              |
| 4:3:210:ARG:CG  | 4:7:69:TYR:CD2[1_554]  | 1.07                     | 1.13              |
| 4:3:110:LEU:CA  | 4:8:192:ILE:CB[1_554]  | 1.07                     | 1.13              |
| 4:3:311:ASP:N   | 4:7:140:LEU:O[1_554]   | 1.07                     | 1.13              |
| 4:4:253:GLU:OE1 | 4:8:214:GLU:CA[1_554]  | 1.07                     | 1.13              |
| 4:3:340:TRP:CE3 | 4:7:121:GLN:CB[1_554]  | 1.07                     | 1.13              |
| 4:5:60:SER:C    | 4:9:66:THR:OG1[1_554]  | 1.07                     | 1.13              |
| 4:4:311:ASP:C   | 4:8:141:SER:O[1_554]   | 1.07                     | 1.13              |
| 4:3:293:LEU:CB  | 4:7:169:TYR:CE2[1_554] | 1.07                     | 1.13              |
| 4:3:18:LYS:CG   | 4:7:79:TRP:CE3[1_554]  | 1.07                     | 1.13              |
| 4:3:26:ALA:CA   | 4:7:122:ILE:CA[1_554]  | 1.07                     | 1.13              |
| 4:4:277:THR:O   | 4:8:174:ALA:C[1_554]   | 1.07                     | 1.13              |
| 4:4:109:PRO:C   | 4:9:195:GLU:CD[1_554]  | 1.07                     | 1.13              |
| 4:3:275:HIS:N   | 4:7:162:ASN:C[1_554]   | 1.07                     | 1.13              |
| 4:5:189:LEU:N   | 4:9:182:GLY:O[1_554]   | 1.07                     | 1.13              |
| 4:5:188:TYR:N   | 4:9:183:ARG:C[1_554]   | 1.07                     | 1.13              |
| 4:4:243:PRO:CA  | 4:8:60:SER:CB[1_554]   | 1.07                     | 1.13              |
| 4:3:185:LEU:O   | 4:7:157:ASP:O[1_554]   | 1.07                     | 1.13              |
| 4:3:333:PRO:CA  | 4:7:104:LEU:C[1_554]   | 1.07                     | 1.13              |
| 4:5:266:PHE:CA  | 4:9:261:LEU:CA[1_554]  | 1.07                     | 1.13              |
| 4:3:338:SER:O   | 4:7:116:ARG:C[1_554]   | 1.07                     | 1.13              |
| 4:5:199:SER:N   | 4:9:205:GLU:O[1_554]   | 1.07                     | 1.13              |
| 4:3:286:ASP:CA  | 4:8:270:GLU:OE1[1_554] | 1.07                     | 1.13              |
| 4:2:115:ASN:CA  | 4:7:250:ILE:N[1_554]   | 1.07                     | 1.13              |
| 4:5:110:LEU:N   | 4:V:195:GLU:CD[1_554]  | 1.07                     | 1.13              |
| 4:3:214:GLU:N   | 4:7:16:LEU:N[1_554]    | 1.07                     | 1.13              |
| 4:5:113:LYS:CG  | 4:V:252:ASN:O[1_554]   | 1.07                     | 1.13              |
| 4:3:157:ASP:OD1 | 4:7:72:GLU:CA[1_554]   | 1.07                     | 1.13              |
| 4:3:254:ARG:NH2 | 4:7:337:TYR:OH[1_554]  | 1.07                     | 1.13              |
| 4:4:291:LYS:CD  | 4:V:64:ILE:CG1[1_554]  | 1.07                     | 1.13              |
| 4:2:177:ARG:CZ  | 4:7:194:THR:CG2[1_554] | 1.07                     | 1.13              |
| 4:5:314:GLN:CA  | 4:9:142:LEU:CD1[1_554] | 1.07                     | 1.13              |
| 4:2:79:TRP:CD1  | 4:7:247:VAL:O[1_554]   | 1.07                     | 1.13              |
| 4:3:151:ILE:CG2 | 4:7:170:ALA:O[1_554]   | 1.07                     | 1.13              |
| 4:3:273:GLY:N   | 4:7:162:ASN:OD1[1_554] | 1.07                     | 1.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:30:VAL:CA   | 4:7:79:TRP:C[1_554]    | 1.07                     | 1.13              |
| 4:5:227:MET:CB  | 4:9:307:PRO:C[1_554]   | 1.07                     | 1.13              |
| 4:3:211:ASP:O   | 4:7:32:PRO:N[1_554]    | 1.07                     | 1.13              |
| 4:4:333:PRO:CB  | 4:8:104:LEU:CA[1_554]  | 1.07                     | 1.13              |
| 4:4:267:ILE:N   | 4:8:180:LEU:CD1[1_554] | 1.07                     | 1.13              |
| 4:4:367:PRO:CD  | 4:9:235:SER:CA[1_554]  | 1.07                     | 1.13              |
| 4:3:308:GLY:C   | 4:7:339:VAL:N[1_554]   | 1.07                     | 1.13              |
| 4:5:24:ASP:CA   | 4:9:124:PHE:C[1_554]   | 1.08                     | 1.12              |
| 4:5:325:MET:SD  | 4:9:166:TYR:CZ[1_554]  | 1.08                     | 1.12              |
| 4:4:341:ILE:CA  | 4:8:120:THR:CB[1_554]  | 1.08                     | 1.12              |
| 4:5:193:LEU:CD2 | 4:9:210:ARG:CG[1_554]  | 1.08                     | 1.12              |
| 4:4:144:ALA:N   | 4:8:370:VAL:C[1_554]   | 1.08                     | 1.12              |
| 4:4:366:GLY:O   | 4:9:234:SER:CA[1_554]  | 1.08                     | 1.12              |
| 4:3:210:ARG:CB  | 4:7:69:TYR:CE2[1_554]  | 1.08                     | 1.12              |
| 4:3:219:VAL:C   | 4:7:335:ARG:O[1_554]   | 1.08                     | 1.12              |
| 4:5:191:LYS:C   | 4:9:186:THR:CA[1_554]  | 1.08                     | 1.12              |
| 4:3:204:ALA:C   | 4:7:62:ARG:CB[1_554]   | 1.08                     | 1.12              |
| 4:3:258:PRO:C   | 4:7:155:SER:C[1_554]   | 1.08                     | 1.12              |
| 4:5:75:ILE:CB   | 4:V:198:TYR:N[1_554]   | 1.08                     | 1.12              |
| 4:5:338:SER:OG  | 4:9:134:VAL:CG1[1_554] | 1.08                     | 1.12              |
| 4:5:194:THR:CA  | 4:9:209:VAL:CB[1_554]  | 1.08                     | 1.12              |
| 4:2:109:PRO:N   | 4:7:195:GLU:CG[1_554]  | 1.08                     | 1.12              |
| 4:5:25:ASP:CB   | 4:9:129:VAL:CG2[1_554] | 1.08                     | 1.12              |
| 4:4:265:SER:CB  | 4:8:261:LEU:O[1_554]   | 1.08                     | 1.12              |
| 4:5:262:PHE:CZ  | 4:9:153:LEU:O[1_554]   | 1.08                     | 1.12              |
| 4:3:331:ALA:C   | 4:7:135:ALA:CB[1_554]  | 1.08                     | 1.12              |
| 4:4:280:ASN:CG  | 4:8:281:SER:O[1_554]   | 1.08                     | 1.12              |
| 4:5:199:SER:CB  | 4:9:206:ARG:N[1_554]   | 1.08                     | 1.12              |
| 4:4:369:ILE:CA  | 4:9:229:THR:O[1_554]   | 1.08                     | 1.12              |
| 4:4:258:PRO:O   | 4:8:155:SER:N[1_554]   | 1.08                     | 1.12              |
| 4:4:367:PRO:CB  | 4:9:234:SER:O[1_554]   | 1.08                     | 1.12              |
| 4:3:182:GLY:N   | 4:7:73:HIS:CA[1_554]   | 1.08                     | 1.12              |
| 4:4:345:ILE:O   | 4:8:366:GLY:CA[1_554]  | 1.08                     | 1.12              |
| 4:5:205:GLU:CG  | 4:9:203:THR:OG1[1_554] | 1.08                     | 1.12              |
| 4:3:75:ILE:CG2  | 4:8:198:TYR:CG[1_554]  | 1.08                     | 1.12              |
| 4:2:116:ARG:C   | 4:7:237:GLU:OE2[1_554] | 1.09                     | 1.11              |
| 4:3:205:GLU:CA  | 4:7:62:ARG:CD[1_554]   | 1.09                     | 1.11              |
| 4:4:110:LEU:CA  | 4:9:192:ILE:CA[1_554]  | 1.09                     | 1.11              |
| 4:3:208:ILE:CB  | 4:7:59:GLN:NE2[1_554]  | 1.09                     | 1.11              |
| 4:5:318:THR:OG1 | 4:9:296:ASN:CG[1_554]  | 1.09                     | 1.11              |
| 4:3:312:ARG:NH2 | 4:7:299:MET:CG[1_554]  | 1.09                     | 1.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:169:TYR:OH  | 4:9:266:PHE:CE1[1_554] | 1.09                     | 1.11              |
| 4:4:187:ASP:N   | 4:8:183:ARG:CG[1_554]  | 1.09                     | 1.11              |
| 4:5:270:GLU:C   | 4:9:272:ALA:CB[1_554]  | 1.09                     | 1.11              |
| 4:5:18:LYS:CA   | 4:9:79:TRP:CE3[1_554]  | 1.09                     | 1.11              |
| 4:5:290:ARG:NE  | 4:9:286:ASP:CG[1_554]  | 1.09                     | 1.11              |
| 4:4:214:GLU:OE2 | 4:8:33:SER:OG[1_554]   | 1.09                     | 1.11              |
| 4:3:282:ILE:CG1 | 4:7:171:LEU:CD2[1_554] | 1.09                     | 1.11              |
| 4:5:270:GLU:CA  | 4:9:272:ALA:N[1_554]   | 1.09                     | 1.11              |
| 4:5:276:GLU:CD  | 4:9:279:TYR:N[1_554]   | 1.09                     | 1.11              |
| 4:3:313:MET:CG  | 4:7:138:ALA:CB[1_554]  | 1.09                     | 1.11              |
| 4:5:331:ALA:O   | 4:9:140:LEU:CD2[1_554] | 1.09                     | 1.11              |
| 4:4:274:ILE:CA  | 4:8:162:ASN:N[1_554]   | 1.09                     | 1.11              |
| 4:4:140:LEU:N   | 4:8:371:HIS:CE1[1_554] | 1.09                     | 1.11              |
| 4:5:214:GLU:CB  | 4:9:16:LEU:C[1_554]    | 1.09                     | 1.11              |
| 4:4:305:MET:O   | 4:8:11:ASP:OD2[1_554]  | 1.09                     | 1.11              |
| 4:4:271:SER:C   | 4:8:277:THR:OG1[1_554] | 1.09                     | 1.11              |
| 4:4:185:LEU:O   | 4:8:157:ASP:O[1_554]   | 1.09                     | 1.11              |
| 4:3:277:THR:O   | 4:7:174:ALA:C[1_554]   | 1.09                     | 1.11              |
| 4:3:192:ILE:CB  | 4:7:213:LYS:CE[1_554]  | 1.09                     | 1.11              |
| 4:5:310:ALA:CA  | 4:9:141:SER:C[1_554]   | 1.09                     | 1.11              |
| 4:4:75:ILE:CA   | 4:9:198:TYR:N[1_554]   | 1.09                     | 1.11              |
| 4:3:111:ASN:OD1 | 4:8:196:ARG:CG[1_554]  | 1.09                     | 1.11              |
| 4:5:282:ILE:CG1 | 4:9:171:LEU:CD1[1_554] | 1.09                     | 1.11              |
| 4:3:31:PHE:C    | 4:7:78:ASN:CG[1_554]   | 1.09                     | 1.11              |
| 4:3:253:GLU:OE1 | 4:7:214:GLU:CB[1_554]  | 1.10                     | 1.10              |
| 4:5:347:ALA:N   | 4:9:366:GLY:C[1_554]   | 1.10                     | 1.10              |
| 4:2:173:HIS:CB  | 4:7:267:ILE:CG1[1_554] | 1.10                     | 1.10              |
| 4:4:210:ARG:CZ  | 4:8:33:SER:O[1_554]    | 1.10                     | 1.10              |
| 4:3:157:ASP:OD2 | 4:7:72:GLU:CB[1_554]   | 1.10                     | 1.10              |
| 4:3:193:LEU:CB  | 4:7:210:ARG:CG[1_554]  | 1.10                     | 1.10              |
| 4:3:338:SER:C   | 4:7:116:ARG:CA[1_554]  | 1.10                     | 1.10              |
| 4:2:74:GLY:C    | 4:7:198:TYR:N[1_554]   | 1.10                     | 1.10              |
| 4:5:369:ILE:CG2 | 4:V:232:SER:N[1_554]   | 1.10                     | 1.10              |
| 4:5:299:MET:SD  | 4:9:139:VAL:N[1_554]   | 1.10                     | 1.10              |
| 4:5:157:ASP:N   | 4:9:75:ILE:N[1_554]    | 1.10                     | 1.10              |
| 4:5:117:GLU:OE2 | 4:V:236:LEU:CD1[1_554] | 1.10                     | 1.10              |
| 4:5:372:ARG:N   | 4:V:227:MET:O[1_554]   | 1.10                     | 1.10              |
| 4:3:357:ILE:CG1 | 4:8:231:ALA:C[1_554]   | 1.10                     | 1.10              |
| 4:4:196:ARG:CD  | 4:8:211:ASP:C[1_554]   | 1.10                     | 1.10              |
| 4:3:114:ALA:C   | 4:8:250:ILE:C[1_554]   | 1.10                     | 1.10              |
| 4:1:287:ILE:O   | 4:7:63:GLY:O[1_554]    | 1.10                     | 1.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:188:TYR:C   | 4:7:183:ARG:N[1_554]   | 1.10                     | 1.10              |
| 4:3:316:GLU:C   | 4:7:151:ILE:N[1_554]   | 1.10                     | 1.10              |
| 4:4:24:ASP:CG   | 4:8:125:GLU:CB[1_554]  | 1.10                     | 1.10              |
| 4:4:180:LEU:CD2 | 4:8:178:LEU:O[1_554]   | 1.10                     | 1.10              |
| 4:5:339:VAL:CA  | 4:9:116:ARG:CB[1_554]  | 1.10                     | 1.10              |
| 4:2:166:TYR:CD1 | 4:8:40:HIS:NE2[1_554]  | 1.10                     | 1.10              |
| 4:3:310:ALA:C   | 4:7:140:LEU:C[1_554]   | 1.10                     | 1.10              |
| 4:5:253:GLU:OE1 | 4:9:213:LYS:C[1_554]   | 1.10                     | 1.10              |
| 4:5:372:ARG:O   | 4:V:227:MET:CB[1_554]  | 1.10                     | 1.10              |
| 4:4:173:HIS:CA  | 4:9:267:ILE:CA[1_554]  | 1.10                     | 1.10              |
| 4:3:372:ARG:CG  | 4:8:227:MET:CA[1_554]  | 1.10                     | 1.10              |
| 4:4:173:HIS:N   | 4:9:266:PHE:O[1_554]   | 1.10                     | 1.10              |
| 4:4:277:THR:N   | 4:8:281:SER:OG[1_554]  | 1.10                     | 1.10              |
| 4:3:335:ARG:NE  | 4:7:106:THR:CB[1_554]  | 1.10                     | 1.10              |
| 4:4:310:ALA:CB  | 4:8:140:LEU:C[1_554]   | 1.10                     | 1.10              |
| 4:3:185:LEU:CA  | 4:7:158:GLY:CA[1_554]  | 1.10                     | 1.10              |
| 4:3:117:GLU:OE1 | 4:8:236:LEU:O[1_554]   | 1.10                     | 1.10              |
| 4:5:281:SER:OG  | 4:9:173:HIS:N[1_554]   | 1.10                     | 1.10              |
| 4:5:198:TYR:CD1 | 4:9:208:ILE:CA[1_554]  | 1.10                     | 1.10              |
| 4:5:265:SER:O   | 4:9:260:THR:O[1_554]   | 1.10                     | 1.10              |
| 4:5:295:ALA:C   | 4:9:167:GLU:O[1_554]   | 1.10                     | 1.10              |
| 4:5:153:LEU:CD1 | 4:9:163:VAL:CG2[1_554] | 1.10                     | 1.10              |
| 4:4:340:TRP:CG  | 4:8:118:LYS:CA[1_554]  | 1.10                     | 1.10              |
| 4:4:220:ALA:CB  | 4:8:335:ARG:CB[1_554]  | 1.10                     | 1.10              |
| 4:5:327:ILE:O   | 4:9:148:THR:OG1[1_554] | 1.10                     | 1.10              |
| 4:3:334:GLU:CA  | 4:7:105:LEU:CD1[1_554] | 1.10                     | 1.10              |
| 4:5:305:MET:O   | 4:9:11:ASP:OD2[1_554]  | 1.11                     | 1.09              |
| 4:3:256:ARG:O   | 4:7:303:THR:CA[1_554]  | 1.11                     | 1.09              |
| 4:5:162:ASN:N   | 4:9:110:LEU:CD2[1_554] | 1.11                     | 1.09              |
| 4:4:178:LEU:CD2 | 4:8:177:ARG:CA[1_554]  | 1.11                     | 1.09              |
| 4:5:315:LYS:O   | 4:9:296:ASN:C[1_554]   | 1.11                     | 1.09              |
| 4:3:341:ILE:N   | 4:7:117:GLU:C[1_554]   | 1.11                     | 1.09              |
| 4:3:186:THR:C   | 4:7:183:ARG:CD[1_554]  | 1.11                     | 1.09              |
| 4:3:223:PHE:C   | 4:7:335:ARG:CZ[1_554]  | 1.11                     | 1.09              |
| 4:5:113:LYS:CB  | 4:V:253:GLU:N[1_554]   | 1.11                     | 1.09              |
| 4:4:288:ASP:O   | 4:V:64:ILE:N[1_554]    | 1.11                     | 1.09              |
| 4:4:110:LEU:CB  | 4:9:192:ILE:N[1_554]   | 1.11                     | 1.09              |
| 4:3:305:MET:O   | 4:7:11:ASP:OD1[1_554]  | 1.11                     | 1.09              |
| 4:4:223:PHE:C   | 4:8:335:ARG:NH2[1_554] | 1.11                     | 1.09              |
| 4:5:160:THR:CG2 | 4:9:161:HIS:CD2[1_554] | 1.11                     | 1.09              |
| 4:3:242:LEU:O   | 4:7:60:SER:CB[1_554]   | 1.11                     | 1.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:313:MET:CA  | 4:8:152:VAL:CG2[1_554] | 1.11                     | 1.09              |
| 4:3:117:GLU:CA  | 4:8:237:GLU:CG[1_554]  | 1.11                     | 1.09              |
| 4:5:331:ALA:CB  | 4:9:140:LEU:CB[1_554]  | 1.11                     | 1.09              |
| 4:3:317:ILE:CD1 | 4:7:165:ILE:CA[1_554]  | 1.11                     | 1.09              |
| 4:4:110:LEU:C   | 4:9:192:ILE:C[1_554]   | 1.11                     | 1.09              |
| 4:3:109:PRO:C   | 4:8:195:GLU:OE1[1_554] | 1.11                     | 1.09              |
| 4:5:312:ARG:C   | 4:9:298:VAL:CG1[1_554] | 1.11                     | 1.09              |
| 4:5:141:SER:C   | 4:9:116:ARG:CZ[1_554]  | 1.11                     | 1.09              |
| 4:3:144:ALA:O   | 4:7:370:VAL:CA[1_554]  | 1.11                     | 1.09              |
| 4:3:204:ALA:O   | 4:7:62:ARG:CB[1_554]   | 1.11                     | 1.09              |
| 4:4:188:TYR:CZ  | 4:8:185:LEU:CD2[1_554] | 1.11                     | 1.09              |
| 4:4:24:ASP:CA   | 4:8:125:GLU:CG[1_554]  | 1.11                     | 1.09              |
| 4:3:270:GLU:N   | 4:7:272:ALA:O[1_554]   | 1.11                     | 1.09              |
| 4:4:267:ILE:C   | 4:8:180:LEU:CD2[1_554] | 1.11                     | 1.09              |
| 4:3:111:ASN:ND2 | 4:8:196:ARG:CG[1_554]  | 1.11                     | 1.09              |
| 4:3:215:LYS:CB  | 4:7:31:PHE:CA[1_554]   | 1.11                     | 1.09              |
| 4:3:304:THR:N   | 4:7:137:GLN:NE2[1_554] | 1.11                     | 1.09              |
| 4:3:326:LYS:CA  | 4:7:167:GLU:OE1[1_554] | 1.11                     | 1.09              |
| 4:5:288:ASP:C   | 4:W:64:ILE:N[1_554]    | 1.11                     | 1.09              |
| 4:5:166:TYR:CG  | 4:W:40:HIS:ND1[1_554]  | 1.11                     | 1.09              |
| 4:5:199:SER:C   | 4:9:206:ARG:CB[1_554]  | 1.11                     | 1.09              |
| 4:4:263:GLN:CA  | 4:8:274:ILE:CG1[1_554] | 1.11                     | 1.09              |
| 4:4:259:GLU:OE1 | 4:8:304:THR:C[1_554]   | 1.11                     | 1.09              |
| 4:4:255:PHE:CD1 | 4:8:305:MET:CG[1_554]  | 1.12                     | 1.08              |
| 4:4:367:PRO:O   | 4:9:236:LEU:CD2[1_554] | 1.12                     | 1.08              |
| 4:3:335:ARG:CZ  | 4:7:106:THR:CB[1_554]  | 1.12                     | 1.08              |
| 4:4:140:LEU:CA  | 4:8:371:HIS:CG[1_554]  | 1.12                     | 1.08              |
| 4:3:299:MET:N   | 4:7:136:ILE:CG1[1_554] | 1.12                     | 1.08              |
| 4:5:194:THR:O   | 4:9:209:VAL:CG2[1_554] | 1.12                     | 1.08              |
| 4:2:109:PRO:CA  | 4:7:195:GLU:OE1[1_554] | 1.12                     | 1.08              |
| 4:3:218:TYR:CD2 | 4:7:337:TYR:CG[1_554]  | 1.12                     | 1.08              |
| 4:3:283:MET:CB  | 4:7:286:ASP:N[1_554]   | 1.12                     | 1.08              |
| 4:5:136:ILE:N   | 4:9:113:LYS:CE[1_554]  | 1.12                     | 1.08              |
| 4:5:27:PRO:CA   | 4:9:122:ILE:CB[1_554]  | 1.12                     | 1.08              |
| 4:5:334:GLU:C   | 4:9:105:LEU:C[1_554]   | 1.12                     | 1.08              |
| 4:4:243:PRO:CA  | 4:8:60:SER:CA[1_554]   | 1.12                     | 1.08              |
| 4:5:317:ILE:N   | 4:9:151:ILE:N[1_554]   | 1.12                     | 1.08              |
| 4:3:258:PRO:O   | 4:7:155:SER:CA[1_554]  | 1.12                     | 1.08              |
| 4:3:31:PHE:CA   | 4:7:78:ASN:OD1[1_554]  | 1.12                     | 1.08              |
| 4:3:320:LEU:CG  | 4:7:293:LEU:CB[1_554]  | 1.12                     | 1.08              |
| 4:5:277:THR:OG1 | 4:9:176:MET:CG[1_554]  | 1.12                     | 1.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:276:GLU:CG  | 4:9:278:THR:C[1_554]   | 1.12                     | 1.08              |
| 4:5:309:ILE:CA  | 4:9:141:SER:OG[1_554]  | 1.12                     | 1.08              |
| 4:3:299:MET:CE  | 4:7:136:ILE:C[1_554]   | 1.12                     | 1.08              |
| 4:5:188:TYR:CE1 | 4:9:185:LEU:CD1[1_554] | 1.12                     | 1.08              |
| 4:4:299:MET:CA  | 4:8:136:ILE:CG1[1_554] | 1.12                     | 1.08              |
| 4:3:139:VAL:CB  | 4:7:113:LYS:CD[1_554]  | 1.12                     | 1.08              |
| 4:4:284:LYS:C   | 4:9:268:GLY:O[1_554]   | 1.12                     | 1.08              |
| 4:4:204:ALA:CA  | 4:8:62:ARG:CB[1_554]   | 1.12                     | 1.08              |
| 4:4:218:TYR:CD1 | 4:8:337:TYR:CE1[1_554] | 1.12                     | 1.08              |
| 4:5:115:ASN:CG  | 4:V:196:ARG:CD[1_554]  | 1.12                     | 1.08              |
| 4:4:154:ASP:N   | 4:8:109:PRO:O[1_554]   | 1.12                     | 1.08              |
| 4:3:253:GLU:CD  | 4:7:214:GLU:CB[1_554]  | 1.12                     | 1.08              |
| 4:4:140:LEU:N   | 4:8:371:HIS:NE2[1_554] | 1.12                     | 1.08              |
| 4:5:205:GLU:N   | 4:9:62:ARG:CD[1_554]   | 1.12                     | 1.08              |
| 4:3:156:GLY:CA  | 4:7:75:ILE:CA[1_554]   | 1.13                     | 1.07              |
| 4:5:160:THR:CG2 | 4:9:161:HIS:NE2[1_554] | 1.13                     | 1.07              |
| 4:5:159:VAL:CA  | 4:9:177:ARG:CZ[1_554]  | 1.13                     | 1.07              |
| 4:5:75:ILE:O    | 4:V:197:GLY:O[1_554]   | 1.13                     | 1.07              |
| 4:5:309:ILE:CD1 | 4:9:154:ASP:OD2[1_554] | 1.13                     | 1.07              |
| 4:3:345:ILE:CA  | 4:7:367:PRO:N[1_554]   | 1.13                     | 1.07              |
| 4:5:223:PHE:CE2 | 4:9:304:THR:CB[1_554]  | 1.13                     | 1.07              |
| 4:5:305:MET:CB  | 4:9:11:ASP:CG[1_554]   | 1.13                     | 1.07              |
| 4:4:253:GLU:OE1 | 4:8:214:GLU:N[1_554]   | 1.13                     | 1.07              |
| 4:5:259:GLU:CD  | 4:9:309:ILE:CD1[1_554] | 1.13                     | 1.07              |
| 4:5:320:LEU:N   | 4:9:293:LEU:C[1_554]   | 1.13                     | 1.07              |
| 4:3:222:ASP:CB  | 4:7:332:PRO:N[1_554]   | 1.13                     | 1.07              |
| 4:5:250:ILE:CB  | 4:9:214:GLU:OE1[1_554] | 1.13                     | 1.07              |
| 4:5:308:GLY:CA  | 4:9:338:SER:OG[1_554]  | 1.13                     | 1.07              |
| 4:5:166:TYR:OH  | 4:W:39:ARG:CA[1_554]   | 1.13                     | 1.07              |
| 4:4:188:TYR:OH  | 4:8:185:LEU:CD2[1_554] | 1.13                     | 1.07              |
| 4:4:19:ALA:CA   | 4:8:118:LYS:NZ[1_554]  | 1.13                     | 1.07              |
| 4:3:141:SER:N   | 4:7:371:HIS:ND1[1_554] | 1.13                     | 1.07              |
| 4:4:370:VAL:CG1 | 4:9:230:ALA:O[1_554]   | 1.13                     | 1.07              |
| 4:3:333:PRO:CB  | 4:7:104:LEU:CA[1_554]  | 1.13                     | 1.07              |
| 4:5:273:GLY:O   | 4:9:162:ASN:CG[1_554]  | 1.13                     | 1.07              |
| 4:4:188:TYR:CD2 | 4:8:182:GLY:N[1_554]   | 1.13                     | 1.07              |
| 4:5:294:TYR:OH  | 4:9:289:ILE:CD1[1_554] | 1.13                     | 1.07              |
| 4:4:219:VAL:CG1 | 4:8:300:SER:CB[1_554]  | 1.13                     | 1.07              |
| 4:5:111:ASN:OD1 | 4:V:196:ARG:CA[1_554]  | 1.13                     | 1.07              |
| 4:5:314:GLN:N   | 4:9:142:LEU:CD1[1_554] | 1.13                     | 1.07              |
| 4:5:110:LEU:CG  | 4:V:191:LYS:CD[1_554]  | 1.13                     | 1.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:193:LEU:CD2 | 4:8:210:ARG:NE[1_554]  | 1.13                     | 1.07              |
| 4:4:189:LEU:N   | 4:8:183:ARG:N[1_554]   | 1.13                     | 1.07              |
| 4:3:75:ILE:N    | 4:8:197:GLY:C[1_554]   | 1.13                     | 1.07              |
| 4:5:335:ARG:CB  | 4:9:106:THR:CA[1_554]  | 1.13                     | 1.07              |
| 4:3:188:TYR:CD2 | 4:7:182:GLY:CA[1_554]  | 1.13                     | 1.07              |
| 4:4:32:PRO:N    | 4:8:78:ASN:ND2[1_554]  | 1.13                     | 1.07              |
| 4:5:26:ALA:CB   | 4:9:123:MET:SD[1_554]  | 1.13                     | 1.07              |
| 4:3:266:PHE:CG  | 4:7:261:LEU:CD1[1_554] | 1.13                     | 1.07              |
| 4:3:337:TYR:C   | 4:7:119:MET:CG[1_554]  | 1.13                     | 1.07              |
| 4:5:262:PHE:CB  | 4:9:153:LEU:CD2[1_554] | 1.14                     | 1.06              |
| 4:5:205:GLU:CA  | 4:9:62:ARG:CZ[1_554]   | 1.14                     | 1.06              |
| 4:4:41:GLN:CG   | 4:7:224:GLU:OE1[1_554] | 1.14                     | 1.06              |
| 4:2:288:ASP:O   | 4:8:64:ILE:C[1_554]    | 1.14                     | 1.06              |
| 4:3:277:THR:CG2 | 4:7:175:ILE:O[1_554]   | 1.14                     | 1.06              |
| 4:4:310:ALA:N   | 4:8:141:SER:N[1_554]   | 1.14                     | 1.06              |
| 1:D:637:LYS:CG  | 4:5:311:ASP:OD1[1_556] | 1.14                     | 1.06              |
| 4:4:154:ASP:OD1 | 4:8:111:ASN:CA[1_554]  | 1.14                     | 1.06              |
| 4:5:19:ALA:O    | 4:9:122:ILE:CG1[1_554] | 1.14                     | 1.06              |
| 4:4:300:SER:CB  | 4:8:107:GLU:OE1[1_554] | 1.14                     | 1.06              |
| 4:3:357:ILE:CG2 | 4:8:232:SER:O[1_554]   | 1.14                     | 1.06              |
| 4:3:154:ASP:N   | 4:7:109:PRO:C[1_554]   | 1.14                     | 1.06              |
| 4:4:294:TYR:CA  | 4:8:166:TYR:O[1_554]   | 1.14                     | 1.06              |
| 4:4:142:LEU:C   | 4:8:372:ARG:CB[1_554]  | 1.14                     | 1.06              |
| 4:3:312:ARG:CZ  | 4:7:299:MET:CA[1_554]  | 1.14                     | 1.06              |
| 4:4:188:TYR:CE1 | 4:8:185:LEU:CG[1_554]  | 1.14                     | 1.06              |
| 4:5:227:MET:SD  | 4:9:307:PRO:N[1_554]   | 1.14                     | 1.06              |
| 4:4:218:TYR:CE1 | 4:8:337:TYR:CD1[1_554] | 1.14                     | 1.06              |
| 4:5:192:ILE:O   | 4:9:213:LYS:CB[1_554]  | 1.14                     | 1.06              |
| 4:5:279:TYR:N   | 4:9:164:PRO:CG[1_554]  | 1.14                     | 1.06              |
| 4:4:275:HIS:N   | 4:8:163:VAL:N[1_554]   | 1.14                     | 1.06              |
| 4:3:113:LYS:O   | 4:8:251:GLY:CA[1_554]  | 1.14                     | 1.06              |
| 4:4:226:GLU:OE2 | 4:8:333:PRO:O[1_554]   | 1.14                     | 1.06              |
| 4:5:178:LEU:CG  | 4:9:177:ARG:C[1_554]   | 1.14                     | 1.06              |
| 4:3:255:PHE:C   | 4:7:302:GLY:CA[1_554]  | 1.14                     | 1.06              |
| 4:4:156:GLY:CA  | 4:8:75:ILE:N[1_554]    | 1.14                     | 1.06              |
| 4:5:198:TYR:CD2 | 4:9:208:ILE:O[1_554]   | 1.14                     | 1.06              |
| 4:5:274:ILE:CG1 | 4:9:161:HIS:CB[1_554]  | 1.14                     | 1.06              |
| 4:3:223:PHE:O   | 4:7:335:ARG:CZ[1_554]  | 1.14                     | 1.06              |
| 4:4:197:GLY:O   | 4:8:208:ILE:CG2[1_554] | 1.14                     | 1.06              |
| 4:5:328:LYS:N   | 4:9:148:THR:O[1_554]   | 1.14                     | 1.06              |
| 4:4:213:LYS:C   | 4:8:16:LEU:N[1_554]    | 1.14                     | 1.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:290:ARG:NE  | 4:9:286:ASP:CB[1_554]  | 1.14                     | 1.06              |
| 4:5:26:ALA:O    | 4:9:122:ILE:C[1_554]   | 1.14                     | 1.06              |
| 4:3:321:ALA:O   | 4:7:292:ASP:CB[1_554]  | 1.14                     | 1.06              |
| 4:5:18:LYS:CB   | 4:9:79:TRP:CZ3[1_554]  | 1.14                     | 1.06              |
| 4:4:26:ALA:CB   | 4:8:123:MET:N[1_554]   | 1.14                     | 1.06              |
| 4:2:75:ILE:CG2  | 4:7:198:TYR:CD2[1_554] | 1.15                     | 1.05              |
| 4:5:299:MET:CA  | 4:9:136:ILE:CA[1_554]  | 1.15                     | 1.05              |
| 4:4:117:GLU:N   | 4:9:237:GLU:OE2[1_554] | 1.15                     | 1.05              |
| 4:3:286:ASP:CA  | 4:8:270:GLU:OE2[1_554] | 1.15                     | 1.05              |
| 4:5:271:SER:C   | 4:9:277:THR:OG1[1_554] | 1.15                     | 1.05              |
| 4:4:210:ARG:O   | 4:8:15:GLY:O[1_554]    | 1.15                     | 1.05              |
| 4:5:277:THR:O   | 4:9:174:ALA:C[1_554]   | 1.15                     | 1.05              |
| 4:2:115:ASN:CG  | 4:7:249:THR:O[1_554]   | 1.15                     | 1.05              |
| 4:2:287:ILE:O   | 4:8:63:GLY:C[1_554]    | 1.15                     | 1.05              |
| 4:5:173:HIS:O   | 4:V:267:ILE:O[1_554]   | 1.15                     | 1.05              |
| 4:4:258:PRO:O   | 4:8:155:SER:CA[1_554]  | 1.15                     | 1.05              |
| 4:5:312:ARG:CG  | 4:9:299:MET:CA[1_554]  | 1.15                     | 1.05              |
| 4:2:117:GLU:CA  | 4:7:237:GLU:CB[1_554]  | 1.15                     | 1.05              |
| 4:3:154:ASP:CA  | 4:7:111:ASN:N[1_554]   | 1.15                     | 1.05              |
| 4:5:109:PRO:O   | 4:V:195:GLU:OE1[1_554] | 1.15                     | 1.05              |
| 4:5:294:TYR:OH  | 4:9:289:ILE:CG1[1_554] | 1.15                     | 1.05              |
| 4:5:200:PHE:N   | 4:9:206:ARG:CG[1_554]  | 1.15                     | 1.05              |
| 4:3:199:SER:N   | 4:7:206:ARG:C[1_554]   | 1.15                     | 1.05              |
| 4:3:262:PHE:CG  | 4:7:153:LEU:O[1_554]   | 1.15                     | 1.05              |
| 4:3:173:HIS:CB  | 4:8:267:ILE:CG1[1_554] | 1.15                     | 1.05              |
| 4:5:196:ARG:C   | 4:9:212:ILE:CB[1_554]  | 1.15                     | 1.05              |
| 4:3:226:GLU:OE2 | 4:7:333:PRO:O[1_554]   | 1.15                     | 1.05              |
| 4:3:334:GLU:OE2 | 4:7:133:TYR:N[1_554]   | 1.15                     | 1.05              |
| 4:4:143:TYR:N   | 4:8:372:ARG:N[1_554]   | 1.15                     | 1.05              |
| 4:3:115:ASN:N   | 4:8:250:ILE:CA[1_554]  | 1.15                     | 1.05              |
| 4:4:144:ALA:N   | 4:8:371:HIS:N[1_554]   | 1.15                     | 1.05              |
| 4:3:335:ARG:NH2 | 4:7:106:THR:CG2[1_554] | 1.15                     | 1.05              |
| 4:4:255:PHE:CE1 | 4:8:305:MET:CA[1_554]  | 1.15                     | 1.05              |
| 4:5:161:HIS:C   | 4:9:110:LEU:CG[1_554]  | 1.15                     | 1.05              |
| 4:3:326:LYS:C   | 4:7:167:GLU:CA[1_554]  | 1.15                     | 1.05              |
| 4:3:144:ALA:C   | 4:7:370:VAL:O[1_554]   | 1.15                     | 1.05              |
| 4:4:337:TYR:CE1 | 4:8:86:TRP:CH2[1_554]  | 1.15                     | 1.05              |
| 4:3:337:TYR:CA  | 4:7:119:MET:CG[1_554]  | 1.16                     | 1.04              |
| 4:3:319:ALA:C   | 4:7:292:ASP:O[1_554]   | 1.16                     | 1.04              |
| 4:2:172:PRO:CG  | 4:7:266:PHE:CD2[1_554] | 1.16                     | 1.04              |
| 4:5:186:THR:C   | 4:9:183:ARG:CG[1_554]  | 1.16                     | 1.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:249:THR:CA  | 4:9:211:ASP:OD2[1_554] | 1.16                     | 1.04              |
| 4:4:196:ARG:CB  | 4:8:212:ILE:N[1_554]   | 1.16                     | 1.04              |
| 4:3:177:ARG:CZ  | 4:8:194:THR:CG2[1_554] | 1.16                     | 1.04              |
| 4:4:337:TYR:CA  | 4:8:119:MET:CB[1_554]  | 1.16                     | 1.04              |
| 4:3:15:GLY:CA   | 4:7:77:THR:CB[1_554]   | 1.16                     | 1.04              |
| 4:5:237:GLU:OE1 | 4:9:215:LYS:CE[1_554]  | 1.16                     | 1.04              |
| 4:5:211:ASP:CB  | 4:9:32:PRO:CG[1_554]   | 1.16                     | 1.04              |
| 4:5:316:GLU:C   | 4:9:296:ASN:O[1_554]   | 1.16                     | 1.04              |
| 4:4:308:GLY:N   | 4:8:339:VAL:N[1_554]   | 1.16                     | 1.04              |
| 4:3:263:GLN:C   | 4:7:274:ILE:CD1[1_554] | 1.16                     | 1.04              |
| 4:3:366:GLY:C   | 4:8:235:SER:N[1_554]   | 1.16                     | 1.04              |
| 4:4:325:MET:CG  | 4:8:166:TYR:CZ[1_554]  | 1.16                     | 1.04              |
| 4:5:23:GLY:N    | 4:9:362:TYR:CD2[1_554] | 1.16                     | 1.04              |
| 4:4:157:ASP:CG  | 4:8:72:GLU:CA[1_554]   | 1.16                     | 1.04              |
| 4:4:256:ARG:O   | 4:8:303:THR:CA[1_554]  | 1.16                     | 1.04              |
| 4:3:208:ILE:CD1 | 4:7:59:GLN:CA[1_554]   | 1.16                     | 1.04              |
| 4:5:32:PRO:CA   | 4:9:78:ASN:CB[1_554]   | 1.16                     | 1.04              |
| 4:2:291:LYS:CD  | 4:8:64:ILE:CG1[1_554]  | 1.16                     | 1.04              |
| 4:4:317:ILE:C   | 4:8:150:GLY:CA[1_554]  | 1.16                     | 1.04              |
| 4:3:199:SER:CB  | 4:7:206:ARG:N[1_554]   | 1.16                     | 1.04              |
| 4:5:332:PRO:C   | 4:9:104:LEU:CD2[1_554] | 1.16                     | 1.04              |
| 4:5:349:LEU:CB  | 4:9:365:ALA:CB[1_554]  | 1.16                     | 1.04              |
| 4:5:326:LYS:CG  | 4:9:167:GLU:OE1[1_554] | 1.16                     | 1.04              |
| 4:2:77:THR:CB   | 4:7:246:GLN:OE1[1_554] | 1.16                     | 1.04              |
| 4:1:326:LYS:CD  | 4:7:43:VAL:O[1_554]    | 1.16                     | 1.04              |
| 4:4:267:ILE:CA  | 4:8:180:LEU:CD1[1_554] | 1.16                     | 1.04              |
| 4:5:24:ASP:CG   | 4:9:125:GLU:N[1_554]   | 1.16                     | 1.04              |
| 4:5:204:ALA:C   | 4:9:62:ARG:CG[1_554]   | 1.16                     | 1.04              |
| 4:5:294:TYR:CD2 | 4:9:166:TYR:CD1[1_554] | 1.16                     | 1.04              |
| 4:5:15:GLY:N    | 4:9:77:THR:CB[1_554]   | 1.17                     | 1.03              |
| 4:4:270:GLU:O   | 4:8:272:ALA:CB[1_554]  | 1.17                     | 1.03              |
| 4:5:211:ASP:CG  | 4:9:32:PRO:CG[1_554]   | 1.17                     | 1.03              |
| 4:5:278:THR:OG1 | 4:9:163:VAL:C[1_554]   | 1.17                     | 1.03              |
| 4:3:255:PHE:CA  | 4:7:302:GLY:CA[1_554]  | 1.17                     | 1.03              |
| 4:5:286:ASP:CA  | 4:V:270:GLU:CD[1_554]  | 1.17                     | 1.03              |
| 4:4:187:ASP:O   | 4:8:183:ARG:O[1_554]   | 1.17                     | 1.03              |
| 4:3:116:ARG:N   | 4:8:196:ARG:NH2[1_554] | 1.17                     | 1.03              |
| 4:1:291:LYS:CD  | 4:7:64:ILE:O[1_554]    | 1.17                     | 1.03              |
| 4:3:281:SER:O   | 4:7:173:HIS:NE2[1_554] | 1.17                     | 1.03              |
| 4:2:110:LEU:C   | 4:7:192:ILE:C[1_554]   | 1.17                     | 1.03              |
| 4:5:334:GLU:N   | 4:9:105:LEU:N[1_554]   | 1.17                     | 1.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:302:GLY:O   | 4:8:12:ASN:O[1_554]    | 1.17                     | 1.03              |
| 4:3:242:LEU:C   | 4:7:60:SER:CB[1_554]   | 1.17                     | 1.03              |
| 4:5:250:ILE:CG2 | 4:9:214:GLU:OE1[1_554] | 1.17                     | 1.03              |
| 4:5:26:ALA:C    | 4:9:123:MET:CA[1_554]  | 1.17                     | 1.03              |
| 4:5:166:TYR:OH  | 4:W:39:ARG:C[1_554]    | 1.17                     | 1.03              |
| 4:3:283:MET:CB  | 4:7:285:CYS:C[1_554]   | 1.17                     | 1.03              |
| 4:5:196:ARG:CG  | 4:9:212:ILE:N[1_554]   | 1.17                     | 1.03              |
| 4:4:268:GLY:C   | 4:8:264:PRO:CB[1_554]  | 1.17                     | 1.03              |
| 4:3:144:ALA:N   | 4:7:371:HIS:CA[1_554]  | 1.17                     | 1.03              |
| 4:4:204:ALA:C   | 4:8:62:ARG:CG[1_554]   | 1.17                     | 1.03              |
| 4:3:23:GLY:C    | 4:7:125:GLU:OE2[1_554] | 1.17                     | 1.03              |
| 4:5:28:ARG:O    | 4:9:83:GLU:CD[1_554]   | 1.17                     | 1.03              |
| 4:3:153:LEU:CD2 | 4:7:109:PRO:CG[1_554]  | 1.17                     | 1.03              |
| 4:5:151:ILE:CD1 | 4:9:171:LEU:C[1_554]   | 1.17                     | 1.03              |
| 4:3:288:ASP:O   | 4:9:64:ILE:C[1_554]    | 1.17                     | 1.03              |
| 4:4:332:PRO:CD  | 4:8:135:ALA:N[1_554]   | 1.17                     | 1.03              |
| 4:4:334:GLU:OE2 | 4:8:133:TYR:N[1_554]   | 1.17                     | 1.03              |
| 4:4:154:ASP:CG  | 4:8:111:ASN:N[1_554]   | 1.17                     | 1.03              |
| 4:3:111:ASN:OD1 | 4:8:196:ARG:CB[1_554]  | 1.17                     | 1.03              |
| 4:3:139:VAL:N   | 4:7:113:LYS:CG[1_554]  | 1.17                     | 1.03              |
| 4:4:106:THR:CB  | 4:8:114:ALA:CB[1_554]  | 1.17                     | 1.03              |
| 4:4:214:GLU:C   | 4:8:16:LEU:C[1_554]    | 1.17                     | 1.03              |
| 4:3:243:PRO:CB  | 4:7:60:SER:C[1_554]    | 1.17                     | 1.03              |
| 4:4:349:LEU:CD2 | 4:8:365:ALA:CA[1_554]  | 1.17                     | 1.03              |
| 4:5:288:ASP:CA  | 4:W:62:ARG:C[1_554]    | 1.17                     | 1.03              |
| 4:5:333:PRO:CG  | 4:9:104:LEU:CB[1_554]  | 1.17                     | 1.03              |
| 4:5:281:SER:N   | 4:9:174:ALA:CB[1_554]  | 1.17                     | 1.03              |
| 4:3:254:ARG:CZ  | 4:7:337:TYR:OH[1_554]  | 1.17                     | 1.03              |
| 4:5:297:ASN:CG  | 4:9:165:ILE:CG1[1_554] | 1.17                     | 1.03              |
| 4:3:262:PHE:C   | 4:7:153:LEU:CD1[1_554] | 1.18                     | 1.02              |
| 4:5:278:THR:CB  | 4:9:164:PRO:CD[1_554]  | 1.18                     | 1.02              |
| 4:5:191:LYS:CA  | 4:9:187:ASP:N[1_554]   | 1.18                     | 1.02              |
| 4:5:266:PHE:CG  | 4:9:261:LEU:CD1[1_554] | 1.18                     | 1.02              |
| 4:3:367:PRO:CD  | 4:8:235:SER:C[1_554]   | 1.18                     | 1.02              |
| 4:3:320:LEU:CB  | 4:7:293:LEU:CG[1_554]  | 1.18                     | 1.02              |
| 4:3:166:TYR:CD1 | 4:9:40:HIS:CE1[1_554]  | 1.18                     | 1.02              |
| 4:4:274:ILE:C   | 4:8:163:VAL:N[1_554]   | 1.18                     | 1.02              |
| 4:3:188:TYR:CA  | 4:7:184:ASP:N[1_554]   | 1.18                     | 1.02              |
| 4:4:339:VAL:CA  | 4:8:116:ARG:CA[1_554]  | 1.18                     | 1.02              |
| 4:2:357:ILE:CG2 | 4:7:232:SER:C[1_554]   | 1.18                     | 1.02              |
| 4:2:117:GLU:CD  | 4:7:236:LEU:O[1_554]   | 1.18                     | 1.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:325:MET:SD  | 4:8:166:TYR:CE2[1_554] | 1.18                     | 1.02              |
| 4:4:286:ASP:CB  | 4:9:270:GLU:OE1[1_554] | 1.18                     | 1.02              |
| 4:3:207:GLU:OE1 | 4:7:67:LEU:CA[1_554]   | 1.18                     | 1.02              |
| 4:2:287:ILE:N   | 4:7:270:GLU:OE1[1_554] | 1.18                     | 1.02              |
| 4:5:143:TYR:CA  | 4:9:372:ARG:CB[1_554]  | 1.18                     | 1.02              |
| 4:5:274:ILE:O   | 4:9:162:ASN:O[1_554]   | 1.18                     | 1.02              |
| 4:5:166:TYR:CE2 | 4:W:39:ARG:O[1_554]    | 1.18                     | 1.02              |
| 4:4:186:THR:CA  | 4:8:183:ARG:NE[1_554]  | 1.18                     | 1.02              |
| 4:4:110:LEU:C   | 4:9:192:ILE:CA[1_554]  | 1.18                     | 1.02              |
| 4:5:227:MET:CA  | 4:9:307:PRO:CA[1_554]  | 1.18                     | 1.02              |
| 4:4:151:ILE:CD1 | 4:8:172:PRO:N[1_554]   | 1.18                     | 1.02              |
| 4:3:306:TYR:C   | 4:7:11:ASP:OD2[1_554]  | 1.18                     | 1.02              |
| 4:3:271:SER:C   | 4:7:277:THR:OG1[1_554] | 1.18                     | 1.02              |
| 4:4:195:GLU:CG  | 4:8:189:LEU:CD2[1_554] | 1.18                     | 1.02              |
| 4:4:327:ILE:CB  | 4:8:148:THR:O[1_554]   | 1.18                     | 1.02              |
| 4:4:340:TRP:CH2 | 4:8:121:GLN:CG[1_554]  | 1.18                     | 1.02              |
| 4:4:371:HIS:C   | 4:9:230:ALA:CB[1_554]  | 1.18                     | 1.02              |
| 4:5:272:ALA:O   | 4:9:277:THR:CG2[1_554] | 1.18                     | 1.02              |
| 4:5:191:LYS:CB  | 4:9:187:ASP:N[1_554]   | 1.18                     | 1.02              |
| 4:5:193:LEU:C   | 4:9:209:VAL:C[1_554]   | 1.18                     | 1.02              |
| 4:3:341:ILE:CG1 | 4:7:120:THR:N[1_554]   | 1.18                     | 1.02              |
| 4:1:292:ASP:OD1 | 4:7:40:HIS:CB[1_554]   | 1.18                     | 1.02              |
| 4:3:27:PRO:N    | 4:7:122:ILE:CG1[1_554] | 1.18                     | 1.02              |
| 4:3:274:ILE:CD1 | 4:7:161:HIS:CG[1_554]  | 1.18                     | 1.02              |
| 4:4:136:ILE:O   | 4:8:113:LYS:CB[1_554]  | 1.18                     | 1.02              |
| 4:5:349:LEU:N   | 4:9:365:ALA:CA[1_554]  | 1.18                     | 1.02              |
| 4:5:219:VAL:CB  | 4:9:301:GLY:N[1_554]   | 1.18                     | 1.02              |
| 4:3:162:ASN:CA  | 4:7:110:LEU:CD2[1_554] | 1.18                     | 1.02              |
| 4:4:333:PRO:CA  | 4:8:105:LEU:N[1_554]   | 1.18                     | 1.02              |
| 4:3:267:ILE:CG1 | 4:7:180:LEU:CG[1_554]  | 1.18                     | 1.02              |
| 4:4:24:ASP:N    | 4:8:125:GLU:CG[1_554]  | 1.18                     | 1.02              |
| 4:3:262:PHE:CG  | 4:7:154:ASP:N[1_554]   | 1.19                     | 1.01              |
| 4:5:56:ASP:CB   | 4:9:37:ARG:CZ[1_554]   | 1.19                     | 1.01              |
| 4:4:369:ILE:O   | 4:9:229:THR:C[1_554]   | 1.19                     | 1.01              |
| 4:3:112:PRO:CD  | 4:8:193:LEU:CD1[1_554] | 1.19                     | 1.01              |
| 4:2:367:PRO:CA  | 4:7:235:SER:C[1_554]   | 1.19                     | 1.01              |
| 4:4:192:ILE:CG1 | 4:8:213:LYS:CE[1_554]  | 1.19                     | 1.01              |
| 4:4:372:ARG:CG  | 4:9:227:MET:CB[1_554]  | 1.19                     | 1.01              |
| 4:4:256:ARG:NH1 | 4:8:306:TYR:CE1[1_554] | 1.19                     | 1.01              |
| 4:5:345:ILE:CB  | 4:9:369:ILE:CG2[1_554] | 1.19                     | 1.01              |
| 4:3:72:GLU:O    | 4:8:198:TYR:C[1_554]   | 1.19                     | 1.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:366:GLY:C   | 4:9:234:SER:CB[1_554]  | 1.19                     | 1.01              |
| 4:4:269:MET:C   | 4:8:272:ALA:O[1_554]   | 1.19                     | 1.01              |
| 4:4:260:THR:N   | 4:8:155:SER:CB[1_554]  | 1.19                     | 1.01              |
| 4:5:343:GLY:C   | 4:9:367:PRO:CA[1_554]  | 1.19                     | 1.01              |
| 4:4:308:GLY:CA  | 4:8:338:SER:CA[1_554]  | 1.19                     | 1.01              |
| 4:5:268:GLY:CA  | 4:9:264:PRO:CB[1_554]  | 1.19                     | 1.01              |
| 4:4:325:MET:CG  | 4:8:166:TYR:CE2[1_554] | 1.19                     | 1.01              |
| 4:5:157:ASP:CA  | 4:9:72:GLU:O[1_554]    | 1.19                     | 1.01              |
| 4:4:172:PRO:CG  | 4:9:266:PHE:CB[1_554]  | 1.19                     | 1.01              |
| 4:3:214:GLU:O   | 4:7:16:LEU:C[1_554]    | 1.19                     | 1.01              |
| 4:3:161:HIS:CA  | 4:7:110:LEU:CD1[1_554] | 1.19                     | 1.01              |
| 4:4:204:ALA:C   | 4:8:62:ARG:CB[1_554]   | 1.19                     | 1.01              |
| 4:3:189:LEU:N   | 4:7:183:ARG:N[1_554]   | 1.19                     | 1.01              |
| 4:2:108:ALA:CA  | 4:7:195:GLU:C[1_554]   | 1.19                     | 1.01              |
| 4:5:312:ARG:NE  | 4:9:299:MET:CG[1_554]  | 1.19                     | 1.01              |
| 4:4:304:THR:OG1 | 4:8:107:GLU:O[1_554]   | 1.19                     | 1.01              |
| 4:4:153:LEU:C   | 4:8:109:PRO:O[1_554]   | 1.19                     | 1.01              |
| 4:5:294:TYR:CG  | 4:9:166:TYR:CB[1_554]  | 1.19                     | 1.01              |
| 4:3:220:ALA:CB  | 4:7:335:ARG:CB[1_554]  | 1.19                     | 1.01              |
| 4:3:280:ASN:CG  | 4:7:281:SER:O[1_554]   | 1.19                     | 1.01              |
| 4:1:326:LYS:CD  | 4:7:43:VAL:C[1_554]    | 1.19                     | 1.01              |
| 4:5:157:ASP:OD1 | 4:9:71:ILE:O[1_554]    | 1.19                     | 1.01              |
| 4:4:320:LEU:C   | 4:8:293:LEU:N[1_554]   | 1.19                     | 1.01              |
| 4:3:226:GLU:OE1 | 4:7:333:PRO:C[1_554]   | 1.19                     | 1.01              |
| 4:4:77:THR:O    | 4:9:246:GLN:NE2[1_554] | 1.19                     | 1.01              |
| 4:5:136:ILE:C   | 4:9:113:LYS:CG[1_554]  | 1.19                     | 1.01              |
| 4:4:310:ALA:CA  | 4:8:140:LEU:C[1_554]   | 1.19                     | 1.01              |
| 4:2:171:LEU:O   | 4:7:266:PHE:O[1_554]   | 1.19                     | 1.01              |
| 4:5:255:PHE:C   | 4:9:302:GLY:O[1_554]   | 1.19                     | 1.01              |
| 4:2:291:LYS:CB  | 4:8:64:ILE:CD1[1_554]  | 1.20                     | 1.00              |
| 4:4:274:ILE:O   | 4:8:162:ASN:C[1_554]   | 1.20                     | 1.00              |
| 4:4:319:ALA:CB  | 4:8:296:ASN:N[1_554]   | 1.20                     | 1.00              |
| 4:5:266:PHE:CD1 | 4:9:261:LEU:CB[1_554]  | 1.20                     | 1.00              |
| 4:4:117:GLU:C   | 4:9:237:GLU:CD[1_554]  | 1.20                     | 1.00              |
| 4:3:113:LYS:CG  | 4:8:254:ARG:N[1_554]   | 1.20                     | 1.00              |
| 4:4:208:ILE:CG1 | 4:8:59:GLN:CB[1_554]   | 1.20                     | 1.00              |
| 4:4:312:ARG:NE  | 4:8:299:MET:C[1_554]   | 1.20                     | 1.00              |
| 4:2:172:PRO:CG  | 4:7:266:PHE:CG[1_554]  | 1.20                     | 1.00              |
| 4:3:280:ASN:N   | 4:7:174:ALA:CB[1_554]  | 1.20                     | 1.00              |
| 4:3:157:ASP:OD1 | 4:7:72:GLU:N[1_554]    | 1.20                     | 1.00              |
| 4:5:19:ALA:CB   | 4:9:118:LYS:NZ[1_554]  | 1.20                     | 1.00              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:24:ASP:O    | 4:9:124:PHE:CG[1_554]  | 1.20                     | 1.00              |
| 4:5:185:LEU:CA  | 4:9:157:ASP:O[1_554]   | 1.20                     | 1.00              |
| 4:3:173:HIS:CA  | 4:8:267:ILE:CG2[1_554] | 1.20                     | 1.00              |
| 4:5:24:ASP:CA   | 4:9:124:PHE:CA[1_554]  | 1.20                     | 1.00              |
| 4:4:194:THR:CB  | 4:8:209:VAL:CG1[1_554] | 1.20                     | 1.00              |
| 4:5:279:TYR:OH  | 4:9:290:ARG:CG[1_554]  | 1.20                     | 1.00              |
| 4:3:297:ASN:OD1 | 4:7:170:ALA:N[1_554]   | 1.20                     | 1.00              |
| 4:4:334:GLU:CA  | 4:8:105:LEU:CG[1_554]  | 1.20                     | 1.00              |
| 4:2:173:HIS:CD2 | 4:7:264:PRO:O[1_554]   | 1.20                     | 1.00              |
| 4:4:185:LEU:N   | 4:8:158:GLY:CA[1_554]  | 1.20                     | 1.00              |
| 4:3:267:ILE:CB  | 4:7:180:LEU:CB[1_554]  | 1.20                     | 1.00              |
| 4:3:317:ILE:CA  | 4:7:150:GLY:C[1_554]   | 1.20                     | 1.00              |
| 4:5:310:ALA:CB  | 4:9:140:LEU:O[1_554]   | 1.20                     | 1.00              |
| 4:5:250:ILE:CG2 | 4:9:214:GLU:CD[1_554]  | 1.20                     | 1.00              |
| 4:4:137:GLN:CB  | 4:8:112:PRO:C[1_554]   | 1.20                     | 1.00              |
| 4:5:312:ARG:CG  | 4:9:299:MET:C[1_554]   | 1.20                     | 1.00              |
| 4:3:207:GLU:CD  | 4:7:67:LEU:C[1_554]    | 1.20                     | 1.00              |
| 4:3:26:ALA:CA   | 4:7:122:ILE:N[1_554]   | 1.20                     | 1.00              |
| 4:3:269:MET:C   | 4:7:272:ALA:O[1_554]   | 1.20                     | 1.00              |
| 4:5:320:LEU:CA  | 4:9:294:TYR:N[1_554]   | 1.20                     | 1.00              |
| 4:3:115:ASN:OD1 | 4:8:249:THR:O[1_554]   | 1.20                     | 1.00              |
| 4:3:319:ALA:O   | 4:7:292:ASP:O[1_554]   | 1.20                     | 1.00              |
| 4:5:198:TYR:CB  | 4:9:209:VAL:N[1_554]   | 1.20                     | 1.00              |
| 4:4:177:ARG:NH1 | 4:9:194:THR:CG2[1_554] | 1.20                     | 1.00              |
| 4:3:193:LEU:CG  | 4:7:210:ARG:CD[1_554]  | 1.21                     | 0.99              |
| 4:5:283:MET:SD  | 4:9:286:ASP:O[1_554]   | 1.21                     | 0.99              |
| 4:4:112:PRO:C   | 4:9:253:GLU:CG[1_554]  | 1.21                     | 0.99              |
| 4:5:178:LEU:O   | 4:9:177:ARG:CG[1_554]  | 1.21                     | 0.99              |
| 4:5:173:HIS:CB  | 4:V:267:ILE:CA[1_554]  | 1.21                     | 0.99              |
| 4:4:287:ILE:O   | 4:V:63:GLY:N[1_554]    | 1.21                     | 0.99              |
| 4:4:18:LYS:CG   | 4:8:79:TRP:CZ3[1_554]  | 1.21                     | 0.99              |
| 4:5:193:LEU:CB  | 4:9:210:ARG:CB[1_554]  | 1.21                     | 0.99              |
| 4:4:161:HIS:CA  | 4:8:110:LEU:CG[1_554]  | 1.21                     | 0.99              |
| 4:3:192:ILE:N   | 4:7:186:THR:OG1[1_554] | 1.21                     | 0.99              |
| 4:3:304:THR:OG1 | 4:7:107:GLU:C[1_554]   | 1.21                     | 0.99              |
| 4:5:304:THR:CA  | 4:9:137:GLN:OE1[1_554] | 1.21                     | 0.99              |
| 4:4:314:GLN:CB  | 4:8:142:LEU:C[1_554]   | 1.21                     | 0.99              |
| 4:5:31:PHE:CD1  | 4:9:80:ASP:N[1_554]    | 1.21                     | 0.99              |
| 4:4:293:LEU:CB  | 4:8:169:TYR:CE2[1_554] | 1.21                     | 0.99              |
| 4:4:139:VAL:O   | 4:8:371:HIS:NE2[1_554] | 1.21                     | 0.99              |
| 4:5:317:ILE:CG2 | 4:9:150:GLY:O[1_554]   | 1.21                     | 0.99              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:112:PRO:O   | 4:V:253:GLU:OE1[1_554] | 1.21                     | 0.99              |
| 4:3:154:ASP:N   | 4:7:110:LEU:N[1_554]   | 1.21                     | 0.99              |
| 4:3:369:ILE:C   | 4:8:229:THR:C[1_554]   | 1.21                     | 0.99              |
| 4:3:274:ILE:CG1 | 4:7:161:HIS:CB[1_554]  | 1.21                     | 0.99              |
| 4:5:310:ALA:CB  | 4:9:141:SER:N[1_554]   | 1.21                     | 0.99              |
| 4:4:111:ASN:CG  | 4:9:196:ARG:CG[1_554]  | 1.21                     | 0.99              |
| 4:3:294:TYR:OH  | 4:7:289:ILE:CD1[1_554] | 1.21                     | 0.99              |
| 4:5:310:ALA:O   | 4:9:142:LEU:CA[1_554]  | 1.21                     | 0.99              |
| 4:3:223:PHE:CG  | 4:7:304:THR:OG1[1_554] | 1.21                     | 0.99              |
| 4:4:194:THR:C   | 4:8:209:VAL:CG2[1_554] | 1.21                     | 0.99              |
| 4:5:18:LYS:O    | 4:9:118:LYS:CG[1_554]  | 1.21                     | 0.99              |
| 4:3:335:ARG:NH1 | 4:7:106:THR:CG2[1_554] | 1.21                     | 0.99              |
| 4:5:313:MET:CA  | 4:9:152:VAL:CG2[1_554] | 1.21                     | 0.99              |
| 4:4:188:TYR:CA  | 4:8:184:ASP:N[1_554]   | 1.21                     | 0.99              |
| 4:5:161:HIS:CB  | 4:9:110:LEU:CG[1_554]  | 1.21                     | 0.99              |
| 4:3:328:LYS:O   | 4:7:168:GLY:O[1_554]   | 1.21                     | 0.99              |
| 4:3:329:ILE:CA  | 4:7:139:VAL:CG1[1_554] | 1.21                     | 0.99              |
| 4:4:319:ALA:CB  | 4:8:296:ASN:CA[1_554]  | 1.21                     | 0.99              |
| 4:5:109:PRO:C   | 4:V:195:GLU:OE1[1_554] | 1.21                     | 0.99              |
| 4:3:272:ALA:C   | 4:7:277:THR:CG2[1_554] | 1.21                     | 0.99              |
| 4:5:300:SER:C   | 4:9:107:GLU:O[1_554]   | 1.21                     | 0.99              |
| 4:4:223:PHE:CA  | 4:8:335:ARG:NE[1_554]  | 1.21                     | 0.99              |
| 4:4:213:LYS:NZ  | 4:8:14:SER:C[1_554]    | 1.21                     | 0.99              |
| 4:5:314:GLN:OE1 | 4:9:147:ARG:CB[1_554]  | 1.21                     | 0.99              |
| 4:4:264:PRO:CB  | 4:8:178:LEU:CD2[1_554] | 1.22                     | 0.98              |
| 4:5:346:LEU:CB  | 4:9:368:SER:C[1_554]   | 1.22                     | 0.98              |
| 4:4:266:PHE:CB  | 4:8:261:LEU:CG[1_554]  | 1.22                     | 0.98              |
| 4:5:144:ALA:N   | 4:9:370:VAL:O[1_554]   | 1.22                     | 0.98              |
| 4:3:172:PRO:CG  | 4:8:266:PHE:CB[1_554]  | 1.22                     | 0.98              |
| 4:4:75:ILE:O    | 4:9:197:GLY:O[1_554]   | 1.22                     | 0.98              |
| 4:5:312:ARG:CZ  | 4:9:299:MET:SD[1_554]  | 1.22                     | 0.98              |
| 4:4:213:LYS:NZ  | 4:8:14:SER:CA[1_554]   | 1.22                     | 0.98              |
| 4:5:114:ALA:C   | 4:V:196:ARG:NH2[1_554] | 1.22                     | 0.98              |
| 4:5:368:SER:O   | 4:V:229:THR:C[1_554]   | 1.22                     | 0.98              |
| 4:5:164:PRO:CD  | 4:9:172:PRO:CG[1_554]  | 1.22                     | 0.98              |
| 4:4:320:LEU:CB  | 4:8:293:LEU:CA[1_554]  | 1.22                     | 0.98              |
| 4:3:193:LEU:C   | 4:7:210:ARG:N[1_554]   | 1.22                     | 0.98              |
| 4:5:280:ASN:O   | 4:9:284:LYS:O[1_554]   | 1.22                     | 0.98              |
| 4:3:109:PRO:CA  | 4:8:195:GLU:OE1[1_554] | 1.22                     | 0.98              |
| 4:5:242:LEU:CG  | 4:9:207:GLU:OE1[1_554] | 1.22                     | 0.98              |
| 4:5:335:ARG:C   | 4:9:106:THR:C[1_554]   | 1.22                     | 0.98              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:311:ASP:N   | 4:7:140:LEU:C[1_554]   | 1.22                     | 0.98              |
| 4:4:194:THR:O   | 4:8:209:VAL:CG2[1_554] | 1.22                     | 0.98              |
| 4:5:276:GLU:OE1 | 4:9:279:TYR:C[1_554]   | 1.22                     | 0.98              |
| 4:5:30:VAL:CB   | 4:9:83:GLU:N[1_554]    | 1.22                     | 0.98              |
| 4:3:304:THR:O   | 4:7:137:GLN:CG[1_554]  | 1.22                     | 0.98              |
| 4:1:288:ASP:C   | 4:7:39:ARG:NH1[1_554]  | 1.22                     | 0.98              |
| 4:5:221:LEU:CD1 | 4:9:332:PRO:CG[1_554]  | 1.22                     | 0.98              |
| 4:5:220:ALA:CA  | 4:9:335:ARG:CB[1_554]  | 1.22                     | 0.98              |
| 4:2:117:GLU:CB  | 4:7:237:GLU:C[1_554]   | 1.22                     | 0.98              |
| 4:4:207:GLU:OE2 | 4:8:67:LEU:CA[1_554]   | 1.22                     | 0.98              |
| 4:5:326:LYS:C   | 4:9:167:GLU:OE2[1_554] | 1.22                     | 0.98              |
| 4:5:340:TRP:CB  | 4:9:119:MET:N[1_554]   | 1.22                     | 0.98              |
| 4:3:186:THR:CB  | 4:7:183:ARG:NH2[1_554] | 1.22                     | 0.98              |
| 4:4:329:ILE:CG2 | 4:8:139:VAL:CB[1_554]  | 1.22                     | 0.98              |
| 4:5:17:VAL:CA   | 4:9:79:TRP:CD1[1_554]  | 1.22                     | 0.98              |
| 4:5:193:LEU:CB  | 4:9:210:ARG:CA[1_554]  | 1.22                     | 0.98              |
| 4:2:72:GLU:O    | 4:7:198:TYR:C[1_554]   | 1.22                     | 0.98              |
| 4:4:367:PRO:C   | 4:9:236:LEU:CD2[1_554] | 1.22                     | 0.98              |
| 4:4:75:ILE:N    | 4:9:197:GLY:C[1_554]   | 1.22                     | 0.98              |
| 4:2:75:ILE:N    | 4:7:198:TYR:CA[1_554]  | 1.22                     | 0.98              |
| 4:4:30:VAL:C    | 4:8:79:TRP:C[1_554]    | 1.22                     | 0.98              |
| 4:5:274:ILE:CB  | 4:9:161:HIS:C[1_554]   | 1.22                     | 0.98              |
| 4:4:114:ALA:CB  | 4:9:250:ILE:O[1_554]   | 1.22                     | 0.98              |
| 4:3:194:THR:C   | 4:7:209:VAL:CG1[1_554] | 1.22                     | 0.98              |
| 4:3:25:ASP:OD1  | 4:7:124:PHE:CG[1_554]  | 1.22                     | 0.98              |
| 4:2:357:ILE:CG2 | 4:7:232:SER:O[1_554]   | 1.22                     | 0.98              |
| 4:4:308:GLY:CA  | 4:8:339:VAL:N[1_554]   | 1.22                     | 0.98              |
| 4:2:109:PRO:CB  | 4:7:195:GLU:OE2[1_554] | 1.22                     | 0.98              |
| 4:3:276:GLU:CD  | 4:7:278:THR:C[1_554]   | 1.22                     | 0.98              |
| 4:3:26:ALA:CB   | 4:7:122:ILE:O[1_554]   | 1.22                     | 0.98              |
| 4:5:277:THR:CA  | 4:9:281:SER:OG[1_554]  | 1.22                     | 0.98              |
| 4:4:154:ASP:OD2 | 4:8:111:ASN:CA[1_554]  | 1.22                     | 0.98              |
| 4:4:199:SER:N   | 4:8:206:ARG:C[1_554]   | 1.22                     | 0.98              |
| 4:5:28:ARG:CD   | 4:9:126:THR:CB[1_554]  | 1.22                     | 0.98              |
| 4:5:193:LEU:O   | 4:9:210:ARG:N[1_554]   | 1.22                     | 0.98              |
| 4:2:371:HIS:CE1 | 4:7:252:ASN:O[1_554]   | 1.22                     | 0.98              |
| 4:4:299:MET:CA  | 4:8:136:ILE:CB[1_554]  | 1.22                     | 0.98              |
| 4:5:255:PHE:CA  | 4:9:302:GLY:O[1_554]   | 1.23                     | 0.97              |
| 4:5:276:GLU:C   | 4:9:281:SER:OG[1_554]  | 1.23                     | 0.97              |
| 4:3:24:ASP:CB   | 4:7:125:GLU:CB[1_554]  | 1.23                     | 0.97              |
| 4:5:343:GLY:O   | 4:9:367:PRO:CB[1_554]  | 1.23                     | 0.97              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:74:GLY:O    | 4:7:197:GLY:N[1_554]   | 1.23                     | 0.97              |
| 4:5:215:LYS:CA  | 4:9:30:VAL:CG1[1_554]  | 1.23                     | 0.97              |
| 4:5:15:GLY:CA   | 4:9:77:THR:CB[1_554]   | 1.23                     | 0.97              |
| 4:5:299:MET:O   | 4:9:135:ALA:C[1_554]   | 1.23                     | 0.97              |
| 4:4:108:ALA:CB  | 4:9:195:GLU:C[1_554]   | 1.23                     | 0.97              |
| 4:3:30:VAL:CG1  | 4:7:79:TRP:CA[1_554]   | 1.23                     | 0.97              |
| 4:4:215:LYS:C   | 4:8:30:VAL:CG1[1_554]  | 1.23                     | 0.97              |
| 4:4:18:LYS:N    | 4:8:79:TRP:CD1[1_554]  | 1.23                     | 0.97              |
| 4:4:294:TYR:CD1 | 4:8:166:TYR:CA[1_554]  | 1.23                     | 0.97              |
| 4:5:173:HIS:ND1 | 4:V:266:PHE:N[1_554]   | 1.23                     | 0.97              |
| 4:3:191:LYS:CA  | 4:7:186:THR:C[1_554]   | 1.23                     | 0.97              |
| 4:4:222:ASP:N   | 4:8:332:PRO:CD[1_554]  | 1.23                     | 0.97              |
| 4:5:278:THR:OG1 | 4:9:163:VAL:CA[1_554]  | 1.23                     | 0.97              |
| 4:5:136:ILE:O   | 4:9:113:LYS:CG[1_554]  | 1.23                     | 0.97              |
| 4:3:337:TYR:N   | 4:7:119:MET:SD[1_554]  | 1.23                     | 0.97              |
| 4:4:316:GLU:CB  | 4:8:151:ILE:O[1_554]   | 1.23                     | 0.97              |
| 4:4:26:ALA:C    | 4:8:122:ILE:C[1_554]   | 1.23                     | 0.97              |
| 4:3:196:ARG:CB  | 4:7:211:ASP:N[1_554]   | 1.23                     | 0.97              |
| 4:3:153:LEU:C   | 4:7:109:PRO:C[1_554]   | 1.23                     | 0.97              |
| 4:5:310:ALA:C   | 4:9:141:SER:O[1_554]   | 1.23                     | 0.97              |
| 4:3:199:SER:CA  | 4:7:206:ARG:CB[1_554]  | 1.23                     | 0.97              |
| 4:5:316:GLU:OE2 | 4:9:297:ASN:ND2[1_554] | 1.23                     | 0.97              |
| 4:4:270:GLU:N   | 4:8:272:ALA:O[1_554]   | 1.23                     | 0.97              |
| 4:4:180:LEU:CA  | 4:8:179:ASP:OD1[1_554] | 1.23                     | 0.97              |
| 4:4:267:ILE:CD1 | 4:8:180:LEU:N[1_554]   | 1.23                     | 0.97              |
| 4:4:177:ARG:NH1 | 4:9:194:THR:OG1[1_554] | 1.23                     | 0.97              |
| 4:5:321:ALA:O   | 4:9:292:ASP:N[1_554]   | 1.23                     | 0.97              |
| 4:3:326:LYS:O   | 4:7:167:GLU:CA[1_554]  | 1.23                     | 0.97              |
| 4:4:262:PHE:CB  | 4:8:153:LEU:CG[1_554]  | 1.23                     | 0.97              |
| 4:5:211:ASP:CG  | 4:9:32:PRO:N[1_554]    | 1.23                     | 0.97              |
| 4:5:340:TRP:N   | 4:9:116:ARG:O[1_554]   | 1.23                     | 0.97              |
| 4:3:371:HIS:N   | 4:8:230:ALA:CA[1_554]  | 1.23                     | 0.97              |
| 4:4:311:ASP:OD1 | 4:8:144:ALA:CB[1_554]  | 1.23                     | 0.97              |
| 4:4:223:PHE:CD2 | 4:8:304:THR:OG1[1_554] | 1.23                     | 0.97              |
| 4:5:213:LYS:CE  | 4:9:15:GLY:N[1_554]    | 1.23                     | 0.97              |
| 4:2:357:ILE:CG1 | 4:7:232:SER:CA[1_554]  | 1.23                     | 0.97              |
| 4:3:226:GLU:OE1 | 4:7:333:PRO:O[1_554]   | 1.23                     | 0.97              |
| 4:3:262:PHE:CD2 | 4:7:153:LEU:O[1_554]   | 1.23                     | 0.97              |
| 4:5:221:LEU:C   | 4:9:331:ALA:CA[1_554]  | 1.23                     | 0.97              |
| 4:2:116:ARG:CD  | 4:7:252:ASN:CB[1_554]  | 1.23                     | 0.97              |
| 4:5:319:ALA:O   | 4:9:294:TYR:CA[1_554]  | 1.23                     | 0.97              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:329:ILE:CG2 | 4:7:139:VAL:CA[1_554]  | 1.23                     | 0.97              |
| 4:4:186:THR:C   | 4:8:183:ARG:CG[1_554]  | 1.23                     | 0.97              |
| 4:3:293:LEU:C   | 4:7:169:TYR:CG[1_554]  | 1.23                     | 0.97              |
| 4:3:248:ILE:CD1 | 4:7:207:GLU:CG[1_554]  | 1.23                     | 0.97              |
| 4:3:193:LEU:CD2 | 4:7:210:ARG:CD[1_554]  | 1.24                     | 0.96              |
| 4:2:289:ILE:N   | 4:8:39:ARG:NH1[1_554]  | 1.24                     | 0.96              |
| 4:4:178:LEU:CG  | 4:8:177:ARG:N[1_554]   | 1.24                     | 0.96              |
| 4:3:185:LEU:N   | 4:7:158:GLY:CA[1_554]  | 1.24                     | 0.96              |
| 4:4:211:ASP:CA  | 4:8:32:PRO:CA[1_554]   | 1.24                     | 0.96              |
| 4:5:263:GLN:CA  | 4:9:274:ILE:CB[1_554]  | 1.24                     | 0.96              |
| 4:1:292:ASP:CB  | 4:7:40:HIS:CB[1_554]   | 1.24                     | 0.96              |
| 4:4:18:LYS:CD   | 4:8:79:TRP:CD2[1_554]  | 1.24                     | 0.96              |
| 4:5:156:GLY:C   | 4:9:74:GLY:C[1_554]    | 1.24                     | 0.96              |
| 4:4:116:ARG:CG  | 4:9:252:ASN:OD1[1_554] | 1.24                     | 0.96              |
| 4:4:143:TYR:CE2 | 4:8:368:SER:C[1_554]   | 1.24                     | 0.96              |
| 4:3:300:SER:N   | 4:7:107:GLU:CG[1_554]  | 1.24                     | 0.96              |
| 4:3:211:ASP:C   | 4:7:32:PRO:CB[1_554]   | 1.24                     | 0.96              |
| 4:5:195:GLU:CG  | 4:9:189:LEU:CD1[1_554] | 1.24                     | 0.96              |
| 4:5:369:ILE:O   | 4:V:228:ALA:O[1_554]   | 1.24                     | 0.96              |
| 4:4:195:GLU:CG  | 4:8:189:LEU:CG[1_554]  | 1.24                     | 0.96              |
| 4:5:341:ILE:CD1 | 4:9:132:MET:CE[1_554]  | 1.24                     | 0.96              |
| 4:3:15:GLY:C    | 4:7:77:THR:CG2[1_554]  | 1.24                     | 0.96              |
| 4:5:183:ARG:CZ  | 4:9:72:GLU:OE1[1_554]  | 1.24                     | 0.96              |
| 4:5:28:ARG:CG   | 4:9:126:THR:CG2[1_554] | 1.24                     | 0.96              |
| 4:5:252:ASN:OD1 | 4:9:215:LYS:C[1_554]   | 1.24                     | 0.96              |
| 4:3:227:MET:SD  | 4:7:305:MET:C[1_554]   | 1.24                     | 0.96              |
| 4:5:18:LYS:N    | 4:9:79:TRP:CE3[1_554]  | 1.24                     | 0.96              |
| 4:3:186:THR:CB  | 4:7:183:ARG:NE[1_554]  | 1.24                     | 0.96              |
| 4:3:313:MET:CB  | 4:7:138:ALA:O[1_554]   | 1.24                     | 0.96              |
| 4:4:143:TYR:N   | 4:8:371:HIS:C[1_554]   | 1.24                     | 0.96              |
| 4:5:318:THR:OG1 | 4:9:296:ASN:OD1[1_554] | 1.24                     | 0.96              |
| 4:4:221:LEU:O   | 4:8:332:PRO:CA[1_554]  | 1.24                     | 0.96              |
| 4:3:188:TYR:C   | 4:7:183:ARG:CA[1_554]  | 1.24                     | 0.96              |
| 4:3:208:ILE:CA  | 4:7:59:GLN:NE2[1_554]  | 1.24                     | 0.96              |
| 4:4:266:PHE:CG  | 4:8:261:LEU:CG[1_554]  | 1.24                     | 0.96              |
| 4:3:304:THR:CG2 | 4:7:108:ALA:CA[1_554]  | 1.24                     | 0.96              |
| 4:4:218:TYR:CB  | 4:8:336:LYS:C[1_554]   | 1.24                     | 0.96              |
| 4:5:321:ALA:O   | 4:9:292:ASP:CA[1_554]  | 1.24                     | 0.96              |
| 4:3:311:ASP:CA  | 4:7:141:SER:O[1_554]   | 1.24                     | 0.96              |
| 4:3:274:ILE:C   | 4:7:162:ASN:O[1_554]   | 1.24                     | 0.96              |
| 4:3:326:LYS:CA  | 4:7:167:GLU:CD[1_554]  | 1.24                     | 0.96              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:196:ARG:CA  | 4:7:212:ILE:N[1_554]   | 1.24                     | 0.96              |
| 4:5:243:PRO:CA  | 4:9:60:SER:CB[1_554]   | 1.24                     | 0.96              |
| 4:4:273:GLY:CA  | 4:8:162:ASN:CG[1_554]  | 1.24                     | 0.96              |
| 4:3:333:PRO:C   | 4:7:105:LEU:CB[1_554]  | 1.24                     | 0.96              |
| 4:5:188:TYR:CZ  | 4:9:185:LEU:CG[1_554]  | 1.24                     | 0.96              |
| 4:3:218:TYR:OH  | 4:7:27:PRO:CG[1_554]   | 1.24                     | 0.96              |
| 4:3:317:ILE:CD1 | 4:7:165:ILE:CB[1_554]  | 1.24                     | 0.96              |
| 4:3:185:LEU:C   | 4:7:157:ASP:O[1_554]   | 1.24                     | 0.96              |
| 4:4:287:ILE:C   | 4:V:63:GLY:CA[1_554]   | 1.24                     | 0.96              |
| 4:3:294:TYR:CG  | 4:7:166:TYR:CB[1_554]  | 1.25                     | 0.95              |
| 4:5:340:TRP:CZ3 | 4:9:120:THR:C[1_554]   | 1.25                     | 0.95              |
| 4:3:18:LYS:CE   | 4:7:79:TRP:NE1[1_554]  | 1.25                     | 0.95              |
| 4:4:340:TRP:CH2 | 4:8:121:GLN:CB[1_554]  | 1.25                     | 0.95              |
| 4:4:205:GLU:CA  | 4:8:62:ARG:CD[1_554]   | 1.25                     | 0.95              |
| 4:3:227:MET:CG  | 4:7:305:MET:O[1_554]   | 1.25                     | 0.95              |
| 4:4:317:ILE:CD1 | 4:8:165:ILE:C[1_554]   | 1.25                     | 0.95              |
| 4:3:341:ILE:CG1 | 4:7:120:THR:CB[1_554]  | 1.25                     | 0.95              |
| 4:3:218:TYR:CD1 | 4:7:337:TYR:CE1[1_554] | 1.25                     | 0.95              |
| 4:5:262:PHE:CE1 | 4:9:153:LEU:C[1_554]   | 1.25                     | 0.95              |
| 4:4:75:ILE:CG2  | 4:9:198:TYR:CG[1_554]  | 1.25                     | 0.95              |
| 4:4:191:LYS:CD  | 4:8:185:LEU:C[1_554]   | 1.25                     | 0.95              |
| 4:4:274:ILE:CD1 | 4:8:161:HIS:CB[1_554]  | 1.25                     | 0.95              |
| 4:5:112:PRO:O   | 4:V:253:GLU:CD[1_554]  | 1.25                     | 0.95              |
| 4:3:281:SER:OG  | 4:7:173:HIS:CA[1_554]  | 1.25                     | 0.95              |
| 4:3:109:PRO:CB  | 4:8:195:GLU:CD[1_554]  | 1.25                     | 0.95              |
| 4:4:214:GLU:CD  | 4:8:33:SER:CB[1_554]   | 1.25                     | 0.95              |
| 4:4:26:ALA:CB   | 4:8:122:ILE:C[1_554]   | 1.25                     | 0.95              |
| 4:5:337:TYR:CE1 | 4:9:86:TRP:CH2[1_554]  | 1.25                     | 0.95              |
| 4:4:218:TYR:CE2 | 4:8:337:TYR:CG[1_554]  | 1.25                     | 0.95              |
| 4:5:277:THR:CG2 | 4:9:176:MET:N[1_554]   | 1.25                     | 0.95              |
| 4:5:369:ILE:CG1 | 4:V:232:SER:OG[1_554]  | 1.25                     | 0.95              |
| 4:3:336:LYS:NZ  | 4:7:86:TRP:CG[1_554]   | 1.25                     | 0.95              |
| 4:4:25:ASP:CA   | 4:8:124:PHE:CB[1_554]  | 1.25                     | 0.95              |
| 4:5:335:ARG:NH2 | 4:9:339:VAL:CG1[1_554] | 1.25                     | 0.95              |
| 4:5:106:THR:CG2 | 4:9:114:ALA:C[1_554]   | 1.25                     | 0.95              |
| 4:3:31:PHE:O    | 4:7:78:ASN:OD1[1_554]  | 1.25                     | 0.95              |
| 4:5:308:GLY:CA  | 4:9:338:SER:CA[1_554]  | 1.25                     | 0.95              |
| 4:3:314:GLN:O   | 4:7:142:LEU:CD2[1_554] | 1.25                     | 0.95              |
| 4:3:109:PRO:CA  | 4:8:195:GLU:CG[1_554]  | 1.25                     | 0.95              |
| 4:5:293:LEU:CG  | 4:9:169:TYR:CE2[1_554] | 1.25                     | 0.95              |
| 4:3:193:LEU:CA  | 4:7:210:ARG:CA[1_554]  | 1.25                     | 0.95              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:215:LYS:NZ  | 4:9:31:PHE:CB[1_554]   | 1.25                     | 0.95              |
| 4:5:294:TYR:CD2 | 4:9:166:TYR:CG[1_554]  | 1.25                     | 0.95              |
| 4:5:327:ILE:CB  | 4:9:149:THR:CA[1_554]  | 1.25                     | 0.95              |
| 4:3:369:ILE:O   | 4:8:229:THR:O[1_554]   | 1.25                     | 0.95              |
| 4:5:279:TYR:N   | 4:9:164:PRO:CB[1_554]  | 1.25                     | 0.95              |
| 4:2:108:ALA:CB  | 4:7:196:ARG:N[1_554]   | 1.25                     | 0.95              |
| 4:5:312:ARG:NH2 | 4:9:299:MET:SD[1_554]  | 1.25                     | 0.95              |
| 4:5:181:ALA:CA  | 4:9:159:VAL:CG1[1_554] | 1.25                     | 0.95              |
| 4:3:218:TYR:CE1 | 4:7:337:TYR:CE1[1_554] | 1.25                     | 0.95              |
| 4:5:150:GLY:C   | 4:9:169:TYR:CE1[1_554] | 1.25                     | 0.95              |
| 4:4:193:LEU:CA  | 4:8:210:ARG:CB[1_554]  | 1.25                     | 0.95              |
| 4:5:59:GLN:CD   | 4:9:68:LYS:CG[1_554]   | 1.25                     | 0.95              |
| 4:4:200:PHE:CA  | 4:8:206:ARG:CG[1_554]  | 1.25                     | 0.95              |
| 4:3:145:SER:OG  | 4:7:372:ARG:CZ[1_554]  | 1.25                     | 0.95              |
| 4:3:370:VAL:N   | 4:8:229:THR:O[1_554]   | 1.25                     | 0.95              |
| 1:D:542:PHE:CE2 | 4:5:328:LYS:NZ[1_556]  | 1.26                     | 0.94              |
| 4:5:283:MET:CG  | 4:9:286:ASP:C[1_554]   | 1.26                     | 0.94              |
| 4:5:262:PHE:CG  | 4:9:153:LEU:CB[1_554]  | 1.26                     | 0.94              |
| 4:5:276:GLU:OE2 | 4:9:278:THR:C[1_554]   | 1.26                     | 0.94              |
| 4:4:174:ALA:O   | 4:8:173:HIS:CB[1_554]  | 1.26                     | 0.94              |
| 4:5:294:TYR:CA  | 4:9:166:TYR:O[1_554]   | 1.26                     | 0.94              |
| 4:3:26:ALA:N    | 4:7:121:GLN:O[1_554]   | 1.26                     | 0.94              |
| 4:3:277:THR:CA  | 4:7:174:ALA:O[1_554]   | 1.26                     | 0.94              |
| 4:3:259:GLU:CD  | 4:7:304:THR:CA[1_554]  | 1.26                     | 0.94              |
| 4:4:111:ASN:CA  | 4:9:192:ILE:O[1_554]   | 1.26                     | 0.94              |
| 4:3:117:GLU:CD  | 4:8:236:LEU:O[1_554]   | 1.26                     | 0.94              |
| 4:5:319:ALA:O   | 4:9:295:ALA:N[1_554]   | 1.26                     | 0.94              |
| 4:3:259:GLU:CG  | 4:7:304:THR:CA[1_554]  | 1.26                     | 0.94              |
| 4:4:173:HIS:CG  | 4:9:267:ILE:N[1_554]   | 1.26                     | 0.94              |
| 4:5:269:MET:O   | 4:9:272:ALA:O[1_554]   | 1.26                     | 0.94              |
| 4:5:337:TYR:OH  | 4:9:86:TRP:NE1[1_554]  | 1.26                     | 0.94              |
| 4:4:304:THR:O   | 4:8:137:GLN:CG[1_554]  | 1.26                     | 0.94              |
| 4:3:223:PHE:C   | 4:7:335:ARG:NH2[1_554] | 1.26                     | 0.94              |
| 4:1:288:ASP:CA  | 4:7:39:ARG:NH1[1_554]  | 1.26                     | 0.94              |
| 4:5:347:ALA:CB  | 4:9:367:PRO:CD[1_554]  | 1.26                     | 0.94              |
| 4:4:211:ASP:O   | 4:8:32:PRO:CA[1_554]   | 1.26                     | 0.94              |
| 4:4:56:ASP:OD1  | 4:8:80:ASP:OD1[1_554]  | 1.26                     | 0.94              |
| 4:5:305:MET:C   | 4:9:11:ASP:OD2[1_554]  | 1.26                     | 0.94              |
| 4:4:304:THR:CA  | 4:8:137:GLN:OE1[1_554] | 1.26                     | 0.94              |
| 4:2:172:PRO:CD  | 4:7:266:PHE:CG[1_554]  | 1.26                     | 0.94              |
| 4:2:74:GLY:O    | 4:7:197:GLY:C[1_554]   | 1.26                     | 0.94              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:326:LYS:CB  | 4:8:167:GLU:OE1[1_554] | 1.26                     | 0.94              |
| 4:5:157:ASP:O   | 4:9:73:HIS:N[1_554]    | 1.26                     | 0.94              |
| 4:3:187:ASP:N   | 4:7:183:ARG:CG[1_554]  | 1.26                     | 0.94              |
| 4:5:26:ALA:N    | 4:9:123:MET:CB[1_554]  | 1.26                     | 0.94              |
| 4:3:259:GLU:N   | 4:7:155:SER:O[1_554]   | 1.26                     | 0.94              |
| 4:3:214:GLU:CA  | 4:7:16:LEU:C[1_554]    | 1.26                     | 0.94              |
| 4:1:292:ASP:CG  | 4:7:40:HIS:CA[1_554]   | 1.26                     | 0.94              |
| 4:3:275:HIS:CA  | 4:7:163:VAL:N[1_554]   | 1.26                     | 0.94              |
| 4:4:199:SER:C   | 4:8:206:ARG:CB[1_554]  | 1.26                     | 0.94              |
| 4:4:144:ALA:CA  | 4:8:370:VAL:CA[1_554]  | 1.26                     | 0.94              |
| 4:3:173:HIS:CB  | 4:8:267:ILE:CB[1_554]  | 1.26                     | 0.94              |
| 4:4:200:PHE:N   | 4:8:206:ARG:CB[1_554]  | 1.26                     | 0.94              |
| 4:3:24:ASP:CA   | 4:7:125:GLU:CD[1_554]  | 1.26                     | 0.94              |
| 4:3:317:ILE:N   | 4:7:150:GLY:C[1_554]   | 1.26                     | 0.94              |
| 4:3:300:SER:CA  | 4:7:107:GLU:CD[1_554]  | 1.26                     | 0.94              |
| 4:4:340:TRP:CZ2 | 4:8:121:GLN:CD[1_554]  | 1.26                     | 0.94              |
| 4:3:294:TYR:CB  | 4:7:166:TYR:O[1_554]   | 1.26                     | 0.94              |
| 4:5:26:ALA:N    | 4:9:123:MET:CA[1_554]  | 1.27                     | 0.93              |
| 4:3:116:ARG:O   | 4:8:237:GLU:OE2[1_554] | 1.27                     | 0.93              |
| 4:5:113:LYS:N   | 4:V:253:GLU:CD[1_554]  | 1.27                     | 0.93              |
| 4:5:348:SER:N   | 4:9:366:GLY:N[1_554]   | 1.27                     | 0.93              |
| 4:4:117:GLU:OE1 | 4:9:236:LEU:O[1_554]   | 1.27                     | 0.93              |
| 4:5:343:GLY:C   | 4:9:367:PRO:CB[1_554]  | 1.27                     | 0.93              |
| 4:3:312:ARG:N   | 4:7:141:SER:C[1_554]   | 1.27                     | 0.93              |
| 4:3:188:TYR:OH  | 4:7:185:LEU:CD2[1_554] | 1.27                     | 0.93              |
| 4:2:116:ARG:CD  | 4:7:252:ASN:OD1[1_554] | 1.27                     | 0.93              |
| 4:4:188:TYR:CD2 | 4:8:182:GLY:CA[1_554]  | 1.27                     | 0.93              |
| 4:5:255:PHE:CG  | 4:9:305:MET:CA[1_554]  | 1.27                     | 0.93              |
| 4:5:310:ALA:C   | 4:9:142:LEU:N[1_554]   | 1.27                     | 0.93              |
| 4:4:309:ILE:CA  | 4:8:141:SER:OG[1_554]  | 1.27                     | 0.93              |
| 4:4:335:ARG:NE  | 4:8:106:THR:CB[1_554]  | 1.27                     | 0.93              |
| 4:3:19:ALA:N    | 4:7:118:LYS:NZ[1_554]  | 1.27                     | 0.93              |
| 4:4:294:TYR:C   | 4:8:166:TYR:O[1_554]   | 1.27                     | 0.93              |
| 4:3:304:THR:C   | 4:7:137:GLN:CD[1_554]  | 1.27                     | 0.93              |
| 4:3:173:HIS:CA  | 4:8:267:ILE:CB[1_554]  | 1.27                     | 0.93              |
| 4:3:340:TRP:N   | 4:7:118:LYS:N[1_554]   | 1.27                     | 0.93              |
| 4:3:277:THR:O   | 4:7:175:ILE:N[1_554]   | 1.27                     | 0.93              |
| 4:3:185:LEU:CB  | 4:7:158:GLY:CA[1_554]  | 1.27                     | 0.93              |
| 4:5:249:THR:OG1 | 4:9:215:LYS:NZ[1_554]  | 1.27                     | 0.93              |
| 4:1:289:ILE:N   | 4:7:39:ARG:NE[1_554]   | 1.27                     | 0.93              |
| 4:5:112:PRO:CA  | 4:V:253:GLU:CG[1_554]  | 1.27                     | 0.93              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:293:LEU:C   | 4:7:169:TYR:CD2[1_554] | 1.27                     | 0.93              |
| 4:3:274:ILE:CD1 | 4:7:161:HIS:CD2[1_554] | 1.27                     | 0.93              |
| 4:4:337:TYR:CE2 | 4:8:86:TRP:CZ3[1_554]  | 1.27                     | 0.93              |
| 4:4:318:THR:CA  | 4:8:149:THR:C[1_554]   | 1.27                     | 0.93              |
| 4:5:340:TRP:CG  | 4:9:119:MET:N[1_554]   | 1.27                     | 0.93              |
| 4:5:341:ILE:CG2 | 4:9:132:MET:SD[1_554]  | 1.27                     | 0.93              |
| 4:3:75:ILE:CA   | 4:8:198:TYR:N[1_554]   | 1.27                     | 0.93              |
| 4:4:116:ARG:N   | 4:9:196:ARG:NH1[1_554] | 1.27                     | 0.93              |
| 4:2:367:PRO:CD  | 4:7:235:SER:O[1_554]   | 1.27                     | 0.93              |
| 4:4:178:LEU:CG  | 4:8:177:ARG:C[1_554]   | 1.27                     | 0.93              |
| 4:4:309:ILE:CB  | 4:8:339:VAL:CG2[1_554] | 1.27                     | 0.93              |
| 4:5:294:TYR:CB  | 4:9:166:TYR:CG[1_554]  | 1.27                     | 0.93              |
| 4:3:30:VAL:O    | 4:7:80:ASP:N[1_554]    | 1.27                     | 0.93              |
| 4:3:261:LEU:O   | 4:7:161:HIS:N[1_554]   | 1.27                     | 0.93              |
| 4:5:160:THR:CB  | 4:9:161:HIS:NE2[1_554] | 1.27                     | 0.93              |
| 4:2:117:GLU:CA  | 4:7:237:GLU:CA[1_554]  | 1.27                     | 0.93              |
| 4:4:173:HIS:CB  | 4:9:267:ILE:CB[1_554]  | 1.27                     | 0.93              |
| 4:2:367:PRO:C   | 4:7:236:LEU:CA[1_554]  | 1.27                     | 0.93              |
| 4:2:173:HIS:CA  | 4:7:267:ILE:CB[1_554]  | 1.27                     | 0.93              |
| 4:5:21:PHE:CA   | 4:9:125:GLU:CD[1_554]  | 1.27                     | 0.93              |
| 4:4:109:PRO:CA  | 4:9:195:GLU:CG[1_554]  | 1.27                     | 0.93              |
| 4:4:344:SER:C   | 4:8:367:PRO:N[1_554]   | 1.27                     | 0.93              |
| 4:4:220:ALA:CB  | 4:8:335:ARG:CG[1_554]  | 1.28                     | 0.92              |
| 4:3:265:SER:O   | 4:7:261:LEU:CA[1_554]  | 1.28                     | 0.92              |
| 4:3:193:LEU:CD1 | 4:7:210:ARG:NE[1_554]  | 1.28                     | 0.92              |
| 4:4:258:PRO:CA  | 4:8:155:SER:C[1_554]   | 1.28                     | 0.92              |
| 4:4:257:CYS:CA  | 4:8:303:THR:OG1[1_554] | 1.28                     | 0.92              |
| 4:3:194:THR:CB  | 4:7:209:VAL:CG1[1_554] | 1.28                     | 0.92              |
| 4:3:327:ILE:N   | 4:7:167:GLU:CA[1_554]  | 1.28                     | 0.92              |
| 4:4:273:GLY:C   | 4:8:162:ASN:CB[1_554]  | 1.28                     | 0.92              |
| 4:3:194:THR:O   | 4:7:209:VAL:CA[1_554]  | 1.28                     | 0.92              |
| 4:4:270:GLU:CB  | 4:8:272:ALA:N[1_554]   | 1.28                     | 0.92              |
| 4:5:62:ARG:NH1  | 4:9:67:LEU:N[1_554]    | 1.28                     | 0.92              |
| 4:3:336:LYS:NZ  | 4:7:86:TRP:NE1[1_554]  | 1.28                     | 0.92              |
| 4:2:288:ASP:OD1 | 4:8:65:LEU:O[1_554]    | 1.28                     | 0.92              |
| 4:5:270:GLU:C   | 4:9:272:ALA:CA[1_554]  | 1.28                     | 0.92              |
| 4:3:368:SER:CA  | 4:8:236:LEU:CB[1_554]  | 1.28                     | 0.92              |
| 4:5:340:TRP:CZ2 | 4:9:122:ILE:N[1_554]   | 1.28                     | 0.92              |
| 4:4:279:TYR:CD1 | 4:8:293:LEU:CD2[1_554] | 1.28                     | 0.92              |
| 4:2:113:LYS:CD  | 4:7:254:ARG:C[1_554]   | 1.28                     | 0.92              |
| 4:5:274:ILE:CD1 | 4:9:161:HIS:CB[1_554]  | 1.28                     | 0.92              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:371:HIS:CE1 | 4:8:252:ASN:O[1_554]   | 1.28                     | 0.92              |
| 4:5:342:GLY:CA  | 4:9:370:VAL:CG1[1_554] | 1.28                     | 0.92              |
| 4:5:188:TYR:CG  | 4:9:181:ALA:O[1_554]   | 1.28                     | 0.92              |
| 4:4:222:ASP:CB  | 4:8:331:ALA:O[1_554]   | 1.28                     | 0.92              |
| 4:4:112:PRO:CA  | 4:9:253:GLU:CG[1_554]  | 1.28                     | 0.92              |
| 4:5:315:LYS:O   | 4:9:296:ASN:CA[1_554]  | 1.28                     | 0.92              |
| 4:3:222:ASP:CG  | 4:7:331:ALA:O[1_554]   | 1.28                     | 0.92              |
| 4:4:345:ILE:CB  | 4:8:366:GLY:O[1_554]   | 1.28                     | 0.92              |
| 4:4:139:VAL:C   | 4:8:371:HIS:CE1[1_554] | 1.28                     | 0.92              |
| 4:4:310:ALA:C   | 4:8:141:SER:N[1_554]   | 1.28                     | 0.92              |
| 4:5:317:ILE:CG1 | 4:9:150:GLY:O[1_554]   | 1.28                     | 0.92              |
| 4:4:166:TYR:CD1 | 4:V:40:HIS:ND1[1_554]  | 1.28                     | 0.92              |
| 4:3:268:GLY:C   | 4:7:264:PRO:CB[1_554]  | 1.28                     | 0.92              |
| 4:3:74:GLY:C    | 4:8:197:GLY:CA[1_554]  | 1.28                     | 0.92              |
| 4:4:311:ASP:N   | 4:8:141:SER:C[1_554]   | 1.28                     | 0.92              |
| 4:4:277:THR:CA  | 4:8:174:ALA:O[1_554]   | 1.28                     | 0.92              |
| 4:4:273:GLY:N   | 4:8:162:ASN:OD1[1_554] | 1.28                     | 0.92              |
| 4:4:140:LEU:CA  | 4:8:371:HIS:ND1[1_554] | 1.28                     | 0.92              |
| 4:3:193:LEU:CB  | 4:7:210:ARG:CB[1_554]  | 1.28                     | 0.92              |
| 4:5:322:PRO:CB  | 4:9:291:LYS:NZ[1_554]  | 1.28                     | 0.92              |
| 4:5:262:PHE:CE1 | 4:9:153:LEU:N[1_554]   | 1.28                     | 0.92              |
| 4:5:145:SER:OG  | 4:9:372:ARG:NH1[1_554] | 1.28                     | 0.92              |
| 4:5:243:PRO:CB  | 4:9:60:SER:C[1_554]    | 1.28                     | 0.92              |
| 4:3:370:VAL:O   | 4:8:230:ALA:CB[1_554]  | 1.28                     | 0.92              |
| 4:4:115:ASN:C   | 4:9:196:ARG:CZ[1_554]  | 1.28                     | 0.92              |
| 4:4:210:ARG:CG  | 4:8:69:TYR:CD2[1_554]  | 1.28                     | 0.92              |
| 4:4:17:VAL:C    | 4:8:79:TRP:CG[1_554]   | 1.28                     | 0.92              |
| 4:5:31:PHE:CA   | 4:9:81:ASP:N[1_554]    | 1.28                     | 0.92              |
| 4:5:24:ASP:OD2  | 4:9:125:GLU:C[1_554]   | 1.28                     | 0.92              |
| 4:5:312:ARG:C   | 4:9:298:VAL:CB[1_554]  | 1.28                     | 0.92              |
| 4:3:315:LYS:CD  | 4:7:147:ARG:CD[1_554]  | 1.28                     | 0.92              |
| 4:3:75:ILE:CG1  | 4:8:193:LEU:O[1_554]   | 1.28                     | 0.92              |
| 4:3:204:ALA:CB  | 4:7:62:ARG:CA[1_554]   | 1.28                     | 0.92              |
| 4:4:345:ILE:N   | 4:8:367:PRO:CA[1_554]  | 1.28                     | 0.92              |
| 4:5:180:LEU:CB  | 4:9:179:ASP:N[1_554]   | 1.28                     | 0.92              |
| 4:4:299:MET:N   | 4:8:136:ILE:CG1[1_554] | 1.28                     | 0.92              |
| 4:4:214:GLU:C   | 4:8:17:VAL:N[1_554]    | 1.28                     | 0.92              |
| 4:5:349:LEU:CA  | 4:9:365:ALA:N[1_554]   | 1.28                     | 0.92              |
| 4:4:222:ASP:CB  | 4:8:331:ALA:C[1_554]   | 1.28                     | 0.92              |
| 4:4:191:LYS:CG  | 4:8:185:LEU:C[1_554]   | 1.28                     | 0.92              |
| 4:5:28:ARG:O    | 4:9:83:GLU:OE2[1_554]  | 1.28                     | 0.92              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:299:MET:CB  | 4:8:136:ILE:C[1_554]   | 1.28                     | 0.92              |
| 4:5:184:ASP:OD1 | 4:9:73:HIS:CE1[1_554]  | 1.28                     | 0.92              |
| 4:3:270:GLU:CB  | 4:7:272:ALA:N[1_554]   | 1.28                     | 0.92              |
| 4:4:151:ILE:CD1 | 4:8:171:LEU:C[1_554]   | 1.28                     | 0.92              |
| 4:5:31:PHE:CG   | 4:9:80:ASP:N[1_554]    | 1.28                     | 0.92              |
| 4:5:137:GLN:NE2 | 4:9:112:PRO:CB[1_554]  | 1.28                     | 0.92              |
| 4:2:372:ARG:NE  | 4:7:227:MET:O[1_554]   | 1.28                     | 0.92              |
| 4:4:316:GLU:O   | 4:8:151:ILE:N[1_554]   | 1.29                     | 0.91              |
| 4:3:109:PRO:O   | 4:8:195:GLU:OE1[1_554] | 1.29                     | 0.91              |
| 4:4:192:ILE:N   | 4:8:186:THR:CA[1_554]  | 1.29                     | 0.91              |
| 4:4:291:LYS:CG  | 4:V:64:ILE:CD1[1_554]  | 1.29                     | 0.91              |
| 4:5:28:ARG:CA   | 4:9:126:THR:OG1[1_554] | 1.29                     | 0.91              |
| 4:4:190:MET:O   | 4:8:186:THR:CG2[1_554] | 1.29                     | 0.91              |
| 4:5:196:ARG:C   | 4:9:212:ILE:CG1[1_554] | 1.29                     | 0.91              |
| 4:3:338:SER:CB  | 4:7:116:ARG:CG[1_554]  | 1.29                     | 0.91              |
| 4:3:340:TRP:NE1 | 4:7:118:LYS:CD[1_554]  | 1.29                     | 0.91              |
| 4:5:258:PRO:O   | 4:9:155:SER:CB[1_554]  | 1.29                     | 0.91              |
| 4:5:22:ALA:C    | 4:9:362:TYR:CE2[1_554] | 1.29                     | 0.91              |
| 4:4:27:PRO:CD   | 4:8:122:ILE:CB[1_554]  | 1.29                     | 0.91              |
| 4:3:144:ALA:C   | 4:7:370:VAL:CA[1_554]  | 1.29                     | 0.91              |
| 4:5:305:MET:CE  | 4:9:11:ASP:CB[1_554]   | 1.29                     | 0.91              |
| 4:5:255:PHE:CB  | 4:9:305:MET:CB[1_554]  | 1.29                     | 0.91              |
| 4:3:339:VAL:CA  | 4:7:116:ARG:N[1_554]   | 1.29                     | 0.91              |
| 4:5:305:MET:CE  | 4:9:11:ASP:CA[1_554]   | 1.29                     | 0.91              |
| 4:3:367:PRO:N   | 4:8:234:SER:C[1_554]   | 1.29                     | 0.91              |
| 4:4:188:TYR:C   | 4:8:183:ARG:N[1_554]   | 1.29                     | 0.91              |
| 4:3:143:TYR:CA  | 4:7:372:ARG:N[1_554]   | 1.29                     | 0.91              |
| 4:5:145:SER:CB  | 4:9:372:ARG:NH1[1_554] | 1.29                     | 0.91              |
| 4:3:25:ASP:CG   | 4:7:124:PHE:CB[1_554]  | 1.29                     | 0.91              |
| 4:3:340:TRP:CH2 | 4:7:121:GLN:CD[1_554]  | 1.29                     | 0.91              |
| 4:3:336:LYS:NZ  | 4:7:86:TRP:CD1[1_554]  | 1.29                     | 0.91              |
| 4:4:161:HIS:C   | 4:8:110:LEU:CD2[1_554] | 1.29                     | 0.91              |
| 4:2:116:ARG:N   | 4:7:196:ARG:NH2[1_554] | 1.29                     | 0.91              |
| 4:3:180:LEU:CD2 | 4:7:178:LEU:C[1_554]   | 1.29                     | 0.91              |
| 4:5:340:TRP:CG  | 4:9:118:LYS:C[1_554]   | 1.29                     | 0.91              |
| 4:3:75:ILE:C    | 4:8:197:GLY:O[1_554]   | 1.29                     | 0.91              |
| 4:4:220:ALA:N   | 4:8:335:ARG:O[1_554]   | 1.29                     | 0.91              |
| 4:4:315:LYS:CD  | 4:8:147:ARG:CZ[1_554]  | 1.29                     | 0.91              |
| 4:3:369:ILE:O   | 4:8:229:THR:CA[1_554]  | 1.29                     | 0.91              |
| 4:5:137:GLN:CG  | 4:9:112:PRO:O[1_554]   | 1.29                     | 0.91              |
| 4:5:255:PHE:O   | 4:9:304:THR:N[1_554]   | 1.29                     | 0.91              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:278:THR:N   | 4:9:164:PRO:CD[1_554]  | 1.29                     | 0.91              |
| 4:3:313:MET:CE  | 4:7:163:VAL:CB[1_554]  | 1.29                     | 0.91              |
| 4:4:334:GLU:N   | 4:8:105:LEU:N[1_554]   | 1.29                     | 0.91              |
| 4:3:282:ILE:N   | 4:7:173:HIS:NE2[1_554] | 1.29                     | 0.91              |
| 4:4:199:SER:CA  | 4:8:206:ARG:N[1_554]   | 1.29                     | 0.91              |
| 4:3:142:LEU:O   | 4:7:372:ARG:CA[1_554]  | 1.29                     | 0.91              |
| 4:1:292:ASP:OD1 | 4:7:40:HIS:C[1_554]    | 1.29                     | 0.91              |
| 4:3:140:LEU:C   | 4:7:371:HIS:CG[1_554]  | 1.29                     | 0.91              |
| 4:5:213:LYS:C   | 4:9:16:LEU:CD2[1_554]  | 1.29                     | 0.91              |
| 4:4:18:LYS:N    | 4:8:79:TRP:CG[1_554]   | 1.29                     | 0.91              |
| 4:3:335:ARG:CD  | 4:7:106:THR:CA[1_554]  | 1.29                     | 0.91              |
| 4:3:341:ILE:O   | 4:7:367:PRO:CB[1_554]  | 1.29                     | 0.91              |
| 4:3:261:LEU:CB  | 4:7:154:ASP:O[1_554]   | 1.29                     | 0.91              |
| 4:4:294:TYR:CD2 | 4:8:166:TYR:CG[1_554]  | 1.29                     | 0.91              |
| 4:2:372:ARG:O   | 4:7:255:PHE:CE1[1_554] | 1.29                     | 0.91              |
| 4:5:317:ILE:CD1 | 4:9:165:ILE:O[1_554]   | 1.29                     | 0.91              |
| 4:2:370:VAL:C   | 4:7:230:ALA:CA[1_554]  | 1.29                     | 0.91              |
| 4:3:286:ASP:C   | 4:8:270:GLU:OE1[1_554] | 1.29                     | 0.91              |
| 4:3:161:HIS:C   | 4:7:110:LEU:CD2[1_554] | 1.29                     | 0.91              |
| 4:3:169:TYR:OH  | 4:8:266:PHE:CD1[1_554] | 1.29                     | 0.91              |
| 4:4:267:ILE:CB  | 4:8:180:LEU:CB[1_554]  | 1.29                     | 0.91              |
| 4:5:141:SER:CB  | 4:9:116:ARG:NE[1_554]  | 1.30                     | 0.90              |
| 4:3:17:VAL:C    | 4:7:79:TRP:CD1[1_554]  | 1.30                     | 0.90              |
| 4:3:25:ASP:CB   | 4:7:124:PHE:CB[1_554]  | 1.30                     | 0.90              |
| 4:5:349:LEU:CB  | 4:9:365:ALA:CA[1_554]  | 1.30                     | 0.90              |
| 4:3:118:LYS:CB  | 4:8:249:THR:OG1[1_554] | 1.30                     | 0.90              |
| 4:4:25:ASP:N    | 4:8:124:PHE:C[1_554]   | 1.30                     | 0.90              |
| 4:5:11:ASP:CG   | 4:9:115:ASN:CA[1_554]  | 1.30                     | 0.90              |
| 4:4:208:ILE:CG2 | 4:8:59:GLN:OE1[1_554]  | 1.30                     | 0.90              |
| 4:4:188:TYR:CB  | 4:8:181:ALA:O[1_554]   | 1.30                     | 0.90              |
| 4:4:113:LYS:O   | 4:9:251:GLY:C[1_554]   | 1.30                     | 0.90              |
| 4:3:218:TYR:CG  | 4:7:337:TYR:CD1[1_554] | 1.30                     | 0.90              |
| 4:5:345:ILE:CG2 | 4:9:369:ILE:CG1[1_554] | 1.30                     | 0.90              |
| 4:3:294:TYR:O   | 4:7:169:TYR:N[1_554]   | 1.30                     | 0.90              |
| 4:4:294:TYR:CB  | 4:8:166:TYR:O[1_554]   | 1.30                     | 0.90              |
| 4:3:186:THR:C   | 4:7:183:ARG:NE[1_554]  | 1.30                     | 0.90              |
| 4:2:109:PRO:CG  | 4:7:195:GLU:CG[1_554]  | 1.30                     | 0.90              |
| 4:4:161:HIS:CB  | 4:8:110:LEU:CB[1_554]  | 1.30                     | 0.90              |
| 4:4:187:ASP:CA  | 4:8:183:ARG:CG[1_554]  | 1.30                     | 0.90              |
| 4:5:311:ASP:OD1 | 4:9:145:SER:N[1_554]   | 1.30                     | 0.90              |
| 4:4:161:HIS:O   | 4:8:110:LEU:CG[1_554]  | 1.30                     | 0.90              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:325:MET:SD  | 4:7:166:TYR:CE2[1_554] | 1.30                     | 0.90              |
| 4:5:154:ASP:OD2 | 4:9:111:ASN:N[1_554]   | 1.30                     | 0.90              |
| 4:4:305:MET:CE  | 4:8:10:CYS:O[1_554]    | 1.30                     | 0.90              |
| 4:3:189:LEU:N   | 4:7:183:ARG:CA[1_554]  | 1.30                     | 0.90              |
| 4:4:27:PRO:CG   | 4:8:122:ILE:CD1[1_554] | 1.30                     | 0.90              |
| 4:3:262:PHE:CD1 | 4:7:153:LEU:C[1_554]   | 1.30                     | 0.90              |
| 4:2:110:LEU:CD1 | 4:7:191:LYS:CG[1_554]  | 1.30                     | 0.90              |
| 4:3:74:GLY:O    | 4:8:197:GLY:N[1_554]   | 1.30                     | 0.90              |
| 4:3:339:VAL:CB  | 4:7:115:ASN:N[1_554]   | 1.30                     | 0.90              |
| 4:5:318:THR:O   | 4:9:292:ASP:O[1_554]   | 1.30                     | 0.90              |
| 4:4:144:ALA:CA  | 4:8:370:VAL:O[1_554]   | 1.30                     | 0.90              |
| 4:5:220:ALA:CA  | 4:9:335:ARG:CD[1_554]  | 1.30                     | 0.90              |
| 4:4:370:VAL:C   | 4:9:231:ALA:N[1_554]   | 1.30                     | 0.90              |
| 4:5:20:GLY:N    | 4:9:121:GLN:OE1[1_554] | 1.30                     | 0.90              |
| 4:3:289:ILE:N   | 4:9:63:GLY:O[1_554]    | 1.30                     | 0.90              |
| 4:4:120:THR:CG2 | 4:9:233:SER:CB[1_554]  | 1.30                     | 0.90              |
| 4:4:186:THR:CB  | 4:8:183:ARG:NH2[1_554] | 1.30                     | 0.90              |
| 4:4:137:GLN:C   | 4:8:113:LYS:CA[1_554]  | 1.30                     | 0.90              |
| 4:4:180:LEU:CG  | 4:8:178:LEU:O[1_554]   | 1.30                     | 0.90              |
| 4:4:243:PRO:CD  | 4:8:60:SER:CA[1_554]   | 1.30                     | 0.90              |
| 4:5:257:CYS:N   | 4:9:303:THR:CA[1_554]  | 1.30                     | 0.90              |
| 4:5:192:ILE:N   | 4:9:186:THR:CA[1_554]  | 1.30                     | 0.90              |
| 1:D:637:LYS:CD  | 4:5:311:ASP:CG[1_556]  | 1.30                     | 0.90              |
| 4:4:180:LEU:CD1 | 4:8:160:THR:N[1_554]   | 1.30                     | 0.90              |
| 4:5:309:ILE:C   | 4:9:141:SER:OG[1_554]  | 1.30                     | 0.90              |
| 4:3:113:LYS:CG  | 4:8:254:ARG:CA[1_554]  | 1.30                     | 0.90              |
| 4:3:188:TYR:CG  | 4:7:181:ALA:C[1_554]   | 1.30                     | 0.90              |
| 4:4:340:TRP:CZ3 | 4:8:121:GLN:C[1_554]   | 1.30                     | 0.90              |
| 4:5:331:ALA:C   | 4:9:140:LEU:CD2[1_554] | 1.30                     | 0.90              |
| 4:4:196:ARG:NE  | 4:8:211:ASP:CG[1_554]  | 1.30                     | 0.90              |
| 4:3:370:VAL:CA  | 4:8:230:ALA:O[1_554]   | 1.30                     | 0.90              |
| 4:4:280:ASN:OD1 | 4:8:281:SER:CA[1_554]  | 1.30                     | 0.90              |
| 4:5:188:TYR:CE2 | 4:9:185:LEU:CD2[1_554] | 1.30                     | 0.90              |
| 4:3:336:LYS:NZ  | 4:7:86:TRP:CE2[1_554]  | 1.31                     | 0.89              |
| 4:4:77:THR:CG2  | 4:9:246:GLN:OE1[1_554] | 1.31                     | 0.89              |
| 4:4:340:TRP:CG  | 4:8:118:LYS:C[1_554]   | 1.31                     | 0.89              |
| 4:4:221:LEU:C   | 4:8:332:PRO:N[1_554]   | 1.31                     | 0.89              |
| 4:4:372:ARG:CB  | 4:9:227:MET:CA[1_554]  | 1.31                     | 0.89              |
| 4:3:140:LEU:CD2 | 4:7:117:GLU:OE2[1_554] | 1.31                     | 0.89              |
| 4:4:293:LEU:CA  | 4:8:169:TYR:CD2[1_554] | 1.31                     | 0.89              |
| 4:3:143:TYR:N   | 4:7:371:HIS:C[1_554]   | 1.31                     | 0.89              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:204:ALA:C   | 4:8:62:ARG:CD[1_554]   | 1.31                     | 0.89              |
| 4:2:75:ILE:C    | 4:7:198:TYR:CD1[1_554] | 1.31                     | 0.89              |
| 4:4:41:GLN:CG   | 4:7:224:GLU:OE2[1_554] | 1.31                     | 0.89              |
| 4:3:320:LEU:O   | 4:7:289:ILE:O[1_554]   | 1.31                     | 0.89              |
| 4:4:345:ILE:O   | 4:8:366:GLY:N[1_554]   | 1.31                     | 0.89              |
| 4:4:312:ARG:CZ  | 4:8:299:MET:CA[1_554]  | 1.31                     | 0.89              |
| 4:5:267:ILE:CB  | 4:9:180:LEU:CG[1_554]  | 1.31                     | 0.89              |
| 4:5:188:TYR:CD1 | 4:9:185:LEU:CD1[1_554] | 1.31                     | 0.89              |
| 4:5:56:ASP:OD2  | 4:9:81:ASP:OD1[1_554]  | 1.31                     | 0.89              |
| 4:5:349:LEU:CG  | 4:9:365:ALA:CB[1_554]  | 1.31                     | 0.89              |
| 4:5:173:HIS:CG  | 4:V:267:ILE:N[1_554]   | 1.31                     | 0.89              |
| 4:3:264:PRO:CB  | 4:7:178:LEU:CD2[1_554] | 1.31                     | 0.89              |
| 4:3:281:SER:CB  | 4:7:173:HIS:N[1_554]   | 1.31                     | 0.89              |
| 4:5:195:GLU:CA  | 4:9:189:LEU:CG[1_554]  | 1.31                     | 0.89              |
| 4:4:222:ASP:N   | 4:8:332:PRO:N[1_554]   | 1.31                     | 0.89              |
| 4:3:156:GLY:CA  | 4:7:75:ILE:N[1_554]    | 1.31                     | 0.89              |
| 4:5:193:LEU:C   | 4:9:210:ARG:N[1_554]   | 1.31                     | 0.89              |
| 4:3:205:GLU:CB  | 4:7:62:ARG:NE[1_554]   | 1.31                     | 0.89              |
| 4:5:113:LYS:CG  | 4:V:252:ASN:C[1_554]   | 1.31                     | 0.89              |
| 4:5:56:ASP:CG   | 4:9:81:ASP:OD1[1_554]  | 1.31                     | 0.89              |
| 4:3:260:THR:O   | 4:7:160:THR:OG1[1_554] | 1.31                     | 0.89              |
| 4:5:166:TYR:CZ  | 4:W:39:ARG:C[1_554]    | 1.31                     | 0.89              |
| 4:4:315:LYS:NZ  | 4:8:296:ASN:OD1[1_554] | 1.31                     | 0.89              |
| 4:3:188:TYR:CA  | 4:7:183:ARG:C[1_554]   | 1.31                     | 0.89              |
| 4:5:342:GLY:N   | 4:9:370:VAL:CG1[1_554] | 1.31                     | 0.89              |
| 4:2:117:GLU:O   | 4:7:237:GLU:CB[1_554]  | 1.31                     | 0.89              |
| 4:5:286:ASP:CB  | 4:V:270:GLU:CD[1_554]  | 1.31                     | 0.89              |
| 4:4:345:ILE:C   | 4:8:366:GLY:O[1_554]   | 1.31                     | 0.89              |
| 4:5:19:ALA:N    | 4:9:122:ILE:CD1[1_554] | 1.31                     | 0.89              |
| 4:4:143:TYR:CA  | 4:8:372:ARG:CA[1_554]  | 1.31                     | 0.89              |
| 4:3:178:LEU:CG  | 4:7:177:ARG:N[1_554]   | 1.31                     | 0.89              |
| 4:4:175:ILE:CD1 | 4:9:191:LYS:NZ[1_554]  | 1.31                     | 0.89              |
| 4:5:369:ILE:CB  | 4:V:232:SER:CB[1_554]  | 1.31                     | 0.89              |
| 4:3:333:PRO:C   | 4:7:105:LEU:CA[1_554]  | 1.31                     | 0.89              |
| 4:3:213:LYS:CE  | 4:7:15:GLY:N[1_554]    | 1.31                     | 0.89              |
| 4:3:267:ILE:CG1 | 4:7:180:LEU:CB[1_554]  | 1.31                     | 0.89              |
| 4:5:157:ASP:OD1 | 4:9:71:ILE:C[1_554]    | 1.31                     | 0.89              |
| 4:3:30:VAL:CG2  | 4:7:79:TRP:O[1_554]    | 1.31                     | 0.89              |
| 4:3:250:ILE:CG1 | 4:7:210:ARG:NH2[1_554] | 1.31                     | 0.89              |
| 4:2:286:ASP:CA  | 4:7:270:GLU:OE1[1_554] | 1.31                     | 0.89              |
| 4:5:158:GLY:C   | 4:9:177:ARG:NH2[1_554] | 1.31                     | 0.89              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:281:SER:O   | 4:7:173:HIS:CG[1_554]  | 1.31                     | 0.89              |
| 4:4:253:GLU:CD  | 4:8:214:GLU:CG[1_554]  | 1.31                     | 0.89              |
| 4:4:243:PRO:N   | 4:8:60:SER:CB[1_554]   | 1.31                     | 0.89              |
| 4:3:311:ASP:OD2 | 4:7:144:ALA:CB[1_554]  | 1.31                     | 0.89              |
| 4:3:214:GLU:CG  | 4:7:33:SER:CB[1_554]   | 1.31                     | 0.89              |
| 4:2:79:TRP:CH2  | 4:7:249:THR:CG2[1_554] | 1.31                     | 0.89              |
| 4:5:25:ASP:OD2  | 4:9:129:VAL:C[1_554]   | 1.32                     | 0.88              |
| 4:5:337:TYR:N   | 4:9:119:MET:CE[1_554]  | 1.32                     | 0.88              |
| 4:3:140:LEU:O   | 4:7:371:HIS:CG[1_554]  | 1.32                     | 0.88              |
| 4:5:178:LEU:CG  | 4:9:177:ARG:N[1_554]   | 1.32                     | 0.88              |
| 4:5:18:LYS:CB   | 4:9:79:TRP:CE3[1_554]  | 1.32                     | 0.88              |
| 4:3:340:TRP:CZ3 | 4:7:121:GLN:CG[1_554]  | 1.32                     | 0.88              |
| 4:4:339:VAL:O   | 4:8:117:GLU:CA[1_554]  | 1.32                     | 0.88              |
| 4:5:227:MET:C   | 4:9:307:PRO:CB[1_554]  | 1.32                     | 0.88              |
| 4:3:151:ILE:CG1 | 4:7:172:PRO:CD[1_554]  | 1.32                     | 0.88              |
| 4:5:193:LEU:CA  | 4:9:210:ARG:CA[1_554]  | 1.32                     | 0.88              |
| 4:3:180:LEU:N   | 4:7:179:ASP:OD1[1_554] | 1.32                     | 0.88              |
| 4:4:162:ASN:OD1 | 4:8:175:ILE:CB[1_554]  | 1.32                     | 0.88              |
| 4:4:207:GLU:OE2 | 4:8:68:LYS:N[1_554]    | 1.32                     | 0.88              |
| 4:3:266:PHE:CA  | 4:7:261:LEU:CD2[1_554] | 1.32                     | 0.88              |
| 4:5:17:VAL:C    | 4:9:79:TRP:CD2[1_554]  | 1.32                     | 0.88              |
| 4:4:273:GLY:C   | 4:8:162:ASN:CG[1_554]  | 1.32                     | 0.88              |
| 4:4:317:ILE:CD1 | 4:8:165:ILE:CA[1_554]  | 1.32                     | 0.88              |
| 4:2:118:LYS:CB  | 4:7:249:THR:OG1[1_554] | 1.32                     | 0.88              |
| 4:3:243:PRO:CA  | 4:7:60:SER:C[1_554]    | 1.32                     | 0.88              |
| 4:4:274:ILE:CD1 | 4:8:161:HIS:CG[1_554]  | 1.32                     | 0.88              |
| 4:3:291:LYS:CG  | 4:9:64:ILE:CG1[1_554]  | 1.32                     | 0.88              |
| 4:3:191:LYS:CG  | 4:7:186:THR:N[1_554]   | 1.32                     | 0.88              |
| 4:3:184:ASP:OD1 | 4:7:73:HIS:NE2[1_554]  | 1.32                     | 0.88              |
| 4:4:173:HIS:CB  | 4:9:267:ILE:CG1[1_554] | 1.32                     | 0.88              |
| 4:4:262:PHE:CD1 | 4:8:153:LEU:CA[1_554]  | 1.32                     | 0.88              |
| 4:4:297:ASN:OD1 | 4:8:170:ALA:CA[1_554]  | 1.32                     | 0.88              |
| 4:2:113:LYS:CG  | 4:7:254:ARG:C[1_554]   | 1.32                     | 0.88              |
| 4:3:255:PHE:C   | 4:7:302:GLY:O[1_554]   | 1.32                     | 0.88              |
| 4:5:188:TYR:OH  | 4:9:185:LEU:CD2[1_554] | 1.32                     | 0.88              |
| 4:2:76:ILE:N    | 4:7:198:TYR:CE1[1_554] | 1.32                     | 0.88              |
| 4:3:186:THR:C   | 4:7:183:ARG:CG[1_554]  | 1.32                     | 0.88              |
| 4:3:341:ILE:CG2 | 4:7:120:THR:CB[1_554]  | 1.32                     | 0.88              |
| 4:3:199:SER:N   | 4:7:207:GLU:N[1_554]   | 1.32                     | 0.88              |
| 4:5:262:PHE:CD1 | 4:9:153:LEU:CB[1_554]  | 1.32                     | 0.88              |
| 4:5:340:TRP:CZ2 | 4:9:121:GLN:CA[1_554]  | 1.32                     | 0.88              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:25:ASP:CA   | 4:8:124:PHE:N[1_554]   | 1.32                     | 0.88              |
| 4:4:153:LEU:CD2 | 4:8:109:PRO:CG[1_554]  | 1.32                     | 0.88              |
| 4:4:196:ARG:CD  | 4:8:211:ASP:O[1_554]   | 1.32                     | 0.88              |
| 4:5:267:ILE:CD1 | 4:9:180:LEU:CB[1_554]  | 1.32                     | 0.88              |
| 4:4:178:LEU:O   | 4:8:177:ARG:CD[1_554]  | 1.32                     | 0.88              |
| 4:5:312:ARG:O   | 4:9:298:VAL:CA[1_554]  | 1.32                     | 0.88              |
| 4:5:113:LYS:NZ  | 4:V:254:ARG:C[1_554]   | 1.32                     | 0.88              |
| 4:4:205:GLU:CB  | 4:8:62:ARG:NE[1_554]   | 1.32                     | 0.88              |
| 4:5:304:THR:N   | 4:9:137:GLN:CD[1_554]  | 1.32                     | 0.88              |
| 4:4:215:LYS:CB  | 4:8:31:PHE:CA[1_554]   | 1.32                     | 0.88              |
| 4:3:274:ILE:C   | 4:7:163:VAL:N[1_554]   | 1.32                     | 0.88              |
| 4:4:333:PRO:CG  | 4:8:104:LEU:N[1_554]   | 1.32                     | 0.88              |
| 4:3:173:HIS:CD2 | 4:8:264:PRO:O[1_554]   | 1.32                     | 0.88              |
| 4:4:263:GLN:C   | 4:8:274:ILE:CG1[1_554] | 1.32                     | 0.88              |
| 4:5:18:LYS:NZ   | 4:9:76:ILE:CB[1_554]   | 1.33                     | 0.87              |
| 4:5:20:GLY:O    | 4:9:121:GLN:CD[1_554]  | 1.33                     | 0.87              |
| 4:1:291:LYS:CA  | 4:7:64:ILE:CG2[1_554]  | 1.33                     | 0.87              |
| 4:5:280:ASN:CG  | 4:9:281:SER:O[1_554]   | 1.33                     | 0.87              |
| 4:3:269:MET:CB  | 4:7:178:LEU:CD1[1_554] | 1.33                     | 0.87              |
| 4:4:218:TYR:CD1 | 4:8:337:TYR:CD1[1_554] | 1.33                     | 0.87              |
| 4:3:305:MET:O   | 4:7:11:ASP:CB[1_554]   | 1.33                     | 0.87              |
| 4:3:218:TYR:CB  | 4:7:336:LYS:C[1_554]   | 1.33                     | 0.87              |
| 4:3:304:THR:CB  | 4:7:107:GLU:O[1_554]   | 1.33                     | 0.87              |
| 4:5:322:PRO:C   | 4:9:291:LYS:NZ[1_554]  | 1.33                     | 0.87              |
| 4:3:255:PHE:O   | 4:7:302:GLY:C[1_554]   | 1.33                     | 0.87              |
| 4:4:113:LYS:CD  | 4:9:255:PHE:N[1_554]   | 1.33                     | 0.87              |
| 4:4:342:GLY:O   | 4:8:368:SER:N[1_554]   | 1.33                     | 0.87              |
| 4:4:371:HIS:N   | 4:9:230:ALA:CB[1_554]  | 1.33                     | 0.87              |
| 4:3:198:TYR:CG  | 4:7:207:GLU:C[1_554]   | 1.33                     | 0.87              |
| 4:4:114:ALA:C   | 4:9:250:ILE:C[1_554]   | 1.33                     | 0.87              |
| 4:5:270:GLU:N   | 4:9:271:SER:C[1_554]   | 1.33                     | 0.87              |
| 4:4:279:TYR:C   | 4:8:285:CYS:SG[1_554]  | 1.33                     | 0.87              |
| 4:5:188:TYR:C   | 4:9:182:GLY:O[1_554]   | 1.33                     | 0.87              |
| 4:4:275:HIS:N   | 4:8:162:ASN:C[1_554]   | 1.33                     | 0.87              |
| 4:5:262:PHE:CD2 | 4:9:153:LEU:O[1_554]   | 1.33                     | 0.87              |
| 4:3:333:PRO:CG  | 4:7:104:LEU:CA[1_554]  | 1.33                     | 0.87              |
| 4:5:333:PRO:CD  | 4:9:104:LEU:CD1[1_554] | 1.33                     | 0.87              |
| 4:5:294:TYR:O   | 4:9:167:GLU:N[1_554]   | 1.33                     | 0.87              |
| 4:3:115:ASN:N   | 4:8:250:ILE:N[1_554]   | 1.33                     | 0.87              |
| 4:5:21:PHE:C    | 4:9:125:GLU:CD[1_554]  | 1.33                     | 0.87              |
| 4:5:336:LYS:CD  | 4:9:12:ASN:CG[1_554]   | 1.33                     | 0.87              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:173:HIS:ND1 | 4:9:266:PHE:N[1_554]   | 1.33                     | 0.87              |
| 4:1:292:ASP:CG  | 4:7:40:HIS:CG[1_554]   | 1.33                     | 0.87              |
| 4:5:326:LYS:CB  | 4:9:167:GLU:CD[1_554]  | 1.33                     | 0.87              |
| 4:4:180:LEU:N   | 4:8:179:ASP:OD1[1_554] | 1.33                     | 0.87              |
| 4:5:17:VAL:CA   | 4:9:79:TRP:CG[1_554]   | 1.33                     | 0.87              |
| 4:4:334:GLU:C   | 4:8:105:LEU:CB[1_554]  | 1.33                     | 0.87              |
| 4:2:177:ARG:NH1 | 4:7:194:THR:CB[1_554]  | 1.33                     | 0.87              |
| 4:5:274:ILE:N   | 4:9:162:ASN:N[1_554]   | 1.33                     | 0.87              |
| 4:4:25:ASP:N    | 4:8:125:GLU:N[1_554]   | 1.33                     | 0.87              |
| 4:4:24:ASP:CB   | 4:8:125:GLU:CG[1_554]  | 1.33                     | 0.87              |
| 4:3:270:GLU:O   | 4:7:272:ALA:CB[1_554]  | 1.33                     | 0.87              |
| 4:4:156:GLY:O   | 4:8:74:GLY:N[1_554]    | 1.33                     | 0.87              |
| 4:4:108:ALA:CA  | 4:9:195:GLU:O[1_554]   | 1.33                     | 0.87              |
| 4:5:305:MET:CA  | 4:9:11:ASP:OD1[1_554]  | 1.33                     | 0.87              |
| 4:4:106:THR:CG2 | 4:8:114:ALA:CB[1_554]  | 1.33                     | 0.87              |
| 4:4:265:SER:C   | 4:8:261:LEU:C[1_554]   | 1.33                     | 0.87              |
| 4:2:372:ARG:CD  | 4:7:227:MET:CB[1_554]  | 1.33                     | 0.87              |
| 4:5:257:CYS:CA  | 4:9:303:THR:CB[1_554]  | 1.33                     | 0.87              |
| 4:4:198:TYR:CB  | 4:8:207:GLU:C[1_554]   | 1.33                     | 0.87              |
| 4:3:110:LEU:C   | 4:8:192:ILE:CA[1_554]  | 1.33                     | 0.87              |
| 4:3:117:GLU:O   | 4:8:237:GLU:CG[1_554]  | 1.33                     | 0.87              |
| 4:4:267:ILE:CG1 | 4:8:180:LEU:CB[1_554]  | 1.33                     | 0.87              |
| 4:3:111:ASN:O   | 4:8:253:GLU:CG[1_554]  | 1.33                     | 0.87              |
| 4:4:304:THR:C   | 4:8:137:GLN:CD[1_554]  | 1.33                     | 0.87              |
| 4:4:371:HIS:ND1 | 4:9:252:ASN:CA[1_554]  | 1.33                     | 0.87              |
| 4:3:371:HIS:CE1 | 4:8:252:ASN:C[1_554]   | 1.33                     | 0.87              |
| 4:4:315:LYS:CD  | 4:8:147:ARG:CD[1_554]  | 1.33                     | 0.87              |
| 4:5:335:ARG:CA  | 4:9:106:THR:CA[1_554]  | 1.33                     | 0.87              |
| 4:5:349:LEU:N   | 4:9:365:ALA:N[1_554]   | 1.33                     | 0.87              |
| 4:5:333:PRO:CD  | 4:9:104:LEU:CG[1_554]  | 1.33                     | 0.87              |
| 4:4:207:GLU:CB  | 4:8:67:LEU:CD1[1_554]  | 1.33                     | 0.87              |
| 4:4:311:ASP:OD1 | 4:8:144:ALA:N[1_554]   | 1.33                     | 0.87              |
| 4:3:27:PRO:CA   | 4:7:122:ILE:CG1[1_554] | 1.33                     | 0.87              |
| 4:5:173:HIS:C   | 4:V:267:ILE:CA[1_554]  | 1.34                     | 0.86              |
| 4:2:116:ARG:CG  | 4:7:252:ASN:CG[1_554]  | 1.34                     | 0.86              |
| 4:4:277:THR:CG2 | 4:8:175:ILE:CA[1_554]  | 1.34                     | 0.86              |
| 4:4:188:TYR:C   | 4:8:182:GLY:C[1_554]   | 1.34                     | 0.86              |
| 4:2:75:ILE:CG2  | 4:7:198:TYR:CG[1_554]  | 1.34                     | 0.86              |
| 4:5:111:ASN:OD1 | 4:V:196:ARG:CB[1_554]  | 1.34                     | 0.86              |
| 4:4:220:ALA:N   | 4:8:335:ARG:C[1_554]   | 1.34                     | 0.86              |
| 4:3:115:ASN:CB  | 4:8:249:THR:O[1_554]   | 1.34                     | 0.86              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:27:PRO:CG   | 4:7:122:ILE:CG1[1_554] | 1.34                     | 0.86              |
| 4:4:262:PHE:CB  | 4:8:153:LEU:CB[1_554]  | 1.34                     | 0.86              |
| 4:2:357:ILE:CB  | 4:7:232:SER:CA[1_554]  | 1.34                     | 0.86              |
| 1:D:542:PHE:CZ  | 4:5:328:LYS:NZ[1_556]  | 1.34                     | 0.86              |
| 4:4:301:GLY:N   | 4:8:107:GLU:CB[1_554]  | 1.34                     | 0.86              |
| 4:4:340:TRP:CZ3 | 4:8:121:GLN:CB[1_554]  | 1.34                     | 0.86              |
| 4:4:344:SER:C   | 4:8:367:PRO:CD[1_554]  | 1.34                     | 0.86              |
| 4:3:166:TYR:CZ  | 4:9:39:ARG:O[1_554]    | 1.34                     | 0.86              |
| 4:3:213:LYS:NZ  | 4:7:14:SER:CA[1_554]   | 1.34                     | 0.86              |
| 4:3:259:GLU:CD  | 4:7:304:THR:C[1_554]   | 1.34                     | 0.86              |
| 4:4:114:ALA:CA  | 4:9:251:GLY:N[1_554]   | 1.34                     | 0.86              |
| 4:4:136:ILE:N   | 4:8:113:LYS:NZ[1_554]  | 1.34                     | 0.86              |
| 4:3:317:ILE:CD1 | 4:7:165:ILE:C[1_554]   | 1.34                     | 0.86              |
| 4:5:297:ASN:N   | 4:9:168:GLY:C[1_554]   | 1.34                     | 0.86              |
| 4:3:335:ARG:CG  | 4:7:106:THR:CA[1_554]  | 1.34                     | 0.86              |
| 4:3:243:PRO:CD  | 4:7:60:SER:CA[1_554]   | 1.34                     | 0.86              |
| 4:4:208:ILE:CG2 | 4:8:59:GLN:CG[1_554]   | 1.34                     | 0.86              |
| 4:5:137:GLN:CA  | 4:9:113:LYS:CA[1_554]  | 1.34                     | 0.86              |
| 4:5:208:ILE:CG1 | 4:9:59:GLN:CG[1_554]   | 1.34                     | 0.86              |
| 4:3:113:LYS:CB  | 4:8:254:ARG:CB[1_554]  | 1.34                     | 0.86              |
| 4:2:326:LYS:CD  | 4:8:44:MET:CA[1_554]   | 1.34                     | 0.86              |
| 4:5:253:GLU:OE2 | 4:9:214:GLU:CA[1_554]  | 1.34                     | 0.86              |
| 4:5:173:HIS:CB  | 4:V:267:ILE:N[1_554]   | 1.34                     | 0.86              |
| 4:3:25:ASP:CB   | 4:7:124:PHE:C[1_554]   | 1.34                     | 0.86              |
| 4:5:183:ARG:NE  | 4:9:72:GLU:OE1[1_554]  | 1.34                     | 0.86              |
| 4:4:328:LYS:O   | 4:8:168:GLY:O[1_554]   | 1.34                     | 0.86              |
| 4:3:178:LEU:CG  | 4:7:177:ARG:C[1_554]   | 1.34                     | 0.86              |
| 4:4:207:GLU:OE1 | 4:8:67:LEU:CA[1_554]   | 1.34                     | 0.86              |
| 4:2:357:ILE:CB  | 4:7:232:SER:O[1_554]   | 1.34                     | 0.86              |
| 4:3:371:HIS:CB  | 4:8:236:LEU:CD1[1_554] | 1.34                     | 0.86              |
| 4:4:154:ASP:CB  | 4:8:110:LEU:C[1_554]   | 1.34                     | 0.86              |
| 4:5:193:LEU:O   | 4:9:209:VAL:CA[1_554]  | 1.34                     | 0.86              |
| 4:4:326:LYS:N   | 4:8:167:GLU:CG[1_554]  | 1.34                     | 0.86              |
| 4:4:115:ASN:CG  | 4:9:249:THR:O[1_554]   | 1.34                     | 0.86              |
| 4:4:198:TYR:C   | 4:8:205:GLU:O[1_554]   | 1.34                     | 0.86              |
| 4:5:304:THR:CB  | 4:9:137:GLN:CG[1_554]  | 1.34                     | 0.86              |
| 4:5:204:ALA:CB  | 4:9:62:ARG:CG[1_554]   | 1.34                     | 0.86              |
| 4:5:367:PRO:CD  | 4:V:234:SER:N[1_554]   | 1.34                     | 0.86              |
| 4:3:272:ALA:CA  | 4:7:277:THR:CG2[1_554] | 1.34                     | 0.86              |
| 4:4:304:THR:C   | 4:8:137:GLN:CG[1_554]  | 1.34                     | 0.86              |
| 4:5:164:PRO:CG  | 4:9:172:PRO:CG[1_554]  | 1.34                     | 0.86              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:283:MET:CB  | 4:9:286:ASP:N[1_554]   | 1.34                     | 0.86              |
| 4:4:184:ASP:OD1 | 4:8:73:HIS:CE1[1_554]  | 1.34                     | 0.86              |
| 4:3:243:PRO:N   | 4:7:60:SER:N[1_554]    | 1.34                     | 0.86              |
| 4:5:249:THR:CB  | 4:9:215:LYS:NZ[1_554]  | 1.34                     | 0.86              |
| 4:3:188:TYR:CD1 | 4:7:181:ALA:O[1_554]   | 1.34                     | 0.86              |
| 4:3:357:ILE:CG2 | 4:8:232:SER:CA[1_554]  | 1.34                     | 0.86              |
| 4:4:195:GLU:CB  | 4:8:189:LEU:CD2[1_554] | 1.34                     | 0.86              |
| 4:4:320:LEU:O   | 4:8:289:ILE:O[1_554]   | 1.34                     | 0.86              |
| 4:5:207:GLU:OE2 | 4:9:67:LEU:CA[1_554]   | 1.35                     | 0.85              |
| 4:4:325:MET:O   | 4:8:167:GLU:OE2[1_554] | 1.35                     | 0.85              |
| 4:3:273:GLY:CA  | 4:7:162:ASN:CG[1_554]  | 1.35                     | 0.85              |
| 4:3:139:VAL:O   | 4:7:371:HIS:CD2[1_554] | 1.35                     | 0.85              |
| 4:3:344:SER:N   | 4:7:367:PRO:CG[1_554]  | 1.35                     | 0.85              |
| 4:5:222:ASP:N   | 4:9:331:ALA:CB[1_554]  | 1.35                     | 0.85              |
| 4:3:277:THR:N   | 4:7:281:SER:OG[1_554]  | 1.35                     | 0.85              |
| 4:5:369:ILE:CB  | 4:V:232:SER:OG[1_554]  | 1.35                     | 0.85              |
| 4:4:300:SER:CB  | 4:8:107:GLU:CG[1_554]  | 1.35                     | 0.85              |
| 4:3:339:VAL:C   | 4:7:117:GLU:N[1_554]   | 1.35                     | 0.85              |
| 4:2:371:HIS:CB  | 4:7:236:LEU:CD1[1_554] | 1.35                     | 0.85              |
| 4:3:140:LEU:O   | 4:7:371:HIS:CB[1_554]  | 1.35                     | 0.85              |
| 4:5:220:ALA:N   | 4:9:335:ARG:CB[1_554]  | 1.35                     | 0.85              |
| 4:2:115:ASN:C   | 4:7:196:ARG:NH2[1_554] | 1.35                     | 0.85              |
| 4:5:219:VAL:CG1 | 4:9:300:SER:C[1_554]   | 1.35                     | 0.85              |
| 4:3:278:THR:CG2 | 4:7:164:PRO:O[1_554]   | 1.35                     | 0.85              |
| 4:3:334:GLU:CG  | 4:7:132:MET:CE[1_554]  | 1.35                     | 0.85              |
| 4:4:183:ARG:NE  | 4:8:72:GLU:CD[1_554]   | 1.35                     | 0.85              |
| 4:2:372:ARG:CG  | 4:7:227:MET:N[1_554]   | 1.35                     | 0.85              |
| 4:4:141:SER:N   | 4:8:371:HIS:ND1[1_554] | 1.35                     | 0.85              |
| 4:3:220:ALA:N   | 4:7:335:ARG:C[1_554]   | 1.35                     | 0.85              |
| 4:5:340:TRP:CE3 | 4:9:120:THR:C[1_554]   | 1.35                     | 0.85              |
| 4:4:192:ILE:CB  | 4:8:213:LYS:CE[1_554]  | 1.35                     | 0.85              |
| 4:4:338:SER:OG  | 4:8:134:VAL:CG1[1_554] | 1.35                     | 0.85              |
| 4:2:366:GLY:CA  | 4:7:235:SER:OG[1_554]  | 1.35                     | 0.85              |
| 4:5:29:ALA:N    | 4:9:83:GLU:OE1[1_554]  | 1.35                     | 0.85              |
| 4:3:172:PRO:C   | 4:8:266:PHE:O[1_554]   | 1.35                     | 0.85              |
| 4:3:198:TYR:N   | 4:7:209:VAL:N[1_554]   | 1.35                     | 0.85              |
| 4:5:305:MET:CG  | 4:9:11:ASP:OD1[1_554]  | 1.35                     | 0.85              |
| 4:5:32:PRO:CG   | 4:9:81:ASP:OD2[1_554]  | 1.35                     | 0.85              |
| 4:5:332:PRO:N   | 4:9:135:ALA:CB[1_554]  | 1.35                     | 0.85              |
| 4:4:15:GLY:N    | 4:8:77:THR:CB[1_554]   | 1.35                     | 0.85              |
| 4:4:223:PHE:CG  | 4:8:304:THR:OG1[1_554] | 1.35                     | 0.85              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:157:ASP:OD1 | 4:7:72:GLU:CB[1_554]   | 1.35                     | 0.85              |
| 4:3:256:ARG:C   | 4:7:303:THR:N[1_554]   | 1.35                     | 0.85              |
| 4:3:18:LYS:N    | 4:7:79:TRP:CD1[1_554]  | 1.35                     | 0.85              |
| 4:4:30:VAL:C    | 4:8:80:ASP:CA[1_554]   | 1.35                     | 0.85              |
| 4:4:340:TRP:CE3 | 4:8:121:GLN:N[1_554]   | 1.35                     | 0.85              |
| 4:3:315:LYS:N   | 4:7:142:LEU:CG[1_554]  | 1.35                     | 0.85              |
| 4:5:156:GLY:C   | 4:9:75:ILE:N[1_554]    | 1.35                     | 0.85              |
| 4:5:266:PHE:CE2 | 4:9:261:LEU:CD1[1_554] | 1.35                     | 0.85              |
| 4:2:111:ASN:O   | 4:7:253:GLU:CB[1_554]  | 1.35                     | 0.85              |
| 4:2:173:HIS:CB  | 4:7:267:ILE:CB[1_554]  | 1.35                     | 0.85              |
| 4:5:151:ILE:CG2 | 4:9:170:ALA:C[1_554]   | 1.35                     | 0.85              |
| 4:3:317:ILE:CG2 | 4:7:165:ILE:N[1_554]   | 1.35                     | 0.85              |
| 4:4:173:HIS:O   | 4:9:267:ILE:O[1_554]   | 1.35                     | 0.85              |
| 4:5:178:LEU:O   | 4:9:177:ARG:CD[1_554]  | 1.35                     | 0.85              |
| 4:4:258:PRO:C   | 4:8:155:SER:C[1_554]   | 1.35                     | 0.85              |
| 4:5:294:TYR:C   | 4:9:167:GLU:N[1_554]   | 1.35                     | 0.85              |
| 4:3:16:LEU:CB   | 4:7:78:ASN:N[1_554]    | 1.35                     | 0.85              |
| 4:3:222:ASP:CB  | 4:7:331:ALA:C[1_554]   | 1.35                     | 0.85              |
| 4:4:326:LYS:N   | 4:8:167:GLU:CD[1_554]  | 1.35                     | 0.85              |
| 4:3:260:THR:O   | 4:7:160:THR:CG2[1_554] | 1.36                     | 0.84              |
| 4:1:326:LYS:CB  | 4:7:43:VAL:O[1_554]    | 1.36                     | 0.84              |
| 4:5:215:LYS:C   | 4:9:30:VAL:CG1[1_554]  | 1.36                     | 0.84              |
| 4:3:142:LEU:C   | 4:7:371:HIS:O[1_554]   | 1.36                     | 0.84              |
| 4:3:267:ILE:CD1 | 4:7:180:LEU:CA[1_554]  | 1.36                     | 0.84              |
| 4:3:178:LEU:CD2 | 4:7:177:ARG:N[1_554]   | 1.36                     | 0.84              |
| 4:3:274:ILE:CA  | 4:7:162:ASN:N[1_554]   | 1.36                     | 0.84              |
| 4:5:196:ARG:NH1 | 4:9:215:LYS:CB[1_554]  | 1.36                     | 0.84              |
| 4:5:325:MET:CG  | 4:9:166:TYR:CE1[1_554] | 1.36                     | 0.84              |
| 4:5:196:ARG:CB  | 4:9:212:ILE:CA[1_554]  | 1.36                     | 0.84              |
| 4:3:276:GLU:OE1 | 4:7:278:THR:O[1_554]   | 1.36                     | 0.84              |
| 4:3:26:ALA:CA   | 4:7:122:ILE:C[1_554]   | 1.36                     | 0.84              |
| 4:4:227:MET:CE  | 4:8:306:TYR:C[1_554]   | 1.36                     | 0.84              |
| 4:3:26:ALA:CB   | 4:7:123:MET:N[1_554]   | 1.36                     | 0.84              |
| 4:4:191:LYS:C   | 4:8:186:THR:CB[1_554]  | 1.36                     | 0.84              |
| 4:3:215:LYS:CD  | 4:7:31:PHE:CG[1_554]   | 1.36                     | 0.84              |
| 4:5:189:LEU:CA  | 4:9:182:GLY:O[1_554]   | 1.36                     | 0.84              |
| 4:3:204:ALA:CB  | 4:7:62:ARG:O[1_554]    | 1.36                     | 0.84              |
| 4:5:317:ILE:CA  | 4:9:150:GLY:C[1_554]   | 1.36                     | 0.84              |
| 4:1:288:ASP:N   | 4:7:39:ARG:NH1[1_554]  | 1.36                     | 0.84              |
| 4:3:332:PRO:CD  | 4:7:135:ALA:N[1_554]   | 1.36                     | 0.84              |
| 4:4:154:ASP:OD2 | 4:8:111:ASN:O[1_554]   | 1.36                     | 0.84              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:279:TYR:O   | 4:8:285:CYS:SG[1_554]  | 1.36                     | 0.84              |
| 4:5:339:VAL:C   | 4:9:116:ARG:O[1_554]   | 1.36                     | 0.84              |
| 4:4:304:THR:CA  | 4:8:137:GLN:NE2[1_554] | 1.36                     | 0.84              |
| 4:2:114:ALA:CA  | 4:7:250:ILE:O[1_554]   | 1.36                     | 0.84              |
| 4:3:18:LYS:CE   | 4:7:79:TRP:CZ2[1_554]  | 1.36                     | 0.84              |
| 4:3:25:ASP:OD1  | 4:7:124:PHE:CD1[1_554] | 1.36                     | 0.84              |
| 4:5:154:ASP:CG  | 4:9:111:ASN:N[1_554]   | 1.36                     | 0.84              |
| 4:3:32:PRO:CD   | 4:7:78:ASN:ND2[1_554]  | 1.36                     | 0.84              |
| 4:3:315:LYS:CG  | 4:7:145:SER:OG[1_554]  | 1.36                     | 0.84              |
| 4:4:18:LYS:O    | 4:8:118:LYS:CE[1_554]  | 1.36                     | 0.84              |
| 4:5:294:TYR:CG  | 4:9:166:TYR:CD1[1_554] | 1.36                     | 0.84              |
| 4:4:137:GLN:CD  | 4:8:112:PRO:CB[1_554]  | 1.36                     | 0.84              |
| 4:5:195:GLU:CG  | 4:9:189:LEU:CG[1_554]  | 1.36                     | 0.84              |
| 4:4:18:LYS:CG   | 4:8:79:TRP:CD2[1_554]  | 1.36                     | 0.84              |
| 4:5:299:MET:O   | 4:9:136:ILE:CA[1_554]  | 1.36                     | 0.84              |
| 4:3:277:THR:CB  | 4:7:175:ILE:C[1_554]   | 1.36                     | 0.84              |
| 4:5:269:MET:C   | 4:9:272:ALA:O[1_554]   | 1.36                     | 0.84              |
| 4:3:192:ILE:CG2 | 4:7:213:LYS:CD[1_554]  | 1.36                     | 0.84              |
| 4:3:333:PRO:O   | 4:7:105:LEU:CA[1_554]  | 1.36                     | 0.84              |
| 4:4:267:ILE:CB  | 4:8:180:LEU:CG[1_554]  | 1.36                     | 0.84              |
| 4:3:210:ARG:CB  | 4:7:69:TYR:CD2[1_554]  | 1.36                     | 0.84              |
| 4:3:157:ASP:C   | 4:7:72:GLU:O[1_554]    | 1.36                     | 0.84              |
| 4:5:227:MET:CG  | 4:9:307:PRO:CA[1_554]  | 1.36                     | 0.84              |
| 4:4:218:TYR:CE2 | 4:8:337:TYR:CE2[1_554] | 1.36                     | 0.84              |
| 4:3:333:PRO:C   | 4:7:105:LEU:N[1_554]   | 1.36                     | 0.84              |
| 4:3:319:ALA:CB  | 4:7:296:ASN:CA[1_554]  | 1.36                     | 0.84              |
| 4:3:218:TYR:CD1 | 4:7:337:TYR:CD1[1_554] | 1.36                     | 0.84              |
| 4:5:334:GLU:CD  | 4:9:133:TYR:O[1_554]   | 1.36                     | 0.84              |
| 4:5:313:MET:CG  | 4:9:152:VAL:CG2[1_554] | 1.36                     | 0.84              |
| 4:5:346:LEU:CG  | 4:9:368:SER:OG[1_554]  | 1.36                     | 0.84              |
| 4:3:116:ARG:CB  | 4:8:252:ASN:OD1[1_554] | 1.36                     | 0.84              |
| 4:5:156:GLY:C   | 4:9:74:GLY:CA[1_554]   | 1.36                     | 0.84              |
| 4:5:258:PRO:CB  | 4:9:155:SER:O[1_554]   | 1.36                     | 0.84              |
| 4:5:366:GLY:C   | 4:V:234:SER:N[1_554]   | 1.36                     | 0.84              |
| 4:3:214:GLU:N   | 4:7:16:LEU:CA[1_554]   | 1.36                     | 0.84              |
| 4:5:141:SER:CA  | 4:9:116:ARG:CD[1_554]  | 1.37                     | 0.83              |
| 4:5:180:LEU:CB  | 4:9:178:LEU:O[1_554]   | 1.37                     | 0.83              |
| 4:4:333:PRO:CB  | 4:8:104:LEU:O[1_554]   | 1.37                     | 0.83              |
| 4:4:243:PRO:CG  | 4:8:59:GLN:O[1_554]    | 1.37                     | 0.83              |
| 4:5:338:SER:CA  | 4:9:134:VAL:CG2[1_554] | 1.37                     | 0.83              |
| 4:3:198:TYR:CG  | 4:7:208:ILE:CA[1_554]  | 1.37                     | 0.83              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:141:SER:OG  | 4:9:107:GLU:OE1[1_554] | 1.37                     | 0.83              |
| 4:3:345:ILE:CG2 | 4:7:366:GLY:O[1_554]   | 1.37                     | 0.83              |
| 4:3:109:PRO:CD  | 4:8:195:GLU:CG[1_554]  | 1.37                     | 0.83              |
| 4:5:26:ALA:N    | 4:9:123:MET:C[1_554]   | 1.37                     | 0.83              |
| 4:2:369:ILE:CG2 | 4:7:234:SER:CA[1_554]  | 1.37                     | 0.83              |
| 4:3:187:ASP:CA  | 4:7:183:ARG:CG[1_554]  | 1.37                     | 0.83              |
| 4:5:263:GLN:CG  | 4:9:274:ILE:CG2[1_554] | 1.37                     | 0.83              |
| 4:4:215:LYS:CD  | 4:8:31:PHE:CA[1_554]   | 1.37                     | 0.83              |
| 4:4:227:MET:CE  | 4:8:306:TYR:CB[1_554]  | 1.37                     | 0.83              |
| 4:4:177:ARG:CZ  | 4:9:194:THR:CG2[1_554] | 1.37                     | 0.83              |
| 4:3:308:GLY:N   | 4:7:340:TRP:N[1_554]   | 1.37                     | 0.83              |
| 4:5:286:ASP:CA  | 4:V:270:GLU:OE1[1_554] | 1.37                     | 0.83              |
| 4:2:112:PRO:CG  | 4:7:193:LEU:CD2[1_554] | 1.37                     | 0.83              |
| 4:4:308:GLY:O   | 4:8:338:SER:CB[1_554]  | 1.37                     | 0.83              |
| 4:5:218:TYR:CB  | 4:9:336:LYS:CA[1_554]  | 1.37                     | 0.83              |
| 4:5:188:TYR:CA  | 4:9:184:ASP:N[1_554]   | 1.37                     | 0.83              |
| 4:3:333:PRO:O   | 4:7:105:LEU:CG[1_554]  | 1.37                     | 0.83              |
| 4:4:281:SER:OG  | 4:8:173:HIS:CA[1_554]  | 1.37                     | 0.83              |
| 4:3:193:LEU:CG  | 4:7:210:ARG:NE[1_554]  | 1.37                     | 0.83              |
| 4:4:207:GLU:CB  | 4:8:67:LEU:CB[1_554]   | 1.37                     | 0.83              |
| 4:3:305:MET:C   | 4:7:11:ASP:CG[1_554]   | 1.37                     | 0.83              |
| 4:5:335:ARG:CG  | 4:9:106:THR:CG2[1_554] | 1.37                     | 0.83              |
| 4:5:250:ILE:CG1 | 4:9:214:GLU:OE1[1_554] | 1.37                     | 0.83              |
| 4:3:372:ARG:CA  | 4:8:226:GLU:O[1_554]   | 1.37                     | 0.83              |
| 4:3:294:TYR:CD1 | 4:7:166:TYR:CA[1_554]  | 1.37                     | 0.83              |
| 4:3:265:SER:C   | 4:7:261:LEU:CA[1_554]  | 1.37                     | 0.83              |
| 4:5:215:LYS:CE  | 4:9:31:PHE:CB[1_554]   | 1.37                     | 0.83              |
| 4:4:211:ASP:CA  | 4:8:32:PRO:CB[1_554]   | 1.37                     | 0.83              |
| 4:3:110:LEU:O   | 4:8:192:ILE:C[1_554]   | 1.37                     | 0.83              |
| 4:5:141:SER:O   | 4:9:116:ARG:CZ[1_554]  | 1.37                     | 0.83              |
| 4:5:181:ALA:O   | 4:9:158:GLY:O[1_554]   | 1.37                     | 0.83              |
| 4:3:221:LEU:C   | 4:7:332:PRO:CD[1_554]  | 1.37                     | 0.83              |
| 4:5:249:THR:CG2 | 4:9:215:LYS:NZ[1_554]  | 1.37                     | 0.83              |
| 4:3:113:LYS:CD  | 4:8:255:PHE:N[1_554]   | 1.37                     | 0.83              |
| 4:3:191:LYS:CE  | 4:7:185:LEU:CA[1_554]  | 1.37                     | 0.83              |
| 4:4:299:MET:CA  | 4:8:136:ILE:CA[1_554]  | 1.37                     | 0.83              |
| 4:5:295:ALA:N   | 4:9:166:TYR:O[1_554]   | 1.37                     | 0.83              |
| 4:5:189:LEU:N   | 4:9:183:ARG:N[1_554]   | 1.37                     | 0.83              |
| 4:4:277:THR:CG2 | 4:8:175:ILE:O[1_554]   | 1.37                     | 0.83              |
| 4:5:115:ASN:CA  | 4:V:196:ARG:NH1[1_554] | 1.37                     | 0.83              |
| 4:5:185:LEU:CB  | 4:9:158:GLY:N[1_554]   | 1.37                     | 0.83              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:195:GLU:C   | 4:7:209:VAL:O[1_554]   | 1.37                     | 0.83              |
| 4:5:222:ASP:CA  | 4:9:331:ALA:CB[1_554]  | 1.37                     | 0.83              |
| 4:3:30:VAL:O    | 4:7:80:ASP:CB[1_554]   | 1.37                     | 0.83              |
| 4:3:173:HIS:CE1 | 4:8:265:SER:C[1_554]   | 1.37                     | 0.83              |
| 4:3:261:LEU:CA  | 4:7:154:ASP:O[1_554]   | 1.37                     | 0.83              |
| 4:5:113:LYS:CA  | 4:V:253:GLU:N[1_554]   | 1.37                     | 0.83              |
| 4:5:348:SER:OG  | 4:9:362:TYR:C[1_554]   | 1.37                     | 0.83              |
| 4:3:208:ILE:CG2 | 4:7:59:GLN:NE2[1_554]  | 1.37                     | 0.83              |
| 4:3:198:TYR:C   | 4:7:206:ARG:C[1_554]   | 1.37                     | 0.83              |
| 4:4:327:ILE:CG1 | 4:8:149:THR:CA[1_554]  | 1.37                     | 0.83              |
| 4:4:340:TRP:NE1 | 4:8:118:LYS:CD[1_554]  | 1.37                     | 0.83              |
| 4:3:336:LYS:NZ  | 4:7:86:TRP:CD2[1_554]  | 1.37                     | 0.83              |
| 4:5:307:PRO:CA  | 4:9:337:TYR:C[1_554]   | 1.37                     | 0.83              |
| 4:3:340:TRP:CB  | 4:7:118:LYS:CB[1_554]  | 1.37                     | 0.83              |
| 4:4:267:ILE:CD1 | 4:8:180:LEU:CA[1_554]  | 1.37                     | 0.83              |
| 4:4:312:ARG:CD  | 4:8:299:MET:CA[1_554]  | 1.37                     | 0.83              |
| 4:3:218:TYR:CD2 | 4:7:337:TYR:CD1[1_554] | 1.37                     | 0.83              |
| 4:3:219:VAL:CG1 | 4:7:300:SER:CB[1_554]  | 1.38                     | 0.82              |
| 4:3:186:THR:O   | 4:7:183:ARG:CG[1_554]  | 1.38                     | 0.82              |
| 4:5:157:ASP:O   | 4:9:73:HIS:CA[1_554]   | 1.38                     | 0.82              |
| 4:4:281:SER:OG  | 4:8:172:PRO:C[1_554]   | 1.38                     | 0.82              |
| 4:3:262:PHE:CB  | 4:7:153:LEU:C[1_554]   | 1.38                     | 0.82              |
| 4:4:367:PRO:CD  | 4:9:234:SER:C[1_554]   | 1.38                     | 0.82              |
| 4:4:272:ALA:CA  | 4:8:277:THR:CG2[1_554] | 1.38                     | 0.82              |
| 4:4:188:TYR:CA  | 4:8:183:ARG:C[1_554]   | 1.38                     | 0.82              |
| 4:4:72:GLU:O    | 4:9:198:TYR:C[1_554]   | 1.38                     | 0.82              |
| 4:3:117:GLU:C   | 4:8:237:GLU:CD[1_554]  | 1.38                     | 0.82              |
| 4:4:143:TYR:C   | 4:8:372:ARG:N[1_554]   | 1.38                     | 0.82              |
| 4:5:249:THR:O   | 4:9:211:ASP:OD2[1_554] | 1.38                     | 0.82              |
| 4:3:173:HIS:N   | 4:8:266:PHE:C[1_554]   | 1.38                     | 0.82              |
| 4:5:183:ARG:CD  | 4:9:72:GLU:OE2[1_554]  | 1.38                     | 0.82              |
| 4:3:243:PRO:N   | 4:7:60:SER:CB[1_554]   | 1.38                     | 0.82              |
| 4:4:367:PRO:N   | 4:9:235:SER:N[1_554]   | 1.38                     | 0.82              |
| 4:5:340:TRP:CE2 | 4:9:118:LYS:O[1_554]   | 1.38                     | 0.82              |
| 4:3:340:TRP:CG  | 4:7:118:LYS:CA[1_554]  | 1.38                     | 0.82              |
| 4:4:367:PRO:N   | 4:9:234:SER:O[1_554]   | 1.38                     | 0.82              |
| 4:5:11:ASP:OD1  | 4:9:115:ASN:CA[1_554]  | 1.38                     | 0.82              |
| 4:3:281:SER:OG  | 4:7:172:PRO:C[1_554]   | 1.38                     | 0.82              |
| 4:5:173:HIS:O   | 4:V:267:ILE:C[1_554]   | 1.38                     | 0.82              |
| 4:5:221:LEU:CA  | 4:9:332:PRO:CD[1_554]  | 1.38                     | 0.82              |
| 4:4:75:ILE:CD1  | 4:9:193:LEU:O[1_554]   | 1.38                     | 0.82              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:186:THR:OG1 | 4:9:183:ARG:NH2[1_554] | 1.38                     | 0.82              |
| 4:4:259:GLU:CG  | 4:8:304:THR:CA[1_554]  | 1.38                     | 0.82              |
| 4:4:265:SER:C   | 4:8:261:LEU:CA[1_554]  | 1.38                     | 0.82              |
| 4:3:336:LYS:N   | 4:7:119:MET:CE[1_554]  | 1.38                     | 0.82              |
| 4:5:266:PHE:CB  | 4:9:261:LEU:CD2[1_554] | 1.38                     | 0.82              |
| 4:4:160:THR:CG2 | 4:8:161:HIS:NE2[1_554] | 1.38                     | 0.82              |
| 4:5:110:LEU:CG  | 4:V:191:LYS:CE[1_554]  | 1.38                     | 0.82              |
| 4:5:185:LEU:CB  | 4:9:157:ASP:C[1_554]   | 1.38                     | 0.82              |
| 4:4:339:VAL:C   | 4:8:116:ARG:C[1_554]   | 1.38                     | 0.82              |
| 4:5:191:LYS:CA  | 4:9:186:THR:O[1_554]   | 1.38                     | 0.82              |
| 4:5:160:THR:OG1 | 4:9:161:HIS:CE1[1_554] | 1.38                     | 0.82              |
| 4:3:220:ALA:CA  | 4:7:335:ARG:C[1_554]   | 1.38                     | 0.82              |
| 4:3:329:ILE:CG2 | 4:7:139:VAL:CG1[1_554] | 1.38                     | 0.82              |
| 4:3:137:GLN:OE1 | 4:7:112:PRO:CB[1_554]  | 1.38                     | 0.82              |
| 4:5:204:ALA:CB  | 4:9:62:ARG:CB[1_554]   | 1.38                     | 0.82              |
| 4:3:341:ILE:CD1 | 4:7:120:THR:CA[1_554]  | 1.38                     | 0.82              |
| 4:3:282:ILE:CG1 | 4:7:171:LEU:CG[1_554]  | 1.38                     | 0.82              |
| 4:3:213:LYS:C   | 4:7:16:LEU:CA[1_554]   | 1.38                     | 0.82              |
| 4:5:266:PHE:CA  | 4:9:261:LEU:N[1_554]   | 1.38                     | 0.82              |
| 4:4:215:LYS:CE  | 4:8:31:PHE:CB[1_554]   | 1.38                     | 0.82              |
| 4:4:158:GLY:O   | 4:8:177:ARG:NH2[1_554] | 1.38                     | 0.82              |
| 4:4:162:ASN:CA  | 4:8:110:LEU:CD2[1_554] | 1.38                     | 0.82              |
| 4:2:368:SER:N   | 4:7:236:LEU:N[1_554]   | 1.38                     | 0.82              |
| 4:3:263:GLN:NE2 | 4:7:153:LEU:CD2[1_554] | 1.38                     | 0.82              |
| 4:5:294:TYR:CA  | 4:9:166:TYR:CA[1_554]  | 1.38                     | 0.82              |
| 4:4:261:LEU:CA  | 4:8:154:ASP:O[1_554]   | 1.38                     | 0.82              |
| 4:4:75:ILE:C    | 4:9:197:GLY:C[1_554]   | 1.39                     | 0.81              |
| 4:4:15:GLY:C    | 4:8:77:THR:CB[1_554]   | 1.39                     | 0.81              |
| 4:4:173:HIS:CA  | 4:9:267:ILE:CB[1_554]  | 1.39                     | 0.81              |
| 4:3:208:ILE:CD1 | 4:7:59:GLN:N[1_554]    | 1.39                     | 0.81              |
| 4:3:340:TRP:CA  | 4:7:117:GLU:C[1_554]   | 1.39                     | 0.81              |
| 4:2:75:ILE:CB   | 4:7:198:TYR:CG[1_554]  | 1.39                     | 0.81              |
| 4:3:153:LEU:CG  | 4:7:109:PRO:CB[1_554]  | 1.39                     | 0.81              |
| 4:5:262:PHE:CD1 | 4:9:153:LEU:C[1_554]   | 1.39                     | 0.81              |
| 4:4:218:TYR:CZ  | 4:8:337:TYR:CE2[1_554] | 1.39                     | 0.81              |
| 4:4:56:ASP:OD2  | 4:8:81:ASP:OD1[1_554]  | 1.39                     | 0.81              |
| 4:4:278:THR:N   | 4:8:164:PRO:CD[1_554]  | 1.39                     | 0.81              |
| 4:5:173:HIS:C   | 4:V:267:ILE:C[1_554]   | 1.39                     | 0.81              |
| 4:3:111:ASN:CA  | 4:8:192:ILE:O[1_554]   | 1.39                     | 0.81              |
| 4:5:327:ILE:C   | 4:9:148:THR:C[1_554]   | 1.39                     | 0.81              |
| 4:4:144:ALA:C   | 4:8:370:VAL:O[1_554]   | 1.39                     | 0.81              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:191:LYS:CB  | 4:8:186:THR:C[1_554]   | 1.39                     | 0.81              |
| 4:3:277:THR:C   | 4:7:175:ILE:N[1_554]   | 1.39                     | 0.81              |
| 4:5:265:SER:C   | 4:9:261:LEU:C[1_554]   | 1.39                     | 0.81              |
| 4:4:314:GLN:C   | 4:8:142:LEU:CD1[1_554] | 1.39                     | 0.81              |
| 4:5:210:ARG:NE  | 4:9:33:SER:O[1_554]    | 1.39                     | 0.81              |
| 4:4:187:ASP:O   | 4:8:183:ARG:C[1_554]   | 1.39                     | 0.81              |
| 4:3:199:SER:C   | 4:7:206:ARG:CB[1_554]  | 1.39                     | 0.81              |
| 4:4:188:TYR:N   | 4:8:184:ASP:N[1_554]   | 1.39                     | 0.81              |
| 4:5:267:ILE:CB  | 4:9:180:LEU:CD1[1_554] | 1.39                     | 0.81              |
| 4:2:75:ILE:N    | 4:7:197:GLY:C[1_554]   | 1.39                     | 0.81              |
| 4:3:192:ILE:N   | 4:7:186:THR:CB[1_554]  | 1.39                     | 0.81              |
| 4:2:108:ALA:CB  | 4:7:195:GLU:O[1_554]   | 1.39                     | 0.81              |
| 4:3:367:PRO:CA  | 4:8:234:SER:C[1_554]   | 1.39                     | 0.81              |
| 4:4:208:ILE:CB  | 4:8:59:GLN:CD[1_554]   | 1.39                     | 0.81              |
| 4:3:327:ILE:CG2 | 4:7:148:THR:C[1_554]   | 1.39                     | 0.81              |
| 4:3:196:ARG:CD  | 4:7:211:ASP:C[1_554]   | 1.39                     | 0.81              |
| 4:5:26:ALA:O    | 4:9:123:MET:N[1_554]   | 1.39                     | 0.81              |
| 4:3:185:LEU:CA  | 4:7:158:GLY:N[1_554]   | 1.39                     | 0.81              |
| 4:3:77:THR:C    | 4:8:246:GLN:NE2[1_554] | 1.39                     | 0.81              |
| 4:3:25:ASP:N    | 4:7:125:GLU:N[1_554]   | 1.39                     | 0.81              |
| 4:3:196:ARG:CD  | 4:7:211:ASP:CA[1_554]  | 1.39                     | 0.81              |
| 4:5:196:ARG:CB  | 4:9:212:ILE:N[1_554]   | 1.39                     | 0.81              |
| 4:5:151:ILE:CG1 | 4:9:170:ALA:O[1_554]   | 1.39                     | 0.81              |
| 4:4:274:ILE:N   | 4:8:161:HIS:C[1_554]   | 1.39                     | 0.81              |
| 4:4:320:LEU:N   | 4:8:293:LEU:CA[1_554]  | 1.39                     | 0.81              |
| 4:3:316:GLU:C   | 4:7:150:GLY:C[1_554]   | 1.39                     | 0.81              |
| 4:4:294:TYR:CG  | 4:8:166:TYR:CG[1_554]  | 1.39                     | 0.81              |
| 4:4:300:SER:OG  | 4:8:107:GLU:CD[1_554]  | 1.39                     | 0.81              |
| 4:3:294:TYR:CE1 | 4:7:166:TYR:CB[1_554]  | 1.39                     | 0.81              |
| 4:3:310:ALA:CA  | 4:7:140:LEU:N[1_554]   | 1.39                     | 0.81              |
| 4:4:297:ASN:ND2 | 4:8:170:ALA:CB[1_554]  | 1.39                     | 0.81              |
| 1:A:637:LYS:CD  | 4:4:311:ASP:CB[1_556]  | 1.39                     | 0.81              |
| 4:3:255:PHE:CD1 | 4:7:305:MET:CB[1_554]  | 1.39                     | 0.81              |
| 4:4:186:THR:C   | 4:8:183:ARG:CD[1_554]  | 1.39                     | 0.81              |
| 4:3:187:ASP:O   | 4:7:183:ARG:O[1_554]   | 1.39                     | 0.81              |
| 4:5:18:LYS:N    | 4:9:79:TRP:CG[1_554]   | 1.39                     | 0.81              |
| 4:5:312:ARG:NH2 | 4:9:299:MET:CG[1_554]  | 1.39                     | 0.81              |
| 4:5:336:LYS:N   | 4:9:106:THR:O[1_554]   | 1.39                     | 0.81              |
| 4:4:156:GLY:CA  | 4:8:75:ILE:CA[1_554]   | 1.39                     | 0.81              |
| 4:3:182:GLY:N   | 4:7:73:HIS:C[1_554]    | 1.39                     | 0.81              |
| 4:4:372:ARG:C   | 4:9:227:MET:N[1_554]   | 1.40                     | 0.80              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:342:GLY:O   | 4:8:367:PRO:C[1_554]   | 1.40                     | 0.80              |
| 4:2:115:ASN:CB  | 4:7:249:THR:C[1_554]   | 1.40                     | 0.80              |
| 4:3:26:ALA:C    | 4:7:122:ILE:N[1_554]   | 1.40                     | 0.80              |
| 4:4:319:ALA:CB  | 4:8:296:ASN:CB[1_554]  | 1.40                     | 0.80              |
| 4:3:191:LYS:CG  | 4:7:185:LEU:C[1_554]   | 1.40                     | 0.80              |
| 4:5:198:TYR:C   | 4:9:205:GLU:O[1_554]   | 1.40                     | 0.80              |
| 4:4:276:GLU:OE1 | 4:8:278:THR:O[1_554]   | 1.40                     | 0.80              |
| 4:3:117:GLU:N   | 4:8:237:GLU:OE2[1_554] | 1.40                     | 0.80              |
| 4:4:259:GLU:CG  | 4:8:304:THR:CB[1_554]  | 1.40                     | 0.80              |
| 4:4:196:ARG:NE  | 4:8:211:ASP:OD1[1_554] | 1.40                     | 0.80              |
| 4:4:269:MET:CB  | 4:8:178:LEU:CD1[1_554] | 1.40                     | 0.80              |
| 4:4:196:ARG:CG  | 4:8:211:ASP:O[1_554]   | 1.40                     | 0.80              |
| 4:5:294:TYR:O   | 4:9:166:TYR:C[1_554]   | 1.40                     | 0.80              |
| 4:3:207:GLU:CG  | 4:7:67:LEU:CB[1_554]   | 1.40                     | 0.80              |
| 4:5:32:PRO:C    | 4:9:78:ASN:CB[1_554]   | 1.40                     | 0.80              |
| 4:3:173:HIS:CA  | 4:8:267:ILE:CA[1_554]  | 1.40                     | 0.80              |
| 4:5:187:ASP:C   | 4:9:184:ASP:N[1_554]   | 1.40                     | 0.80              |
| 4:4:112:PRO:O   | 4:9:253:GLU:CD[1_554]  | 1.40                     | 0.80              |
| 4:5:346:LEU:CG  | 4:9:368:SER:CA[1_554]  | 1.40                     | 0.80              |
| 4:4:255:PHE:O   | 4:8:302:GLY:C[1_554]   | 1.40                     | 0.80              |
| 4:4:185:LEU:CA  | 4:8:157:ASP:O[1_554]   | 1.40                     | 0.80              |
| 4:5:196:ARG:O   | 4:9:212:ILE:CD1[1_554] | 1.40                     | 0.80              |
| 4:4:59:GLN:CG   | 4:8:68:LYS:CD[1_554]   | 1.40                     | 0.80              |
| 4:5:115:ASN:C   | 4:V:196:ARG:NH1[1_554] | 1.40                     | 0.80              |
| 4:4:274:ILE:C   | 4:8:162:ASN:O[1_554]   | 1.40                     | 0.80              |
| 4:2:326:LYS:CD  | 4:8:44:MET:C[1_554]    | 1.40                     | 0.80              |
| 4:2:76:ILE:N    | 4:7:198:TYR:CD1[1_554] | 1.40                     | 0.80              |
| 4:3:253:GLU:CG  | 4:7:214:GLU:CD[1_554]  | 1.40                     | 0.80              |
| 4:3:137:GLN:O   | 4:7:113:LYS:CB[1_554]  | 1.40                     | 0.80              |
| 4:4:260:THR:O   | 4:8:160:THR:CG2[1_554] | 1.40                     | 0.80              |
| 4:5:210:ARG:CD  | 4:9:69:TYR:CD2[1_554]  | 1.40                     | 0.80              |
| 4:4:153:LEU:C   | 4:8:109:PRO:C[1_554]   | 1.40                     | 0.80              |
| 4:4:59:GLN:CB   | 4:8:68:LYS:CD[1_554]   | 1.40                     | 0.80              |
| 4:3:309:ILE:N   | 4:7:339:VAL:CA[1_554]  | 1.40                     | 0.80              |
| 4:4:220:ALA:C   | 4:8:335:ARG:CB[1_554]  | 1.40                     | 0.80              |
| 4:3:289:ILE:CG2 | 4:9:39:ARG:CZ[1_554]   | 1.40                     | 0.80              |
| 4:3:192:ILE:N   | 4:7:186:THR:CA[1_554]  | 1.40                     | 0.80              |
| 4:3:112:PRO:O   | 4:8:253:GLU:OE2[1_554] | 1.40                     | 0.80              |
| 4:5:227:MET:CG  | 4:9:307:PRO:N[1_554]   | 1.40                     | 0.80              |
| 4:3:333:PRO:N   | 4:7:105:LEU:N[1_554]   | 1.40                     | 0.80              |
| 4:2:286:ASP:C   | 4:7:270:GLU:CD[1_554]  | 1.40                     | 0.80              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:27:PRO:CA   | 4:9:122:ILE:CG2[1_554] | 1.40                     | 0.80              |
| 4:4:188:TYR:N   | 4:8:183:ARG:C[1_554]   | 1.40                     | 0.80              |
| 4:3:345:ILE:CB  | 4:7:366:GLY:C[1_554]   | 1.40                     | 0.80              |
| 4:5:349:LEU:C   | 4:9:364:GLU:O[1_554]   | 1.40                     | 0.80              |
| 4:5:265:SER:CA  | 4:9:261:LEU:O[1_554]   | 1.40                     | 0.80              |
| 4:4:185:LEU:C   | 4:8:157:ASP:C[1_554]   | 1.40                     | 0.80              |
| 4:5:219:VAL:CG2 | 4:9:300:SER:C[1_554]   | 1.40                     | 0.80              |
| 4:3:223:PHE:CA  | 4:7:335:ARG:CD[1_554]  | 1.40                     | 0.80              |
| 4:4:154:ASP:N   | 4:8:110:LEU:N[1_554]   | 1.40                     | 0.80              |
| 4:5:17:VAL:O    | 4:9:79:TRP:CA[1_554]   | 1.40                     | 0.80              |
| 4:5:191:LYS:C   | 4:9:186:THR:C[1_554]   | 1.40                     | 0.80              |
| 4:4:289:ILE:CG2 | 4:V:39:ARG:CZ[1_554]   | 1.40                     | 0.80              |
| 4:3:277:THR:CG2 | 4:7:175:ILE:CA[1_554]  | 1.40                     | 0.80              |
| 4:4:266:PHE:N   | 4:8:261:LEU:CA[1_554]  | 1.40                     | 0.80              |
| 4:5:218:TYR:CA  | 4:9:336:LYS:CB[1_554]  | 1.40                     | 0.80              |
| 4:3:336:LYS:CD  | 4:7:86:TRP:CZ2[1_554]  | 1.40                     | 0.80              |
| 4:3:280:ASN:OD1 | 4:7:281:SER:CA[1_554]  | 1.40                     | 0.80              |
| 4:2:369:ILE:N   | 4:7:234:SER:OG[1_554]  | 1.40                     | 0.80              |
| 4:4:185:LEU:CA  | 4:8:158:GLY:CA[1_554]  | 1.40                     | 0.80              |
| 4:4:185:LEU:CD1 | 4:8:159:VAL:N[1_554]   | 1.40                     | 0.80              |
| 4:4:286:ASP:N   | 4:9:270:GLU:CD[1_554]  | 1.40                     | 0.80              |
| 4:3:154:ASP:N   | 4:7:109:PRO:O[1_554]   | 1.40                     | 0.80              |
| 4:4:112:PRO:C   | 4:9:253:GLU:CD[1_554]  | 1.40                     | 0.80              |
| 4:4:191:LYS:CA  | 4:8:186:THR:CA[1_554]  | 1.41                     | 0.79              |
| 4:5:24:ASP:OD2  | 4:9:125:GLU:CB[1_554]  | 1.41                     | 0.79              |
| 4:5:189:LEU:C   | 4:9:186:THR:OG1[1_554] | 1.41                     | 0.79              |
| 4:5:196:ARG:CG  | 4:9:212:ILE:C[1_554]   | 1.41                     | 0.79              |
| 4:4:75:ILE:CG1  | 4:9:193:LEU:O[1_554]   | 1.41                     | 0.79              |
| 4:5:143:TYR:CE2 | 4:9:369:ILE:O[1_554]   | 1.41                     | 0.79              |
| 4:3:207:GLU:OE2 | 4:7:67:LEU:O[1_554]    | 1.41                     | 0.79              |
| 4:5:60:SER:O    | 4:9:66:THR:OG1[1_554]  | 1.41                     | 0.79              |
| 4:4:269:MET:O   | 4:8:272:ALA:O[1_554]   | 1.41                     | 0.79              |
| 4:5:334:GLU:C   | 4:9:105:LEU:CB[1_554]  | 1.41                     | 0.79              |
| 4:3:314:GLN:CA  | 4:7:142:LEU:CG[1_554]  | 1.41                     | 0.79              |
| 4:4:371:HIS:ND1 | 4:9:252:ASN:CB[1_554]  | 1.41                     | 0.79              |
| 4:5:180:LEU:CD1 | 4:9:160:THR:N[1_554]   | 1.41                     | 0.79              |
| 4:5:116:ARG:N   | 4:V:196:ARG:NH1[1_554] | 1.41                     | 0.79              |
| 4:4:215:LYS:CG  | 4:8:31:PHE:CB[1_554]   | 1.41                     | 0.79              |
| 4:5:184:ASP:O   | 4:9:184:ASP:OD1[1_554] | 1.41                     | 0.79              |
| 4:3:273:GLY:C   | 4:7:162:ASN:CB[1_554]  | 1.41                     | 0.79              |
| 4:4:213:LYS:CB  | 4:8:15:GLY:CA[1_554]   | 1.41                     | 0.79              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:173:HIS:CG  | 4:8:267:ILE:N[1_554]   | 1.41                     | 0.79              |
| 4:3:267:ILE:O   | 4:7:180:LEU:CD2[1_554] | 1.41                     | 0.79              |
| 4:4:109:PRO:CA  | 4:9:195:GLU:OE2[1_554] | 1.41                     | 0.79              |
| 4:3:30:VAL:CA   | 4:7:80:ASP:N[1_554]    | 1.41                     | 0.79              |
| 4:5:335:ARG:O   | 4:9:106:THR:C[1_554]   | 1.41                     | 0.79              |
| 4:4:340:TRP:CD1 | 4:8:118:LYS:CD[1_554]  | 1.41                     | 0.79              |
| 4:5:335:ARG:C   | 4:9:106:THR:O[1_554]   | 1.41                     | 0.79              |
| 4:5:296:ASN:C   | 4:9:168:GLY:O[1_554]   | 1.41                     | 0.79              |
| 4:5:114:ALA:CB  | 4:V:250:ILE:CA[1_554]  | 1.41                     | 0.79              |
| 4:5:326:LYS:CB  | 4:9:167:GLU:OE2[1_554] | 1.41                     | 0.79              |
| 4:5:307:PRO:CB  | 4:9:337:TYR:C[1_554]   | 1.41                     | 0.79              |
| 4:5:157:ASP:O   | 4:9:73:HIS:CB[1_554]   | 1.41                     | 0.79              |
| 4:4:293:LEU:CG  | 4:8:169:TYR:CE2[1_554] | 1.41                     | 0.79              |
| 4:4:113:LYS:CG  | 4:9:254:ARG:N[1_554]   | 1.41                     | 0.79              |
| 4:4:293:LEU:CB  | 4:8:169:TYR:CD2[1_554] | 1.41                     | 0.79              |
| 4:4:339:VAL:CB  | 4:8:115:ASN:C[1_554]   | 1.41                     | 0.79              |
| 4:5:276:GLU:CD  | 4:9:278:THR:O[1_554]   | 1.41                     | 0.79              |
| 4:2:357:ILE:CD1 | 4:7:232:SER:N[1_554]   | 1.41                     | 0.79              |
| 4:4:259:GLU:CB  | 4:8:304:THR:CA[1_554]  | 1.41                     | 0.79              |
| 4:5:208:ILE:CA  | 4:9:59:GLN:NE2[1_554]  | 1.41                     | 0.79              |
| 4:4:198:TYR:CD1 | 4:8:208:ILE:CA[1_554]  | 1.41                     | 0.79              |
| 4:3:277:THR:CB  | 4:7:176:MET:N[1_554]   | 1.41                     | 0.79              |
| 4:5:222:ASP:N   | 4:9:331:ALA:N[1_554]   | 1.41                     | 0.79              |
| 4:5:137:GLN:OE1 | 4:9:112:PRO:CD[1_554]  | 1.41                     | 0.79              |
| 4:5:320:LEU:CB  | 4:9:293:LEU:CB[1_554]  | 1.41                     | 0.79              |
| 4:3:111:ASN:CG  | 4:8:196:ARG:CB[1_554]  | 1.41                     | 0.79              |
| 4:3:260:THR:O   | 4:7:160:THR:CB[1_554]  | 1.41                     | 0.79              |
| 4:3:318:THR:OG1 | 4:7:149:THR:O[1_554]   | 1.41                     | 0.79              |
| 4:5:173:HIS:N   | 4:V:267:ILE:N[1_554]   | 1.41                     | 0.79              |
| 4:5:154:ASP:N   | 4:9:109:PRO:O[1_554]   | 1.41                     | 0.79              |
| 4:2:79:TRP:NE1  | 4:7:247:VAL:O[1_554]   | 1.41                     | 0.79              |
| 4:4:74:GLY:C    | 4:9:197:GLY:CA[1_554]  | 1.41                     | 0.79              |
| 4:5:313:MET:SD  | 4:9:152:VAL:N[1_554]   | 1.41                     | 0.79              |
| 4:2:371:HIS:N   | 4:7:236:LEU:CD1[1_554] | 1.41                     | 0.79              |
| 4:4:313:MET:CB  | 4:8:138:ALA:O[1_554]   | 1.41                     | 0.79              |
| 4:3:366:GLY:O   | 4:8:234:SER:CA[1_554]  | 1.41                     | 0.79              |
| 4:4:211:ASP:C   | 4:8:32:PRO:CB[1_554]   | 1.41                     | 0.79              |
| 4:5:258:PRO:CD  | 4:9:303:THR:N[1_554]   | 1.41                     | 0.79              |
| 4:4:184:ASP:OD1 | 4:8:73:HIS:NE2[1_554]  | 1.42                     | 0.78              |
| 4:4:213:LYS:O   | 4:8:16:LEU:CB[1_554]   | 1.42                     | 0.78              |
| 4:4:157:ASP:CG  | 4:8:72:GLU:N[1_554]    | 1.42                     | 0.78              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:160:THR:OG1 | 4:9:161:HIS:NE2[1_554] | 1.42                     | 0.78              |
| 4:4:140:LEU:O   | 4:8:371:HIS:CA[1_554]  | 1.42                     | 0.78              |
| 4:4:196:ARG:CA  | 4:8:212:ILE:N[1_554]   | 1.42                     | 0.78              |
| 4:4:214:GLU:OE1 | 4:8:33:SER:OG[1_554]   | 1.42                     | 0.78              |
| 4:5:219:VAL:N   | 4:9:335:ARG:O[1_554]   | 1.42                     | 0.78              |
| 4:5:316:GLU:OE1 | 4:9:297:ASN:CB[1_554]  | 1.42                     | 0.78              |
| 4:3:115:ASN:ND2 | 4:8:198:TYR:CE2[1_554] | 1.42                     | 0.78              |
| 4:5:210:ARG:NH2 | 4:9:33:SER:O[1_554]    | 1.42                     | 0.78              |
| 4:5:253:GLU:OE2 | 4:9:214:GLU:CB[1_554]  | 1.42                     | 0.78              |
| 4:3:142:LEU:CA  | 4:7:371:HIS:O[1_554]   | 1.42                     | 0.78              |
| 4:5:312:ARG:CG  | 4:9:299:MET:N[1_554]   | 1.42                     | 0.78              |
| 4:4:218:TYR:CZ  | 4:8:337:TYR:CD2[1_554] | 1.42                     | 0.78              |
| 4:3:75:ILE:CA   | 4:8:197:GLY:C[1_554]   | 1.42                     | 0.78              |
| 4:4:219:VAL:CG1 | 4:8:300:SER:CA[1_554]  | 1.42                     | 0.78              |
| 4:3:308:GLY:N   | 4:7:339:VAL:C[1_554]   | 1.42                     | 0.78              |
| 4:5:157:ASP:OD1 | 4:9:72:GLU:N[1_554]    | 1.42                     | 0.78              |
| 4:4:214:GLU:OE1 | 4:8:33:SER:CA[1_554]   | 1.42                     | 0.78              |
| 4:5:11:ASP:O    | 4:9:79:TRP:CE2[1_554]  | 1.42                     | 0.78              |
| 4:3:213:LYS:CE  | 4:7:14:SER:CA[1_554]   | 1.42                     | 0.78              |
| 4:5:334:GLU:CB  | 4:9:105:LEU:N[1_554]   | 1.42                     | 0.78              |
| 4:5:267:ILE:CG1 | 4:9:180:LEU:CB[1_554]  | 1.42                     | 0.78              |
| 4:5:141:SER:CA  | 4:9:116:ARG:CZ[1_554]  | 1.42                     | 0.78              |
| 4:3:27:PRO:CD   | 4:7:122:ILE:CG1[1_554] | 1.42                     | 0.78              |
| 4:4:295:ALA:CA  | 4:8:167:GLU:O[1_554]   | 1.42                     | 0.78              |
| 4:3:27:PRO:CB   | 4:7:122:ILE:CD1[1_554] | 1.42                     | 0.78              |
| 4:3:205:GLU:N   | 4:7:62:ARG:CD[1_554]   | 1.42                     | 0.78              |
| 4:3:173:HIS:N   | 4:8:266:PHE:O[1_554]   | 1.42                     | 0.78              |
| 4:5:333:PRO:C   | 4:9:104:LEU:O[1_554]   | 1.42                     | 0.78              |
| 4:5:154:ASP:CA  | 4:9:109:PRO:C[1_554]   | 1.42                     | 0.78              |
| 4:3:196:ARG:CD  | 4:7:211:ASP:CB[1_554]  | 1.42                     | 0.78              |
| 4:4:259:GLU:CA  | 4:8:304:THR:CG2[1_554] | 1.42                     | 0.78              |
| 4:2:284:LYS:C   | 4:7:268:GLY:C[1_554]   | 1.42                     | 0.78              |
| 4:3:113:LYS:O   | 4:8:251:GLY:N[1_554]   | 1.42                     | 0.78              |
| 4:3:118:LYS:N   | 4:8:237:GLU:CD[1_554]  | 1.42                     | 0.78              |
| 4:2:372:ARG:CD  | 4:7:227:MET:CA[1_554]  | 1.42                     | 0.78              |
| 4:3:316:GLU:OE1 | 4:7:151:ILE:O[1_554]   | 1.42                     | 0.78              |
| 4:4:166:TYR:OH  | 4:V:39:ARG:CA[1_554]   | 1.42                     | 0.78              |
| 4:3:32:PRO:N    | 4:7:78:ASN:CG[1_554]   | 1.42                     | 0.78              |
| 4:5:20:GLY:CA   | 4:9:121:GLN:NE2[1_554] | 1.42                     | 0.78              |
| 4:5:283:MET:CA  | 4:9:286:ASP:N[1_554]   | 1.42                     | 0.78              |
| 4:5:30:VAL:CA   | 4:9:79:TRP:O[1_554]    | 1.42                     | 0.78              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:178:LEU:CD1 | 4:7:177:ARG:O[1_554]   | 1.42                     | 0.78              |
| 4:4:240:TYR:CE2 | 4:8:56:ASP:OD2[1_554]  | 1.42                     | 0.78              |
| 4:3:16:LEU:CD1  | 4:7:78:ASN:CA[1_554]   | 1.42                     | 0.78              |
| 4:5:273:GLY:N   | 4:9:277:THR:CG2[1_554] | 1.43                     | 0.77              |
| 4:5:266:PHE:CG  | 4:9:261:LEU:CB[1_554]  | 1.43                     | 0.77              |
| 4:4:309:ILE:O   | 4:8:141:SER:CB[1_554]  | 1.43                     | 0.77              |
| 4:5:221:LEU:CB  | 4:9:332:PRO:CG[1_554]  | 1.43                     | 0.77              |
| 4:4:193:LEU:C   | 4:8:210:ARG:CA[1_554]  | 1.43                     | 0.77              |
| 4:5:173:HIS:CE1 | 4:V:265:SER:O[1_554]   | 1.43                     | 0.77              |
| 4:3:314:GLN:O   | 4:7:142:LEU:CG[1_554]  | 1.43                     | 0.77              |
| 4:2:357:ILE:CA  | 4:7:232:SER:CA[1_554]  | 1.43                     | 0.77              |
| 4:5:31:PHE:CB   | 4:9:81:ASP:N[1_554]    | 1.43                     | 0.77              |
| 4:3:166:TYR:CG  | 4:9:40:HIS:NE2[1_554]  | 1.43                     | 0.77              |
| 4:3:268:GLY:O   | 4:7:264:PRO:CB[1_554]  | 1.43                     | 0.77              |
| 4:3:307:PRO:N   | 4:7:11:ASP:OD2[1_554]  | 1.43                     | 0.77              |
| 4:4:335:ARG:CD  | 4:8:106:THR:CA[1_554]  | 1.43                     | 0.77              |
| 4:3:340:TRP:CB  | 4:7:118:LYS:N[1_554]   | 1.43                     | 0.77              |
| 4:3:226:GLU:OE1 | 4:7:333:PRO:CA[1_554]  | 1.43                     | 0.77              |
| 4:3:215:LYS:CG  | 4:7:31:PHE:CG[1_554]   | 1.43                     | 0.77              |
| 4:5:156:GLY:O   | 4:9:73:HIS:C[1_554]    | 1.43                     | 0.77              |
| 4:5:190:MET:C   | 4:9:186:THR:CB[1_554]  | 1.43                     | 0.77              |
| 4:3:110:LEU:CB  | 4:8:192:ILE:CA[1_554]  | 1.43                     | 0.77              |
| 4:3:297:ASN:CG  | 4:7:170:ALA:CB[1_554]  | 1.43                     | 0.77              |
| 4:4:332:PRO:CD  | 4:8:135:ALA:CA[1_554]  | 1.43                     | 0.77              |
| 4:5:368:SER:C   | 4:V:230:ALA:N[1_554]   | 1.43                     | 0.77              |
| 4:3:263:GLN:CA  | 4:7:274:ILE:CG1[1_554] | 1.43                     | 0.77              |
| 4:4:110:LEU:C   | 4:9:192:ILE:O[1_554]   | 1.43                     | 0.77              |
| 4:4:110:LEU:CB  | 4:9:192:ILE:CA[1_554]  | 1.43                     | 0.77              |
| 4:5:320:LEU:O   | 4:9:290:ARG:O[1_554]   | 1.43                     | 0.77              |
| 4:5:173:HIS:CB  | 4:V:267:ILE:CB[1_554]  | 1.43                     | 0.77              |
| 4:5:173:HIS:CE1 | 4:V:265:SER:CA[1_554]  | 1.43                     | 0.77              |
| 4:5:194:THR:N   | 4:9:209:VAL:CG1[1_554] | 1.43                     | 0.77              |
| 4:4:371:HIS:N   | 4:9:230:ALA:C[1_554]   | 1.43                     | 0.77              |
| 4:4:334:GLU:CA  | 4:8:105:LEU:CB[1_554]  | 1.43                     | 0.77              |
| 4:3:267:ILE:CB  | 4:7:180:LEU:CG[1_554]  | 1.43                     | 0.77              |
| 4:3:184:ASP:N   | 4:7:73:HIS:CE1[1_554]  | 1.43                     | 0.77              |
| 4:5:350:SER:N   | 4:9:364:GLU:O[1_554]   | 1.43                     | 0.77              |
| 4:4:151:ILE:CG1 | 4:8:172:PRO:CD[1_554]  | 1.43                     | 0.77              |
| 4:5:291:LYS:NZ  | 4:W:64:ILE:CD1[1_554]  | 1.43                     | 0.77              |
| 4:4:223:PHE:CA  | 4:8:335:ARG:CZ[1_554]  | 1.43                     | 0.77              |
| 4:3:321:ALA:O   | 4:7:292:ASP:OD2[1_554] | 1.43                     | 0.77              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:370:VAL:N   | 4:9:229:THR:O[1_554]   | 1.43                     | 0.77              |
| 4:3:213:LYS:CE  | 4:7:14:SER:O[1_554]    | 1.43                     | 0.77              |
| 4:5:296:ASN:N   | 4:9:169:TYR:N[1_554]   | 1.43                     | 0.77              |
| 4:4:173:HIS:NE2 | 4:9:265:SER:C[1_554]   | 1.43                     | 0.77              |
| 4:4:293:LEU:O   | 4:8:169:TYR:CG[1_554]  | 1.43                     | 0.77              |
| 4:4:180:LEU:O   | 4:8:159:VAL:CG1[1_554] | 1.43                     | 0.77              |
| 4:3:275:HIS:O   | 4:7:164:PRO:N[1_554]   | 1.43                     | 0.77              |
| 4:3:266:PHE:CA  | 4:7:261:LEU:CG[1_554]  | 1.43                     | 0.77              |
| 4:3:338:SER:O   | 4:7:116:ARG:O[1_554]   | 1.43                     | 0.77              |
| 4:4:312:ARG:CZ  | 4:8:299:MET:CB[1_554]  | 1.43                     | 0.77              |
| 4:3:311:ASP:O   | 4:7:142:LEU:CA[1_554]  | 1.43                     | 0.77              |
| 4:4:180:LEU:CD2 | 4:8:178:LEU:C[1_554]   | 1.43                     | 0.77              |
| 4:5:25:ASP:N    | 4:9:124:PHE:CA[1_554]  | 1.43                     | 0.77              |
| 4:2:291:LYS:CG  | 4:8:64:ILE:CG1[1_554]  | 1.43                     | 0.77              |
| 4:5:339:VAL:CB  | 4:9:116:ARG:N[1_554]   | 1.43                     | 0.77              |
| 4:3:274:ILE:N   | 4:7:161:HIS:C[1_554]   | 1.43                     | 0.77              |
| 4:3:315:LYS:N   | 4:7:142:LEU:CD1[1_554] | 1.43                     | 0.77              |
| 4:5:210:ARG:NH1 | 4:9:33:SER:O[1_554]    | 1.43                     | 0.77              |
| 4:3:113:LYS:CD  | 4:8:254:ARG:C[1_554]   | 1.43                     | 0.77              |
| 4:5:109:PRO:CA  | 4:V:195:GLU:OE2[1_554] | 1.43                     | 0.77              |
| 4:4:329:ILE:CA  | 4:8:139:VAL:CG1[1_554] | 1.43                     | 0.77              |
| 4:4:173:HIS:O   | 4:9:267:ILE:C[1_554]   | 1.43                     | 0.77              |
| 4:3:197:GLY:O   | 4:7:208:ILE:CB[1_554]  | 1.43                     | 0.77              |
| 4:3:213:LYS:O   | 4:7:16:LEU:N[1_554]    | 1.43                     | 0.77              |
| 4:4:294:TYR:O   | 4:8:168:GLY:N[1_554]   | 1.43                     | 0.77              |
| 4:5:370:VAL:N   | 4:V:231:ALA:N[1_554]   | 1.43                     | 0.77              |
| 4:4:191:LYS:CG  | 4:8:186:THR:N[1_554]   | 1.43                     | 0.77              |
| 4:5:180:LEU:CG  | 4:9:178:LEU:C[1_554]   | 1.43                     | 0.77              |
| 4:3:253:GLU:OE1 | 4:7:214:GLU:CA[1_554]  | 1.43                     | 0.77              |
| 4:4:185:LEU:CA  | 4:8:158:GLY:N[1_554]   | 1.44                     | 0.76              |
| 4:3:372:ARG:O   | 4:8:255:PHE:CZ[1_554]  | 1.44                     | 0.76              |
| 4:3:116:ARG:CD  | 4:8:252:ASN:OD1[1_554] | 1.44                     | 0.76              |
| 4:4:259:GLU:C   | 4:8:155:SER:CB[1_554]  | 1.44                     | 0.76              |
| 4:3:367:PRO:N   | 4:8:235:SER:CA[1_554]  | 1.44                     | 0.76              |
| 4:5:345:ILE:C   | 4:9:369:ILE:CG2[1_554] | 1.44                     | 0.76              |
| 4:5:263:GLN:CB  | 4:9:274:ILE:CG2[1_554] | 1.44                     | 0.76              |
| 4:4:276:GLU:CG  | 4:8:278:THR:O[1_554]   | 1.44                     | 0.76              |
| 4:4:320:LEU:CG  | 4:8:293:LEU:CB[1_554]  | 1.44                     | 0.76              |
| 4:3:137:GLN:O   | 4:7:113:LYS:N[1_554]   | 1.44                     | 0.76              |
| 4:5:349:LEU:N   | 4:9:365:ALA:C[1_554]   | 1.44                     | 0.76              |
| 4:4:279:TYR:N   | 4:8:164:PRO:CG[1_554]  | 1.44                     | 0.76              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:143:TYR:CE2 | 4:7:368:SER:CB[1_554]  | 1.44                     | 0.76              |
| 4:4:193:LEU:CG  | 4:8:210:ARG:CD[1_554]  | 1.44                     | 0.76              |
| 4:3:298:VAL:CG1 | 4:7:116:ARG:NH2[1_554] | 1.44                     | 0.76              |
| 4:5:220:ALA:CB  | 4:9:335:ARG:CG[1_554]  | 1.44                     | 0.76              |
| 4:4:16:LEU:CD1  | 4:8:78:ASN:O[1_554]    | 1.44                     | 0.76              |
| 4:5:284:LYS:O   | 4:V:268:GLY:C[1_554]   | 1.44                     | 0.76              |
| 4:4:346:LEU:CB  | 4:8:368:SER:CB[1_554]  | 1.44                     | 0.76              |
| 4:4:198:TYR:N   | 4:8:209:VAL:N[1_554]   | 1.44                     | 0.76              |
| 4:5:280:ASN:OD1 | 4:9:281:SER:CA[1_554]  | 1.44                     | 0.76              |
| 4:5:166:TYR:CD1 | 4:W:40:HIS:CE1[1_554]  | 1.44                     | 0.76              |
| 4:4:288:ASP:C   | 4:V:63:GLY:C[1_554]    | 1.44                     | 0.76              |
| 4:4:333:PRO:CA  | 4:8:104:LEU:O[1_554]   | 1.44                     | 0.76              |
| 4:5:187:ASP:O   | 4:9:183:ARG:C[1_554]   | 1.44                     | 0.76              |
| 4:4:300:SER:O   | 4:8:108:ALA:N[1_554]   | 1.44                     | 0.76              |
| 4:4:189:LEU:N   | 4:8:183:ARG:CA[1_554]  | 1.44                     | 0.76              |
| 4:4:182:GLY:CA  | 4:8:14:SER:OG[1_554]   | 1.44                     | 0.76              |
| 4:5:339:VAL:O   | 4:9:117:GLU:N[1_554]   | 1.44                     | 0.76              |
| 4:4:222:ASP:C   | 4:8:331:ALA:C[1_554]   | 1.44                     | 0.76              |
| 4:3:214:GLU:N   | 4:7:15:GLY:C[1_554]    | 1.44                     | 0.76              |
| 4:5:295:ALA:CB  | 4:9:167:GLU:O[1_554]   | 1.44                     | 0.76              |
| 4:5:340:TRP:CA  | 4:9:116:ARG:O[1_554]   | 1.44                     | 0.76              |
| 4:5:76:ILE:N    | 4:V:197:GLY:O[1_554]   | 1.44                     | 0.76              |
| 4:2:169:TYR:OH  | 4:7:266:PHE:CZ[1_554]  | 1.44                     | 0.76              |
| 4:5:181:ALA:O   | 4:9:159:VAL:N[1_554]   | 1.44                     | 0.76              |
| 4:5:262:PHE:CB  | 4:9:153:LEU:CB[1_554]  | 1.44                     | 0.76              |
| 4:3:16:LEU:N    | 4:7:77:THR:O[1_554]    | 1.44                     | 0.76              |
| 4:4:310:ALA:CB  | 4:8:140:LEU:CB[1_554]  | 1.44                     | 0.76              |
| 4:5:157:ASP:C   | 4:9:72:GLU:C[1_554]    | 1.44                     | 0.76              |
| 4:3:143:TYR:C   | 4:7:372:ARG:N[1_554]   | 1.44                     | 0.76              |
| 4:4:187:ASP:C   | 4:8:183:ARG:C[1_554]   | 1.44                     | 0.76              |
| 4:4:145:SER:OG  | 4:8:372:ARG:NH1[1_554] | 1.44                     | 0.76              |
| 4:4:337:TYR:OH  | 4:8:86:TRP:CE3[1_554]  | 1.44                     | 0.76              |
| 4:5:219:VAL:CB  | 4:9:300:SER:C[1_554]   | 1.44                     | 0.76              |
| 4:5:371:HIS:N   | 4:V:231:ALA:N[1_554]   | 1.44                     | 0.76              |
| 4:2:284:LYS:O   | 4:7:269:MET:N[1_554]   | 1.44                     | 0.76              |
| 4:5:218:TYR:CG  | 4:9:336:LYS:CB[1_554]  | 1.44                     | 0.76              |
| 4:3:258:PRO:CA  | 4:7:155:SER:C[1_554]   | 1.44                     | 0.76              |
| 4:3:213:LYS:CD  | 4:7:15:GLY:N[1_554]    | 1.44                     | 0.76              |
| 4:5:281:SER:C   | 4:9:173:HIS:NE2[1_554] | 1.44                     | 0.76              |
| 4:5:178:LEU:CB  | 4:9:177:ARG:CA[1_554]  | 1.44                     | 0.76              |
| 4:5:200:PHE:CB  | 4:9:206:ARG:CD[1_554]  | 1.44                     | 0.76              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:141:SER:N   | 4:9:116:ARG:CD[1_554]  | 1.44                     | 0.76              |
| 4:4:263:GLN:NE2 | 4:8:153:LEU:CD2[1_554] | 1.44                     | 0.76              |
| 4:4:221:LEU:O   | 4:8:332:PRO:N[1_554]   | 1.44                     | 0.76              |
| 4:4:288:ASP:O   | 4:V:64:ILE:C[1_554]    | 1.44                     | 0.76              |
| 4:2:113:LYS:CB  | 4:7:254:ARG:CA[1_554]  | 1.44                     | 0.76              |
| 4:4:17:VAL:O    | 4:8:79:TRP:CG[1_554]   | 1.44                     | 0.76              |
| 4:3:311:ASP:CA  | 4:7:141:SER:C[1_554]   | 1.44                     | 0.76              |
| 4:5:155:SER:C   | 4:9:108:ALA:CB[1_554]  | 1.45                     | 0.75              |
| 4:5:331:ALA:CA  | 4:9:140:LEU:CG[1_554]  | 1.45                     | 0.75              |
| 4:4:211:ASP:CB  | 4:8:32:PRO:CB[1_554]   | 1.45                     | 0.75              |
| 4:3:172:PRO:CG  | 4:8:266:PHE:CD2[1_554] | 1.45                     | 0.75              |
| 4:5:211:ASP:CA  | 4:9:32:PRO:CB[1_554]   | 1.45                     | 0.75              |
| 4:3:340:TRP:CZ3 | 4:7:121:GLN:CA[1_554]  | 1.45                     | 0.75              |
| 4:3:191:LYS:CB  | 4:7:186:THR:C[1_554]   | 1.45                     | 0.75              |
| 4:4:367:PRO:N   | 4:9:234:SER:CA[1_554]  | 1.45                     | 0.75              |
| 4:5:154:ASP:OD2 | 4:9:111:ASN:CB[1_554]  | 1.45                     | 0.75              |
| 4:4:188:TYR:CE1 | 4:8:185:LEU:CD2[1_554] | 1.45                     | 0.75              |
| 4:4:286:ASP:CA  | 4:9:270:GLU:OE2[1_554] | 1.45                     | 0.75              |
| 4:4:186:THR:O   | 4:8:183:ARG:CG[1_554]  | 1.45                     | 0.75              |
| 4:3:243:PRO:CD  | 4:7:59:GLN:O[1_554]    | 1.45                     | 0.75              |
| 4:4:337:TYR:N   | 4:8:119:MET:SD[1_554]  | 1.45                     | 0.75              |
| 4:4:113:LYS:O   | 4:9:251:GLY:CA[1_554]  | 1.45                     | 0.75              |
| 4:4:338:SER:O   | 4:8:116:ARG:O[1_554]   | 1.45                     | 0.75              |
| 4:3:223:PHE:CD2 | 4:7:304:THR:OG1[1_554] | 1.45                     | 0.75              |
| 4:5:157:ASP:OD1 | 4:9:72:GLU:CA[1_554]   | 1.45                     | 0.75              |
| 4:5:362:TYR:CD1 | 4:V:232:SER:O[1_554]   | 1.45                     | 0.75              |
| 4:4:315:LYS:NZ  | 4:8:147:ARG:NH1[1_554] | 1.45                     | 0.75              |
| 4:5:345:ILE:CG2 | 4:9:369:ILE:CB[1_554]  | 1.45                     | 0.75              |
| 4:5:23:GLY:CA   | 4:9:362:TYR:CD2[1_554] | 1.45                     | 0.75              |
| 4:3:273:GLY:C   | 4:7:162:ASN:N[1_554]   | 1.45                     | 0.75              |
| 4:3:370:VAL:CG1 | 4:8:230:ALA:O[1_554]   | 1.45                     | 0.75              |
| 4:3:143:TYR:N   | 4:7:372:ARG:N[1_554]   | 1.45                     | 0.75              |
| 4:4:340:TRP:CD2 | 4:8:118:LYS:O[1_554]   | 1.45                     | 0.75              |
| 4:4:136:ILE:CB  | 4:8:113:LYS:NZ[1_554]  | 1.45                     | 0.75              |
| 4:5:193:LEU:CG  | 4:9:210:ARG:CA[1_554]  | 1.45                     | 0.75              |
| 4:5:338:SER:OG  | 4:9:134:VAL:CB[1_554]  | 1.45                     | 0.75              |
| 4:4:141:SER:CA  | 4:8:116:ARG:CD[1_554]  | 1.45                     | 0.75              |
| 4:5:28:ARG:CG   | 4:9:126:THR:CB[1_554]  | 1.45                     | 0.75              |
| 4:5:220:ALA:C   | 4:9:335:ARG:CD[1_554]  | 1.45                     | 0.75              |
| 4:5:340:TRP:CB  | 4:9:119:MET:CA[1_554]  | 1.45                     | 0.75              |
| 4:3:328:LYS:N   | 4:7:168:GLY:N[1_554]   | 1.45                     | 0.75              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:27:PRO:CD   | 4:7:122:ILE:CB[1_554]  | 1.45                     | 0.75              |
| 4:3:260:THR:C   | 4:7:160:THR:OG1[1_554] | 1.45                     | 0.75              |
| 4:5:295:ALA:C   | 4:9:167:GLU:C[1_554]   | 1.45                     | 0.75              |
| 4:2:75:ILE:CG1  | 4:7:193:LEU:O[1_554]   | 1.45                     | 0.75              |
| 4:4:277:THR:O   | 4:8:175:ILE:N[1_554]   | 1.45                     | 0.75              |
| 4:4:193:LEU:CG  | 4:8:210:ARG:CB[1_554]  | 1.45                     | 0.75              |
| 4:4:318:THR:N   | 4:8:150:GLY:CA[1_554]  | 1.45                     | 0.75              |
| 4:5:221:LEU:C   | 4:9:332:PRO:N[1_554]   | 1.45                     | 0.75              |
| 4:5:335:ARG:N   | 4:9:106:THR:N[1_554]   | 1.45                     | 0.75              |
| 4:5:344:SER:O   | 4:9:362:TYR:CE1[1_554] | 1.45                     | 0.75              |
| 4:3:344:SER:OG  | 4:7:362:TYR:OH[1_554]  | 1.45                     | 0.75              |
| 4:4:140:LEU:CD2 | 4:8:117:GLU:CD[1_554]  | 1.45                     | 0.75              |
| 4:5:204:ALA:O   | 4:9:62:ARG:CD[1_554]   | 1.45                     | 0.75              |
| 4:5:173:HIS:CA  | 4:V:267:ILE:N[1_554]   | 1.45                     | 0.75              |
| 4:5:275:HIS:O   | 4:9:151:ILE:CG1[1_554] | 1.45                     | 0.75              |
| 4:2:169:TYR:OH  | 4:7:266:PHE:CD1[1_554] | 1.45                     | 0.75              |
| 4:4:268:GLY:CA  | 4:8:264:PRO:CA[1_554]  | 1.45                     | 0.75              |
| 4:3:180:LEU:CG  | 4:7:178:LEU:O[1_554]   | 1.45                     | 0.75              |
| 4:5:335:ARG:CA  | 4:9:106:THR:N[1_554]   | 1.45                     | 0.75              |
| 4:5:262:PHE:CD1 | 4:9:153:LEU:N[1_554]   | 1.45                     | 0.75              |
| 4:1:288:ASP:C   | 4:7:39:ARG:CZ[1_554]   | 1.45                     | 0.75              |
| 4:3:304:THR:C   | 4:7:137:GLN:NE2[1_554] | 1.45                     | 0.75              |
| 4:3:108:ALA:N   | 4:8:195:GLU:O[1_554]   | 1.45                     | 0.75              |
| 4:3:306:TYR:N   | 4:7:11:ASP:OD1[1_554]  | 1.46                     | 0.74              |
| 4:4:267:ILE:O   | 4:8:180:LEU:CD2[1_554] | 1.46                     | 0.74              |
| 4:5:75:ILE:CD1  | 4:V:196:ARG:N[1_554]   | 1.46                     | 0.74              |
| 4:5:140:LEU:CB  | 4:9:371:HIS:ND1[1_554] | 1.46                     | 0.74              |
| 4:2:291:LYS:NZ  | 4:8:64:ILE:O[1_554]    | 1.46                     | 0.74              |
| 4:4:196:ARG:CG  | 4:8:212:ILE:N[1_554]   | 1.46                     | 0.74              |
| 4:5:137:GLN:CB  | 4:9:112:PRO:CA[1_554]  | 1.46                     | 0.74              |
| 4:3:327:ILE:CB  | 4:7:148:THR:C[1_554]   | 1.46                     | 0.74              |
| 4:3:188:TYR:C   | 4:7:182:GLY:C[1_554]   | 1.46                     | 0.74              |
| 4:3:193:LEU:CD2 | 4:7:210:ARG:NE[1_554]  | 1.46                     | 0.74              |
| 4:3:282:ILE:CB  | 4:7:171:LEU:CD2[1_554] | 1.46                     | 0.74              |
| 4:4:328:LYS:N   | 4:8:168:GLY:N[1_554]   | 1.46                     | 0.74              |
| 4:5:310:ALA:CA  | 4:9:141:SER:N[1_554]   | 1.46                     | 0.74              |
| 4:4:299:MET:CB  | 4:8:136:ILE:CB[1_554]  | 1.46                     | 0.74              |
| 4:3:79:TRP:CH2  | 4:8:249:THR:CG2[1_554] | 1.46                     | 0.74              |
| 4:4:308:GLY:N   | 4:8:338:SER:C[1_554]   | 1.46                     | 0.74              |
| 4:4:267:ILE:CB  | 4:8:180:LEU:CD1[1_554] | 1.46                     | 0.74              |
| 4:2:74:GLY:C    | 4:7:197:GLY:CA[1_554]  | 1.46                     | 0.74              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:338:SER:OG  | 4:8:134:VAL:CB[1_554]  | 1.46                     | 0.74              |
| 4:5:112:PRO:O   | 4:V:253:GLU:OE2[1_554] | 1.46                     | 0.74              |
| 4:5:316:GLU:CD  | 4:9:297:ASN:ND2[1_554] | 1.46                     | 0.74              |
| 4:4:304:THR:N   | 4:8:137:GLN:CD[1_554]  | 1.46                     | 0.74              |
| 4:5:113:LYS:NZ  | 4:V:255:PHE:N[1_554]   | 1.46                     | 0.74              |
| 4:3:311:ASP:N   | 4:7:141:SER:N[1_554]   | 1.46                     | 0.74              |
| 4:3:212:ILE:N   | 4:7:32:PRO:CB[1_554]   | 1.46                     | 0.74              |
| 4:5:200:PHE:CB  | 4:9:206:ARG:NE[1_554]  | 1.46                     | 0.74              |
| 4:3:270:GLU:CA  | 4:7:272:ALA:O[1_554]   | 1.46                     | 0.74              |
| 4:4:227:MET:SD  | 4:8:305:MET:O[1_554]   | 1.46                     | 0.74              |
| 4:3:310:ALA:CA  | 4:7:140:LEU:CA[1_554]  | 1.46                     | 0.74              |
| 4:2:368:SER:CA  | 4:7:236:LEU:CB[1_554]  | 1.46                     | 0.74              |
| 4:5:59:GLN:CB   | 4:9:68:LYS:CG[1_554]   | 1.46                     | 0.74              |
| 4:3:243:PRO:CB  | 4:7:61:LYS:CA[1_554]   | 1.46                     | 0.74              |
| 4:5:313:MET:CE  | 4:9:163:VAL:O[1_554]   | 1.46                     | 0.74              |
| 4:4:140:LEU:C   | 4:8:371:HIS:CG[1_554]  | 1.46                     | 0.74              |
| 4:5:227:MET:CE  | 4:9:306:TYR:CB[1_554]  | 1.46                     | 0.74              |
| 4:4:114:ALA:N   | 4:9:250:ILE:C[1_554]   | 1.46                     | 0.74              |
| 4:4:199:SER:CA  | 4:8:206:ARG:CB[1_554]  | 1.46                     | 0.74              |
| 4:5:318:THR:C   | 4:9:292:ASP:O[1_554]   | 1.46                     | 0.74              |
| 4:5:296:ASN:O   | 4:9:169:TYR:CA[1_554]  | 1.46                     | 0.74              |
| 4:3:194:THR:O   | 4:7:209:VAL:CG2[1_554] | 1.46                     | 0.74              |
| 4:4:305:MET:O   | 4:8:11:ASP:CB[1_554]   | 1.46                     | 0.74              |
| 4:5:259:GLU:CG  | 4:9:309:ILE:CD1[1_554] | 1.46                     | 0.74              |
| 4:5:299:MET:SD  | 4:9:138:ALA:C[1_554]   | 1.46                     | 0.74              |
| 4:3:240:TYR:CD2 | 4:7:56:ASP:OD2[1_554]  | 1.46                     | 0.74              |
| 4:4:368:SER:N   | 4:9:234:SER:OG[1_554]  | 1.46                     | 0.74              |
| 4:4:300:SER:CA  | 4:8:107:GLU:CB[1_554]  | 1.46                     | 0.74              |
| 4:4:136:ILE:O   | 4:8:113:LYS:CG[1_554]  | 1.46                     | 0.74              |
| 4:3:74:GLY:C    | 4:8:197:GLY:C[1_554]   | 1.46                     | 0.74              |
| 4:3:313:MET:CB  | 4:7:138:ALA:C[1_554]   | 1.46                     | 0.74              |
| 4:4:277:THR:CG2 | 4:8:176:MET:N[1_554]   | 1.46                     | 0.74              |
| 4:4:339:VAL:N   | 4:8:116:ARG:CB[1_554]  | 1.46                     | 0.74              |
| 4:5:312:ARG:N   | 4:9:298:VAL:CG1[1_554] | 1.46                     | 0.74              |
| 4:3:192:ILE:CG1 | 4:7:213:LYS:CE[1_554]  | 1.46                     | 0.74              |
| 4:3:223:PHE:CZ  | 4:7:301:GLY:N[1_554]   | 1.46                     | 0.74              |
| 4:5:221:LEU:CD2 | 4:9:332:PRO:CB[1_554]  | 1.46                     | 0.74              |
| 4:5:198:TYR:CE1 | 4:9:208:ILE:CB[1_554]  | 1.46                     | 0.74              |
| 4:4:262:PHE:CA  | 4:8:153:LEU:CG[1_554]  | 1.46                     | 0.74              |
| 4:5:367:PRO:CD  | 4:V:234:SER:C[1_554]   | 1.46                     | 0.74              |
| 4:3:222:ASP:C   | 4:7:331:ALA:C[1_554]   | 1.46                     | 0.74              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:180:LEU:CB  | 4:8:179:ASP:N[1_554]   | 1.46                     | 0.74              |
| 4:4:191:LYS:CA  | 4:8:187:ASP:N[1_554]   | 1.46                     | 0.74              |
| 4:5:218:TYR:OH  | 4:9:337:TYR:CD2[1_554] | 1.46                     | 0.74              |
| 4:4:253:GLU:OE1 | 4:8:214:GLU:CB[1_554]  | 1.46                     | 0.74              |
| 1:D:637:LYS:CE  | 4:5:311:ASP:OD1[1_556] | 1.47                     | 0.73              |
| 4:4:114:ALA:C   | 4:9:251:GLY:N[1_554]   | 1.47                     | 0.73              |
| 4:4:207:GLU:CB  | 4:8:67:LEU:CG[1_554]   | 1.47                     | 0.73              |
| 4:3:316:GLU:O   | 4:7:150:GLY:C[1_554]   | 1.47                     | 0.73              |
| 4:3:213:LYS:CG  | 4:7:15:GLY:N[1_554]    | 1.47                     | 0.73              |
| 4:4:300:SER:C   | 4:8:107:GLU:CB[1_554]  | 1.47                     | 0.73              |
| 4:3:338:SER:C   | 4:7:116:ARG:O[1_554]   | 1.47                     | 0.73              |
| 4:4:169:TYR:OH  | 4:9:266:PHE:CD1[1_554] | 1.47                     | 0.73              |
| 4:3:310:ALA:CA  | 4:7:141:SER:N[1_554]   | 1.47                     | 0.73              |
| 4:4:340:TRP:O   | 4:8:117:GLU:C[1_554]   | 1.47                     | 0.73              |
| 4:4:188:TYR:CG  | 4:8:181:ALA:C[1_554]   | 1.47                     | 0.73              |
| 4:4:151:ILE:CD1 | 4:8:172:PRO:CD[1_554]  | 1.47                     | 0.73              |
| 4:2:113:LYS:CG  | 4:7:254:ARG:CB[1_554]  | 1.47                     | 0.73              |
| 4:3:369:ILE:N   | 4:8:234:SER:OG[1_554]  | 1.47                     | 0.73              |
| 4:4:153:LEU:CG  | 4:8:109:PRO:CG[1_554]  | 1.47                     | 0.73              |
| 4:3:30:VAL:CG1  | 4:7:79:TRP:C[1_554]    | 1.47                     | 0.73              |
| 4:5:213:LYS:O   | 4:9:16:LEU:CD2[1_554]  | 1.47                     | 0.73              |
| 4:5:275:HIS:C   | 4:9:151:ILE:CG1[1_554] | 1.47                     | 0.73              |
| 4:5:339:VAL:CB  | 4:9:116:ARG:CA[1_554]  | 1.47                     | 0.73              |
| 4:3:258:PRO:CA  | 4:7:155:SER:O[1_554]   | 1.47                     | 0.73              |
| 4:4:143:TYR:N   | 4:8:371:HIS:O[1_554]   | 1.47                     | 0.73              |
| 4:3:339:VAL:N   | 4:7:116:ARG:C[1_554]   | 1.47                     | 0.73              |
| 4:4:256:ARG:O   | 4:8:303:THR:CG2[1_554] | 1.47                     | 0.73              |
| 4:5:277:THR:CA  | 4:9:174:ALA:O[1_554]   | 1.47                     | 0.73              |
| 4:3:300:SER:CA  | 4:7:107:GLU:CB[1_554]  | 1.47                     | 0.73              |
| 4:5:337:TYR:OH  | 4:9:86:TRP:CD2[1_554]  | 1.47                     | 0.73              |
| 4:4:110:LEU:CA  | 4:9:192:ILE:CB[1_554]  | 1.47                     | 0.73              |
| 4:3:180:LEU:CB  | 4:7:179:ASP:N[1_554]   | 1.47                     | 0.73              |
| 4:4:326:LYS:C   | 4:8:167:GLU:CG[1_554]  | 1.47                     | 0.73              |
| 4:4:317:ILE:CD1 | 4:8:165:ILE:CB[1_554]  | 1.47                     | 0.73              |
| 4:3:216:LEU:CA  | 4:7:30:VAL:CG1[1_554]  | 1.47                     | 0.73              |
| 4:4:188:TYR:CE1 | 4:8:185:LEU:CB[1_554]  | 1.47                     | 0.73              |
| 4:2:289:ILE:CG2 | 4:8:39:ARG:NE[1_554]   | 1.47                     | 0.73              |
| 4:3:262:PHE:CD1 | 4:7:154:ASP:N[1_554]   | 1.47                     | 0.73              |
| 4:5:261:LEU:CB  | 4:9:154:ASP:C[1_554]   | 1.47                     | 0.73              |
| 4:5:253:GLU:CG  | 4:9:214:GLU:N[1_554]   | 1.47                     | 0.73              |
| 4:4:371:HIS:CE1 | 4:9:252:ASN:CA[1_554]  | 1.47                     | 0.73              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:307:PRO:CB  | 4:7:340:TRP:CB[1_554]  | 1.47                     | 0.73              |
| 4:5:192:ILE:CB  | 4:9:213:LYS:CG[1_554]  | 1.47                     | 0.73              |
| 4:5:367:PRO:CD  | 4:V:234:SER:CA[1_554]  | 1.47                     | 0.73              |
| 4:4:143:TYR:N   | 4:8:372:ARG:CA[1_554]  | 1.47                     | 0.73              |
| 4:3:325:MET:CB  | 4:7:166:TYR:CZ[1_554]  | 1.47                     | 0.73              |
| 4:5:300:SER:OG  | 4:9:107:GLU:CG[1_554]  | 1.47                     | 0.73              |
| 4:5:270:GLU:N   | 4:9:272:ALA:N[1_554]   | 1.47                     | 0.73              |
| 4:3:188:TYR:CE1 | 4:7:185:LEU:CG[1_554]  | 1.47                     | 0.73              |
| 4:3:173:HIS:NE2 | 4:8:265:SER:C[1_554]   | 1.47                     | 0.73              |
| 4:3:213:LYS:O   | 4:7:16:LEU:CB[1_554]   | 1.47                     | 0.73              |
| 4:4:218:TYR:CZ  | 4:8:337:TYR:CZ[1_554]  | 1.47                     | 0.73              |
| 4:4:139:VAL:CB  | 4:8:113:LYS:CD[1_554]  | 1.47                     | 0.73              |
| 4:2:166:TYR:OH  | 4:8:39:ARG:O[1_554]    | 1.47                     | 0.73              |
| 4:3:259:GLU:OE1 | 4:7:305:MET:N[1_554]   | 1.47                     | 0.73              |
| 4:4:159:VAL:O   | 4:8:177:ARG:NH1[1_554] | 1.47                     | 0.73              |
| 4:5:167:GLU:OE2 | 4:W:40:HIS:C[1_554]    | 1.47                     | 0.73              |
| 4:3:195:GLU:CG  | 4:7:189:LEU:CG[1_554]  | 1.47                     | 0.73              |
| 4:5:273:GLY:C   | 4:9:162:ASN:CB[1_554]  | 1.47                     | 0.73              |
| 4:5:30:VAL:O    | 4:9:80:ASP:O[1_554]    | 1.47                     | 0.73              |
| 4:4:357:ILE:CG2 | 4:9:232:SER:CA[1_554]  | 1.47                     | 0.73              |
| 4:5:110:LEU:O   | 4:V:192:ILE:O[1_554]   | 1.47                     | 0.73              |
| 4:5:151:ILE:N   | 4:9:169:TYR:CD1[1_554] | 1.47                     | 0.73              |
| 4:3:332:PRO:CB  | 4:7:133:TYR:C[1_554]   | 1.47                     | 0.73              |
| 4:3:259:GLU:OE1 | 4:7:304:THR:CA[1_554]  | 1.47                     | 0.73              |
| 4:5:316:GLU:CA  | 4:9:296:ASN:O[1_554]   | 1.47                     | 0.73              |
| 4:4:188:TYR:C   | 4:8:182:GLY:O[1_554]   | 1.47                     | 0.73              |
| 4:3:299:MET:CB  | 4:7:136:ILE:CB[1_554]  | 1.47                     | 0.73              |
| 4:3:340:TRP:CZ2 | 4:7:121:GLN:CG[1_554]  | 1.47                     | 0.73              |
| 4:5:320:LEU:N   | 4:9:294:TYR:N[1_554]   | 1.47                     | 0.73              |
| 4:5:340:TRP:O   | 4:9:120:THR:CB[1_554]  | 1.47                     | 0.73              |
| 4:5:112:PRO:C   | 4:V:253:GLU:OE2[1_554] | 1.48                     | 0.72              |
| 4:5:115:ASN:ND2 | 4:V:196:ARG:CD[1_554]  | 1.48                     | 0.72              |
| 4:5:335:ARG:O   | 4:9:106:THR:O[1_554]   | 1.48                     | 0.72              |
| 4:3:114:ALA:N   | 4:8:250:ILE:C[1_554]   | 1.48                     | 0.72              |
| 4:4:255:PHE:CA  | 4:8:302:GLY:CA[1_554]  | 1.48                     | 0.72              |
| 4:3:326:LYS:CD  | 4:9:45:VAL:N[1_554]    | 1.48                     | 0.72              |
| 4:5:314:GLN:CD  | 4:9:147:ARG:C[1_554]   | 1.48                     | 0.72              |
| 4:5:137:GLN:CB  | 4:9:113:LYS:N[1_554]   | 1.48                     | 0.72              |
| 4:3:154:ASP:CG  | 4:7:111:ASN:N[1_554]   | 1.48                     | 0.72              |
| 4:5:343:GLY:O   | 4:9:367:PRO:N[1_554]   | 1.48                     | 0.72              |
| 4:3:213:LYS:O   | 4:7:16:LEU:CA[1_554]   | 1.48                     | 0.72              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:18:LYS:CG   | 4:9:79:TRP:CZ3[1_554]  | 1.48                     | 0.72              |
| 4:4:259:GLU:CB  | 4:8:304:THR:N[1_554]   | 1.48                     | 0.72              |
| 4:4:279:TYR:N   | 4:8:164:PRO:CB[1_554]  | 1.48                     | 0.72              |
| 4:2:111:ASN:N   | 4:7:192:ILE:C[1_554]   | 1.48                     | 0.72              |
| 4:5:208:ILE:CG2 | 4:9:59:GLN:OE1[1_554]  | 1.48                     | 0.72              |
| 4:4:262:PHE:C   | 4:8:153:LEU:CG[1_554]  | 1.48                     | 0.72              |
| 4:4:311:ASP:N   | 4:8:141:SER:CA[1_554]  | 1.48                     | 0.72              |
| 4:5:274:ILE:O   | 4:9:163:VAL:N[1_554]   | 1.48                     | 0.72              |
| 4:4:312:ARG:CZ  | 4:8:299:MET:CG[1_554]  | 1.48                     | 0.72              |
| 4:1:289:ILE:N   | 4:7:39:ARG:NH2[1_554]  | 1.48                     | 0.72              |
| 4:3:243:PRO:CA  | 4:7:61:LYS:N[1_554]    | 1.48                     | 0.72              |
| 4:3:188:TYR:N   | 4:7:183:ARG:CB[1_554]  | 1.48                     | 0.72              |
| 4:3:259:GLU:CB  | 4:7:304:THR:N[1_554]   | 1.48                     | 0.72              |
| 4:4:162:ASN:CG  | 4:8:175:ILE:CB[1_554]  | 1.48                     | 0.72              |
| 4:4:137:GLN:OE1 | 4:8:112:PRO:CG[1_554]  | 1.48                     | 0.72              |
| 4:2:73:HIS:C    | 4:7:198:TYR:O[1_554]   | 1.48                     | 0.72              |
| 4:5:282:ILE:CD1 | 4:9:171:LEU:CG[1_554]  | 1.48                     | 0.72              |
| 4:4:265:SER:C   | 4:8:261:LEU:O[1_554]   | 1.48                     | 0.72              |
| 4:3:153:LEU:CG  | 4:7:109:PRO:CA[1_554]  | 1.48                     | 0.72              |
| 4:5:174:ALA:C   | 4:9:173:HIS:CB[1_554]  | 1.48                     | 0.72              |
| 4:5:192:ILE:CG1 | 4:9:213:LYS:CE[1_554]  | 1.48                     | 0.72              |
| 4:5:215:LYS:CG  | 4:9:31:PHE:CA[1_554]   | 1.48                     | 0.72              |
| 4:5:266:PHE:N   | 4:9:261:LEU:C[1_554]   | 1.48                     | 0.72              |
| 4:5:297:ASN:ND2 | 4:9:165:ILE:CG1[1_554] | 1.48                     | 0.72              |
| 4:3:16:LEU:CA   | 4:7:78:ASN:N[1_554]    | 1.48                     | 0.72              |
| 4:4:273:GLY:C   | 4:8:162:ASN:OD1[1_554] | 1.48                     | 0.72              |
| 4:3:255:PHE:CE1 | 4:7:305:MET:CG[1_554]  | 1.48                     | 0.72              |
| 4:5:283:MET:CG  | 4:9:286:ASP:CA[1_554]  | 1.48                     | 0.72              |
| 4:5:151:ILE:CA  | 4:9:170:ALA:O[1_554]   | 1.48                     | 0.72              |
| 4:4:26:ALA:CB   | 4:8:123:MET:CA[1_554]  | 1.48                     | 0.72              |
| 4:3:331:ALA:C   | 4:7:135:ALA:CA[1_554]  | 1.48                     | 0.72              |
| 4:4:270:GLU:C   | 4:8:272:ALA:CB[1_554]  | 1.48                     | 0.72              |
| 4:3:72:GLU:O    | 4:8:199:SER:N[1_554]   | 1.48                     | 0.72              |
| 4:4:41:GLN:CB   | 4:7:224:GLU:CG[1_554]  | 1.48                     | 0.72              |
| 4:3:188:TYR:CZ  | 4:7:185:LEU:CD2[1_554] | 1.48                     | 0.72              |
| 4:2:116:ARG:C   | 4:7:237:GLU:CD[1_554]  | 1.48                     | 0.72              |
| 4:5:194:THR:CA  | 4:9:209:VAL:CG2[1_554] | 1.48                     | 0.72              |
| 4:4:288:ASP:C   | 4:V:64:ILE:N[1_554]    | 1.48                     | 0.72              |
| 4:2:370:VAL:CB  | 4:7:230:ALA:O[1_554]   | 1.48                     | 0.72              |
| 4:4:215:LYS:CG  | 4:8:31:PHE:N[1_554]    | 1.48                     | 0.72              |
| 4:3:193:LEU:C   | 4:7:210:ARG:CA[1_554]  | 1.48                     | 0.72              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:300:SER:O   | 4:9:108:ALA:N[1_554]   | 1.48                     | 0.72              |
| 4:5:318:THR:CB  | 4:9:296:ASN:CG[1_554]  | 1.48                     | 0.72              |
| 4:5:325:MET:CG  | 4:9:166:TYR:CZ[1_554]  | 1.48                     | 0.72              |
| 4:2:109:PRO:N   | 4:7:195:GLU:CB[1_554]  | 1.48                     | 0.72              |
| 4:2:114:ALA:C   | 4:7:250:ILE:O[1_554]   | 1.48                     | 0.72              |
| 4:4:268:GLY:O   | 4:8:264:PRO:CB[1_554]  | 1.48                     | 0.72              |
| 4:3:186:THR:OG1 | 4:7:183:ARG:CZ[1_554]  | 1.48                     | 0.72              |
| 4:5:166:TYR:CB  | 4:W:40:HIS:CE1[1_554]  | 1.48                     | 0.72              |
| 4:2:288:ASP:O   | 4:8:64:ILE:CA[1_554]   | 1.48                     | 0.72              |
| 4:4:215:LYS:CE  | 4:8:31:PHE:CG[1_554]   | 1.48                     | 0.72              |
| 4:5:319:ALA:C   | 4:9:295:ALA:N[1_554]   | 1.48                     | 0.72              |
| 4:3:180:LEU:CD1 | 4:7:160:THR:N[1_554]   | 1.48                     | 0.72              |
| 4:5:27:PRO:CB   | 4:9:122:ILE:CB[1_554]  | 1.48                     | 0.72              |
| 4:4:226:GLU:OE1 | 4:8:333:PRO:CA[1_554]  | 1.48                     | 0.72              |
| 4:4:288:ASP:CA  | 4:V:62:ARG:O[1_554]    | 1.48                     | 0.72              |
| 4:4:196:ARG:CG  | 4:8:211:ASP:CA[1_554]  | 1.48                     | 0.72              |
| 4:4:178:LEU:CD1 | 4:8:177:ARG:O[1_554]   | 1.48                     | 0.72              |
| 4:5:113:LYS:C   | 4:V:252:ASN:N[1_554]   | 1.48                     | 0.72              |
| 4:4:178:LEU:CD2 | 4:8:177:ARG:N[1_554]   | 1.48                     | 0.72              |
| 4:5:346:LEU:CA  | 4:9:369:ILE:N[1_554]   | 1.48                     | 0.72              |
| 4:4:226:GLU:CD  | 4:8:333:PRO:O[1_554]   | 1.49                     | 0.71              |
| 4:3:286:ASP:N   | 4:8:270:GLU:CD[1_554]  | 1.49                     | 0.71              |
| 4:5:223:PHE:CZ  | 4:9:304:THR:CB[1_554]  | 1.49                     | 0.71              |
| 4:4:193:LEU:CG  | 4:8:210:ARG:CG[1_554]  | 1.49                     | 0.71              |
| 4:3:215:LYS:CE  | 4:7:31:PHE:CD2[1_554]  | 1.49                     | 0.71              |
| 4:4:75:ILE:CB   | 4:9:198:TYR:CB[1_554]  | 1.49                     | 0.71              |
| 4:4:243:PRO:CA  | 4:8:60:SER:C[1_554]    | 1.49                     | 0.71              |
| 4:4:333:PRO:CD  | 4:8:104:LEU:CB[1_554]  | 1.49                     | 0.71              |
| 4:4:369:ILE:CG1 | 4:9:232:SER:CB[1_554]  | 1.49                     | 0.71              |
| 4:3:142:LEU:N   | 4:7:371:HIS:O[1_554]   | 1.49                     | 0.71              |
| 4:5:281:SER:C   | 4:9:173:HIS:CD2[1_554] | 1.49                     | 0.71              |
| 4:5:199:SER:N   | 4:9:205:GLU:C[1_554]   | 1.49                     | 0.71              |
| 4:5:256:ARG:CG  | 4:9:306:TYR:CD1[1_554] | 1.49                     | 0.71              |
| 4:4:136:ILE:CA  | 4:8:113:LYS:NZ[1_554]  | 1.49                     | 0.71              |
| 4:5:286:ASP:CG  | 4:V:270:GLU:OE1[1_554] | 1.49                     | 0.71              |
| 4:4:212:ILE:O   | 4:8:16:LEU:CG[1_554]   | 1.49                     | 0.71              |
| 4:5:218:TYR:CD1 | 4:9:336:LYS:CG[1_554]  | 1.49                     | 0.71              |
| 4:3:287:ILE:O   | 4:9:63:GLY:N[1_554]    | 1.49                     | 0.71              |
| 4:5:277:THR:O   | 4:9:174:ALA:O[1_554]   | 1.49                     | 0.71              |
| 4:5:299:MET:O   | 4:9:135:ALA:O[1_554]   | 1.49                     | 0.71              |
| 4:2:73:HIS:CD2  | 4:7:199:SER:OG[1_554]  | 1.49                     | 0.71              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:75:ILE:CG1  | 4:V:194:THR:C[1_554]   | 1.49                     | 0.71              |
| 4:4:303:THR:OG1 | 4:8:74:GLY:CA[1_554]   | 1.49                     | 0.71              |
| 4:3:269:MET:O   | 4:7:272:ALA:O[1_554]   | 1.49                     | 0.71              |
| 4:5:219:VAL:C   | 4:9:335:ARG:CB[1_554]  | 1.49                     | 0.71              |
| 4:5:347:ALA:CA  | 4:9:366:GLY:CA[1_554]  | 1.49                     | 0.71              |
| 4:3:308:GLY:O   | 4:7:141:SER:OG[1_554]  | 1.49                     | 0.71              |
| 4:5:227:MET:CG  | 4:9:306:TYR:O[1_554]   | 1.49                     | 0.71              |
| 4:1:291:LYS:CE  | 4:7:64:ILE:O[1_554]    | 1.49                     | 0.71              |
| 4:4:309:ILE:C   | 4:8:141:SER:OG[1_554]  | 1.49                     | 0.71              |
| 4:3:156:GLY:O   | 4:7:75:ILE:N[1_554]    | 1.49                     | 0.71              |
| 4:5:300:SER:OG  | 4:9:107:GLU:CD[1_554]  | 1.49                     | 0.71              |
| 4:4:213:LYS:NZ  | 4:8:14:SER:CB[1_554]   | 1.49                     | 0.71              |
| 4:4:115:ASN:ND2 | 4:9:198:TYR:CE2[1_554] | 1.49                     | 0.71              |
| 4:2:75:ILE:CD1  | 4:7:193:LEU:C[1_554]   | 1.49                     | 0.71              |
| 4:3:108:ALA:CB  | 4:8:195:GLU:CA[1_554]  | 1.49                     | 0.71              |
| 4:2:372:ARG:C   | 4:7:255:PHE:CZ[1_554]  | 1.49                     | 0.71              |
| 4:3:110:LEU:C   | 4:8:192:ILE:O[1_554]   | 1.49                     | 0.71              |
| 4:5:186:THR:N   | 4:9:157:ASP:O[1_554]   | 1.49                     | 0.71              |
| 4:3:314:GLN:CB  | 4:7:143:TYR:N[1_554]   | 1.49                     | 0.71              |
| 4:3:213:LYS:C   | 4:7:15:GLY:C[1_554]    | 1.49                     | 0.71              |
| 4:3:371:HIS:CE1 | 4:8:252:ASN:CA[1_554]  | 1.49                     | 0.71              |
| 4:3:188:TYR:CD2 | 4:7:181:ALA:C[1_554]   | 1.49                     | 0.71              |
| 4:4:261:LEU:O   | 4:8:161:HIS:O[1_554]   | 1.49                     | 0.71              |
| 4:2:73:HIS:O    | 4:7:198:TYR:O[1_554]   | 1.49                     | 0.71              |
| 4:5:140:LEU:CD1 | 4:9:113:LYS:O[1_554]   | 1.49                     | 0.71              |
| 4:4:312:ARG:CD  | 4:8:299:MET:C[1_554]   | 1.49                     | 0.71              |
| 4:4:256:ARG:N   | 4:8:302:GLY:C[1_554]   | 1.49                     | 0.71              |
| 4:3:308:GLY:N   | 4:7:339:VAL:N[1_554]   | 1.49                     | 0.71              |
| 4:5:215:LYS:CD  | 4:9:30:VAL:O[1_554]    | 1.49                     | 0.71              |
| 4:4:26:ALA:C    | 4:8:122:ILE:N[1_554]   | 1.49                     | 0.71              |
| 4:5:157:ASP:CA  | 4:9:72:GLU:C[1_554]    | 1.49                     | 0.71              |
| 4:4:185:LEU:CA  | 4:8:157:ASP:C[1_554]   | 1.49                     | 0.71              |
| 4:3:191:LYS:CE  | 4:7:185:LEU:C[1_554]   | 1.49                     | 0.71              |
| 4:3:276:GLU:CB  | 4:7:281:SER:CB[1_554]  | 1.49                     | 0.71              |
| 4:3:256:ARG:CA  | 4:7:303:THR:CA[1_554]  | 1.49                     | 0.71              |
| 4:4:320:LEU:N   | 4:8:293:LEU:N[1_554]   | 1.49                     | 0.71              |
| 4:4:322:PRO:C   | 4:8:292:ASP:OD2[1_554] | 1.49                     | 0.71              |
| 4:3:159:VAL:O   | 4:7:177:ARG:NH1[1_554] | 1.49                     | 0.71              |
| 4:3:137:GLN:C   | 4:7:113:LYS:CA[1_554]  | 1.49                     | 0.71              |
| 4:2:173:HIS:C   | 4:7:267:ILE:CB[1_554]  | 1.49                     | 0.71              |
| 4:3:303:THR:CB  | 4:7:74:GLY:CA[1_554]   | 1.49                     | 0.71              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:339:VAL:O   | 4:7:117:GLU:CB[1_554]  | 1.49                     | 0.71              |
| 4:4:370:VAL:C   | 4:9:230:ALA:CA[1_554]  | 1.49                     | 0.71              |
| 4:4:313:MET:CE  | 4:8:163:VAL:CB[1_554]  | 1.50                     | 0.70              |
| 4:3:59:GLN:CG   | 4:7:68:LYS:CG[1_554]   | 1.50                     | 0.70              |
| 4:4:372:ARG:CA  | 4:9:227:MET:C[1_554]   | 1.50                     | 0.70              |
| 4:2:369:ILE:O   | 4:7:229:THR:C[1_554]   | 1.50                     | 0.70              |
| 4:3:344:SER:CB  | 4:7:367:PRO:CG[1_554]  | 1.50                     | 0.70              |
| 4:3:174:ALA:O   | 4:7:173:HIS:CB[1_554]  | 1.50                     | 0.70              |
| 4:2:371:HIS:CA  | 4:7:236:LEU:CD1[1_554] | 1.50                     | 0.70              |
| 4:4:311:ASP:CG  | 4:8:144:ALA:CA[1_554]  | 1.50                     | 0.70              |
| 4:5:294:TYR:CB  | 4:9:166:TYR:CB[1_554]  | 1.50                     | 0.70              |
| 4:4:280:ASN:N   | 4:8:174:ALA:CB[1_554]  | 1.50                     | 0.70              |
| 4:4:260:THR:O   | 4:8:160:THR:OG1[1_554] | 1.50                     | 0.70              |
| 4:5:315:LYS:CD  | 4:9:147:ARG:CZ[1_554]  | 1.50                     | 0.70              |
| 4:4:182:GLY:N   | 4:8:73:HIS:CA[1_554]   | 1.50                     | 0.70              |
| 4:2:172:PRO:CG  | 4:7:266:PHE:CB[1_554]  | 1.50                     | 0.70              |
| 4:4:340:TRP:CG  | 4:8:118:LYS:O[1_554]   | 1.50                     | 0.70              |
| 4:4:258:PRO:N   | 4:8:155:SER:O[1_554]   | 1.50                     | 0.70              |
| 4:3:243:PRO:CD  | 4:7:60:SER:N[1_554]    | 1.50                     | 0.70              |
| 4:2:114:ALA:N   | 4:7:250:ILE:CG2[1_554] | 1.50                     | 0.70              |
| 4:3:357:ILE:CD1 | 4:8:232:SER:N[1_554]   | 1.50                     | 0.70              |
| 4:4:137:GLN:CB  | 4:8:112:PRO:CA[1_554]  | 1.50                     | 0.70              |
| 4:5:299:MET:CE  | 4:9:137:GLN:O[1_554]   | 1.50                     | 0.70              |
| 4:5:301:GLY:CA  | 4:9:108:ALA:N[1_554]   | 1.50                     | 0.70              |
| 4:5:32:PRO:N    | 4:9:78:ASN:ND2[1_554]  | 1.50                     | 0.70              |
| 4:5:316:GLU:OE1 | 4:9:297:ASN:ND2[1_554] | 1.50                     | 0.70              |
| 4:3:315:LYS:CE  | 4:7:147:ARG:NH1[1_554] | 1.50                     | 0.70              |
| 4:5:309:ILE:CG2 | 4:9:339:VAL:CG2[1_554] | 1.50                     | 0.70              |
| 4:4:26:ALA:O    | 4:8:122:ILE:CA[1_554]  | 1.50                     | 0.70              |
| 4:5:183:ARG:NE  | 4:9:72:GLU:OE2[1_554]  | 1.50                     | 0.70              |
| 4:5:215:LYS:N   | 4:9:16:LEU:CG[1_554]   | 1.50                     | 0.70              |
| 4:5:338:SER:CA  | 4:9:134:VAL:CB[1_554]  | 1.50                     | 0.70              |
| 4:5:196:ARG:CZ  | 4:9:211:ASP:O[1_554]   | 1.50                     | 0.70              |
| 4:4:194:THR:C   | 4:8:209:VAL:CG1[1_554] | 1.50                     | 0.70              |
| 4:3:305:MET:CE  | 4:7:10:CYS:O[1_554]    | 1.50                     | 0.70              |
| 4:4:339:VAL:CG1 | 4:8:114:ALA:C[1_554]   | 1.50                     | 0.70              |
| 4:4:189:LEU:O   | 4:8:186:THR:OG1[1_554] | 1.50                     | 0.70              |
| 4:3:207:GLU:CB  | 4:7:67:LEU:CG[1_554]   | 1.50                     | 0.70              |
| 4:4:321:ALA:C   | 4:8:292:ASP:CB[1_554]  | 1.50                     | 0.70              |
| 4:5:191:LYS:N   | 4:9:186:THR:C[1_554]   | 1.50                     | 0.70              |
| 4:5:181:ALA:N   | 4:9:159:VAL:CG1[1_554] | 1.50                     | 0.70              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:166:TYR:CE1 | 4:W:40:HIS:ND1[1_554]  | 1.50                     | 0.70              |
| 4:3:320:LEU:CB  | 4:7:293:LEU:CA[1_554]  | 1.50                     | 0.70              |
| 4:4:198:TYR:CD1 | 4:8:208:ILE:CB[1_554]  | 1.50                     | 0.70              |
| 4:5:31:PHE:O    | 4:9:78:ASN:O[1_554]    | 1.50                     | 0.70              |
| 4:4:308:GLY:C   | 4:8:339:VAL:N[1_554]   | 1.50                     | 0.70              |
| 4:3:255:PHE:O   | 4:7:301:GLY:O[1_554]   | 1.50                     | 0.70              |
| 4:3:208:ILE:CG1 | 4:7:59:GLN:CB[1_554]   | 1.50                     | 0.70              |
| 4:3:184:ASP:OD1 | 4:7:73:HIS:CE1[1_554]  | 1.50                     | 0.70              |
| 4:4:204:ALA:O   | 4:8:62:ARG:CG[1_554]   | 1.50                     | 0.70              |
| 4:4:120:THR:CG2 | 4:9:233:SER:OG[1_554]  | 1.50                     | 0.70              |
| 4:5:32:PRO:CD   | 4:9:81:ASP:OD2[1_554]  | 1.50                     | 0.70              |
| 4:3:196:ARG:C   | 4:7:208:ILE:O[1_554]   | 1.50                     | 0.70              |
| 4:3:345:ILE:CG1 | 4:7:366:GLY:O[1_554]   | 1.50                     | 0.70              |
| 4:3:255:PHE:CE1 | 4:7:305:MET:CA[1_554]  | 1.50                     | 0.70              |
| 4:4:366:GLY:C   | 4:9:234:SER:C[1_554]   | 1.50                     | 0.70              |
| 4:5:21:PHE:C    | 4:9:125:GLU:CG[1_554]  | 1.50                     | 0.70              |
| 4:5:262:PHE:CE1 | 4:9:153:LEU:CA[1_554]  | 1.50                     | 0.70              |
| 4:3:178:LEU:O   | 4:7:177:ARG:CD[1_554]  | 1.50                     | 0.70              |
| 4:4:328:LYS:N   | 4:8:168:GLY:CA[1_554]  | 1.50                     | 0.70              |
| 4:5:137:GLN:OE1 | 4:9:112:PRO:CB[1_554]  | 1.50                     | 0.70              |
| 4:4:345:ILE:CG1 | 4:8:369:ILE:CG2[1_554] | 1.50                     | 0.70              |
| 4:4:144:ALA:N   | 4:8:370:VAL:O[1_554]   | 1.50                     | 0.70              |
| 4:2:367:PRO:N   | 4:7:235:SER:O[1_554]   | 1.50                     | 0.70              |
| 4:4:317:ILE:CA  | 4:8:150:GLY:CA[1_554]  | 1.50                     | 0.70              |
| 4:5:143:TYR:CE2 | 4:9:369:ILE:C[1_554]   | 1.50                     | 0.70              |
| 4:4:326:LYS:C   | 4:8:167:GLU:CD[1_554]  | 1.50                     | 0.70              |
| 4:5:314:GLN:CG  | 4:9:142:LEU:O[1_554]   | 1.50                     | 0.70              |
| 4:2:371:HIS:ND1 | 4:7:252:ASN:CA[1_554]  | 1.50                     | 0.70              |
| 4:3:151:ILE:CD1 | 4:7:171:LEU:C[1_554]   | 1.50                     | 0.70              |
| 4:5:219:VAL:O   | 4:9:335:ARG:CA[1_554]  | 1.50                     | 0.70              |
| 4:2:288:ASP:C   | 4:8:39:ARG:NH1[1_554]  | 1.50                     | 0.70              |
| 4:3:299:MET:CG  | 4:7:136:ILE:CG2[1_554] | 1.50                     | 0.70              |
| 4:3:266:PHE:CB  | 4:7:261:LEU:CG[1_554]  | 1.50                     | 0.70              |
| 4:3:265:SER:O   | 4:7:261:LEU:C[1_554]   | 1.50                     | 0.70              |
| 4:3:173:HIS:O   | 4:8:267:ILE:O[1_554]   | 1.50                     | 0.70              |
| 4:3:256:ARG:CA  | 4:7:302:GLY:O[1_554]   | 1.50                     | 0.70              |
| 4:3:262:PHE:C   | 4:7:153:LEU:CG[1_554]  | 1.50                     | 0.70              |
| 4:4:114:ALA:CB  | 4:9:250:ILE:C[1_554]   | 1.50                     | 0.70              |
| 4:4:214:GLU:OE1 | 4:8:33:SER:CB[1_554]   | 1.50                     | 0.70              |
| 4:4:311:ASP:CA  | 4:8:141:SER:C[1_554]   | 1.50                     | 0.70              |
| 4:3:208:ILE:CG2 | 4:7:59:GLN:OE1[1_554]  | 1.50                     | 0.70              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:16:LEU:C    | 4:7:77:THR:O[1_554]    | 1.50                     | 0.70              |
| 4:5:278:THR:OG1 | 4:9:164:PRO:N[1_554]   | 1.50                     | 0.70              |
| 4:3:258:PRO:N   | 4:7:156:GLY:CA[1_554]  | 1.50                     | 0.70              |
| 4:4:304:THR:CA  | 4:8:137:GLN:CG[1_554]  | 1.50                     | 0.70              |
| 4:5:213:LYS:NZ  | 4:9:14:SER:C[1_554]    | 1.50                     | 0.70              |
| 4:5:333:PRO:CA  | 4:9:104:LEU:CD2[1_554] | 1.50                     | 0.70              |
| 4:4:332:PRO:N   | 4:8:135:ALA:N[1_554]   | 1.50                     | 0.70              |
| 4:4:338:SER:C   | 4:8:116:ARG:CA[1_554]  | 1.50                     | 0.70              |
| 4:4:333:PRO:CD  | 4:8:104:LEU:CA[1_554]  | 1.51                     | 0.69              |
| 4:4:342:GLY:CA  | 4:8:367:PRO:O[1_554]   | 1.51                     | 0.69              |
| 4:5:222:ASP:N   | 4:9:331:ALA:C[1_554]   | 1.51                     | 0.69              |
| 4:5:339:VAL:O   | 4:9:116:ARG:O[1_554]   | 1.51                     | 0.69              |
| 4:4:322:PRO:N   | 4:8:292:ASP:OD2[1_554] | 1.51                     | 0.69              |
| 4:3:222:ASP:O   | 4:7:332:PRO:O[1_554]   | 1.51                     | 0.69              |
| 4:5:221:LEU:CA  | 4:9:332:PRO:N[1_554]   | 1.51                     | 0.69              |
| 4:3:27:PRO:N    | 4:7:122:ILE:CB[1_554]  | 1.51                     | 0.69              |
| 4:4:151:ILE:CD1 | 4:8:171:LEU:CA[1_554]  | 1.51                     | 0.69              |
| 4:5:299:MET:N   | 4:9:136:ILE:CB[1_554]  | 1.51                     | 0.69              |
| 4:3:218:TYR:CE2 | 4:7:337:TYR:CD1[1_554] | 1.51                     | 0.69              |
| 4:3:259:GLU:OE1 | 4:7:304:THR:O[1_554]   | 1.51                     | 0.69              |
| 4:4:180:LEU:CB  | 4:8:178:LEU:C[1_554]   | 1.51                     | 0.69              |
| 4:4:315:LYS:N   | 4:8:142:LEU:CD1[1_554] | 1.51                     | 0.69              |
| 4:3:199:SER:N   | 4:7:206:ARG:CA[1_554]  | 1.51                     | 0.69              |
| 4:5:196:ARG:CA  | 4:9:212:ILE:CG2[1_554] | 1.51                     | 0.69              |
| 4:5:183:ARG:CG  | 4:9:72:GLU:OE2[1_554]  | 1.51                     | 0.69              |
| 4:2:372:ARG:CG  | 4:7:227:MET:CB[1_554]  | 1.51                     | 0.69              |
| 4:5:221:LEU:CG  | 4:9:332:PRO:CD[1_554]  | 1.51                     | 0.69              |
| 4:3:339:VAL:CG2 | 4:7:112:PRO:O[1_554]   | 1.51                     | 0.69              |
| 4:3:277:THR:C   | 4:7:174:ALA:C[1_554]   | 1.51                     | 0.69              |
| 4:4:183:ARG:CZ  | 4:8:72:GLU:OE1[1_554]  | 1.51                     | 0.69              |
| 4:3:265:SER:C   | 4:7:261:LEU:C[1_554]   | 1.51                     | 0.69              |
| 4:3:223:PHE:CE2 | 4:7:300:SER:C[1_554]   | 1.51                     | 0.69              |
| 4:4:192:ILE:CG2 | 4:8:213:LYS:CD[1_554]  | 1.51                     | 0.69              |
| 4:3:310:ALA:CB  | 4:7:140:LEU:N[1_554]   | 1.51                     | 0.69              |
| 4:4:340:TRP:CB  | 4:8:119:MET:N[1_554]   | 1.51                     | 0.69              |
| 4:4:367:PRO:CG  | 4:9:234:SER:O[1_554]   | 1.51                     | 0.69              |
| 4:4:265:SER:O   | 4:8:260:THR:O[1_554]   | 1.51                     | 0.69              |
| 4:5:227:MET:CG  | 4:9:307:PRO:C[1_554]   | 1.51                     | 0.69              |
| 4:5:22:ALA:CA   | 4:9:362:TYR:CZ[1_554]  | 1.51                     | 0.69              |
| 4:3:200:PHE:N   | 4:7:206:ARG:CB[1_554]  | 1.51                     | 0.69              |
| 4:4:367:PRO:CA  | 4:9:234:SER:C[1_554]   | 1.51                     | 0.69              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:218:TYR:CZ  | 4:9:337:TYR:CE2[1_554] | 1.51                     | 0.69              |
| 4:5:281:SER:CB  | 4:9:174:ALA:N[1_554]   | 1.51                     | 0.69              |
| 4:3:368:SER:N   | 4:8:236:LEU:CB[1_554]  | 1.51                     | 0.69              |
| 4:5:139:VAL:O   | 4:9:371:HIS:O[1_554]   | 1.51                     | 0.69              |
| 4:3:308:GLY:N   | 4:7:339:VAL:CA[1_554]  | 1.51                     | 0.69              |
| 4:4:218:TYR:CZ  | 4:8:337:TYR:CG[1_554]  | 1.51                     | 0.69              |
| 4:3:110:LEU:N   | 4:8:192:ILE:CA[1_554]  | 1.51                     | 0.69              |
| 4:3:337:TYR:CZ  | 4:7:86:TRP:CH2[1_554]  | 1.51                     | 0.69              |
| 4:4:111:ASN:CG  | 4:9:196:ARG:CB[1_554]  | 1.51                     | 0.69              |
| 4:3:274:ILE:CD1 | 4:7:161:HIS:CB[1_554]  | 1.51                     | 0.69              |
| 4:5:243:PRO:CG  | 4:9:60:SER:CA[1_554]   | 1.51                     | 0.69              |
| 4:4:178:LEU:CB  | 4:8:177:ARG:N[1_554]   | 1.51                     | 0.69              |
| 4:3:207:GLU:OE1 | 4:7:67:LEU:N[1_554]    | 1.51                     | 0.69              |
| 4:5:186:THR:OG1 | 4:9:157:ASP:OD2[1_554] | 1.51                     | 0.69              |
| 4:5:28:ARG:CB   | 4:9:126:THR:CB[1_554]  | 1.51                     | 0.69              |
| 4:5:115:ASN:CA  | 4:V:196:ARG:NE[1_554]  | 1.51                     | 0.69              |
| 4:3:24:ASP:CB   | 4:7:125:GLU:CG[1_554]  | 1.51                     | 0.69              |
| 4:4:188:TYR:N   | 4:8:183:ARG:CA[1_554]  | 1.51                     | 0.69              |
| 4:5:193:LEU:CG  | 4:9:210:ARG:CG[1_554]  | 1.51                     | 0.69              |
| 4:3:315:LYS:CE  | 4:7:147:ARG:CD[1_554]  | 1.51                     | 0.69              |
| 4:3:154:ASP:OD2 | 4:7:111:ASN:O[1_554]   | 1.51                     | 0.69              |
| 4:4:115:ASN:CB  | 4:9:196:ARG:CZ[1_554]  | 1.51                     | 0.69              |
| 4:5:295:ALA:CA  | 4:9:167:GLU:CA[1_554]  | 1.51                     | 0.69              |
| 4:4:270:GLU:CA  | 4:8:272:ALA:N[1_554]   | 1.51                     | 0.69              |
| 4:3:367:PRO:CG  | 4:8:235:SER:CA[1_554]  | 1.51                     | 0.69              |
| 4:4:18:LYS:CD   | 4:8:79:TRP:CE3[1_554]  | 1.51                     | 0.69              |
| 4:5:185:LEU:O   | 4:9:157:ASP:O[1_554]   | 1.51                     | 0.69              |
| 4:5:300:SER:OG  | 4:9:107:GLU:OE2[1_554] | 1.51                     | 0.69              |
| 4:4:305:MET:O   | 4:8:11:ASP:OD1[1_554]  | 1.51                     | 0.69              |
| 4:3:115:ASN:CA  | 4:8:196:ARG:NH2[1_554] | 1.51                     | 0.69              |
| 4:5:283:MET:CG  | 4:9:286:ASP:N[1_554]   | 1.51                     | 0.69              |
| 4:5:370:VAL:N   | 4:V:231:ALA:C[1_554]   | 1.52                     | 0.68              |
| 4:5:272:ALA:CA  | 4:9:277:THR:CB[1_554]  | 1.52                     | 0.68              |
| 4:5:269:MET:CA  | 4:9:271:SER:OG[1_554]  | 1.52                     | 0.68              |
| 4:5:150:GLY:CA  | 4:9:169:TYR:CD1[1_554] | 1.52                     | 0.68              |
| 4:3:116:ARG:CD  | 4:8:252:ASN:CG[1_554]  | 1.52                     | 0.68              |
| 4:4:337:TYR:CA  | 4:8:119:MET:SD[1_554]  | 1.52                     | 0.68              |
| 4:5:320:LEU:CA  | 4:9:293:LEU:C[1_554]   | 1.52                     | 0.68              |
| 4:2:109:PRO:CB  | 4:7:195:GLU:CG[1_554]  | 1.52                     | 0.68              |
| 4:3:293:LEU:CA  | 4:7:169:TYR:CD2[1_554] | 1.52                     | 0.68              |
| 4:3:110:LEU:O   | 4:8:193:LEU:N[1_554]   | 1.52                     | 0.68              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:326:LYS:CE  | 4:V:45:VAL:CA[1_554]   | 1.52                     | 0.68              |
| 4:4:326:LYS:C   | 4:8:167:GLU:CA[1_554]  | 1.52                     | 0.68              |
| 4:5:155:SER:N   | 4:9:108:ALA:CB[1_554]  | 1.52                     | 0.68              |
| 4:3:341:ILE:CB  | 4:7:120:THR:OG1[1_554] | 1.52                     | 0.68              |
| 4:5:24:ASP:CA   | 4:9:124:PHE:CB[1_554]  | 1.52                     | 0.68              |
| 4:3:187:ASP:O   | 4:7:183:ARG:C[1_554]   | 1.52                     | 0.68              |
| 4:5:310:ALA:N   | 4:9:141:SER:OG[1_554]  | 1.52                     | 0.68              |
| 4:4:137:GLN:CB  | 4:8:113:LYS:N[1_554]   | 1.52                     | 0.68              |
| 4:4:143:TYR:CE2 | 4:8:368:SER:O[1_554]   | 1.52                     | 0.68              |
| 4:5:137:GLN:CB  | 4:9:112:PRO:O[1_554]   | 1.52                     | 0.68              |
| 4:4:117:GLU:CA  | 4:9:237:GLU:CG[1_554]  | 1.52                     | 0.68              |
| 4:5:153:LEU:C   | 4:9:109:PRO:CA[1_554]  | 1.52                     | 0.68              |
| 4:3:242:LEU:C   | 4:7:60:SER:CA[1_554]   | 1.52                     | 0.68              |
| 4:5:180:LEU:CD2 | 4:9:178:LEU:CB[1_554]  | 1.52                     | 0.68              |
| 4:5:317:ILE:CG1 | 4:9:150:GLY:N[1_554]   | 1.52                     | 0.68              |
| 4:4:142:LEU:N   | 4:8:371:HIS:O[1_554]   | 1.52                     | 0.68              |
| 4:5:211:ASP:CA  | 4:9:32:PRO:CA[1_554]   | 1.52                     | 0.68              |
| 4:5:333:PRO:N   | 4:9:104:LEU:CG[1_554]  | 1.52                     | 0.68              |
| 4:3:161:HIS:C   | 4:7:110:LEU:CB[1_554]  | 1.52                     | 0.68              |
| 4:3:117:GLU:C   | 4:8:237:GLU:CB[1_554]  | 1.52                     | 0.68              |
| 4:3:357:ILE:CB  | 4:8:232:SER:CA[1_554]  | 1.52                     | 0.68              |
| 4:3:261:LEU:C   | 4:7:154:ASP:O[1_554]   | 1.52                     | 0.68              |
| 4:5:214:GLU:OE1 | 4:9:33:SER:CB[1_554]   | 1.52                     | 0.68              |
| 4:5:320:LEU:CD1 | 4:9:282:ILE:CG1[1_554] | 1.52                     | 0.68              |
| 4:3:30:VAL:C    | 4:7:80:ASP:CA[1_554]   | 1.52                     | 0.68              |
| 4:5:157:ASP:CB  | 4:9:72:GLU:N[1_554]    | 1.52                     | 0.68              |
| 4:3:259:GLU:CB  | 4:7:304:THR:CG2[1_554] | 1.52                     | 0.68              |
| 4:4:154:ASP:OD2 | 4:8:112:PRO:N[1_554]   | 1.52                     | 0.68              |
| 4:4:166:TYR:CB  | 4:V:40:HIS:NE2[1_554]  | 1.52                     | 0.68              |
| 4:5:136:ILE:CG1 | 4:9:113:LYS:NZ[1_554]  | 1.52                     | 0.68              |
| 4:5:338:SER:CA  | 4:9:134:VAL:CG1[1_554] | 1.52                     | 0.68              |
| 4:4:345:ILE:N   | 4:8:366:GLY:C[1_554]   | 1.52                     | 0.68              |
| 4:5:314:GLN:CA  | 4:9:142:LEU:CG[1_554]  | 1.52                     | 0.68              |
| 4:3:16:LEU:CD2  | 4:7:70:PRO:O[1_554]    | 1.52                     | 0.68              |
| 4:5:303:THR:C   | 4:9:137:GLN:OE1[1_554] | 1.52                     | 0.68              |
| 4:2:367:PRO:CD  | 4:7:235:SER:C[1_554]   | 1.52                     | 0.68              |
| 4:3:287:ILE:C   | 4:9:63:GLY:CA[1_554]   | 1.52                     | 0.68              |
| 4:3:112:PRO:CG  | 4:8:193:LEU:CG[1_554]  | 1.52                     | 0.68              |
| 4:5:287:ILE:C   | 4:W:63:GLY:CA[1_554]   | 1.52                     | 0.68              |
| 4:3:345:ILE:CA  | 4:7:366:GLY:O[1_554]   | 1.52                     | 0.68              |
| 4:3:312:ARG:NE  | 4:7:300:SER:N[1_554]   | 1.52                     | 0.68              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:276:GLU:OE2 | 4:8:279:TYR:N[1_554]   | 1.52                     | 0.68              |
| 4:4:274:ILE:N   | 4:8:162:ASN:CA[1_554]  | 1.52                     | 0.68              |
| 4:4:317:ILE:N   | 4:8:151:ILE:N[1_554]   | 1.52                     | 0.68              |
| 4:4:178:LEU:CB  | 4:8:177:ARG:CB[1_554]  | 1.52                     | 0.68              |
| 4:4:268:GLY:CA  | 4:8:264:PRO:CB[1_554]  | 1.52                     | 0.68              |
| 4:5:223:PHE:N   | 4:9:331:ALA:CB[1_554]  | 1.52                     | 0.68              |
| 4:5:312:ARG:CD  | 4:9:299:MET:CB[1_554]  | 1.52                     | 0.68              |
| 4:5:340:TRP:CG  | 4:9:118:LYS:O[1_554]   | 1.52                     | 0.68              |
| 4:4:26:ALA:CB   | 4:8:122:ILE:O[1_554]   | 1.52                     | 0.68              |
| 4:5:21:PHE:CB   | 4:9:125:GLU:CD[1_554]  | 1.52                     | 0.68              |
| 4:5:262:PHE:O   | 4:9:153:LEU:CD1[1_554] | 1.52                     | 0.68              |
| 4:3:322:PRO:CA  | 4:7:292:ASP:OD2[1_554] | 1.52                     | 0.68              |
| 4:3:326:LYS:CA  | 4:7:167:GLU:CG[1_554]  | 1.52                     | 0.68              |
| 4:3:211:ASP:CA  | 4:7:32:PRO:C[1_554]    | 1.52                     | 0.68              |
| 4:5:372:ARG:CA  | 4:V:227:MET:C[1_554]   | 1.52                     | 0.68              |
| 4:5:180:LEU:CD2 | 4:9:178:LEU:O[1_554]   | 1.53                     | 0.67              |
| 4:3:27:PRO:CB   | 4:7:122:ILE:CG1[1_554] | 1.53                     | 0.67              |
| 4:4:265:SER:O   | 4:8:261:LEU:CA[1_554]  | 1.53                     | 0.67              |
| 4:4:326:LYS:C   | 4:8:167:GLU:CB[1_554]  | 1.53                     | 0.67              |
| 4:4:16:LEU:CD2  | 4:8:70:PRO:O[1_554]    | 1.53                     | 0.67              |
| 4:4:326:LYS:O   | 4:8:167:GLU:CG[1_554]  | 1.53                     | 0.67              |
| 4:5:312:ARG:CG  | 4:9:299:MET:O[1_554]   | 1.53                     | 0.67              |
| 4:3:243:PRO:CA  | 4:7:60:SER:CA[1_554]   | 1.53                     | 0.67              |
| 4:4:255:PHE:CE2 | 4:8:305:MET:CE[1_554]  | 1.53                     | 0.67              |
| 4:2:113:LYS:N   | 4:7:250:ILE:CG2[1_554] | 1.53                     | 0.67              |
| 4:5:289:ILE:CA  | 4:W:63:GLY:O[1_554]    | 1.53                     | 0.67              |
| 4:4:266:PHE:CA  | 4:8:261:LEU:CG[1_554]  | 1.53                     | 0.67              |
| 4:5:154:ASP:CA  | 4:9:108:ALA:O[1_554]   | 1.53                     | 0.67              |
| 4:4:281:SER:O   | 4:8:173:HIS:CG[1_554]  | 1.53                     | 0.67              |
| 4:5:222:ASP:C   | 4:9:331:ALA:CB[1_554]  | 1.53                     | 0.67              |
| 4:5:263:GLN:N   | 4:9:274:ILE:CG1[1_554] | 1.53                     | 0.67              |
| 4:3:281:SER:C   | 4:7:173:HIS:CG[1_554]  | 1.53                     | 0.67              |
| 4:3:73:HIS:CD2  | 4:8:199:SER:OG[1_554]  | 1.53                     | 0.67              |
| 4:5:208:ILE:CD1 | 4:9:59:GLN:CB[1_554]   | 1.53                     | 0.67              |
| 4:4:117:GLU:OE1 | 4:9:236:LEU:C[1_554]   | 1.53                     | 0.67              |
| 4:4:226:GLU:CB  | 4:8:335:ARG:NH1[1_554] | 1.53                     | 0.67              |
| 4:5:287:ILE:O   | 4:W:63:GLY:N[1_554]    | 1.53                     | 0.67              |
| 1:A:637:LYS:NZ  | 4:4:311:ASP:C[1_556]   | 1.53                     | 0.67              |
| 4:5:272:ALA:N   | 4:9:277:THR:OG1[1_554] | 1.53                     | 0.67              |
| 4:5:218:TYR:CD2 | 4:9:336:LYS:CG[1_554]  | 1.53                     | 0.67              |
| 4:4:204:ALA:CB  | 4:8:62:ARG:CB[1_554]   | 1.53                     | 0.67              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:213:LYS:NZ  | 4:7:14:SER:C[1_554]    | 1.53                     | 0.67              |
| 4:5:258:PRO:CA  | 4:9:155:SER:C[1_554]   | 1.53                     | 0.67              |
| 4:5:205:GLU:OE2 | 4:9:203:THR:CG2[1_554] | 1.53                     | 0.67              |
| 4:4:214:GLU:N   | 4:8:15:GLY:C[1_554]    | 1.53                     | 0.67              |
| 4:4:164:PRO:CG  | 4:8:172:PRO:CG[1_554]  | 1.53                     | 0.67              |
| 4:4:160:THR:N   | 4:8:177:ARG:NH1[1_554] | 1.53                     | 0.67              |
| 4:5:318:THR:OG1 | 4:9:296:ASN:CB[1_554]  | 1.53                     | 0.67              |
| 4:4:210:ARG:NE  | 4:8:33:SER:O[1_554]    | 1.53                     | 0.67              |
| 4:4:154:ASP:CG  | 4:8:111:ASN:CB[1_554]  | 1.53                     | 0.67              |
| 4:3:191:LYS:CE  | 4:7:185:LEU:O[1_554]   | 1.53                     | 0.67              |
| 4:4:337:TYR:OH  | 4:8:86:TRP:CZ3[1_554]  | 1.53                     | 0.67              |
| 4:5:75:ILE:C    | 4:V:197:GLY:CA[1_554]  | 1.53                     | 0.67              |
| 4:3:326:LYS:N   | 4:7:167:GLU:CD[1_554]  | 1.53                     | 0.67              |
| 4:5:296:ASN:C   | 4:9:169:TYR:CA[1_554]  | 1.53                     | 0.67              |
| 4:5:284:LYS:C   | 4:V:268:GLY:O[1_554]   | 1.53                     | 0.67              |
| 4:5:75:ILE:CG1  | 4:V:194:THR:O[1_554]   | 1.53                     | 0.67              |
| 4:4:300:SER:N   | 4:8:107:GLU:CG[1_554]  | 1.53                     | 0.67              |
| 4:4:312:ARG:NE  | 4:8:299:MET:CB[1_554]  | 1.53                     | 0.67              |
| 4:5:32:PRO:O    | 4:9:78:ASN:CG[1_554]   | 1.53                     | 0.67              |
| 4:3:192:ILE:CD1 | 4:7:213:LYS:NZ[1_554]  | 1.53                     | 0.67              |
| 4:3:256:ARG:O   | 4:7:303:THR:OG1[1_554] | 1.53                     | 0.67              |
| 4:4:277:THR:CB  | 4:8:176:MET:N[1_554]   | 1.53                     | 0.67              |
| 4:5:180:LEU:O   | 4:9:159:VAL:CG1[1_554] | 1.53                     | 0.67              |
| 4:3:156:GLY:N   | 4:7:75:ILE:CG1[1_554]  | 1.53                     | 0.67              |
| 4:3:204:ALA:C   | 4:7:62:ARG:CG[1_554]   | 1.53                     | 0.67              |
| 4:4:208:ILE:CD1 | 4:8:59:GLN:CA[1_554]   | 1.53                     | 0.67              |
| 4:4:114:ALA:N   | 4:9:251:GLY:N[1_554]   | 1.53                     | 0.67              |
| 4:5:115:ASN:CB  | 4:V:196:ARG:CZ[1_554]  | 1.53                     | 0.67              |
| 4:3:319:ALA:CB  | 4:7:296:ASN:CG[1_554]  | 1.53                     | 0.67              |
| 4:3:274:ILE:O   | 4:7:162:ASN:C[1_554]   | 1.53                     | 0.67              |
| 4:3:340:TRP:CB  | 4:7:118:LYS:C[1_554]   | 1.53                     | 0.67              |
| 4:3:24:ASP:C    | 4:7:125:GLU:CG[1_554]  | 1.53                     | 0.67              |
| 4:5:151:ILE:CD1 | 4:9:171:LEU:N[1_554]   | 1.53                     | 0.67              |
| 4:4:334:GLU:CD  | 4:8:133:TYR:N[1_554]   | 1.53                     | 0.67              |
| 4:4:199:SER:N   | 4:8:206:ARG:CA[1_554]  | 1.53                     | 0.67              |
| 4:4:25:ASP:CG   | 4:8:124:PHE:CD1[1_554] | 1.53                     | 0.67              |
| 4:4:315:LYS:CG  | 4:8:145:SER:OG[1_554]  | 1.53                     | 0.67              |
| 4:3:253:GLU:OE2 | 4:7:214:GLU:CB[1_554]  | 1.53                     | 0.67              |
| 4:4:306:TYR:O   | 4:8:339:VAL:CB[1_554]  | 1.53                     | 0.67              |
| 4:4:174:ALA:O   | 4:8:173:HIS:CA[1_554]  | 1.53                     | 0.67              |
| 4:5:208:ILE:CG2 | 4:9:59:GLN:CD[1_554]   | 1.53                     | 0.67              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:334:GLU:CA  | 4:9:104:LEU:C[1_554]   | 1.53                     | 0.67              |
| 4:5:220:ALA:CB  | 4:9:335:ARG:CD[1_554]  | 1.53                     | 0.67              |
| 4:4:173:HIS:CD2 | 4:9:264:PRO:O[1_554]   | 1.53                     | 0.67              |
| 4:2:109:PRO:CA  | 4:7:195:GLU:CG[1_554]  | 1.54                     | 0.66              |
| 4:4:260:THR:C   | 4:8:155:SER:OG[1_554]  | 1.54                     | 0.66              |
| 4:4:293:LEU:C   | 4:8:169:TYR:CB[1_554]  | 1.54                     | 0.66              |
| 4:4:113:LYS:CG  | 4:9:252:ASN:O[1_554]   | 1.54                     | 0.66              |
| 4:3:288:ASP:CB  | 4:9:65:LEU:O[1_554]    | 1.54                     | 0.66              |
| 4:3:327:ILE:CD1 | 4:7:149:THR:OG1[1_554] | 1.54                     | 0.66              |
| 4:5:59:GLN:CG   | 4:9:68:LYS:CB[1_554]   | 1.54                     | 0.66              |
| 4:4:312:ARG:CD  | 4:8:299:MET:N[1_554]   | 1.54                     | 0.66              |
| 4:4:27:PRO:CA   | 4:8:122:ILE:CB[1_554]  | 1.54                     | 0.66              |
| 4:5:191:LYS:CG  | 4:9:185:LEU:C[1_554]   | 1.54                     | 0.66              |
| 4:4:185:LEU:CB  | 4:8:158:GLY:CA[1_554]  | 1.54                     | 0.66              |
| 4:3:160:THR:N   | 4:7:177:ARG:NH1[1_554] | 1.54                     | 0.66              |
| 4:5:180:LEU:N   | 4:9:179:ASP:OD1[1_554] | 1.54                     | 0.66              |
| 4:4:255:PHE:CD1 | 4:8:305:MET:CA[1_554]  | 1.54                     | 0.66              |
| 4:5:219:VAL:O   | 4:9:335:ARG:CB[1_554]  | 1.54                     | 0.66              |
| 4:4:204:ALA:O   | 4:8:62:ARG:CB[1_554]   | 1.54                     | 0.66              |
| 4:3:259:GLU:CD  | 4:7:304:THR:O[1_554]   | 1.54                     | 0.66              |
| 4:5:104:LEU:CD2 | 4:9:117:GLU:OE1[1_554] | 1.54                     | 0.66              |
| 4:4:161:HIS:CA  | 4:8:110:LEU:CB[1_554]  | 1.54                     | 0.66              |
| 4:5:273:GLY:CA  | 4:9:162:ASN:CG[1_554]  | 1.54                     | 0.66              |
| 4:4:309:ILE:N   | 4:8:339:VAL:N[1_554]   | 1.54                     | 0.66              |
| 4:5:172:PRO:CA  | 4:V:266:PHE:O[1_554]   | 1.54                     | 0.66              |
| 4:3:278:THR:O   | 4:7:171:LEU:CB[1_554]  | 1.54                     | 0.66              |
| 4:5:267:ILE:C   | 4:9:180:LEU:CD2[1_554] | 1.54                     | 0.66              |
| 4:5:75:ILE:O    | 4:V:197:GLY:C[1_554]   | 1.54                     | 0.66              |
| 4:4:154:ASP:CG  | 4:8:111:ASN:C[1_554]   | 1.54                     | 0.66              |
| 4:3:25:ASP:OD1  | 4:7:124:PHE:CB[1_554]  | 1.54                     | 0.66              |
| 4:3:317:ILE:C   | 4:7:150:GLY:CA[1_554]  | 1.54                     | 0.66              |
| 4:5:218:TYR:O   | 4:9:301:GLY:C[1_554]   | 1.54                     | 0.66              |
| 4:5:223:PHE:CE1 | 4:9:304:THR:OG1[1_554] | 1.54                     | 0.66              |
| 4:5:195:GLU:N   | 4:9:209:VAL:CG2[1_554] | 1.54                     | 0.66              |
| 4:4:194:THR:O   | 4:8:209:VAL:CA[1_554]  | 1.54                     | 0.66              |
| 4:5:258:PRO:CG  | 4:9:302:GLY:N[1_554]   | 1.54                     | 0.66              |
| 4:3:261:LEU:O   | 4:7:161:HIS:O[1_554]   | 1.54                     | 0.66              |
| 4:3:188:TYR:CB  | 4:7:181:ALA:O[1_554]   | 1.54                     | 0.66              |
| 4:3:316:GLU:N   | 4:7:142:LEU:CD1[1_554] | 1.54                     | 0.66              |
| 4:5:319:ALA:CB  | 4:9:295:ALA:CA[1_554]  | 1.54                     | 0.66              |
| 4:5:320:LEU:O   | 4:9:290:ARG:C[1_554]   | 1.54                     | 0.66              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:278:THR:C   | 4:9:164:PRO:CG[1_554]  | 1.54                     | 0.66              |
| 4:4:344:SER:OG  | 4:8:362:TYR:CZ[1_554]  | 1.54                     | 0.66              |
| 4:4:116:ARG:C   | 4:9:237:GLU:OE2[1_554] | 1.54                     | 0.66              |
| 4:3:166:TYR:OH  | 4:9:39:ARG:C[1_554]    | 1.54                     | 0.66              |
| 4:3:341:ILE:O   | 4:7:367:PRO:CA[1_554]  | 1.54                     | 0.66              |
| 4:4:218:TYR:CB  | 4:8:336:LYS:CA[1_554]  | 1.54                     | 0.66              |
| 4:5:227:MET:CG  | 4:9:306:TYR:C[1_554]   | 1.54                     | 0.66              |
| 4:4:282:ILE:CG1 | 4:8:171:LEU:CB[1_554]  | 1.54                     | 0.66              |
| 4:4:249:THR:O   | 4:8:211:ASP:OD2[1_554] | 1.54                     | 0.66              |
| 4:4:243:PRO:CA  | 4:8:60:SER:OG[1_554]   | 1.54                     | 0.66              |
| 4:2:369:ILE:CB  | 4:7:234:SER:CB[1_554]  | 1.54                     | 0.66              |
| 4:4:333:PRO:C   | 4:8:104:LEU:C[1_554]   | 1.54                     | 0.66              |
| 4:5:215:LYS:CG  | 4:9:30:VAL:C[1_554]    | 1.54                     | 0.66              |
| 4:5:255:PHE:CD2 | 4:9:305:MET:CB[1_554]  | 1.54                     | 0.66              |
| 4:5:156:GLY:CA  | 4:9:74:GLY:O[1_554]    | 1.54                     | 0.66              |
| 4:5:166:TYR:OH  | 4:W:39:ARG:N[1_554]    | 1.54                     | 0.66              |
| 4:5:257:CYS:C   | 4:9:303:THR:OG1[1_554] | 1.54                     | 0.66              |
| 4:4:192:ILE:N   | 4:8:186:THR:OG1[1_554] | 1.54                     | 0.66              |
| 4:4:326:LYS:CA  | 4:8:167:GLU:CG[1_554]  | 1.54                     | 0.66              |
| 4:4:288:ASP:CB  | 4:V:65:LEU:O[1_554]    | 1.54                     | 0.66              |
| 4:5:110:LEU:N   | 4:V:195:GLU:OE1[1_554] | 1.54                     | 0.66              |
| 4:5:210:ARG:NH1 | 4:9:33:SER:CB[1_554]   | 1.54                     | 0.66              |
| 4:5:205:GLU:CD  | 4:7:288:ASP:OD2[1_554] | 1.54                     | 0.66              |
| 4:4:173:HIS:CA  | 4:9:267:ILE:CG2[1_554] | 1.54                     | 0.66              |
| 4:5:295:ALA:O   | 4:9:167:GLU:O[1_554]   | 1.54                     | 0.66              |
| 4:5:114:ALA:O   | 4:V:237:GLU:OE2[1_554] | 1.54                     | 0.66              |
| 4:5:274:ILE:CB  | 4:9:161:HIS:O[1_554]   | 1.54                     | 0.66              |
| 4:5:368:SER:O   | 4:V:230:ALA:CA[1_554]  | 1.54                     | 0.66              |
| 4:2:109:PRO:CG  | 4:7:195:GLU:CD[1_554]  | 1.54                     | 0.66              |
| 4:5:278:THR:CG2 | 4:9:164:PRO:CA[1_554]  | 1.54                     | 0.66              |
| 4:4:193:LEU:O   | 4:8:209:VAL:C[1_554]   | 1.54                     | 0.66              |
| 4:4:166:TYR:CD1 | 4:V:40:HIS:CD2[1_554]  | 1.54                     | 0.66              |
| 4:5:197:GLY:CA  | 4:9:212:ILE:CD1[1_554] | 1.54                     | 0.66              |
| 4:5:207:GLU:CD  | 4:9:67:LEU:CB[1_554]   | 1.54                     | 0.66              |
| 4:4:309:ILE:C   | 4:8:141:SER:CB[1_554]  | 1.54                     | 0.66              |
| 4:5:262:PHE:CZ  | 4:9:153:LEU:C[1_554]   | 1.54                     | 0.66              |
| 4:5:18:LYS:CE   | 4:9:79:TRP:CH2[1_554]  | 1.55                     | 0.65              |
| 4:3:282:ILE:CD1 | 4:7:171:LEU:CD2[1_554] | 1.55                     | 0.65              |
| 4:5:200:PHE:CB  | 4:9:206:ARG:CG[1_554]  | 1.55                     | 0.65              |
| 4:4:185:LEU:CB  | 4:8:157:ASP:C[1_554]   | 1.55                     | 0.65              |
| 4:2:111:ASN:C   | 4:7:253:GLU:CG[1_554]  | 1.55                     | 0.65              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:260:THR:C   | 4:8:160:THR:OG1[1_554] | 1.55                     | 0.65              |
| 4:4:112:PRO:C   | 4:9:253:GLU:OE2[1_554] | 1.55                     | 0.65              |
| 4:4:109:PRO:CA  | 4:9:195:GLU:OE1[1_554] | 1.55                     | 0.65              |
| 4:3:15:GLY:N    | 4:7:77:THR:OG1[1_554]  | 1.55                     | 0.65              |
| 4:4:340:TRP:CE3 | 4:8:121:GLN:CA[1_554]  | 1.55                     | 0.65              |
| 4:3:297:ASN:CG  | 4:7:170:ALA:CA[1_554]  | 1.55                     | 0.65              |
| 4:3:207:GLU:OE2 | 4:7:68:LYS:N[1_554]    | 1.55                     | 0.65              |
| 4:5:185:LEU:C   | 4:9:157:ASP:C[1_554]   | 1.55                     | 0.65              |
| 4:4:184:ASP:N   | 4:8:73:HIS:CE1[1_554]  | 1.55                     | 0.65              |
| 4:5:155:SER:CA  | 4:9:108:ALA:CB[1_554]  | 1.55                     | 0.65              |
| 4:5:166:TYR:CG  | 4:W:40:HIS:CG[1_554]   | 1.55                     | 0.65              |
| 4:3:344:SER:C   | 4:7:367:PRO:CG[1_554]  | 1.55                     | 0.65              |
| 4:5:142:LEU:C   | 4:9:372:ARG:CD[1_554]  | 1.55                     | 0.65              |
| 4:3:332:PRO:O   | 4:7:105:LEU:C[1_554]   | 1.55                     | 0.65              |
| 4:2:288:ASP:CG  | 4:8:65:LEU:O[1_554]    | 1.55                     | 0.65              |
| 4:4:204:ALA:O   | 4:8:62:ARG:CD[1_554]   | 1.55                     | 0.65              |
| 4:5:288:ASP:CA  | 4:W:63:GLY:N[1_554]    | 1.55                     | 0.65              |
| 4:4:343:GLY:C   | 4:8:367:PRO:CB[1_554]  | 1.55                     | 0.65              |
| 4:4:214:GLU:CG  | 4:8:33:SER:OG[1_554]   | 1.55                     | 0.65              |
| 4:5:106:THR:CG2 | 4:9:114:ALA:O[1_554]   | 1.55                     | 0.65              |
| 4:5:164:PRO:CD  | 4:9:172:PRO:CB[1_554]  | 1.55                     | 0.65              |
| 4:4:113:LYS:NZ  | 4:9:254:ARG:C[1_554]   | 1.55                     | 0.65              |
| 4:4:322:PRO:CA  | 4:8:291:LYS:NZ[1_554]  | 1.55                     | 0.65              |
| 4:2:175:ILE:CG2 | 4:7:191:LYS:CD[1_554]  | 1.55                     | 0.65              |
| 4:5:320:LEU:C   | 4:9:293:LEU:N[1_554]   | 1.55                     | 0.65              |
| 4:3:26:ALA:CB   | 4:7:122:ILE:CA[1_554]  | 1.55                     | 0.65              |
| 4:5:59:GLN:CB   | 4:9:68:LYS:CE[1_554]   | 1.55                     | 0.65              |
| 4:3:191:LYS:CA  | 4:7:186:THR:CA[1_554]  | 1.55                     | 0.65              |
| 4:4:298:VAL:C   | 4:8:136:ILE:CG1[1_554] | 1.55                     | 0.65              |
| 4:5:32:PRO:CD   | 4:9:81:ASP:CG[1_554]   | 1.55                     | 0.65              |
| 4:5:264:PRO:CA  | 4:9:178:LEU:CD2[1_554] | 1.55                     | 0.65              |
| 4:4:299:MET:CG  | 4:8:136:ILE:C[1_554]   | 1.55                     | 0.65              |
| 4:3:256:ARG:C   | 4:7:303:THR:CB[1_554]  | 1.55                     | 0.65              |
| 4:5:252:ASN:CB  | 4:9:214:GLU:O[1_554]   | 1.55                     | 0.65              |
| 4:4:190:MET:CG  | 4:8:206:ARG:NH2[1_554] | 1.55                     | 0.65              |
| 4:2:113:LYS:CG  | 4:7:254:ARG:N[1_554]   | 1.55                     | 0.65              |
| 4:5:219:VAL:CG1 | 4:9:300:SER:N[1_554]   | 1.55                     | 0.65              |
| 4:3:196:ARG:N   | 4:7:209:VAL:C[1_554]   | 1.55                     | 0.65              |
| 4:5:340:TRP:C   | 4:9:120:THR:OG1[1_554] | 1.55                     | 0.65              |
| 4:3:259:GLU:OE2 | 4:7:304:THR:O[1_554]   | 1.55                     | 0.65              |
| 4:5:282:ILE:CG1 | 4:9:171:LEU:CD2[1_554] | 1.55                     | 0.65              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:205:GLU:CD  | 4:9:203:THR:OG1[1_554] | 1.55                     | 0.65              |
| 4:5:193:LEU:O   | 4:9:209:VAL:O[1_554]   | 1.55                     | 0.65              |
| 4:3:199:SER:CA  | 4:7:206:ARG:N[1_554]   | 1.55                     | 0.65              |
| 4:3:293:LEU:C   | 4:7:169:TYR:CB[1_554]  | 1.55                     | 0.65              |
| 4:5:173:HIS:ND1 | 4:V:265:SER:C[1_554]   | 1.55                     | 0.65              |
| 4:5:270:GLU:CB  | 4:9:272:ALA:N[1_554]   | 1.55                     | 0.65              |
| 4:5:137:GLN:N   | 4:9:113:LYS:CA[1_554]  | 1.55                     | 0.65              |
| 4:4:166:TYR:CE1 | 4:V:40:HIS:ND1[1_554]  | 1.55                     | 0.65              |
| 4:3:185:LEU:O   | 4:7:157:ASP:C[1_554]   | 1.55                     | 0.65              |
| 4:5:334:GLU:N   | 4:9:104:LEU:O[1_554]   | 1.55                     | 0.65              |
| 4:3:111:ASN:N   | 4:8:192:ILE:C[1_554]   | 1.55                     | 0.65              |
| 4:4:18:LYS:CD   | 4:8:79:TRP:CE2[1_554]  | 1.55                     | 0.65              |
| 4:3:338:SER:O   | 4:7:117:GLU:N[1_554]   | 1.55                     | 0.65              |
| 4:3:340:TRP:CZ2 | 4:7:121:GLN:CD[1_554]  | 1.55                     | 0.65              |
| 4:4:218:TYR:CB  | 4:8:336:LYS:O[1_554]   | 1.55                     | 0.65              |
| 4:4:31:PHE:O    | 4:8:78:ASN:CG[1_554]   | 1.55                     | 0.65              |
| 4:4:214:GLU:C   | 4:8:16:LEU:CA[1_554]   | 1.55                     | 0.65              |
| 4:3:222:ASP:CA  | 4:7:331:ALA:CA[1_554]  | 1.55                     | 0.65              |
| 4:4:192:ILE:CA  | 4:8:213:LYS:CD[1_554]  | 1.55                     | 0.65              |
| 4:3:198:TYR:CD2 | 4:7:207:GLU:O[1_554]   | 1.55                     | 0.65              |
| 4:4:110:LEU:CD1 | 4:9:191:LYS:CB[1_554]  | 1.55                     | 0.65              |
| 4:5:117:GLU:CG  | 4:V:252:ASN:ND2[1_554] | 1.55                     | 0.65              |
| 4:4:293:LEU:O   | 4:8:169:TYR:CA[1_554]  | 1.55                     | 0.65              |
| 4:4:30:VAL:O    | 4:8:80:ASP:N[1_554]    | 1.55                     | 0.65              |
| 4:2:174:ALA:N   | 4:7:267:ILE:CA[1_554]  | 1.55                     | 0.65              |
| 4:5:340:TRP:CE3 | 4:9:120:THR:CA[1_554]  | 1.55                     | 0.65              |
| 4:5:311:ASP:N   | 4:9:141:SER:C[1_554]   | 1.56                     | 0.64              |
| 4:5:110:LEU:C   | 4:V:192:ILE:CA[1_554]  | 1.56                     | 0.64              |
| 4:3:115:ASN:O   | 4:8:196:ARG:NH2[1_554] | 1.56                     | 0.64              |
| 4:4:208:ILE:N   | 4:8:59:GLN:NE2[1_554]  | 1.56                     | 0.64              |
| 4:3:273:GLY:C   | 4:7:162:ASN:CA[1_554]  | 1.56                     | 0.64              |
| 4:2:357:ILE:CD1 | 4:7:232:SER:CB[1_554]  | 1.56                     | 0.64              |
| 4:5:166:TYR:CG  | 4:W:40:HIS:CD2[1_554]  | 1.56                     | 0.64              |
| 4:3:340:TRP:CA  | 4:7:118:LYS:CA[1_554]  | 1.56                     | 0.64              |
| 4:5:180:LEU:CD1 | 4:9:178:LEU:O[1_554]   | 1.56                     | 0.64              |
| 4:4:281:SER:N   | 4:8:174:ALA:CB[1_554]  | 1.56                     | 0.64              |
| 4:5:338:SER:CB  | 4:9:134:VAL:CB[1_554]  | 1.56                     | 0.64              |
| 4:5:200:PHE:C   | 4:9:206:ARG:CG[1_554]  | 1.56                     | 0.64              |
| 4:4:305:MET:C   | 4:8:11:ASP:OD2[1_554]  | 1.56                     | 0.64              |
| 4:4:188:TYR:C   | 4:8:183:ARG:CA[1_554]  | 1.56                     | 0.64              |
| 4:3:215:LYS:CG  | 4:7:31:PHE:CB[1_554]   | 1.56                     | 0.64              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:311:ASP:OD1 | 4:7:144:ALA:CA[1_554]  | 1.56                     | 0.64              |
| 4:2:173:HIS:O   | 4:7:267:ILE:CA[1_554]  | 1.56                     | 0.64              |
| 4:5:367:PRO:CA  | 4:V:233:SER:C[1_554]   | 1.56                     | 0.64              |
| 4:3:76:ILE:C    | 4:8:198:TYR:CE1[1_554] | 1.56                     | 0.64              |
| 4:5:191:LYS:CA  | 4:9:186:THR:CA[1_554]  | 1.56                     | 0.64              |
| 4:3:286:ASP:CB  | 4:8:270:GLU:OE1[1_554] | 1.56                     | 0.64              |
| 4:5:11:ASP:O    | 4:9:79:TRP:NE1[1_554]  | 1.56                     | 0.64              |
| 4:5:327:ILE:C   | 4:9:148:THR:CB[1_554]  | 1.56                     | 0.64              |
| 4:4:340:TRP:CZ2 | 4:8:121:GLN:CB[1_554]  | 1.56                     | 0.64              |
| 4:3:188:TYR:CE1 | 4:7:185:LEU:CB[1_554]  | 1.56                     | 0.64              |
| 4:5:286:ASP:N   | 4:V:270:GLU:CD[1_554]  | 1.56                     | 0.64              |
| 4:4:337:TYR:O   | 4:8:119:MET:CG[1_554]  | 1.56                     | 0.64              |
| 4:4:318:THR:N   | 4:8:149:THR:O[1_554]   | 1.56                     | 0.64              |
| 4:5:369:ILE:N   | 4:V:229:THR:C[1_554]   | 1.56                     | 0.64              |
| 4:3:310:ALA:CA  | 4:7:140:LEU:C[1_554]   | 1.56                     | 0.64              |
| 4:5:270:GLU:CA  | 4:9:272:ALA:C[1_554]   | 1.56                     | 0.64              |
| 4:4:153:LEU:CA  | 4:8:109:PRO:O[1_554]   | 1.56                     | 0.64              |
| 4:5:112:PRO:C   | 4:V:253:GLU:CG[1_554]  | 1.56                     | 0.64              |
| 4:3:218:TYR:CE1 | 4:7:337:TYR:CD1[1_554] | 1.56                     | 0.64              |
| 4:4:190:MET:SD  | 4:8:206:ARG:NH2[1_554] | 1.56                     | 0.64              |
| 4:4:277:THR:OG1 | 4:8:176:MET:CG[1_554]  | 1.56                     | 0.64              |
| 4:3:317:ILE:CB  | 4:7:150:GLY:O[1_554]   | 1.56                     | 0.64              |
| 4:4:157:ASP:CA  | 4:8:72:GLU:C[1_554]    | 1.56                     | 0.64              |
| 4:3:171:LEU:O   | 4:8:266:PHE:O[1_554]   | 1.56                     | 0.64              |
| 4:5:300:SER:O   | 4:9:108:ALA:CA[1_554]  | 1.56                     | 0.64              |
| 4:4:282:ILE:CB  | 4:8:171:LEU:CD2[1_554] | 1.56                     | 0.64              |
| 4:2:75:ILE:CA   | 4:7:198:TYR:CG[1_554]  | 1.56                     | 0.64              |
| 4:4:76:ILE:N    | 4:9:197:GLY:O[1_554]   | 1.56                     | 0.64              |
| 4:5:341:ILE:C   | 4:9:370:VAL:CG1[1_554] | 1.56                     | 0.64              |
| 4:4:151:ILE:CB  | 4:8:170:ALA:O[1_554]   | 1.56                     | 0.64              |
| 4:5:114:ALA:CA  | 4:V:251:GLY:CA[1_554]  | 1.56                     | 0.64              |
| 4:4:332:PRO:CD  | 4:8:134:VAL:C[1_554]   | 1.56                     | 0.64              |
| 4:3:111:ASN:O   | 4:8:253:GLU:CB[1_554]  | 1.56                     | 0.64              |
| 4:5:334:GLU:O   | 4:9:105:LEU:CA[1_554]  | 1.56                     | 0.64              |
| 4:5:211:ASP:CB  | 4:9:32:PRO:CA[1_554]   | 1.56                     | 0.64              |
| 4:5:164:PRO:N   | 4:9:172:PRO:CB[1_554]  | 1.56                     | 0.64              |
| 4:3:314:GLN:CB  | 4:7:142:LEU:C[1_554]   | 1.56                     | 0.64              |
| 4:5:346:LEU:N   | 4:9:369:ILE:N[1_554]   | 1.56                     | 0.64              |
| 4:4:194:THR:CA  | 4:8:209:VAL:CB[1_554]  | 1.56                     | 0.64              |
| 4:5:274:ILE:CB  | 4:9:162:ASN:N[1_554]   | 1.56                     | 0.64              |
| 4:5:31:PHE:CG   | 4:9:80:ASP:CB[1_554]   | 1.56                     | 0.64              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:227:MET:CB  | 4:9:307:PRO:CB[1_554]  | 1.56                     | 0.64              |
| 4:4:207:GLU:CG  | 4:8:67:LEU:CB[1_554]   | 1.56                     | 0.64              |
| 4:3:305:MET:CB  | 4:7:12:ASN:N[1_554]    | 1.56                     | 0.64              |
| 1:D:637:LYS:CE  | 4:5:311:ASP:CB[1_556]  | 1.56                     | 0.64              |
| 4:4:265:SER:O   | 4:8:261:LEU:C[1_554]   | 1.56                     | 0.64              |
| 4:4:300:SER:OG  | 4:8:107:GLU:OE2[1_554] | 1.56                     | 0.64              |
| 4:3:161:HIS:CA  | 4:7:110:LEU:CG[1_554]  | 1.56                     | 0.64              |
| 4:3:210:ARG:CA  | 4:7:69:TYR:CE2[1_554]  | 1.56                     | 0.64              |
| 4:5:272:ALA:CA  | 4:9:277:THR:CA[1_554]  | 1.56                     | 0.64              |
| 4:2:112:PRO:CD  | 4:7:193:LEU:CG[1_554]  | 1.56                     | 0.64              |
| 4:3:198:TYR:C   | 4:7:205:GLU:O[1_554]   | 1.56                     | 0.64              |
| 4:4:255:PHE:CD2 | 4:8:305:MET:SD[1_554]  | 1.56                     | 0.64              |
| 4:5:193:LEU:CD2 | 4:9:210:ARG:NE[1_554]  | 1.57                     | 0.63              |
| 4:4:341:ILE:CG1 | 4:8:120:THR:CB[1_554]  | 1.57                     | 0.63              |
| 4:4:186:THR:OG1 | 4:8:183:ARG:CZ[1_554]  | 1.57                     | 0.63              |
| 4:4:274:ILE:O   | 4:8:163:VAL:N[1_554]   | 1.57                     | 0.63              |
| 4:4:115:ASN:CA  | 4:9:196:ARG:CZ[1_554]  | 1.57                     | 0.63              |
| 4:5:258:PRO:N   | 4:9:303:THR:N[1_554]   | 1.57                     | 0.63              |
| 4:5:115:ASN:OD1 | 4:V:196:ARG:NE[1_554]  | 1.57                     | 0.63              |
| 4:3:288:ASP:CG  | 4:9:65:LEU:O[1_554]    | 1.57                     | 0.63              |
| 4:4:162:ASN:N   | 4:8:110:LEU:CG[1_554]  | 1.57                     | 0.63              |
| 4:5:346:LEU:CB  | 4:9:368:SER:CB[1_554]  | 1.57                     | 0.63              |
| 4:3:337:TYR:OH  | 4:7:86:TRP:CZ3[1_554]  | 1.57                     | 0.63              |
| 4:3:265:SER:C   | 4:7:261:LEU:O[1_554]   | 1.57                     | 0.63              |
| 4:4:15:GLY:C    | 4:8:77:THR:CG2[1_554]  | 1.57                     | 0.63              |
| 4:4:110:LEU:O   | 4:9:193:LEU:N[1_554]   | 1.57                     | 0.63              |
| 4:4:282:ILE:N   | 4:8:173:HIS:NE2[1_554] | 1.57                     | 0.63              |
| 4:5:115:ASN:CA  | 4:V:196:ARG:NH2[1_554] | 1.57                     | 0.63              |
| 4:5:210:ARG:CB  | 4:9:69:TYR:CE2[1_554]  | 1.57                     | 0.63              |
| 4:2:357:ILE:CB  | 4:7:233:SER:N[1_554]   | 1.57                     | 0.63              |
| 4:4:227:MET:CE  | 4:8:306:TYR:N[1_554]   | 1.57                     | 0.63              |
| 4:3:302:GLY:O   | 4:7:12:ASN:O[1_554]    | 1.57                     | 0.63              |
| 4:4:248:ILE:CD1 | 4:8:207:GLU:CG[1_554]  | 1.57                     | 0.63              |
| 4:3:325:MET:CG  | 4:7:166:TYR:CZ[1_554]  | 1.57                     | 0.63              |
| 4:3:311:ASP:OD1 | 4:7:144:ALA:N[1_554]   | 1.57                     | 0.63              |
| 4:5:296:ASN:C   | 4:9:168:GLY:C[1_554]   | 1.57                     | 0.63              |
| 4:4:310:ALA:C   | 4:8:141:SER:C[1_554]   | 1.57                     | 0.63              |
| 4:5:344:SER:C   | 4:9:362:TYR:CD1[1_554] | 1.57                     | 0.63              |
| 4:3:200:PHE:CA  | 4:7:206:ARG:CG[1_554]  | 1.57                     | 0.63              |
| 4:3:161:HIS:C   | 4:7:110:LEU:CD1[1_554] | 1.57                     | 0.63              |
| 4:5:210:ARG:O   | 4:9:15:GLY:C[1_554]    | 1.57                     | 0.63              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:371:HIS:C   | 4:8:230:ALA:CB[1_554]  | 1.57                     | 0.63              |
| 4:4:110:LEU:O   | 4:9:192:ILE:CA[1_554]  | 1.57                     | 0.63              |
| 4:3:316:GLU:CD  | 4:7:151:ILE:O[1_554]   | 1.57                     | 0.63              |
| 1:D:637:LYS:NZ  | 4:5:311:ASP:CB[1_556]  | 1.57                     | 0.63              |
| 4:3:339:VAL:CB  | 4:7:116:ARG:N[1_554]   | 1.57                     | 0.63              |
| 4:4:262:PHE:CD2 | 4:8:153:LEU:C[1_554]   | 1.57                     | 0.63              |
| 4:4:156:GLY:O   | 4:8:73:HIS:C[1_554]    | 1.57                     | 0.63              |
| 4:3:370:VAL:O   | 4:8:230:ALA:C[1_554]   | 1.57                     | 0.63              |
| 4:4:310:ALA:C   | 4:8:140:LEU:C[1_554]   | 1.57                     | 0.63              |
| 4:4:370:VAL:CB  | 4:9:230:ALA:O[1_554]   | 1.57                     | 0.63              |
| 4:5:283:MET:CE  | 4:9:286:ASP:O[1_554]   | 1.57                     | 0.63              |
| 1:A:637:LYS:NZ  | 4:4:311:ASP:O[1_556]   | 1.57                     | 0.63              |
| 4:5:56:ASP:CB   | 4:9:37:ARG:NH2[1_554]  | 1.57                     | 0.63              |
| 4:5:109:PRO:CA  | 4:V:195:GLU:CD[1_554]  | 1.57                     | 0.63              |
| 4:4:118:LYS:CA  | 4:9:237:GLU:OE1[1_554] | 1.57                     | 0.63              |
| 4:3:215:LYS:N   | 4:7:31:PHE:O[1_554]    | 1.57                     | 0.63              |
| 4:4:334:GLU:OE2 | 4:8:133:TYR:O[1_554]   | 1.57                     | 0.63              |
| 4:5:243:PRO:CA  | 4:9:60:SER:CA[1_554]   | 1.57                     | 0.63              |
| 4:3:114:ALA:C   | 4:8:250:ILE:N[1_554]   | 1.57                     | 0.63              |
| 4:2:173:HIS:NE2 | 4:7:265:SER:C[1_554]   | 1.57                     | 0.63              |
| 4:5:75:ILE:CA   | 4:V:198:TYR:N[1_554]   | 1.57                     | 0.63              |
| 4:3:178:LEU:CB  | 4:7:177:ARG:CB[1_554]  | 1.57                     | 0.63              |
| 4:4:17:VAL:CA   | 4:8:79:TRP:CD1[1_554]  | 1.57                     | 0.63              |
| 4:1:292:ASP:OD2 | 4:7:40:HIS:CG[1_554]   | 1.57                     | 0.63              |
| 4:5:342:GLY:C   | 4:9:367:PRO:O[1_554]   | 1.57                     | 0.63              |
| 4:4:218:TYR:CE1 | 4:8:337:TYR:CZ[1_554]  | 1.57                     | 0.63              |
| 4:4:139:VAL:O   | 4:8:371:HIS:CD2[1_554] | 1.57                     | 0.63              |
| 4:4:196:ARG:NH1 | 4:8:215:LYS:CG[1_554]  | 1.57                     | 0.63              |
| 4:4:192:ILE:O   | 4:8:213:LYS:CB[1_554]  | 1.57                     | 0.63              |
| 4:3:204:ALA:O   | 4:7:62:ARG:CG[1_554]   | 1.57                     | 0.63              |
| 4:5:309:ILE:O   | 4:9:141:SER:CB[1_554]  | 1.57                     | 0.63              |
| 4:3:211:ASP:CA  | 4:7:33:SER:N[1_554]    | 1.57                     | 0.63              |
| 4:5:276:GLU:O   | 4:9:281:SER:CB[1_554]  | 1.57                     | 0.63              |
| 4:5:300:SER:O   | 4:9:107:GLU:C[1_554]   | 1.57                     | 0.63              |
| 4:5:207:GLU:OE2 | 4:9:67:LEU:C[1_554]    | 1.57                     | 0.63              |
| 4:3:16:LEU:CD1  | 4:7:78:ASN:CB[1_554]   | 1.58                     | 0.62              |
| 4:4:345:ILE:CG2 | 4:8:369:ILE:CB[1_554]  | 1.58                     | 0.62              |
| 4:4:333:PRO:CD  | 4:8:104:LEU:CG[1_554]  | 1.58                     | 0.62              |
| 4:5:367:PRO:CD  | 4:V:234:SER:O[1_554]   | 1.58                     | 0.62              |
| 4:4:371:HIS:CE1 | 4:9:252:ASN:C[1_554]   | 1.58                     | 0.62              |
| 4:4:311:ASP:C   | 4:8:141:SER:C[1_554]   | 1.58                     | 0.62              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:156:GLY:CA  | 4:7:75:ILE:CB[1_554]   | 1.58                     | 0.62              |
| 4:3:213:LYS:CA  | 4:7:15:GLY:C[1_554]    | 1.58                     | 0.62              |
| 4:4:191:LYS:CE  | 4:8:185:LEU:O[1_554]   | 1.58                     | 0.62              |
| 4:4:223:PHE:CE2 | 4:8:304:THR:OG1[1_554] | 1.58                     | 0.62              |
| 4:5:26:ALA:C    | 4:9:122:ILE:C[1_554]   | 1.58                     | 0.62              |
| 4:5:166:TYR:OH  | 4:W:40:HIS:N[1_554]    | 1.58                     | 0.62              |
| 4:3:320:LEU:C   | 4:7:293:LEU:N[1_554]   | 1.58                     | 0.62              |
| 4:4:259:GLU:OE1 | 4:8:304:THR:O[1_554]   | 1.58                     | 0.62              |
| 4:2:117:GLU:OE2 | 4:7:236:LEU:O[1_554]   | 1.58                     | 0.62              |
| 4:3:317:ILE:CG1 | 4:7:165:ILE:CB[1_554]  | 1.58                     | 0.62              |
| 4:5:187:ASP:C   | 4:9:183:ARG:O[1_554]   | 1.58                     | 0.62              |
| 4:5:31:PHE:CD1  | 4:9:80:ASP:CA[1_554]   | 1.58                     | 0.62              |
| 4:3:180:LEU:O   | 4:7:159:VAL:CG1[1_554] | 1.58                     | 0.62              |
| 4:5:276:GLU:OE1 | 4:9:280:ASN:N[1_554]   | 1.58                     | 0.62              |
| 4:5:263:GLN:O   | 4:9:274:ILE:CD1[1_554] | 1.58                     | 0.62              |
| 4:5:193:LEU:CD2 | 4:9:210:ARG:CB[1_554]  | 1.58                     | 0.62              |
| 4:5:145:SER:N   | 4:9:372:ARG:CZ[1_554]  | 1.58                     | 0.62              |
| 4:4:250:ILE:CG1 | 4:8:210:ARG:NH2[1_554] | 1.58                     | 0.62              |
| 4:5:214:GLU:CD  | 4:9:33:SER:CB[1_554]   | 1.58                     | 0.62              |
| 4:3:142:LEU:C   | 4:7:371:HIS:C[1_554]   | 1.58                     | 0.62              |
| 4:5:195:GLU:CB  | 4:9:189:LEU:CD2[1_554] | 1.58                     | 0.62              |
| 4:3:153:LEU:O   | 4:7:108:ALA:O[1_554]   | 1.58                     | 0.62              |
| 4:3:327:ILE:C   | 4:7:168:GLY:N[1_554]   | 1.58                     | 0.62              |
| 4:3:213:LYS:CG  | 4:7:15:GLY:CA[1_554]   | 1.58                     | 0.62              |
| 4:5:198:TYR:CD1 | 4:9:208:ILE:CG1[1_554] | 1.58                     | 0.62              |
| 4:3:191:LYS:CA  | 4:7:187:ASP:N[1_554]   | 1.58                     | 0.62              |
| 4:4:196:ARG:O   | 4:8:212:ILE:CG1[1_554] | 1.58                     | 0.62              |
| 4:5:215:LYS:O   | 4:9:30:VAL:CG1[1_554]  | 1.58                     | 0.62              |
| 4:4:336:LYS:CE  | 4:8:86:TRP:CE2[1_554]  | 1.58                     | 0.62              |
| 4:4:189:LEU:N   | 4:8:182:GLY:C[1_554]   | 1.58                     | 0.62              |
| 4:3:318:THR:CG2 | 4:7:149:THR:N[1_554]   | 1.58                     | 0.62              |
| 4:5:280:ASN:ND2 | 4:9:281:SER:O[1_554]   | 1.58                     | 0.62              |
| 4:3:157:ASP:CG  | 4:7:72:GLU:CA[1_554]   | 1.58                     | 0.62              |
| 4:5:221:LEU:C   | 4:9:331:ALA:O[1_554]   | 1.58                     | 0.62              |
| 4:5:221:LEU:CB  | 4:9:332:PRO:N[1_554]   | 1.58                     | 0.62              |
| 4:4:332:PRO:N   | 4:8:135:ALA:CB[1_554]  | 1.58                     | 0.62              |
| 4:2:75:ILE:CA   | 4:7:198:TYR:CB[1_554]  | 1.58                     | 0.62              |
| 4:5:59:GLN:OE1  | 4:9:67:LEU:O[1_554]    | 1.58                     | 0.62              |
| 4:3:314:GLN:C   | 4:7:142:LEU:CD2[1_554] | 1.58                     | 0.62              |
| 4:4:273:GLY:O   | 4:8:162:ASN:CG[1_554]  | 1.58                     | 0.62              |
| 4:5:224:GLU:CB  | 4:9:310:ALA:CB[1_554]  | 1.58                     | 0.62              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:326:LYS:CB  | 4:9:167:GLU:OE1[1_554] | 1.58                     | 0.62              |
| 4:4:262:PHE:CD1 | 4:8:153:LEU:N[1_554]   | 1.58                     | 0.62              |
| 4:3:265:SER:OG  | 4:7:274:ILE:CB[1_554]  | 1.58                     | 0.62              |
| 4:3:195:GLU:CB  | 4:7:189:LEU:CD2[1_554] | 1.58                     | 0.62              |
| 4:4:219:VAL:O   | 4:8:335:ARG:O[1_554]   | 1.58                     | 0.62              |
| 4:3:266:PHE:CG  | 4:7:261:LEU:CG[1_554]  | 1.58                     | 0.62              |
| 4:3:207:GLU:OE2 | 4:7:67:LEU:CA[1_554]   | 1.58                     | 0.62              |
| 4:5:340:TRP:CD1 | 4:9:119:MET:N[1_554]   | 1.58                     | 0.62              |
| 4:4:15:GLY:C    | 4:8:77:THR:CA[1_554]   | 1.58                     | 0.62              |
| 4:3:345:ILE:CA  | 4:7:366:GLY:CA[1_554]  | 1.58                     | 0.62              |
| 4:3:166:TYR:CD1 | 4:9:40:HIS:CD2[1_554]  | 1.58                     | 0.62              |
| 4:4:21:PHE:O    | 4:8:125:GLU:CD[1_554]  | 1.58                     | 0.62              |
| 4:3:140:LEU:N   | 4:7:371:HIS:NE2[1_554] | 1.58                     | 0.62              |
| 4:4:276:GLU:CB  | 4:8:281:SER:CB[1_554]  | 1.58                     | 0.62              |
| 4:3:304:THR:C   | 4:7:137:GLN:CG[1_554]  | 1.58                     | 0.62              |
| 4:5:173:HIS:CE1 | 4:V:266:PHE:N[1_554]   | 1.58                     | 0.62              |
| 4:3:335:ARG:CG  | 4:7:106:THR:O[1_554]   | 1.58                     | 0.62              |
| 4:5:369:ILE:CG2 | 4:V:232:SER:CB[1_554]  | 1.58                     | 0.62              |
| 4:5:327:ILE:CA  | 4:9:149:THR:OG1[1_554] | 1.58                     | 0.62              |
| 4:5:188:TYR:O   | 4:9:186:THR:N[1_554]   | 1.58                     | 0.62              |
| 4:4:218:TYR:CZ  | 4:8:337:TYR:CD1[1_554] | 1.59                     | 0.61              |
| 4:2:367:PRO:O   | 4:7:236:LEU:CD2[1_554] | 1.59                     | 0.61              |
| 4:4:298:VAL:CG1 | 4:8:116:ARG:NH2[1_554] | 1.59                     | 0.61              |
| 4:4:215:LYS:CG  | 4:8:31:PHE:C[1_554]    | 1.59                     | 0.61              |
| 4:3:140:LEU:O   | 4:7:371:HIS:ND1[1_554] | 1.59                     | 0.61              |
| 4:4:25:ASP:OD1  | 4:8:124:PHE:CE1[1_554] | 1.59                     | 0.61              |
| 4:4:108:ALA:N   | 4:9:195:GLU:O[1_554]   | 1.59                     | 0.61              |
| 4:5:136:ILE:CA  | 4:9:113:LYS:CG[1_554]  | 1.59                     | 0.61              |
| 4:5:311:ASP:OD1 | 4:9:144:ALA:O[1_554]   | 1.59                     | 0.61              |
| 4:4:338:SER:O   | 4:8:116:ARG:C[1_554]   | 1.59                     | 0.61              |
| 4:4:337:TYR:CE2 | 4:8:86:TRP:CH2[1_554]  | 1.59                     | 0.61              |
| 4:3:243:PRO:CD  | 4:7:59:GLN:C[1_554]    | 1.59                     | 0.61              |
| 4:4:186:THR:C   | 4:8:183:ARG:NE[1_554]  | 1.59                     | 0.61              |
| 4:5:340:TRP:CH2 | 4:9:121:GLN:CA[1_554]  | 1.59                     | 0.61              |
| 4:4:320:LEU:CB  | 4:8:293:LEU:CG[1_554]  | 1.59                     | 0.61              |
| 4:4:270:GLU:CA  | 4:8:272:ALA:O[1_554]   | 1.59                     | 0.61              |
| 4:5:256:ARG:O   | 4:9:303:THR:CG2[1_554] | 1.59                     | 0.61              |
| 4:3:267:ILE:CB  | 4:7:180:LEU:CD1[1_554] | 1.59                     | 0.61              |
| 4:3:277:THR:O   | 4:7:174:ALA:CA[1_554]  | 1.59                     | 0.61              |
| 4:5:31:PHE:CB   | 4:9:80:ASP:CA[1_554]   | 1.59                     | 0.61              |
| 4:5:257:CYS:O   | 4:9:303:THR:CB[1_554]  | 1.59                     | 0.61              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:257:CYS:N   | 4:8:303:THR:N[1_554]   | 1.59                     | 0.61              |
| 4:5:329:ILE:CD1 | 4:9:142:LEU:CD2[1_554] | 1.59                     | 0.61              |
| 4:4:145:SER:CA  | 4:8:372:ARG:NH2[1_554] | 1.59                     | 0.61              |
| 4:3:222:ASP:OD1 | 4:7:331:ALA:O[1_554]   | 1.59                     | 0.61              |
| 4:4:311:ASP:N   | 4:8:141:SER:O[1_554]   | 1.59                     | 0.61              |
| 4:3:333:PRO:CG  | 4:7:103:THR:O[1_554]   | 1.59                     | 0.61              |
| 4:3:223:PHE:CE1 | 4:7:301:GLY:O[1_554]   | 1.59                     | 0.61              |
| 4:5:296:ASN:CA  | 4:9:168:GLY:C[1_554]   | 1.59                     | 0.61              |
| 4:3:309:ILE:CB  | 4:7:339:VAL:CG2[1_554] | 1.59                     | 0.61              |
| 4:5:317:ILE:CG1 | 4:9:150:GLY:C[1_554]   | 1.59                     | 0.61              |
| 4:5:322:PRO:O   | 4:9:292:ASP:OD2[1_554] | 1.59                     | 0.61              |
| 4:3:188:TYR:N   | 4:7:184:ASP:N[1_554]   | 1.59                     | 0.61              |
| 4:3:173:HIS:O   | 4:8:267:ILE:C[1_554]   | 1.59                     | 0.61              |
| 4:5:31:PHE:O    | 4:9:78:ASN:CA[1_554]   | 1.59                     | 0.61              |
| 4:5:346:LEU:N   | 4:9:366:GLY:O[1_554]   | 1.59                     | 0.61              |
| 4:5:154:ASP:OD1 | 4:9:111:ASN:CB[1_554]  | 1.59                     | 0.61              |
| 4:3:367:PRO:C   | 4:8:236:LEU:CD2[1_554] | 1.59                     | 0.61              |
| 4:2:367:PRO:O   | 4:7:236:LEU:CG[1_554]  | 1.59                     | 0.61              |
| 4:4:222:ASP:CA  | 4:8:332:PRO:N[1_554]   | 1.59                     | 0.61              |
| 4:5:11:ASP:OD1  | 4:9:115:ASN:CB[1_554]  | 1.59                     | 0.61              |
| 4:4:316:GLU:CB  | 4:8:151:ILE:C[1_554]   | 1.59                     | 0.61              |
| 4:4:329:ILE:C   | 4:8:139:VAL:CG1[1_554] | 1.59                     | 0.61              |
| 4:3:331:ALA:CB  | 4:7:135:ALA:CB[1_554]  | 1.59                     | 0.61              |
| 4:3:333:PRO:CB  | 4:7:104:LEU:N[1_554]   | 1.59                     | 0.61              |
| 4:4:310:ALA:C   | 4:8:141:SER:CA[1_554]  | 1.59                     | 0.61              |
| 4:5:196:ARG:O   | 4:9:212:ILE:CB[1_554]  | 1.59                     | 0.61              |
| 4:4:278:THR:CA  | 4:8:164:PRO:CD[1_554]  | 1.59                     | 0.61              |
| 4:4:243:PRO:CG  | 4:8:59:GLN:C[1_554]    | 1.59                     | 0.61              |
| 4:4:255:PHE:CD2 | 4:8:305:MET:CG[1_554]  | 1.59                     | 0.61              |
| 4:3:314:GLN:OE1 | 4:7:147:ARG:C[1_554]   | 1.59                     | 0.61              |
| 4:5:166:TYR:CD2 | 4:W:40:HIS:NE2[1_554]  | 1.59                     | 0.61              |
| 4:5:113:LYS:CB  | 4:V:252:ASN:O[1_554]   | 1.59                     | 0.61              |
| 4:5:257:CYS:CB  | 4:9:303:THR:OG1[1_554] | 1.59                     | 0.61              |
| 4:3:282:ILE:CG1 | 4:7:171:LEU:CB[1_554]  | 1.59                     | 0.61              |
| 4:3:185:LEU:C   | 4:7:157:ASP:C[1_554]   | 1.59                     | 0.61              |
| 4:5:159:VAL:N   | 4:9:177:ARG:NH2[1_554] | 1.59                     | 0.61              |
| 4:5:190:MET:C   | 4:9:186:THR:CG2[1_554] | 1.59                     | 0.61              |
| 4:5:314:GLN:CD  | 4:9:147:ARG:O[1_554]   | 1.59                     | 0.61              |
| 4:3:243:PRO:CG  | 4:7:59:GLN:O[1_554]    | 1.59                     | 0.61              |
| 4:3:273:GLY:O   | 4:7:162:ASN:CA[1_554]  | 1.59                     | 0.61              |
| 4:3:186:THR:CA  | 4:7:183:ARG:CZ[1_554]  | 1.59                     | 0.61              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:221:LEU:O   | 4:9:332:PRO:N[1_554]   | 1.59                     | 0.61              |
| 4:5:188:TYR:CE1 | 4:9:185:LEU:CD2[1_554] | 1.59                     | 0.61              |
| 4:5:208:ILE:CG2 | 4:9:59:GLN:CG[1_554]   | 1.59                     | 0.61              |
| 4:4:326:LYS:NZ  | 4:V:45:VAL:N[1_554]    | 1.59                     | 0.61              |
| 4:5:195:GLU:CG  | 4:9:189:LEU:CB[1_554]  | 1.59                     | 0.61              |
| 4:5:137:GLN:CA  | 4:9:112:PRO:C[1_554]   | 1.59                     | 0.61              |
| 4:3:313:MET:CA  | 4:7:152:VAL:CG2[1_554] | 1.59                     | 0.61              |
| 4:5:17:VAL:C    | 4:9:79:TRP:CB[1_554]   | 1.59                     | 0.61              |
| 4:4:109:PRO:CB  | 4:9:195:GLU:CD[1_554]  | 1.59                     | 0.61              |
| 4:5:16:LEU:CD1  | 4:9:70:PRO:CB[1_554]   | 1.59                     | 0.61              |
| 4:3:110:LEU:CD1 | 4:8:191:LYS:CB[1_554]  | 1.59                     | 0.61              |
| 4:5:266:PHE:CD2 | 4:9:261:LEU:CG[1_554]  | 1.59                     | 0.61              |
| 4:4:24:ASP:CB   | 4:8:125:GLU:CA[1_554]  | 1.59                     | 0.61              |
| 4:3:188:TYR:N   | 4:7:183:ARG:C[1_554]   | 1.59                     | 0.61              |
| 4:3:190:MET:O   | 4:7:186:THR:CG2[1_554] | 1.59                     | 0.61              |
| 4:3:289:ILE:CG2 | 4:9:39:ARG:NH2[1_554]  | 1.59                     | 0.61              |
| 4:3:223:PHE:CB  | 4:7:335:ARG:NE[1_554]  | 1.59                     | 0.61              |
| 4:5:290:ARG:NE  | 4:9:286:ASP:OD2[1_554] | 1.59                     | 0.61              |
| 4:3:196:ARG:CB  | 4:7:212:ILE:N[1_554]   | 1.59                     | 0.61              |
| 4:5:191:LYS:N   | 4:9:187:ASP:N[1_554]   | 1.59                     | 0.61              |
| 4:5:113:LYS:CB  | 4:V:252:ASN:CA[1_554]  | 1.60                     | 0.60              |
| 4:3:218:TYR:CZ  | 4:7:337:TYR:CD1[1_554] | 1.60                     | 0.60              |
| 4:3:194:THR:C   | 4:7:209:VAL:CG2[1_554] | 1.60                     | 0.60              |
| 4:3:315:LYS:NZ  | 4:7:147:ARG:CD[1_554]  | 1.60                     | 0.60              |
| 4:3:144:ALA:O   | 4:7:370:VAL:CB[1_554]  | 1.60                     | 0.60              |
| 4:5:345:ILE:C   | 4:9:366:GLY:O[1_554]   | 1.60                     | 0.60              |
| 4:5:113:LYS:NZ  | 4:V:254:ARG:CA[1_554]  | 1.60                     | 0.60              |
| 4:4:222:ASP:CA  | 4:8:331:ALA:O[1_554]   | 1.60                     | 0.60              |
| 4:3:222:ASP:N   | 4:7:332:PRO:N[1_554]   | 1.60                     | 0.60              |
| 4:3:258:PRO:CA  | 4:7:156:GLY:N[1_554]   | 1.60                     | 0.60              |
| 4:5:307:PRO:CB  | 4:9:337:TYR:CB[1_554]  | 1.60                     | 0.60              |
| 4:4:218:TYR:CZ  | 4:8:337:TYR:CE1[1_554] | 1.60                     | 0.60              |
| 4:2:173:HIS:O   | 4:7:267:ILE:CB[1_554]  | 1.60                     | 0.60              |
| 4:3:340:TRP:O   | 4:7:117:GLU:O[1_554]   | 1.60                     | 0.60              |
| 4:3:335:ARG:NE  | 4:7:106:THR:CA[1_554]  | 1.60                     | 0.60              |
| 4:3:305:MET:CA  | 4:7:11:ASP:OD1[1_554]  | 1.60                     | 0.60              |
| 4:3:321:ALA:CB  | 4:7:149:THR:CG2[1_554] | 1.60                     | 0.60              |
| 4:4:254:ARG:NH1 | 4:8:336:LYS:NZ[1_554]  | 1.60                     | 0.60              |
| 4:5:297:ASN:OD1 | 4:9:165:ILE:CA[1_554]  | 1.60                     | 0.60              |
| 4:4:72:GLU:O    | 4:9:198:TYR:O[1_554]   | 1.60                     | 0.60              |
| 4:5:308:GLY:C   | 4:9:338:SER:OG[1_554]  | 1.60                     | 0.60              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:219:VAL:CB  | 4:9:300:SER:CA[1_554]  | 1.60                     | 0.60              |
| 4:3:270:GLU:C   | 4:7:272:ALA:CB[1_554]  | 1.60                     | 0.60              |
| 4:3:263:GLN:C   | 4:7:274:ILE:CG1[1_554] | 1.60                     | 0.60              |
| 4:3:114:ALA:C   | 4:8:250:ILE:CA[1_554]  | 1.60                     | 0.60              |
| 4:3:322:PRO:C   | 4:7:292:ASP:OD2[1_554] | 1.60                     | 0.60              |
| 4:4:345:ILE:C   | 4:8:366:GLY:CA[1_554]  | 1.60                     | 0.60              |
| 4:3:289:ILE:N   | 4:9:39:ARG:NH1[1_554]  | 1.60                     | 0.60              |
| 4:3:147:ARG:CG  | 4:7:372:ARG:CG[1_554]  | 1.60                     | 0.60              |
| 4:5:262:PHE:CG  | 4:9:153:LEU:CG[1_554]  | 1.60                     | 0.60              |
| 4:5:259:GLU:CD  | 4:9:309:ILE:CG1[1_554] | 1.60                     | 0.60              |
| 4:4:317:ILE:CD1 | 4:8:165:ILE:O[1_554]   | 1.60                     | 0.60              |
| 4:5:346:LEU:CB  | 4:9:368:SER:N[1_554]   | 1.60                     | 0.60              |
| 4:5:277:THR:C   | 4:9:174:ALA:O[1_554]   | 1.60                     | 0.60              |
| 4:5:307:PRO:C   | 4:9:337:TYR:C[1_554]   | 1.60                     | 0.60              |
| 4:5:288:ASP:N   | 4:W:63:GLY:CA[1_554]   | 1.60                     | 0.60              |
| 4:3:257:CYS:O   | 4:7:156:GLY:O[1_554]   | 1.60                     | 0.60              |
| 4:5:349:LEU:N   | 4:9:366:GLY:N[1_554]   | 1.60                     | 0.60              |
| 4:4:261:LEU:O   | 4:8:161:HIS:N[1_554]   | 1.60                     | 0.60              |
| 4:5:296:ASN:C   | 4:9:169:TYR:N[1_554]   | 1.60                     | 0.60              |
| 4:2:291:LYS:CD  | 4:8:64:ILE:CB[1_554]   | 1.60                     | 0.60              |
| 4:5:30:VAL:CB   | 4:9:82:MET:C[1_554]    | 1.60                     | 0.60              |
| 4:5:330:ILE:N   | 4:9:139:VAL:CG1[1_554] | 1.60                     | 0.60              |
| 4:5:137:GLN:CG  | 4:9:112:PRO:CA[1_554]  | 1.60                     | 0.60              |
| 4:5:267:ILE:CB  | 4:9:180:LEU:CB[1_554]  | 1.60                     | 0.60              |
| 4:4:336:LYS:NZ  | 4:8:86:TRP:CG[1_554]   | 1.60                     | 0.60              |
| 4:5:255:PHE:O   | 4:9:303:THR:C[1_554]   | 1.60                     | 0.60              |
| 4:4:321:ALA:C   | 4:8:292:ASP:OD2[1_554] | 1.60                     | 0.60              |
| 4:5:194:THR:C   | 4:9:209:VAL:CB[1_554]  | 1.60                     | 0.60              |
| 4:4:199:SER:N   | 4:8:207:GLU:N[1_554]   | 1.60                     | 0.60              |
| 4:3:31:PHE:N    | 4:7:80:ASP:N[1_554]    | 1.60                     | 0.60              |
| 4:4:143:TYR:O   | 4:8:369:ILE:O[1_554]   | 1.60                     | 0.60              |
| 4:3:320:LEU:CA  | 4:7:293:LEU:CB[1_554]  | 1.60                     | 0.60              |
| 4:3:317:ILE:CD1 | 4:7:165:ILE:CG2[1_554] | 1.60                     | 0.60              |
| 4:5:249:THR:O   | 4:9:211:ASP:CB[1_554]  | 1.60                     | 0.60              |
| 4:4:338:SER:C   | 4:8:116:ARG:C[1_554]   | 1.60                     | 0.60              |
| 4:3:312:ARG:N   | 4:7:141:SER:O[1_554]   | 1.60                     | 0.60              |
| 4:5:191:LYS:CD  | 4:9:185:LEU:O[1_554]   | 1.60                     | 0.60              |
| 4:4:221:LEU:O   | 4:8:332:PRO:C[1_554]   | 1.60                     | 0.60              |
| 4:5:335:ARG:CG  | 4:9:106:THR:CA[1_554]  | 1.60                     | 0.60              |
| 4:4:193:LEU:CG  | 4:8:210:ARG:NE[1_554]  | 1.60                     | 0.60              |
| 4:5:33:SER:CB   | 4:9:77:THR:O[1_554]    | 1.60                     | 0.60              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:112:PRO:CG  | 4:7:193:LEU:CD1[1_554] | 1.60                     | 0.60              |
| 4:5:166:TYR:CE2 | 4:W:39:ARG:C[1_554]    | 1.60                     | 0.60              |
| 4:5:21:PHE:O    | 4:9:125:GLU:CG[1_554]  | 1.60                     | 0.60              |
| 4:5:151:ILE:CG2 | 4:9:170:ALA:O[1_554]   | 1.60                     | 0.60              |
| 4:5:267:ILE:CD1 | 4:9:180:LEU:CA[1_554]  | 1.60                     | 0.60              |
| 4:5:26:ALA:CA   | 4:9:123:MET:CG[1_554]  | 1.61                     | 0.59              |
| 4:4:278:THR:O   | 4:8:171:LEU:CB[1_554]  | 1.61                     | 0.59              |
| 4:5:299:MET:CA  | 4:9:136:ILE:C[1_554]   | 1.61                     | 0.59              |
| 4:4:317:ILE:CG2 | 4:8:150:GLY:O[1_554]   | 1.61                     | 0.59              |
| 4:4:303:THR:O   | 4:8:137:GLN:OE1[1_554] | 1.61                     | 0.59              |
| 4:4:222:ASP:CG  | 4:8:331:ALA:O[1_554]   | 1.61                     | 0.59              |
| 4:5:310:ALA:CB  | 4:9:141:SER:CA[1_554]  | 1.61                     | 0.59              |
| 4:3:193:LEU:CA  | 4:7:210:ARG:CG[1_554]  | 1.61                     | 0.59              |
| 4:5:162:ASN:OD1 | 4:9:175:ILE:CG2[1_554] | 1.61                     | 0.59              |
| 4:3:204:ALA:CA  | 4:7:62:ARG:CB[1_554]   | 1.61                     | 0.59              |
| 4:3:311:ASP:N   | 4:7:141:SER:CA[1_554]  | 1.61                     | 0.59              |
| 4:4:340:TRP:CB  | 4:8:118:LYS:N[1_554]   | 1.61                     | 0.59              |
| 4:5:256:ARG:C   | 4:9:303:THR:CA[1_554]  | 1.61                     | 0.59              |
| 4:3:335:ARG:C   | 4:7:119:MET:CE[1_554]  | 1.61                     | 0.59              |
| 4:3:18:LYS:CG   | 4:7:79:TRP:CE2[1_554]  | 1.61                     | 0.59              |
| 4:4:188:TYR:CD1 | 4:8:181:ALA:O[1_554]   | 1.61                     | 0.59              |
| 4:3:268:GLY:CA  | 4:7:264:PRO:CA[1_554]  | 1.61                     | 0.59              |
| 4:5:115:ASN:N   | 4:V:196:ARG:NH1[1_554] | 1.61                     | 0.59              |
| 4:4:340:TRP:CD1 | 4:8:118:LYS:CG[1_554]  | 1.61                     | 0.59              |
| 4:3:262:PHE:CB  | 4:7:153:LEU:CA[1_554]  | 1.61                     | 0.59              |
| 4:4:173:HIS:N   | 4:9:267:ILE:N[1_554]   | 1.61                     | 0.59              |
| 4:5:158:GLY:N   | 4:9:72:GLU:O[1_554]    | 1.61                     | 0.59              |
| 4:3:113:LYS:CB  | 4:8:254:ARG:N[1_554]   | 1.61                     | 0.59              |
| 4:5:286:ASP:CA  | 4:V:270:GLU:CG[1_554]  | 1.61                     | 0.59              |
| 4:3:288:ASP:O   | 4:9:64:ILE:N[1_554]    | 1.61                     | 0.59              |
| 4:3:317:ILE:N   | 4:7:150:GLY:O[1_554]   | 1.61                     | 0.59              |
| 4:3:279:TYR:C   | 4:7:285:CYS:SG[1_554]  | 1.61                     | 0.59              |
| 4:4:320:LEU:CA  | 4:8:293:LEU:CB[1_554]  | 1.61                     | 0.59              |
| 4:5:261:LEU:N   | 4:9:155:SER:OG[1_554]  | 1.61                     | 0.59              |
| 4:3:109:PRO:C   | 4:8:195:GLU:CD[1_554]  | 1.61                     | 0.59              |
| 4:5:313:MET:C   | 4:9:142:LEU:CD1[1_554] | 1.61                     | 0.59              |
| 4:3:310:ALA:N   | 4:7:141:SER:N[1_554]   | 1.61                     | 0.59              |
| 4:3:303:THR:OG1 | 4:7:74:GLY:N[1_554]    | 1.61                     | 0.59              |
| 4:4:301:GLY:N   | 4:8:107:GLU:CA[1_554]  | 1.61                     | 0.59              |
| 4:5:16:LEU:CA   | 4:9:78:ASN:N[1_554]    | 1.61                     | 0.59              |
| 4:4:181:ALA:CB  | 4:8:73:HIS:O[1_554]    | 1.61                     | 0.59              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:275:HIS:C   | 4:9:151:ILE:CD1[1_554] | 1.61                     | 0.59              |
| 4:3:311:ASP:C   | 4:7:142:LEU:N[1_554]   | 1.61                     | 0.59              |
| 4:5:343:GLY:O   | 4:9:367:PRO:C[1_554]   | 1.61                     | 0.59              |
| 4:4:213:LYS:CD  | 4:8:15:GLY:N[1_554]    | 1.61                     | 0.59              |
| 4:3:116:ARG:CG  | 4:8:252:ASN:CG[1_554]  | 1.61                     | 0.59              |
| 4:4:286:ASP:CB  | 4:9:270:GLU:CD[1_554]  | 1.61                     | 0.59              |
| 4:4:333:PRO:N   | 4:8:104:LEU:CG[1_554]  | 1.61                     | 0.59              |
| 4:5:349:LEU:CD2 | 4:9:365:ALA:CB[1_554]  | 1.61                     | 0.59              |
| 4:3:331:ALA:C   | 4:7:135:ALA:N[1_554]   | 1.61                     | 0.59              |
| 4:5:321:ALA:C   | 4:9:292:ASP:CB[1_554]  | 1.61                     | 0.59              |
| 4:5:195:GLU:OE1 | 4:9:257:CYS:SG[1_554]  | 1.61                     | 0.59              |
| 4:5:156:GLY:CA  | 4:9:75:ILE:N[1_554]    | 1.61                     | 0.59              |
| 4:5:196:ARG:C   | 4:9:212:ILE:CD1[1_554] | 1.61                     | 0.59              |
| 4:3:207:GLU:CG  | 4:7:67:LEU:CA[1_554]   | 1.61                     | 0.59              |
| 4:3:188:TYR:N   | 4:7:183:ARG:CA[1_554]  | 1.61                     | 0.59              |
| 4:3:370:VAL:O   | 4:8:230:ALA:CA[1_554]  | 1.61                     | 0.59              |
| 4:3:340:TRP:C   | 4:7:118:LYS:N[1_554]   | 1.61                     | 0.59              |
| 4:5:11:ASP:O    | 4:9:79:TRP:CZ2[1_554]  | 1.61                     | 0.59              |
| 4:4:256:ARG:C   | 4:8:303:THR:CB[1_554]  | 1.61                     | 0.59              |
| 4:5:304:THR:CA  | 4:9:137:GLN:CD[1_554]  | 1.61                     | 0.59              |
| 4:5:201:VAL:CG2 | 4:9:203:THR:CA[1_554]  | 1.61                     | 0.59              |
| 4:3:335:ARG:CD  | 4:7:106:THR:C[1_554]   | 1.61                     | 0.59              |
| 4:4:327:ILE:CG1 | 4:8:149:THR:OG1[1_554] | 1.61                     | 0.59              |
| 4:4:211:ASP:CA  | 4:8:32:PRO:C[1_554]    | 1.61                     | 0.59              |
| 4:4:145:SER:N   | 4:8:370:VAL:O[1_554]   | 1.61                     | 0.59              |
| 4:4:227:MET:CB  | 4:8:307:PRO:CA[1_554]  | 1.61                     | 0.59              |
| 4:5:154:ASP:CA  | 4:9:109:PRO:CA[1_554]  | 1.61                     | 0.59              |
| 4:3:325:MET:CG  | 4:7:166:TYR:CD2[1_554] | 1.61                     | 0.59              |
| 4:4:299:MET:CG  | 4:8:136:ILE:CG2[1_554] | 1.61                     | 0.59              |
| 4:5:340:TRP:CG  | 4:9:119:MET:CA[1_554]  | 1.61                     | 0.59              |
| 4:5:193:LEU:CD1 | 4:9:210:ARG:O[1_554]   | 1.61                     | 0.59              |
| 4:5:28:ARG:CD   | 4:9:126:THR:CA[1_554]  | 1.61                     | 0.59              |
| 4:3:274:ILE:CB  | 4:7:161:HIS:CB[1_554]  | 1.61                     | 0.59              |
| 4:3:327:ILE:CA  | 4:7:167:GLU:CA[1_554]  | 1.62                     | 0.58              |
| 4:1:287:ILE:O   | 4:7:63:GLY:C[1_554]    | 1.62                     | 0.58              |
| 4:4:157:ASP:O   | 4:8:72:GLU:C[1_554]    | 1.62                     | 0.58              |
| 4:3:298:VAL:C   | 4:7:136:ILE:CG1[1_554] | 1.62                     | 0.58              |
| 4:5:197:GLY:N   | 4:9:212:ILE:CD1[1_554] | 1.62                     | 0.58              |
| 4:5:214:GLU:N   | 4:9:16:LEU:CB[1_554]   | 1.62                     | 0.58              |
| 4:4:257:CYS:N   | 4:8:303:THR:OG1[1_554] | 1.62                     | 0.58              |
| 4:4:216:LEU:N   | 4:8:30:VAL:CG1[1_554]  | 1.62                     | 0.58              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:277:THR:CG2 | 4:7:176:MET:N[1_554]   | 1.62                     | 0.58              |
| 4:4:25:ASP:N    | 4:8:124:PHE:CA[1_554]  | 1.62                     | 0.58              |
| 4:5:31:PHE:CG   | 4:9:80:ASP:CA[1_554]   | 1.62                     | 0.58              |
| 4:5:326:LYS:O   | 4:9:167:GLU:CG[1_554]  | 1.62                     | 0.58              |
| 4:4:312:ARG:CG  | 4:8:299:MET:O[1_554]   | 1.62                     | 0.58              |
| 4:4:195:GLU:CG  | 4:8:189:LEU:CB[1_554]  | 1.62                     | 0.58              |
| 4:3:214:GLU:CA  | 4:7:16:LEU:CA[1_554]   | 1.62                     | 0.58              |
| 4:4:300:SER:CB  | 4:8:107:GLU:OE2[1_554] | 1.62                     | 0.58              |
| 4:5:164:PRO:CA  | 4:9:172:PRO:CG[1_554]  | 1.62                     | 0.58              |
| 4:5:159:VAL:O   | 4:9:177:ARG:NH1[1_554] | 1.62                     | 0.58              |
| 4:3:297:ASN:CG  | 4:7:170:ALA:N[1_554]   | 1.62                     | 0.58              |
| 4:5:191:LYS:O   | 4:9:186:THR:O[1_554]   | 1.62                     | 0.58              |
| 4:4:187:ASP:N   | 4:8:183:ARG:CB[1_554]  | 1.62                     | 0.58              |
| 4:3:339:VAL:CB  | 4:7:115:ASN:CA[1_554]  | 1.62                     | 0.58              |
| 4:3:273:GLY:N   | 4:7:162:ASN:CG[1_554]  | 1.62                     | 0.58              |
| 4:4:293:LEU:C   | 4:8:169:TYR:CD2[1_554] | 1.62                     | 0.58              |
| 4:4:277:THR:C   | 4:8:174:ALA:C[1_554]   | 1.62                     | 0.58              |
| 4:5:172:PRO:CG  | 4:V:266:PHE:CB[1_554]  | 1.62                     | 0.58              |
| 4:3:173:HIS:O   | 4:8:267:ILE:CA[1_554]  | 1.62                     | 0.58              |
| 4:3:262:PHE:CB  | 4:7:153:LEU:CB[1_554]  | 1.62                     | 0.58              |
| 4:3:326:LYS:CE  | 4:9:44:MET:C[1_554]    | 1.62                     | 0.58              |
| 4:5:154:ASP:C   | 4:9:109:PRO:N[1_554]   | 1.62                     | 0.58              |
| 4:4:319:ALA:O   | 4:8:292:ASP:O[1_554]   | 1.62                     | 0.58              |
| 4:2:79:TRP:CZ2  | 4:7:249:THR:N[1_554]   | 1.62                     | 0.58              |
| 4:4:286:ASP:C   | 4:9:270:GLU:OE1[1_554] | 1.62                     | 0.58              |
| 4:5:113:LYS:CG  | 4:V:253:GLU:N[1_554]   | 1.62                     | 0.58              |
| 4:4:173:HIS:CA  | 4:9:267:ILE:N[1_554]   | 1.62                     | 0.58              |
| 4:4:313:MET:CG  | 4:8:138:ALA:CB[1_554]  | 1.62                     | 0.58              |
| 4:4:294:TYR:CB  | 4:8:166:TYR:C[1_554]   | 1.62                     | 0.58              |
| 4:3:256:ARG:O   | 4:7:303:THR:CG2[1_554] | 1.62                     | 0.58              |
| 4:3:336:LYS:CE  | 4:7:86:TRP:CZ2[1_554]  | 1.62                     | 0.58              |
| 4:4:262:PHE:CG  | 4:8:153:LEU:CA[1_554]  | 1.62                     | 0.58              |
| 4:3:214:GLU:CD  | 4:7:33:SER:CB[1_554]   | 1.62                     | 0.58              |
| 4:4:207:GLU:CD  | 4:8:67:LEU:C[1_554]    | 1.62                     | 0.58              |
| 4:5:366:GLY:C   | 4:V:233:SER:C[1_554]   | 1.62                     | 0.58              |
| 4:3:191:LYS:O   | 4:7:186:THR:CG2[1_554] | 1.62                     | 0.58              |
| 4:3:188:TYR:CE1 | 4:7:185:LEU:CD2[1_554] | 1.62                     | 0.58              |
| 4:3:333:PRO:CA  | 4:7:105:LEU:CA[1_554]  | 1.62                     | 0.58              |
| 4:4:214:GLU:CG  | 4:8:33:SER:CB[1_554]   | 1.62                     | 0.58              |
| 4:3:274:ILE:CG1 | 4:7:161:HIS:CG[1_554]  | 1.62                     | 0.58              |
| 4:2:114:ALA:C   | 4:7:250:ILE:N[1_554]   | 1.62                     | 0.58              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:227:MET:SD  | 4:8:306:TYR:CA[1_554]  | 1.62                     | 0.58              |
| 4:5:62:ARG:NH1  | 4:9:67:LEU:O[1_554]    | 1.62                     | 0.58              |
| 4:5:17:VAL:CB   | 4:9:79:TRP:CD1[1_554]  | 1.62                     | 0.58              |
| 4:4:289:ILE:O   | 4:V:64:ILE:CG2[1_554]  | 1.62                     | 0.58              |
| 4:3:113:LYS:O   | 4:8:252:ASN:N[1_554]   | 1.62                     | 0.58              |
| 4:3:366:GLY:O   | 4:8:234:SER:OG[1_554]  | 1.62                     | 0.58              |
| 4:4:143:TYR:CD2 | 4:8:368:SER:C[1_554]   | 1.62                     | 0.58              |
| 4:4:274:ILE:C   | 4:8:162:ASN:CA[1_554]  | 1.62                     | 0.58              |
| 4:5:283:MET:CG  | 4:9:286:ASP:O[1_554]   | 1.62                     | 0.58              |
| 4:3:258:PRO:O   | 4:7:155:SER:C[1_554]   | 1.62                     | 0.58              |
| 4:3:286:ASP:C   | 4:8:270:GLU:CD[1_554]  | 1.62                     | 0.58              |
| 1:D:637:LYS:CE  | 4:5:311:ASP:CG[1_556]  | 1.62                     | 0.58              |
| 4:4:159:VAL:CA  | 4:8:177:ARG:NH1[1_554] | 1.62                     | 0.58              |
| 4:4:212:ILE:C   | 4:8:16:LEU:CD1[1_554]  | 1.62                     | 0.58              |
| 4:5:336:LYS:CA  | 4:9:106:THR:O[1_554]   | 1.62                     | 0.58              |
| 4:5:147:ARG:O   | 4:9:372:ARG:CG[1_554]  | 1.62                     | 0.58              |
| 4:2:112:PRO:CG  | 4:7:193:LEU:CG[1_554]  | 1.62                     | 0.58              |
| 4:3:181:ALA:C   | 4:7:73:HIS:CA[1_554]   | 1.62                     | 0.58              |
| 4:2:357:ILE:CG1 | 4:7:232:SER:C[1_554]   | 1.62                     | 0.58              |
| 4:5:223:PHE:CG  | 4:9:304:THR:O[1_554]   | 1.62                     | 0.58              |
| 4:5:172:PRO:CG  | 4:V:266:PHE:CA[1_554]  | 1.62                     | 0.58              |
| 4:3:259:GLU:CG  | 4:7:304:THR:CG2[1_554] | 1.62                     | 0.58              |
| 4:2:173:HIS:CG  | 4:7:267:ILE:N[1_554]   | 1.62                     | 0.58              |
| 4:4:173:HIS:C   | 4:9:267:ILE:C[1_554]   | 1.62                     | 0.58              |
| 4:4:273:GLY:C   | 4:8:162:ASN:CA[1_554]  | 1.62                     | 0.58              |
| 4:5:113:LYS:O   | 4:V:252:ASN:CG[1_554]  | 1.62                     | 0.58              |
| 4:4:275:HIS:CA  | 4:8:163:VAL:N[1_554]   | 1.62                     | 0.58              |
| 4:5:166:TYR:CD1 | 4:W:40:HIS:CG[1_554]   | 1.62                     | 0.58              |
| 4:4:283:MET:CG  | 4:8:285:CYS:C[1_554]   | 1.62                     | 0.58              |
| 4:5:304:THR:OG1 | 4:9:137:GLN:CB[1_554]  | 1.62                     | 0.58              |
| 4:3:213:LYS:NZ  | 4:7:14:SER:CB[1_554]   | 1.62                     | 0.58              |
| 4:4:222:ASP:N   | 4:8:331:ALA:C[1_554]   | 1.62                     | 0.58              |
| 4:4:188:TYR:CD2 | 4:8:181:ALA:C[1_554]   | 1.62                     | 0.58              |
| 4:4:288:ASP:C   | 4:V:63:GLY:O[1_554]    | 1.62                     | 0.58              |
| 4:4:266:PHE:CA  | 4:8:261:LEU:CD2[1_554] | 1.63                     | 0.57              |
| 4:3:173:HIS:ND1 | 4:8:266:PHE:N[1_554]   | 1.63                     | 0.57              |
| 4:5:109:PRO:O   | 4:V:195:GLU:CD[1_554]  | 1.63                     | 0.57              |
| 4:3:218:TYR:CE2 | 4:7:337:TYR:CE2[1_554] | 1.63                     | 0.57              |
| 4:4:116:ARG:N   | 4:9:196:ARG:CZ[1_554]  | 1.63                     | 0.57              |
| 4:4:140:LEU:O   | 4:8:371:HIS:CB[1_554]  | 1.63                     | 0.57              |
| 4:3:115:ASN:CB  | 4:8:196:ARG:NE[1_554]  | 1.63                     | 0.57              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:318:THR:OG1 | 4:8:149:THR:O[1_554]   | 1.63                     | 0.57              |
| 4:4:211:ASP:O   | 4:8:31:PHE:C[1_554]    | 1.63                     | 0.57              |
| 4:3:287:ILE:O   | 4:9:63:GLY:C[1_554]    | 1.63                     | 0.57              |
| 4:5:162:ASN:ND2 | 4:9:175:ILE:CB[1_554]  | 1.63                     | 0.57              |
| 4:3:223:PHE:C   | 4:7:335:ARG:NE[1_554]  | 1.63                     | 0.57              |
| 4:4:192:ILE:CD1 | 4:8:213:LYS:NZ[1_554]  | 1.63                     | 0.57              |
| 4:2:113:LYS:NZ  | 4:7:217:CYS:CA[1_554]  | 1.63                     | 0.57              |
| 4:4:15:GLY:C    | 4:8:77:THR:C[1_554]    | 1.63                     | 0.57              |
| 4:2:76:ILE:CA   | 4:7:198:TYR:CE1[1_554] | 1.63                     | 0.57              |
| 4:4:336:LYS:C   | 4:8:119:MET:CE[1_554]  | 1.63                     | 0.57              |
| 4:5:11:ASP:OD1  | 4:9:115:ASN:CG[1_554]  | 1.63                     | 0.57              |
| 4:4:166:TYR:CD1 | 4:V:40:HIS:CG[1_554]   | 1.63                     | 0.57              |
| 4:5:32:PRO:CD   | 4:9:81:ASP:CB[1_554]   | 1.63                     | 0.57              |
| 4:4:17:VAL:O    | 4:8:79:TRP:CA[1_554]   | 1.63                     | 0.57              |
| 4:3:332:PRO:C   | 4:7:105:LEU:O[1_554]   | 1.63                     | 0.57              |
| 4:4:220:ALA:CB  | 4:8:335:ARG:CA[1_554]  | 1.63                     | 0.57              |
| 4:3:59:GLN:CG   | 4:7:68:LYS:CD[1_554]   | 1.63                     | 0.57              |
| 4:3:114:ALA:C   | 4:8:250:ILE:O[1_554]   | 1.63                     | 0.57              |
| 4:4:262:PHE:CG  | 4:8:154:ASP:N[1_554]   | 1.63                     | 0.57              |
| 4:5:261:LEU:CG  | 4:9:154:ASP:O[1_554]   | 1.63                     | 0.57              |
| 4:5:267:ILE:CG2 | 4:9:180:LEU:CD1[1_554] | 1.63                     | 0.57              |
| 4:2:108:ALA:CB  | 4:7:195:GLU:CA[1_554]  | 1.63                     | 0.57              |
| 4:3:177:ARG:NH1 | 4:8:194:THR:OG1[1_554] | 1.63                     | 0.57              |
| 4:3:289:ILE:CG2 | 4:9:39:ARG:NE[1_554]   | 1.63                     | 0.57              |
| 4:4:162:ASN:ND2 | 4:8:175:ILE:CB[1_554]  | 1.63                     | 0.57              |
| 4:5:253:GLU:OE2 | 4:9:214:GLU:C[1_554]   | 1.63                     | 0.57              |
| 4:3:276:GLU:OE2 | 4:7:278:THR:O[1_554]   | 1.63                     | 0.57              |
| 4:4:199:SER:O   | 4:8:203:THR:O[1_554]   | 1.63                     | 0.57              |
| 4:3:309:ILE:CA  | 4:7:339:VAL:CG2[1_554] | 1.63                     | 0.57              |
| 4:5:137:GLN:CD  | 4:9:112:PRO:CA[1_554]  | 1.63                     | 0.57              |
| 4:2:291:LYS:CB  | 4:8:64:ILE:CG1[1_554]  | 1.63                     | 0.57              |
| 4:5:27:PRO:N    | 4:9:123:MET:N[1_554]   | 1.63                     | 0.57              |
| 4:3:257:CYS:SG  | 4:7:157:ASP:CA[1_554]  | 1.63                     | 0.57              |
| 4:4:31:PHE:C    | 4:8:78:ASN:ND2[1_554]  | 1.63                     | 0.57              |
| 4:3:215:LYS:CB  | 4:7:31:PHE:C[1_554]    | 1.63                     | 0.57              |
| 4:3:194:THR:C   | 4:7:209:VAL:CA[1_554]  | 1.63                     | 0.57              |
| 4:4:192:ILE:N   | 4:8:186:THR:CB[1_554]  | 1.63                     | 0.57              |
| 4:5:280:ASN:OD1 | 4:9:280:ASN:O[1_554]   | 1.63                     | 0.57              |
| 4:2:372:ARG:CB  | 4:7:227:MET:CA[1_554]  | 1.63                     | 0.57              |
| 4:5:178:LEU:CD2 | 4:9:177:ARG:CA[1_554]  | 1.63                     | 0.57              |
| 4:4:207:GLU:CD  | 4:8:67:LEU:CB[1_554]   | 1.63                     | 0.57              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:201:VAL:CG2 | 4:8:203:THR:CA[1_554]  | 1.63                     | 0.57              |
| 4:2:111:ASN:ND2 | 4:7:196:ARG:CD[1_554]  | 1.63                     | 0.57              |
| 4:5:75:ILE:CA   | 4:V:197:GLY:N[1_554]   | 1.63                     | 0.57              |
| 4:4:266:PHE:CD2 | 4:8:261:LEU:CD1[1_554] | 1.63                     | 0.57              |
| 4:4:213:LYS:C   | 4:8:16:LEU:CA[1_554]   | 1.63                     | 0.57              |
| 4:4:289:ILE:CG2 | 4:V:39:ARG:NH2[1_554]  | 1.63                     | 0.57              |
| 4:3:262:PHE:CB  | 4:7:153:LEU:CG[1_554]  | 1.63                     | 0.57              |
| 4:3:330:ILE:CG2 | 4:7:133:TYR:OH[1_554]  | 1.63                     | 0.57              |
| 4:4:191:LYS:CE  | 4:8:185:LEU:CA[1_554]  | 1.63                     | 0.57              |
| 4:5:335:ARG:CA  | 4:9:105:LEU:C[1_554]   | 1.63                     | 0.57              |
| 4:5:300:SER:O   | 4:9:107:GLU:O[1_554]   | 1.63                     | 0.57              |
| 4:5:276:GLU:N   | 4:9:151:ILE:CD1[1_554] | 1.63                     | 0.57              |
| 4:3:196:ARG:NE  | 4:7:211:ASP:OD2[1_554] | 1.63                     | 0.57              |
| 4:3:370:VAL:C   | 4:8:230:ALA:CB[1_554]  | 1.63                     | 0.57              |
| 4:5:340:TRP:CH2 | 4:9:121:GLN:O[1_554]   | 1.63                     | 0.57              |
| 4:5:30:VAL:CG1  | 4:9:82:MET:CA[1_554]   | 1.63                     | 0.57              |
| 4:4:291:LYS:CE  | 4:V:64:ILE:CG1[1_554]  | 1.63                     | 0.57              |
| 4:3:108:ALA:CA  | 4:8:195:GLU:C[1_554]   | 1.63                     | 0.57              |
| 4:5:207:GLU:OE2 | 4:9:67:LEU:CB[1_554]   | 1.63                     | 0.57              |
| 4:4:218:TYR:CB  | 4:8:336:LYS:CB[1_554]  | 1.63                     | 0.57              |
| 4:4:115:ASN:N   | 4:9:196:ARG:NH2[1_554] | 1.63                     | 0.57              |
| 4:2:110:LEU:CB  | 4:7:192:ILE:CA[1_554]  | 1.63                     | 0.57              |
| 4:5:196:ARG:CD  | 4:9:212:ILE:N[1_554]   | 1.63                     | 0.57              |
| 4:3:223:PHE:CA  | 4:7:335:ARG:CZ[1_554]  | 1.63                     | 0.57              |
| 4:5:112:PRO:CA  | 4:V:253:GLU:CD[1_554]  | 1.63                     | 0.57              |
| 4:4:153:LEU:CG  | 4:8:109:PRO:CB[1_554]  | 1.63                     | 0.57              |
| 4:5:369:ILE:C   | 4:V:228:ALA:O[1_554]   | 1.63                     | 0.57              |
| 4:3:112:PRO:C   | 4:8:253:GLU:CG[1_554]  | 1.63                     | 0.57              |
| 4:5:280:ASN:CG  | 4:9:281:SER:C[1_554]   | 1.63                     | 0.57              |
| 4:5:205:GLU:OE2 | 4:7:288:ASP:CG[1_554]  | 1.63                     | 0.57              |
| 4:4:339:VAL:N   | 4:8:116:ARG:C[1_554]   | 1.63                     | 0.57              |
| 4:4:311:ASP:N   | 4:8:140:LEU:O[1_554]   | 1.63                     | 0.57              |
| 4:3:300:SER:C   | 4:7:107:GLU:CB[1_554]  | 1.63                     | 0.57              |
| 4:5:348:SER:O   | 4:9:364:GLU:C[1_554]   | 1.64                     | 0.56              |
| 4:5:277:THR:N   | 4:9:281:SER:CB[1_554]  | 1.64                     | 0.56              |
| 4:4:210:ARG:CD  | 4:8:69:TYR:CD2[1_554]  | 1.64                     | 0.56              |
| 4:4:173:HIS:NE2 | 4:9:265:SER:CA[1_554]  | 1.64                     | 0.56              |
| 4:5:188:TYR:C   | 4:9:182:GLY:C[1_554]   | 1.64                     | 0.56              |
| 4:5:317:ILE:CA  | 4:9:151:ILE:N[1_554]   | 1.64                     | 0.56              |
| 4:3:260:THR:CG2 | 4:7:180:LEU:O[1_554]   | 1.64                     | 0.56              |
| 4:5:26:ALA:O    | 4:9:123:MET:CA[1_554]  | 1.64                     | 0.56              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:372:ARG:NE  | 4:7:227:MET:C[1_554]   | 1.64                     | 0.56              |
| 4:5:371:HIS:CA  | 4:V:230:ALA:CB[1_554]  | 1.64                     | 0.56              |
| 4:5:340:TRP:NE1 | 4:9:118:LYS:C[1_554]   | 1.64                     | 0.56              |
| 4:3:162:ASN:N   | 4:7:110:LEU:CG[1_554]  | 1.64                     | 0.56              |
| 4:5:370:VAL:N   | 4:V:231:ALA:CB[1_554]  | 1.64                     | 0.56              |
| 4:5:283:MET:CA  | 4:9:285:CYS:C[1_554]   | 1.64                     | 0.56              |
| 4:5:157:ASP:O   | 4:9:72:GLU:C[1_554]    | 1.64                     | 0.56              |
| 4:3:161:HIS:O   | 4:7:110:LEU:CB[1_554]  | 1.64                     | 0.56              |
| 4:3:143:TYR:CD2 | 4:7:368:SER:O[1_554]   | 1.64                     | 0.56              |
| 4:5:196:ARG:CD  | 4:9:212:ILE:CA[1_554]  | 1.64                     | 0.56              |
| 4:2:292:ASP:OD2 | 4:8:40:HIS:N[1_554]    | 1.64                     | 0.56              |
| 4:4:211:ASP:OD2 | 4:8:55:GLY:CA[1_554]   | 1.64                     | 0.56              |
| 4:4:154:ASP:O   | 4:8:110:LEU:N[1_554]   | 1.64                     | 0.56              |
| 4:4:322:PRO:CA  | 4:8:292:ASP:OD2[1_554] | 1.64                     | 0.56              |
| 4:3:16:LEU:CG   | 4:7:78:ASN:N[1_554]    | 1.64                     | 0.56              |
| 4:3:372:ARG:CA  | 4:8:226:GLU:C[1_554]   | 1.64                     | 0.56              |
| 4:3:79:TRP:CD1  | 4:8:247:VAL:O[1_554]   | 1.64                     | 0.56              |
| 4:5:151:ILE:CB  | 4:9:170:ALA:C[1_554]   | 1.64                     | 0.56              |
| 4:5:278:THR:CA  | 4:9:164:PRO:CG[1_554]  | 1.64                     | 0.56              |
| 4:3:192:ILE:CA  | 4:7:213:LYS:CD[1_554]  | 1.64                     | 0.56              |
| 4:3:322:PRO:N   | 4:7:292:ASP:OD2[1_554] | 1.64                     | 0.56              |
| 4:3:243:PRO:CG  | 4:7:61:LYS:N[1_554]    | 1.64                     | 0.56              |
| 4:4:262:PHE:CD1 | 4:8:154:ASP:N[1_554]   | 1.64                     | 0.56              |
| 4:4:211:ASP:OD2 | 4:8:32:PRO:O[1_554]    | 1.64                     | 0.56              |
| 4:5:140:LEU:CA  | 4:9:371:HIS:CG[1_554]  | 1.64                     | 0.56              |
| 4:3:153:LEU:CG  | 4:7:109:PRO:CG[1_554]  | 1.64                     | 0.56              |
| 4:5:24:ASP:OD2  | 4:9:125:GLU:N[1_554]   | 1.64                     | 0.56              |
| 4:4:223:PHE:CB  | 4:8:335:ARG:NE[1_554]  | 1.64                     | 0.56              |
| 4:3:15:GLY:C    | 4:7:77:THR:CB[1_554]   | 1.64                     | 0.56              |
| 4:4:274:ILE:CD1 | 4:8:161:HIS:CD2[1_554] | 1.64                     | 0.56              |
| 4:5:329:ILE:CG1 | 4:9:142:LEU:CD2[1_554] | 1.64                     | 0.56              |
| 4:4:274:ILE:CA  | 4:8:162:ASN:CA[1_554]  | 1.64                     | 0.56              |
| 4:3:199:SER:C   | 4:7:206:ARG:CG[1_554]  | 1.64                     | 0.56              |
| 4:5:249:THR:C   | 4:9:211:ASP:CG[1_554]  | 1.64                     | 0.56              |
| 4:4:144:ALA:CA  | 4:8:371:HIS:N[1_554]   | 1.64                     | 0.56              |
| 4:2:369:ILE:CA  | 4:7:234:SER:OG[1_554]  | 1.64                     | 0.56              |
| 4:4:294:TYR:CD2 | 4:8:166:TYR:CD2[1_554] | 1.64                     | 0.56              |
| 4:2:112:PRO:C   | 4:7:250:ILE:CG2[1_554] | 1.64                     | 0.56              |
| 4:4:173:HIS:CB  | 4:9:267:ILE:CA[1_554]  | 1.64                     | 0.56              |
| 4:4:18:LYS:C    | 4:8:118:LYS:NZ[1_554]  | 1.64                     | 0.56              |
| 4:3:169:TYR:CZ  | 4:8:266:PHE:CE1[1_554] | 1.64                     | 0.56              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:188:TYR:N   | 4:8:183:ARG:CB[1_554]  | 1.64                     | 0.56              |
| 4:4:195:GLU:N   | 4:8:209:VAL:CG2[1_554] | 1.64                     | 0.56              |
| 4:5:200:PHE:CZ  | 4:9:207:GLU:O[1_554]   | 1.64                     | 0.56              |
| 4:3:75:ILE:CB   | 4:8:198:TYR:CG[1_554]  | 1.64                     | 0.56              |
| 4:4:155:SER:CA  | 4:8:108:ALA:CB[1_554]  | 1.64                     | 0.56              |
| 4:4:243:PRO:CD  | 4:8:60:SER:N[1_554]    | 1.64                     | 0.56              |
| 4:4:205:GLU:OE2 | 4:8:203:THR:CG2[1_554] | 1.64                     | 0.56              |
| 4:5:299:MET:CE  | 4:9:139:VAL:N[1_554]   | 1.64                     | 0.56              |
| 4:5:188:TYR:O   | 4:9:182:GLY:O[1_554]   | 1.64                     | 0.56              |
| 4:3:220:ALA:CB  | 4:7:335:ARG:C[1_554]   | 1.64                     | 0.56              |
| 4:3:315:LYS:NZ  | 4:7:296:ASN:OD1[1_554] | 1.64                     | 0.56              |
| 4:4:299:MET:CG  | 4:8:137:GLN:N[1_554]   | 1.64                     | 0.56              |
| 4:5:274:ILE:N   | 4:9:162:ASN:CG[1_554]  | 1.64                     | 0.56              |
| 4:4:219:VAL:CG1 | 4:8:300:SER:C[1_554]   | 1.64                     | 0.56              |
| 4:2:73:HIS:CG   | 4:7:199:SER:OG[1_554]  | 1.64                     | 0.56              |
| 4:5:346:LEU:CD2 | 4:9:368:SER:CB[1_554]  | 1.64                     | 0.56              |
| 4:4:219:VAL:CA  | 4:8:335:ARG:O[1_554]   | 1.64                     | 0.56              |
| 4:4:314:GLN:N   | 4:8:142:LEU:CA[1_554]  | 1.64                     | 0.56              |
| 4:4:185:LEU:O   | 4:8:157:ASP:C[1_554]   | 1.64                     | 0.56              |
| 4:4:182:GLY:N   | 4:8:73:HIS:C[1_554]    | 1.64                     | 0.56              |
| 4:4:312:ARG:CG  | 4:8:299:MET:C[1_554]   | 1.64                     | 0.56              |
| 4:3:369:ILE:O   | 4:8:230:ALA:N[1_554]   | 1.64                     | 0.56              |
| 4:5:156:GLY:C   | 4:9:74:GLY:N[1_554]    | 1.64                     | 0.56              |
| 4:4:277:THR:CB  | 4:8:175:ILE:C[1_554]   | 1.64                     | 0.56              |
| 4:5:289:ILE:N   | 4:W:64:ILE:N[1_554]    | 1.64                     | 0.56              |
| 4:5:300:SER:C   | 4:9:108:ALA:N[1_554]   | 1.64                     | 0.56              |
| 4:3:270:GLU:CA  | 4:7:272:ALA:N[1_554]   | 1.64                     | 0.56              |
| 4:4:280:ASN:OD1 | 4:8:281:SER:C[1_554]   | 1.64                     | 0.56              |
| 4:4:18:LYS:CB   | 4:8:79:TRP:CD2[1_554]  | 1.64                     | 0.56              |
| 4:5:205:GLU:CA  | 4:9:62:ARG:NH2[1_554]  | 1.64                     | 0.56              |
| 4:4:21:PHE:C    | 4:8:125:GLU:OE1[1_554] | 1.65                     | 0.55              |
| 4:3:161:HIS:CA  | 4:7:110:LEU:CB[1_554]  | 1.65                     | 0.55              |
| 4:4:277:THR:O   | 4:8:174:ALA:CA[1_554]  | 1.65                     | 0.55              |
| 4:5:278:THR:CB  | 4:9:164:PRO:CA[1_554]  | 1.65                     | 0.55              |
| 4:5:301:GLY:N   | 4:9:108:ALA:N[1_554]   | 1.65                     | 0.55              |
| 4:2:173:HIS:NE2 | 4:7:264:PRO:O[1_554]   | 1.65                     | 0.55              |
| 4:4:191:LYS:C   | 4:8:186:THR:C[1_554]   | 1.65                     | 0.55              |
| 4:3:367:PRO:CD  | 4:8:235:SER:N[1_554]   | 1.65                     | 0.55              |
| 4:3:136:ILE:N   | 4:7:113:LYS:NZ[1_554]  | 1.65                     | 0.55              |
| 4:3:17:VAL:O    | 4:7:79:TRP:CB[1_554]   | 1.65                     | 0.55              |
| 4:5:187:ASP:CA  | 4:9:183:ARG:CG[1_554]  | 1.65                     | 0.55              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:299:MET:C   | 4:9:136:ILE:N[1_554]   | 1.65                     | 0.55              |
| 4:5:321:ALA:CA  | 4:9:289:ILE:O[1_554]   | 1.65                     | 0.55              |
| 4:3:255:PHE:CZ  | 4:7:305:MET:CE[1_554]  | 1.65                     | 0.55              |
| 4:4:259:GLU:CD  | 4:8:304:THR:O[1_554]   | 1.65                     | 0.55              |
| 4:3:299:MET:CG  | 4:7:136:ILE:CA[1_554]  | 1.65                     | 0.55              |
| 4:5:336:LYS:CE  | 4:9:10:CYS:SG[1_554]   | 1.65                     | 0.55              |
| 4:4:255:PHE:O   | 4:8:301:GLY:O[1_554]   | 1.65                     | 0.55              |
| 4:5:368:SER:CA  | 4:V:229:THR:O[1_554]   | 1.65                     | 0.55              |
| 4:4:282:ILE:CD1 | 4:8:171:LEU:CD1[1_554] | 1.65                     | 0.55              |
| 4:5:345:ILE:CG2 | 4:9:369:ILE:CG2[1_554] | 1.65                     | 0.55              |
| 4:5:340:TRP:CD2 | 4:9:120:THR:N[1_554]   | 1.65                     | 0.55              |
| 4:5:254:ARG:NH1 | 4:9:336:LYS:NZ[1_554]  | 1.65                     | 0.55              |
| 4:3:268:GLY:CA  | 4:7:264:PRO:CB[1_554]  | 1.65                     | 0.55              |
| 4:5:155:SER:N   | 4:9:108:ALA:C[1_554]   | 1.65                     | 0.55              |
| 4:5:186:THR:CB  | 4:9:183:ARG:CZ[1_554]  | 1.65                     | 0.55              |
| 4:2:117:GLU:N   | 4:7:251:GLY:CA[1_554]  | 1.65                     | 0.55              |
| 4:3:141:SER:N   | 4:7:371:HIS:CE1[1_554] | 1.65                     | 0.55              |
| 4:5:317:ILE:N   | 4:9:150:GLY:C[1_554]   | 1.65                     | 0.55              |
| 4:3:327:ILE:CG1 | 4:7:148:THR:O[1_554]   | 1.65                     | 0.55              |
| 4:5:178:LEU:CD1 | 4:9:177:ARG:O[1_554]   | 1.65                     | 0.55              |
| 4:2:367:PRO:CA  | 4:7:235:SER:CA[1_554]  | 1.65                     | 0.55              |
| 4:3:332:PRO:CG  | 4:7:134:VAL:O[1_554]   | 1.65                     | 0.55              |
| 4:4:108:ALA:CB  | 4:9:195:GLU:CA[1_554]  | 1.65                     | 0.55              |
| 4:3:273:GLY:C   | 4:7:162:ASN:CG[1_554]  | 1.65                     | 0.55              |
| 4:3:334:GLU:CA  | 4:7:105:LEU:CG[1_554]  | 1.65                     | 0.55              |
| 4:5:340:TRP:CH2 | 4:9:122:ILE:N[1_554]   | 1.65                     | 0.55              |
| 4:3:357:ILE:CG1 | 4:8:232:SER:CA[1_554]  | 1.65                     | 0.55              |
| 4:5:204:ALA:C   | 4:9:62:ARG:NE[1_554]   | 1.65                     | 0.55              |
| 4:4:156:GLY:O   | 4:8:75:ILE:N[1_554]    | 1.65                     | 0.55              |
| 4:5:180:LEU:C   | 4:9:159:VAL:CG1[1_554] | 1.65                     | 0.55              |
| 4:5:19:ALA:CA   | 4:9:118:LYS:NZ[1_554]  | 1.65                     | 0.55              |
| 4:2:285:CYS:C   | 4:7:270:GLU:OE2[1_554] | 1.65                     | 0.55              |
| 4:3:277:THR:OG1 | 4:7:176:MET:N[1_554]   | 1.65                     | 0.55              |
| 4:4:180:LEU:C   | 4:8:159:VAL:CG1[1_554] | 1.65                     | 0.55              |
| 4:3:214:GLU:OE1 | 4:7:33:SER:OG[1_554]   | 1.65                     | 0.55              |
| 4:2:284:LYS:CA  | 4:7:268:GLY:O[1_554]   | 1.65                     | 0.55              |
| 4:4:214:GLU:O   | 4:8:16:LEU:C[1_554]    | 1.65                     | 0.55              |
| 4:3:262:PHE:CD2 | 4:7:154:ASP:CA[1_554]  | 1.65                     | 0.55              |
| 4:3:142:LEU:C   | 4:7:372:ARG:CA[1_554]  | 1.65                     | 0.55              |
| 4:4:75:ILE:CB   | 4:9:198:TYR:N[1_554]   | 1.65                     | 0.55              |
| 4:5:157:ASP:CB  | 4:9:72:GLU:O[1_554]    | 1.65                     | 0.55              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:327:ILE:CG2 | 4:9:149:THR:CA[1_554]  | 1.65                     | 0.55              |
| 4:2:369:ILE:CG2 | 4:7:234:SER:OG[1_554]  | 1.65                     | 0.55              |
| 4:5:370:VAL:CB  | 4:V:231:ALA:CA[1_554]  | 1.65                     | 0.55              |
| 4:4:27:PRO:N    | 4:8:122:ILE:N[1_554]   | 1.65                     | 0.55              |
| 4:3:197:GLY:N   | 4:7:208:ILE:O[1_554]   | 1.65                     | 0.55              |
| 4:4:222:ASP:C   | 4:8:331:ALA:O[1_554]   | 1.65                     | 0.55              |
| 4:4:281:SER:CB  | 4:8:173:HIS:N[1_554]   | 1.65                     | 0.55              |
| 4:4:325:MET:SD  | 4:8:166:TYR:CZ[1_554]  | 1.65                     | 0.55              |
| 4:3:185:LEU:CA  | 4:7:157:ASP:O[1_554]   | 1.65                     | 0.55              |
| 4:3:260:THR:C   | 4:7:155:SER:OG[1_554]  | 1.65                     | 0.55              |
| 4:5:14:SER:O    | 4:9:77:THR:CG2[1_554]  | 1.65                     | 0.55              |
| 4:4:41:GLN:CD   | 4:7:224:GLU:OE2[1_554] | 1.65                     | 0.55              |
| 4:5:299:MET:SD  | 4:9:138:ALA:CA[1_554]  | 1.65                     | 0.55              |
| 4:5:278:THR:CB  | 4:9:163:VAL:C[1_554]   | 1.65                     | 0.55              |
| 4:5:198:TYR:CE2 | 4:9:208:ILE:O[1_554]   | 1.65                     | 0.55              |
| 4:4:223:PHE:N   | 4:8:331:ALA:CB[1_554]  | 1.65                     | 0.55              |
| 4:5:255:PHE:CD1 | 4:9:305:MET:CB[1_554]  | 1.65                     | 0.55              |
| 4:5:274:ILE:N   | 4:9:162:ASN:OD1[1_554] | 1.65                     | 0.55              |
| 4:5:208:ILE:CA  | 4:9:59:GLN:CD[1_554]   | 1.65                     | 0.55              |
| 4:5:211:ASP:OD1 | 4:9:32:PRO:N[1_554]    | 1.65                     | 0.55              |
| 4:5:185:LEU:CA  | 4:9:157:ASP:C[1_554]   | 1.65                     | 0.55              |
| 4:3:340:TRP:CH2 | 4:7:121:GLN:CB[1_554]  | 1.65                     | 0.55              |
| 4:3:142:LEU:C   | 4:7:372:ARG:N[1_554]   | 1.65                     | 0.55              |
| 4:3:331:ALA:O   | 4:7:135:ALA:CB[1_554]  | 1.65                     | 0.55              |
| 4:4:144:ALA:CB  | 4:8:370:VAL:C[1_554]   | 1.65                     | 0.55              |
| 4:5:106:THR:OG1 | 4:9:114:ALA:CB[1_554]  | 1.65                     | 0.55              |
| 4:4:342:GLY:C   | 4:8:367:PRO:O[1_554]   | 1.65                     | 0.55              |
| 4:4:255:PHE:CB  | 4:8:305:MET:CG[1_554]  | 1.66                     | 0.54              |
| 4:3:160:THR:CG2 | 4:7:161:HIS:NE2[1_554] | 1.66                     | 0.54              |
| 4:3:332:PRO:N   | 4:7:134:VAL:C[1_554]   | 1.66                     | 0.54              |
| 4:4:321:ALA:O   | 4:8:292:ASP:OD2[1_554] | 1.66                     | 0.54              |
| 4:3:181:ALA:CB  | 4:7:73:HIS:CB[1_554]   | 1.66                     | 0.54              |
| 4:3:253:GLU:OE1 | 4:7:214:GLU:N[1_554]   | 1.66                     | 0.54              |
| 4:4:31:PHE:CA   | 4:8:78:ASN:OD1[1_554]  | 1.66                     | 0.54              |
| 4:5:274:ILE:N   | 4:9:162:ASN:CA[1_554]  | 1.66                     | 0.54              |
| 4:4:299:MET:N   | 4:8:136:ILE:CB[1_554]  | 1.66                     | 0.54              |
| 4:4:111:ASN:ND2 | 4:9:196:ARG:CG[1_554]  | 1.66                     | 0.54              |
| 4:5:137:GLN:OE1 | 4:9:112:PRO:CG[1_554]  | 1.66                     | 0.54              |
| 4:5:337:TYR:CD1 | 4:9:86:TRP:CZ2[1_554]  | 1.66                     | 0.54              |
| 4:4:223:PHE:CD1 | 4:8:304:THR:OG1[1_554] | 1.66                     | 0.54              |
| 4:5:214:GLU:N   | 4:9:16:LEU:N[1_554]    | 1.66                     | 0.54              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:256:ARG:CB  | 4:9:306:TYR:CZ[1_554]  | 1.66                     | 0.54              |
| 4:5:340:TRP:N   | 4:9:116:ARG:C[1_554]   | 1.66                     | 0.54              |
| 4:2:113:LYS:O   | 4:7:251:GLY:CA[1_554]  | 1.66                     | 0.54              |
| 4:4:327:ILE:CB  | 4:8:149:THR:N[1_554]   | 1.66                     | 0.54              |
| 4:4:297:ASN:OD1 | 4:8:170:ALA:N[1_554]   | 1.66                     | 0.54              |
| 4:3:143:TYR:N   | 4:7:371:HIS:O[1_554]   | 1.66                     | 0.54              |
| 4:5:320:LEU:N   | 4:9:293:LEU:CA[1_554]  | 1.66                     | 0.54              |
| 4:3:309:ILE:N   | 4:7:339:VAL:CG2[1_554] | 1.66                     | 0.54              |
| 4:4:304:THR:CB  | 4:8:137:GLN:CG[1_554]  | 1.66                     | 0.54              |
| 4:2:114:ALA:C   | 4:7:250:ILE:C[1_554]   | 1.66                     | 0.54              |
| 4:3:345:ILE:O   | 4:7:366:GLY:CA[1_554]  | 1.66                     | 0.54              |
| 4:4:156:GLY:O   | 4:8:74:GLY:CA[1_554]   | 1.66                     | 0.54              |
| 4:3:156:GLY:N   | 4:7:75:ILE:CD1[1_554]  | 1.66                     | 0.54              |
| 4:4:325:MET:C   | 4:8:167:GLU:OE2[1_554] | 1.66                     | 0.54              |
| 4:3:213:LYS:CB  | 4:7:15:GLY:C[1_554]    | 1.66                     | 0.54              |
| 4:4:341:ILE:CD1 | 4:8:132:MET:CE[1_554]  | 1.66                     | 0.54              |
| 4:5:16:LEU:CB   | 4:9:76:ILE:CG2[1_554]  | 1.66                     | 0.54              |
| 4:3:139:VAL:CA  | 4:7:113:LYS:CD[1_554]  | 1.66                     | 0.54              |
| 4:4:74:GLY:O    | 4:9:197:GLY:N[1_554]   | 1.66                     | 0.54              |
| 4:4:260:THR:CG2 | 4:8:180:LEU:O[1_554]   | 1.66                     | 0.54              |
| 4:3:325:MET:O   | 4:7:167:GLU:CD[1_554]  | 1.66                     | 0.54              |
| 4:4:220:ALA:O   | 4:8:299:MET:O[1_554]   | 1.66                     | 0.54              |
| 4:4:259:GLU:CB  | 4:8:304:THR:CG2[1_554] | 1.66                     | 0.54              |
| 4:5:340:TRP:CE3 | 4:9:120:THR:N[1_554]   | 1.66                     | 0.54              |
| 4:4:180:LEU:CG  | 4:8:178:LEU:C[1_554]   | 1.66                     | 0.54              |
| 4:5:372:ARG:O   | 4:V:227:MET:SD[1_554]  | 1.66                     | 0.54              |
| 4:5:334:GLU:OE1 | 4:9:133:TYR:CA[1_554]  | 1.66                     | 0.54              |
| 4:4:243:PRO:C   | 4:8:60:SER:CB[1_554]   | 1.66                     | 0.54              |
| 4:3:198:TYR:C   | 4:7:206:ARG:O[1_554]   | 1.66                     | 0.54              |
| 4:5:198:TYR:CB  | 4:9:208:ILE:C[1_554]   | 1.66                     | 0.54              |
| 4:4:110:LEU:C   | 4:9:192:ILE:CB[1_554]  | 1.66                     | 0.54              |
| 4:3:326:LYS:CE  | 4:9:45:VAL:CA[1_554]   | 1.66                     | 0.54              |
| 4:5:227:MET:CA  | 4:9:307:PRO:CG[1_554]  | 1.66                     | 0.54              |
| 4:5:190:MET:CE  | 4:9:206:ARG:NH2[1_554] | 1.66                     | 0.54              |
| 4:4:294:TYR:CE1 | 4:8:166:TYR:CB[1_554]  | 1.66                     | 0.54              |
| 4:3:282:ILE:CG2 | 4:7:171:LEU:CD2[1_554] | 1.66                     | 0.54              |
| 4:3:262:PHE:CD2 | 4:7:153:LEU:C[1_554]   | 1.66                     | 0.54              |
| 4:5:345:ILE:CG1 | 4:9:357:ILE:CG2[1_554] | 1.66                     | 0.54              |
| 4:5:188:TYR:CD1 | 4:9:185:LEU:CG[1_554]  | 1.66                     | 0.54              |
| 4:4:196:ARG:CA  | 4:8:212:ILE:CA[1_554]  | 1.66                     | 0.54              |
| 4:3:220:ALA:CA  | 4:7:335:ARG:CB[1_554]  | 1.66                     | 0.54              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:73:HIS:CD2  | 4:9:199:SER:OG[1_554]  | 1.66                     | 0.54              |
| 4:3:215:LYS:N   | 4:7:17:VAL:N[1_554]    | 1.66                     | 0.54              |
| 4:3:27:PRO:N    | 4:7:122:ILE:CA[1_554]  | 1.66                     | 0.54              |
| 4:5:319:ALA:CA  | 4:9:295:ALA:N[1_554]   | 1.66                     | 0.54              |
| 4:5:31:PHE:CB   | 4:9:80:ASP:C[1_554]    | 1.66                     | 0.54              |
| 4:5:190:MET:CG  | 4:9:206:ARG:NH2[1_554] | 1.66                     | 0.54              |
| 4:2:77:THR:CG2  | 4:7:246:GLN:CD[1_554]  | 1.66                     | 0.54              |
| 4:5:322:PRO:CD  | 4:9:289:ILE:CA[1_554]  | 1.66                     | 0.54              |
| 4:3:180:LEU:CD2 | 4:7:178:LEU:CA[1_554]  | 1.66                     | 0.54              |
| 4:4:198:TYR:CG  | 4:8:207:GLU:C[1_554]   | 1.66                     | 0.54              |
| 4:3:190:MET:CG  | 4:7:206:ARG:NH2[1_554] | 1.66                     | 0.54              |
| 4:4:256:ARG:C   | 4:8:303:THR:N[1_554]   | 1.66                     | 0.54              |
| 4:3:188:TYR:CA  | 4:7:183:ARG:N[1_554]   | 1.66                     | 0.54              |
| 4:3:321:ALA:C   | 4:7:292:ASP:OD2[1_554] | 1.66                     | 0.54              |
| 4:3:109:PRO:CA  | 4:8:195:GLU:OE2[1_554] | 1.66                     | 0.54              |
| 4:5:140:LEU:CD2 | 4:9:371:HIS:CB[1_554]  | 1.66                     | 0.54              |
| 4:4:320:LEU:N   | 4:8:292:ASP:C[1_554]   | 1.66                     | 0.54              |
| 4:5:313:MET:SD  | 4:9:152:VAL:CA[1_554]  | 1.66                     | 0.54              |
| 4:3:219:VAL:CG1 | 4:7:300:SER:OG[1_554]  | 1.66                     | 0.54              |
| 4:2:289:ILE:N   | 4:8:39:ARG:CZ[1_554]   | 1.66                     | 0.54              |
| 4:4:372:ARG:C   | 4:9:227:MET:CA[1_554]  | 1.66                     | 0.54              |
| 4:5:214:GLU:OE2 | 4:9:33:SER:CB[1_554]   | 1.66                     | 0.54              |
| 4:4:256:ARG:CA  | 4:8:303:THR:CA[1_554]  | 1.66                     | 0.54              |
| 4:4:317:ILE:N   | 4:8:150:GLY:CA[1_554]  | 1.66                     | 0.54              |
| 4:5:335:ARG:C   | 4:9:106:THR:CA[1_554]  | 1.66                     | 0.54              |
| 4:3:193:LEU:C   | 4:7:210:ARG:CB[1_554]  | 1.66                     | 0.54              |
| 4:5:288:ASP:C   | 4:W:63:GLY:CA[1_554]   | 1.66                     | 0.54              |
| 4:3:316:GLU:CB  | 4:7:151:ILE:C[1_554]   | 1.66                     | 0.54              |
| 4:4:243:PRO:CB  | 4:8:60:SER:CA[1_554]   | 1.66                     | 0.54              |
| 4:5:294:TYR:N   | 4:9:166:TYR:O[1_554]   | 1.66                     | 0.54              |
| 4:4:110:LEU:CD1 | 4:9:191:LYS:CD[1_554]  | 1.66                     | 0.54              |
| 4:4:316:GLU:C   | 4:8:150:GLY:C[1_554]   | 1.66                     | 0.54              |
| 4:3:117:GLU:CB  | 4:8:237:GLU:CB[1_554]  | 1.67                     | 0.53              |
| 4:3:335:ARG:CD  | 4:7:107:GLU:N[1_554]   | 1.67                     | 0.53              |
| 4:3:320:LEU:N   | 4:7:293:LEU:CA[1_554]  | 1.67                     | 0.53              |
| 4:3:188:TYR:CA  | 4:7:183:ARG:CA[1_554]  | 1.67                     | 0.53              |
| 4:3:243:PRO:CA  | 4:7:60:SER:OG[1_554]   | 1.67                     | 0.53              |
| 4:3:283:MET:CG  | 4:7:285:CYS:C[1_554]   | 1.67                     | 0.53              |
| 4:2:113:LYS:O   | 4:7:251:GLY:C[1_554]   | 1.67                     | 0.53              |
| 4:3:278:THR:OG1 | 4:7:163:VAL:CG1[1_554] | 1.67                     | 0.53              |
| 4:3:16:LEU:CD1  | 4:7:78:ASN:O[1_554]    | 1.67                     | 0.53              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:321:ALA:N   | 4:9:292:ASP:C[1_554]   | 1.67                     | 0.53              |
| 4:3:180:LEU:CB  | 4:7:178:LEU:C[1_554]   | 1.67                     | 0.53              |
| 4:5:341:ILE:O   | 4:9:120:THR:CG2[1_554] | 1.67                     | 0.53              |
| 4:5:281:SER:OG  | 4:9:173:HIS:CA[1_554]  | 1.67                     | 0.53              |
| 4:3:337:TYR:N   | 4:7:119:MET:CG[1_554]  | 1.67                     | 0.53              |
| 4:5:173:HIS:CD2 | 4:V:268:GLY:N[1_554]   | 1.67                     | 0.53              |
| 4:3:255:PHE:CD2 | 4:7:305:MET:SD[1_554]  | 1.67                     | 0.53              |
| 4:5:270:GLU:CB  | 4:9:272:ALA:CA[1_554]  | 1.67                     | 0.53              |
| 4:5:297:ASN:O   | 4:9:139:VAL:CG1[1_554] | 1.67                     | 0.53              |
| 4:3:137:GLN:CA  | 4:7:113:LYS:N[1_554]   | 1.67                     | 0.53              |
| 4:5:294:TYR:CB  | 4:9:166:TYR:CA[1_554]  | 1.67                     | 0.53              |
| 4:3:110:LEU:C   | 4:8:192:ILE:CB[1_554]  | 1.67                     | 0.53              |
| 4:5:274:ILE:C   | 4:9:163:VAL:N[1_554]   | 1.67                     | 0.53              |
| 4:4:337:TYR:CZ  | 4:8:86:TRP:CE3[1_554]  | 1.67                     | 0.53              |
| 4:4:117:GLU:O   | 4:9:237:GLU:CG[1_554]  | 1.67                     | 0.53              |
| 4:4:357:ILE:CG1 | 4:9:231:ALA:C[1_554]   | 1.67                     | 0.53              |
| 1:D:637:LYS:NZ  | 4:5:311:ASP:N[1_556]   | 1.67                     | 0.53              |
| 4:3:240:TYR:CE2 | 4:7:56:ASP:OD2[1_554]  | 1.67                     | 0.53              |
| 4:5:166:TYR:C   | 4:W:40:HIS:CD2[1_554]  | 1.67                     | 0.53              |
| 4:5:189:LEU:O   | 4:9:186:THR:CB[1_554]  | 1.67                     | 0.53              |
| 4:5:155:SER:OG  | 4:9:161:HIS:CE1[1_554] | 1.67                     | 0.53              |
| 4:5:200:PHE:N   | 4:9:206:ARG:CA[1_554]  | 1.67                     | 0.53              |
| 4:2:115:ASN:CA  | 4:7:249:THR:O[1_554]   | 1.67                     | 0.53              |
| 4:5:322:PRO:CG  | 4:9:288:ASP:C[1_554]   | 1.67                     | 0.53              |
| 4:4:157:ASP:OD2 | 4:8:72:GLU:CG[1_554]   | 1.67                     | 0.53              |
| 4:4:158:GLY:C   | 4:8:177:ARG:NH2[1_554] | 1.67                     | 0.53              |
| 4:3:333:PRO:C   | 4:7:105:LEU:CG[1_554]  | 1.67                     | 0.53              |
| 4:5:154:ASP:CG  | 4:9:111:ASN:CB[1_554]  | 1.67                     | 0.53              |
| 4:4:213:LYS:NZ  | 4:8:14:SER:O[1_554]    | 1.67                     | 0.53              |
| 4:4:288:ASP:CG  | 4:V:65:LEU:O[1_554]    | 1.67                     | 0.53              |
| 4:5:56:ASP:CA   | 4:9:37:ARG:NH1[1_554]  | 1.67                     | 0.53              |
| 4:3:372:ARG:N   | 4:8:226:GLU:O[1_554]   | 1.67                     | 0.53              |
| 4:5:162:ASN:OD1 | 4:9:175:ILE:CA[1_554]  | 1.67                     | 0.53              |
| 4:4:260:THR:O   | 4:8:160:THR:CB[1_554]  | 1.67                     | 0.53              |
| 4:3:312:ARG:CD  | 4:7:299:MET:C[1_554]   | 1.67                     | 0.53              |
| 4:3:182:GLY:CA  | 4:7:14:SER:OG[1_554]   | 1.67                     | 0.53              |
| 4:3:308:GLY:CA  | 4:7:338:SER:O[1_554]   | 1.67                     | 0.53              |
| 4:3:218:TYR:CZ  | 4:7:337:TYR:CE1[1_554] | 1.67                     | 0.53              |
| 4:3:314:GLN:CD  | 4:7:147:ARG:O[1_554]   | 1.67                     | 0.53              |
| 4:5:249:THR:N   | 4:9:211:ASP:OD2[1_554] | 1.67                     | 0.53              |
| 4:2:372:ARG:CA  | 4:7:226:GLU:C[1_554]   | 1.67                     | 0.53              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:283:MET:CG  | 4:9:285:CYS:C[1_554]   | 1.67                     | 0.53              |
| 4:3:243:PRO:N   | 4:7:60:SER:C[1_554]    | 1.67                     | 0.53              |
| 4:5:204:ALA:CB  | 4:9:62:ARG:CA[1_554]   | 1.67                     | 0.53              |
| 4:5:280:ASN:CB  | 4:9:284:LYS:CB[1_554]  | 1.67                     | 0.53              |
| 4:5:297:ASN:OD1 | 4:9:165:ILE:CG1[1_554] | 1.67                     | 0.53              |
| 4:5:328:LYS:O   | 4:9:168:GLY:CA[1_554]  | 1.67                     | 0.53              |
| 4:1:291:LYS:NZ  | 4:7:40:HIS:N[1_554]    | 1.67                     | 0.53              |
| 4:4:320:LEU:N   | 4:8:292:ASP:O[1_554]   | 1.67                     | 0.53              |
| 4:4:177:ARG:NH2 | 4:9:194:THR:CG2[1_554] | 1.67                     | 0.53              |
| 4:5:173:HIS:CA  | 4:V:267:ILE:CB[1_554]  | 1.67                     | 0.53              |
| 4:5:321:ALA:C   | 4:9:292:ASP:N[1_554]   | 1.67                     | 0.53              |
| 4:4:266:PHE:CD1 | 4:8:261:LEU:CG[1_554]  | 1.67                     | 0.53              |
| 4:4:280:ASN:ND2 | 4:8:281:SER:C[1_554]   | 1.67                     | 0.53              |
| 4:5:191:LYS:CB  | 4:9:186:THR:C[1_554]   | 1.67                     | 0.53              |
| 4:2:78:ASN:N    | 4:7:246:GLN:NE2[1_554] | 1.67                     | 0.53              |
| 4:5:305:MET:CA  | 4:9:11:ASP:CG[1_554]   | 1.67                     | 0.53              |
| 4:3:331:ALA:N   | 4:7:135:ALA:CB[1_554]  | 1.67                     | 0.53              |
| 4:4:335:ARG:CG  | 4:8:106:THR:N[1_554]   | 1.67                     | 0.53              |
| 4:5:288:ASP:CG  | 4:W:62:ARG:O[1_554]    | 1.67                     | 0.53              |
| 4:4:334:GLU:OE2 | 4:8:133:TYR:CA[1_554]  | 1.67                     | 0.53              |
| 4:3:145:SER:OG  | 4:7:372:ARG:CD[1_554]  | 1.67                     | 0.53              |
| 4:3:211:ASP:CG  | 4:7:32:PRO:O[1_554]    | 1.67                     | 0.53              |
| 4:5:33:SER:OG   | 4:9:77:THR:O[1_554]    | 1.67                     | 0.53              |
| 4:5:337:TYR:CE2 | 4:9:86:TRP:CE2[1_554]  | 1.67                     | 0.53              |
| 4:5:114:ALA:O   | 4:V:196:ARG:NH2[1_554] | 1.67                     | 0.53              |
| 4:5:178:LEU:O   | 4:9:177:ARG:CB[1_554]  | 1.67                     | 0.53              |
| 4:5:173:HIS:CB  | 4:V:267:ILE:CG1[1_554] | 1.67                     | 0.53              |
| 4:1:291:LYS:CE  | 4:7:39:ARG:N[1_554]    | 1.68                     | 0.52              |
| 4:3:277:THR:OG1 | 4:7:176:MET:CG[1_554]  | 1.68                     | 0.52              |
| 4:4:337:TYR:CB  | 4:8:119:MET:CA[1_554]  | 1.68                     | 0.52              |
| 4:5:312:ARG:NE  | 4:9:299:MET:CA[1_554]  | 1.68                     | 0.52              |
| 4:4:369:ILE:O   | 4:9:229:THR:CA[1_554]  | 1.68                     | 0.52              |
| 4:3:227:MET:SD  | 4:7:306:TYR:N[1_554]   | 1.68                     | 0.52              |
| 4:5:154:ASP:CB  | 4:9:111:ASN:N[1_554]   | 1.68                     | 0.52              |
| 4:5:15:GLY:C    | 4:9:77:THR:CB[1_554]   | 1.68                     | 0.52              |
| 4:4:259:GLU:CD  | 4:8:304:THR:C[1_554]   | 1.68                     | 0.52              |
| 4:4:173:HIS:O   | 4:9:267:ILE:CA[1_554]  | 1.68                     | 0.52              |
| 4:5:258:PRO:N   | 4:9:155:SER:O[1_554]   | 1.68                     | 0.52              |
| 4:3:279:TYR:CD1 | 4:7:293:LEU:CD2[1_554] | 1.68                     | 0.52              |
| 4:4:243:PRO:CG  | 4:8:60:SER:C[1_554]    | 1.68                     | 0.52              |
| 4:1:289:ILE:N   | 4:7:39:ARG:NH1[1_554]  | 1.68                     | 0.52              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:166:TYR:CZ  | 4:V:39:ARG:C[1_554]    | 1.68                     | 0.52              |
| 4:5:32:PRO:C    | 4:9:78:ASN:CG[1_554]   | 1.68                     | 0.52              |
| 4:3:311:ASP:CB  | 4:7:144:ALA:CB[1_554]  | 1.68                     | 0.52              |
| 4:4:223:PHE:C   | 4:8:335:ARG:CZ[1_554]  | 1.68                     | 0.52              |
| 4:2:75:ILE:C    | 4:7:198:TYR:CG[1_554]  | 1.68                     | 0.52              |
| 4:3:162:ASN:CB  | 4:7:172:PRO:O[1_554]   | 1.68                     | 0.52              |
| 4:3:279:TYR:CB  | 4:7:164:PRO:CB[1_554]  | 1.68                     | 0.52              |
| 4:5:310:ALA:CA  | 4:9:142:LEU:N[1_554]   | 1.68                     | 0.52              |
| 4:3:114:ALA:N   | 4:8:250:ILE:CG2[1_554] | 1.68                     | 0.52              |
| 4:4:41:GLN:CA   | 4:7:224:GLU:OE2[1_554] | 1.68                     | 0.52              |
| 4:2:357:ILE:CG1 | 4:7:233:SER:N[1_554]   | 1.68                     | 0.52              |
| 4:3:255:PHE:CZ  | 4:7:305:MET:CB[1_554]  | 1.68                     | 0.52              |
| 4:3:109:PRO:CB  | 4:8:195:GLU:CG[1_554]  | 1.68                     | 0.52              |
| 4:3:193:LEU:CB  | 4:7:210:ARG:CD[1_554]  | 1.68                     | 0.52              |
| 4:3:372:ARG:O   | 4:8:255:PHE:CE1[1_554] | 1.68                     | 0.52              |
| 4:3:266:PHE:N   | 4:7:261:LEU:CA[1_554]  | 1.68                     | 0.52              |
| 4:4:333:PRO:CG  | 4:8:104:LEU:CB[1_554]  | 1.68                     | 0.52              |
| 4:5:218:TYR:CE1 | 4:9:337:TYR:CZ[1_554]  | 1.68                     | 0.52              |
| 4:5:309:ILE:CD1 | 4:9:154:ASP:CG[1_554]  | 1.68                     | 0.52              |
| 4:5:299:MET:C   | 4:9:136:ILE:CB[1_554]  | 1.68                     | 0.52              |
| 4:2:113:LYS:O   | 4:7:251:GLY:N[1_554]   | 1.68                     | 0.52              |
| 4:5:332:PRO:CD  | 4:9:135:ALA:CA[1_554]  | 1.68                     | 0.52              |
| 4:5:25:ASP:CG   | 4:9:129:VAL:O[1_554]   | 1.68                     | 0.52              |
| 4:4:333:PRO:CB  | 4:8:104:LEU:N[1_554]   | 1.68                     | 0.52              |
| 4:5:114:ALA:N   | 4:V:253:GLU:OE2[1_554] | 1.68                     | 0.52              |
| 4:4:184:ASP:CG  | 4:8:73:HIS:CE1[1_554]  | 1.68                     | 0.52              |
| 4:4:345:ILE:O   | 4:8:365:ALA:C[1_554]   | 1.68                     | 0.52              |
| 4:5:219:VAL:CA  | 4:9:301:GLY:N[1_554]   | 1.68                     | 0.52              |
| 4:3:372:ARG:CA  | 4:8:227:MET:CA[1_554]  | 1.68                     | 0.52              |
| 4:4:210:ARG:NH1 | 4:8:33:SER:O[1_554]    | 1.68                     | 0.52              |
| 4:4:300:SER:CA  | 4:8:107:GLU:CD[1_554]  | 1.68                     | 0.52              |
| 4:5:339:VAL:CG1 | 4:9:115:ASN:C[1_554]   | 1.68                     | 0.52              |
| 4:5:227:MET:SD  | 4:9:306:TYR:CA[1_554]  | 1.68                     | 0.52              |
| 4:4:283:MET:CG  | 4:8:286:ASP:C[1_554]   | 1.68                     | 0.52              |
| 4:5:296:ASN:CA  | 4:9:169:TYR:N[1_554]   | 1.68                     | 0.52              |
| 4:3:317:ILE:O   | 4:7:150:GLY:N[1_554]   | 1.68                     | 0.52              |
| 4:4:273:GLY:C   | 4:8:162:ASN:N[1_554]   | 1.68                     | 0.52              |
| 4:4:173:HIS:CB  | 4:9:267:ILE:N[1_554]   | 1.68                     | 0.52              |
| 4:4:113:LYS:N   | 4:9:253:GLU:CG[1_554]  | 1.68                     | 0.52              |
| 4:3:162:ASN:OD1 | 4:7:175:ILE:CB[1_554]  | 1.68                     | 0.52              |
| 4:5:160:THR:N   | 4:9:177:ARG:CD[1_554]  | 1.68                     | 0.52              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:115:ASN:OD1 | 4:V:249:THR:O[1_554]   | 1.68                     | 0.52              |
| 4:4:370:VAL:CA  | 4:9:230:ALA:O[1_554]   | 1.68                     | 0.52              |
| 4:4:341:ILE:CB  | 4:8:120:THR:CG2[1_554] | 1.68                     | 0.52              |
| 4:5:188:TYR:CE1 | 4:9:185:LEU:CB[1_554]  | 1.68                     | 0.52              |
| 4:5:114:ALA:N   | 4:V:251:GLY:N[1_554]   | 1.68                     | 0.52              |
| 4:4:321:ALA:CB  | 4:8:149:THR:CG2[1_554] | 1.68                     | 0.52              |
| 4:4:340:TRP:CD1 | 4:8:118:LYS:CA[1_554]  | 1.68                     | 0.52              |
| 4:3:221:LEU:O   | 4:7:332:PRO:CB[1_554]  | 1.68                     | 0.52              |
| 4:4:315:LYS:CG  | 4:8:147:ARG:NE[1_554]  | 1.68                     | 0.52              |
| 4:5:308:GLY:N   | 4:9:338:SER:CB[1_554]  | 1.68                     | 0.52              |
| 4:3:278:THR:N   | 4:7:164:PRO:CD[1_554]  | 1.68                     | 0.52              |
| 4:3:155:SER:CB  | 4:7:108:ALA:CB[1_554]  | 1.68                     | 0.52              |
| 4:4:325:MET:CB  | 4:8:166:TYR:CZ[1_554]  | 1.68                     | 0.52              |
| 4:3:213:LYS:NZ  | 4:7:14:SER:O[1_554]    | 1.68                     | 0.52              |
| 4:3:185:LEU:CD1 | 4:7:158:GLY:C[1_554]   | 1.68                     | 0.52              |
| 4:3:222:ASP:CA  | 4:7:332:PRO:CD[1_554]  | 1.68                     | 0.52              |
| 4:3:158:GLY:O   | 4:7:177:ARG:NH2[1_554] | 1.68                     | 0.52              |
| 4:3:196:ARG:CD  | 4:7:211:ASP:CG[1_554]  | 1.68                     | 0.52              |
| 4:4:312:ARG:NH2 | 4:8:299:MET:CB[1_554]  | 1.68                     | 0.52              |
| 4:5:309:ILE:CB  | 4:9:141:SER:OG[1_554]  | 1.68                     | 0.52              |
| 4:2:357:ILE:CD1 | 4:7:232:SER:CA[1_554]  | 1.68                     | 0.52              |
| 4:5:313:MET:SD  | 4:9:152:VAL:CB[1_554]  | 1.68                     | 0.52              |
| 4:3:162:ASN:ND2 | 4:7:175:ILE:CB[1_554]  | 1.68                     | 0.52              |
| 4:5:322:PRO:CA  | 4:9:291:LYS:CE[1_554]  | 1.68                     | 0.52              |
| 4:4:281:SER:O   | 4:8:173:HIS:CE1[1_554] | 1.68                     | 0.52              |
| 4:5:277:THR:CG2 | 4:9:175:ILE:CA[1_554]  | 1.68                     | 0.52              |
| 4:4:161:HIS:C   | 4:8:110:LEU:CD1[1_554] | 1.68                     | 0.52              |
| 4:2:109:PRO:C   | 4:7:195:GLU:OE1[1_554] | 1.68                     | 0.52              |
| 4:5:346:LEU:CD1 | 4:9:368:SER:CB[1_554]  | 1.68                     | 0.52              |
| 4:5:372:ARG:N   | 4:V:227:MET:C[1_554]   | 1.68                     | 0.52              |
| 4:3:327:ILE:CA  | 4:7:168:GLY:N[1_554]   | 1.69                     | 0.51              |
| 4:4:326:LYS:CA  | 4:8:167:GLU:OE2[1_554] | 1.69                     | 0.51              |
| 4:4:255:PHE:CG  | 4:8:305:MET:SD[1_554]  | 1.69                     | 0.51              |
| 4:3:145:SER:N   | 4:7:370:VAL:C[1_554]   | 1.69                     | 0.51              |
| 4:2:173:HIS:O   | 4:7:267:ILE:O[1_554]   | 1.69                     | 0.51              |
| 4:4:178:LEU:O   | 4:8:177:ARG:CG[1_554]  | 1.69                     | 0.51              |
| 4:4:19:ALA:CA   | 4:8:118:LYS:CE[1_554]  | 1.69                     | 0.51              |
| 4:5:321:ALA:O   | 4:9:292:ASP:CB[1_554]  | 1.69                     | 0.51              |
| 4:5:190:MET:CE  | 4:9:206:ARG:CZ[1_554]  | 1.69                     | 0.51              |
| 4:5:347:ALA:N   | 4:9:366:GLY:O[1_554]   | 1.69                     | 0.51              |
| 4:3:196:ARG:CB  | 4:7:211:ASP:CA[1_554]  | 1.69                     | 0.51              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:144:ALA:CA  | 4:7:370:VAL:CA[1_554]  | 1.69                     | 0.51              |
| 4:4:372:ARG:CB  | 4:9:227:MET:CB[1_554]  | 1.69                     | 0.51              |
| 4:5:340:TRP:CD1 | 4:9:118:LYS:CA[1_554]  | 1.69                     | 0.51              |
| 4:2:367:PRO:O   | 4:7:236:LEU:CB[1_554]  | 1.69                     | 0.51              |
| 4:5:259:GLU:OE2 | 4:9:309:ILE:CG2[1_554] | 1.69                     | 0.51              |
| 4:5:274:ILE:CG1 | 4:9:161:HIS:CA[1_554]  | 1.69                     | 0.51              |
| 4:5:305:MET:SD  | 4:9:106:THR:OG1[1_554] | 1.69                     | 0.51              |
| 4:4:372:ARG:CB  | 4:9:227:MET:C[1_554]   | 1.69                     | 0.51              |
| 4:5:319:ALA:O   | 4:9:294:TYR:N[1_554]   | 1.69                     | 0.51              |
| 4:4:137:GLN:CA  | 4:8:113:LYS:CA[1_554]  | 1.69                     | 0.51              |
| 4:3:366:GLY:C   | 4:8:234:SER:C[1_554]   | 1.69                     | 0.51              |
| 4:3:196:ARG:CB  | 4:7:210:ARG:C[1_554]   | 1.69                     | 0.51              |
| 4:5:191:LYS:N   | 4:9:186:THR:CA[1_554]  | 1.69                     | 0.51              |
| 4:5:310:ALA:O   | 4:9:141:SER:C[1_554]   | 1.69                     | 0.51              |
| 4:5:338:SER:OG  | 4:9:134:VAL:CA[1_554]  | 1.69                     | 0.51              |
| 4:3:198:TYR:CA  | 4:7:208:ILE:N[1_554]   | 1.69                     | 0.51              |
| 4:4:198:TYR:CD1 | 4:8:208:ILE:N[1_554]   | 1.69                     | 0.51              |
| 4:5:214:GLU:C   | 4:9:16:LEU:CG[1_554]   | 1.69                     | 0.51              |
| 4:4:186:THR:C   | 4:8:183:ARG:CB[1_554]  | 1.69                     | 0.51              |
| 4:5:331:ALA:CA  | 4:9:140:LEU:CD2[1_554] | 1.69                     | 0.51              |
| 4:4:199:SER:N   | 4:8:206:ARG:N[1_554]   | 1.69                     | 0.51              |
| 4:4:157:ASP:O   | 4:8:72:GLU:O[1_554]    | 1.69                     | 0.51              |
| 4:5:182:GLY:CA  | 4:9:14:SER:OG[1_554]   | 1.69                     | 0.51              |
| 4:4:372:ARG:CA  | 4:9:227:MET:N[1_554]   | 1.69                     | 0.51              |
| 4:4:25:ASP:OD1  | 4:8:124:PHE:CG[1_554]  | 1.69                     | 0.51              |
| 4:4:315:LYS:CE  | 4:8:147:ARG:NE[1_554]  | 1.69                     | 0.51              |
| 4:3:180:LEU:CG  | 4:7:178:LEU:C[1_554]   | 1.69                     | 0.51              |
| 4:3:25:ASP:CG   | 4:7:124:PHE:CA[1_554]  | 1.69                     | 0.51              |
| 4:4:314:GLN:N   | 4:8:142:LEU:CG[1_554]  | 1.69                     | 0.51              |
| 4:4:208:ILE:CG2 | 4:8:59:GLN:NE2[1_554]  | 1.69                     | 0.51              |
| 4:5:145:SER:CA  | 4:9:372:ARG:CZ[1_554]  | 1.69                     | 0.51              |
| 4:4:108:ALA:C   | 4:9:195:GLU:CG[1_554]  | 1.69                     | 0.51              |
| 4:5:110:LEU:N   | 4:V:195:GLU:OE2[1_554] | 1.69                     | 0.51              |
| 4:3:185:LEU:CA  | 4:7:157:ASP:C[1_554]   | 1.69                     | 0.51              |
| 4:5:186:THR:O   | 4:9:183:ARG:CG[1_554]  | 1.69                     | 0.51              |
| 4:3:184:ASP:CG  | 4:7:73:HIS:CE1[1_554]  | 1.69                     | 0.51              |
| 4:4:196:ARG:CB  | 4:8:211:ASP:C[1_554]   | 1.69                     | 0.51              |
| 4:3:30:VAL:O    | 4:7:80:ASP:C[1_554]    | 1.69                     | 0.51              |
| 4:5:167:GLU:CD  | 4:W:41:GLN:N[1_554]    | 1.69                     | 0.51              |
| 4:5:211:ASP:O   | 4:9:16:LEU:CD1[1_554]  | 1.69                     | 0.51              |
| 4:4:195:GLU:O   | 4:8:212:ILE:CG2[1_554] | 1.69                     | 0.51              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:274:ILE:N   | 4:7:162:ASN:CA[1_554]  | 1.69                     | 0.51              |
| 4:5:275:HIS:O   | 4:9:151:ILE:CD1[1_554] | 1.69                     | 0.51              |
| 4:2:117:GLU:C   | 4:7:237:GLU:CG[1_554]  | 1.69                     | 0.51              |
| 4:3:214:GLU:C   | 4:7:16:LEU:CA[1_554]   | 1.69                     | 0.51              |
| 4:2:357:ILE:CG2 | 4:7:233:SER:N[1_554]   | 1.69                     | 0.51              |
| 4:3:189:LEU:CB  | 4:7:157:ASP:OD1[1_554] | 1.69                     | 0.51              |
| 4:5:327:ILE:C   | 4:9:148:THR:O[1_554]   | 1.69                     | 0.51              |
| 4:4:16:LEU:N    | 4:8:78:ASN:N[1_554]    | 1.69                     | 0.51              |
| 4:3:339:VAL:CB  | 4:7:115:ASN:C[1_554]   | 1.69                     | 0.51              |
| 4:4:266:PHE:CE1 | 4:8:261:LEU:CD1[1_554] | 1.69                     | 0.51              |
| 4:5:265:SER:C   | 4:9:261:LEU:O[1_554]   | 1.69                     | 0.51              |
| 4:4:337:TYR:CE1 | 4:8:86:TRP:CZ3[1_554]  | 1.69                     | 0.51              |
| 4:3:256:ARG:C   | 4:7:303:THR:OG1[1_554] | 1.69                     | 0.51              |
| 4:4:278:THR:CB  | 4:8:164:PRO:N[1_554]   | 1.69                     | 0.51              |
| 4:4:275:HIS:N   | 4:8:162:ASN:CA[1_554]  | 1.69                     | 0.51              |
| 4:2:115:ASN:OD1 | 4:7:250:ILE:CD1[1_554] | 1.69                     | 0.51              |
| 4:3:337:TYR:CE2 | 4:7:86:TRP:CH2[1_554]  | 1.69                     | 0.51              |
| 4:4:338:SER:C   | 4:8:116:ARG:O[1_554]   | 1.69                     | 0.51              |
| 4:4:194:THR:C   | 4:8:209:VAL:CA[1_554]  | 1.69                     | 0.51              |
| 4:5:272:ALA:C   | 4:9:277:THR:CB[1_554]  | 1.69                     | 0.51              |
| 4:4:277:THR:C   | 4:8:175:ILE:N[1_554]   | 1.69                     | 0.51              |
| 4:4:24:ASP:N    | 4:8:125:GLU:CD[1_554]  | 1.69                     | 0.51              |
| 4:3:115:ASN:OD1 | 4:8:249:THR:C[1_554]   | 1.69                     | 0.51              |
| 4:4:161:HIS:N   | 4:8:110:LEU:CD1[1_554] | 1.69                     | 0.51              |
| 4:3:288:ASP:C   | 4:9:63:GLY:O[1_554]    | 1.69                     | 0.51              |
| 4:4:112:PRO:CG  | 4:9:193:LEU:CG[1_554]  | 1.69                     | 0.51              |
| 4:5:167:GLU:OE2 | 4:W:41:GLN:CA[1_554]   | 1.69                     | 0.51              |
| 4:3:172:PRO:CD  | 4:8:266:PHE:CG[1_554]  | 1.69                     | 0.51              |
| 4:4:222:ASP:O   | 4:8:331:ALA:O[1_554]   | 1.69                     | 0.51              |
| 4:4:113:LYS:NZ  | 4:9:254:ARG:O[1_554]   | 1.69                     | 0.51              |
| 4:2:77:THR:C    | 4:7:246:GLN:CD[1_554]  | 1.69                     | 0.51              |
| 4:4:340:TRP:CE3 | 4:8:121:GLN:CB[1_554]  | 1.69                     | 0.51              |
| 4:3:325:MET:C   | 4:7:167:GLU:CD[1_554]  | 1.70                     | 0.50              |
| 1:A:637:LYS:CD  | 4:4:311:ASP:CG[1_556]  | 1.70                     | 0.50              |
| 4:4:162:ASN:CG  | 4:8:175:ILE:CG1[1_554] | 1.70                     | 0.50              |
| 4:5:319:ALA:CA  | 4:9:296:ASN:N[1_554]   | 1.70                     | 0.50              |
| 4:3:25:ASP:C    | 4:7:120:THR:O[1_554]   | 1.70                     | 0.50              |
| 4:4:159:VAL:CA  | 4:8:177:ARG:CZ[1_554]  | 1.70                     | 0.50              |
| 4:2:116:ARG:N   | 4:7:251:GLY:N[1_554]   | 1.70                     | 0.50              |
| 4:4:116:ARG:N   | 4:9:196:ARG:NH2[1_554] | 1.70                     | 0.50              |
| 4:4:321:ALA:C   | 4:8:292:ASP:CG[1_554]  | 1.70                     | 0.50              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:339:VAL:N   | 4:8:116:ARG:N[1_554]   | 1.70                     | 0.50              |
| 4:4:199:SER:CA  | 4:8:206:ARG:C[1_554]   | 1.70                     | 0.50              |
| 4:4:191:LYS:N   | 4:8:186:THR:CB[1_554]  | 1.70                     | 0.50              |
| 4:5:327:ILE:CG2 | 4:9:148:THR:C[1_554]   | 1.70                     | 0.50              |
| 4:4:154:ASP:CA  | 4:8:111:ASN:N[1_554]   | 1.70                     | 0.50              |
| 4:5:110:LEU:CD1 | 4:V:191:LYS:CB[1_554]  | 1.70                     | 0.50              |
| 4:4:366:GLY:O   | 4:9:234:SER:N[1_554]   | 1.70                     | 0.50              |
| 4:3:318:THR:CA  | 4:7:149:THR:CA[1_554]  | 1.70                     | 0.50              |
| 4:5:287:ILE:O   | 4:W:63:GLY:CA[1_554]   | 1.70                     | 0.50              |
| 4:3:187:ASP:C   | 4:7:183:ARG:C[1_554]   | 1.70                     | 0.50              |
| 4:3:75:ILE:O    | 4:8:197:GLY:O[1_554]   | 1.70                     | 0.50              |
| 4:3:185:LEU:CG  | 4:7:159:VAL:N[1_554]   | 1.70                     | 0.50              |
| 4:3:273:GLY:C   | 4:7:162:ASN:OD1[1_554] | 1.70                     | 0.50              |
| 4:4:243:PRO:N   | 4:8:60:SER:N[1_554]    | 1.70                     | 0.50              |
| 4:3:183:ARG:NE  | 4:7:72:GLU:CD[1_554]   | 1.70                     | 0.50              |
| 4:5:242:LEU:CD1 | 4:9:207:GLU:OE1[1_554] | 1.70                     | 0.50              |
| 4:5:194:THR:CB  | 4:9:209:VAL:CG1[1_554] | 1.70                     | 0.50              |
| 4:4:335:ARG:CD  | 4:8:106:THR:CB[1_554]  | 1.70                     | 0.50              |
| 4:4:16:LEU:CB   | 4:8:78:ASN:N[1_554]    | 1.70                     | 0.50              |
| 4:4:157:ASP:N   | 4:8:75:ILE:N[1_554]    | 1.70                     | 0.50              |
| 4:5:93:GLU:OE2  | 4:9:80:ASP:OD2[1_554]  | 1.70                     | 0.50              |
| 4:4:218:TYR:CA  | 4:8:336:LYS:C[1_554]   | 1.70                     | 0.50              |
| 4:3:293:LEU:CB  | 4:7:169:TYR:CD2[1_554] | 1.70                     | 0.50              |
| 4:5:143:TYR:CA  | 4:9:372:ARG:CA[1_554]  | 1.70                     | 0.50              |
| 4:5:367:PRO:N   | 4:V:233:SER:CA[1_554]  | 1.70                     | 0.50              |
| 4:3:192:ILE:CB  | 4:7:213:LYS:NZ[1_554]  | 1.70                     | 0.50              |
| 4:5:28:ARG:N    | 4:9:122:ILE:CG2[1_554] | 1.70                     | 0.50              |
| 4:5:278:THR:C   | 4:9:164:PRO:CB[1_554]  | 1.70                     | 0.50              |
| 4:5:347:ALA:N   | 4:9:367:PRO:N[1_554]   | 1.70                     | 0.50              |
| 4:5:270:GLU:N   | 4:9:271:SER:O[1_554]   | 1.70                     | 0.50              |
| 4:3:106:THR:CG2 | 4:7:114:ALA:CB[1_554]  | 1.70                     | 0.50              |
| 4:3:198:TYR:CD1 | 4:7:208:ILE:N[1_554]   | 1.70                     | 0.50              |
| 4:4:291:LYS:NZ  | 4:V:64:ILE:CB[1_554]   | 1.70                     | 0.50              |
| 4:4:341:ILE:CG1 | 4:8:120:THR:N[1_554]   | 1.70                     | 0.50              |
| 4:5:32:PRO:N    | 4:9:78:ASN:CG[1_554]   | 1.70                     | 0.50              |
| 4:4:215:LYS:O   | 4:8:30:VAL:CB[1_554]   | 1.70                     | 0.50              |
| 4:5:16:LEU:N    | 4:9:77:THR:CA[1_554]   | 1.70                     | 0.50              |
| 4:5:106:THR:CB  | 4:9:114:ALA:C[1_554]   | 1.70                     | 0.50              |
| 4:2:172:PRO:CD  | 4:7:266:PHE:CB[1_554]  | 1.70                     | 0.50              |
| 4:3:255:PHE:CE2 | 4:7:305:MET:CE[1_554]  | 1.70                     | 0.50              |
| 4:3:210:ARG:CD  | 4:7:69:TYR:CB[1_554]   | 1.70                     | 0.50              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:110:LEU:CA  | 4:9:192:ILE:CG2[1_554] | 1.70                     | 0.50              |
| 4:4:298:VAL:O   | 4:8:136:ILE:CG1[1_554] | 1.70                     | 0.50              |
| 4:5:24:ASP:OD1  | 4:9:124:PHE:O[1_554]   | 1.70                     | 0.50              |
| 4:3:287:ILE:N   | 4:8:270:GLU:OE1[1_554] | 1.70                     | 0.50              |
| 4:3:336:LYS:CG  | 4:7:86:TRP:CZ2[1_554]  | 1.70                     | 0.50              |
| 4:4:243:PRO:CG  | 4:8:60:SER:N[1_554]    | 1.70                     | 0.50              |
| 4:5:280:ASN:OD1 | 4:9:281:SER:N[1_554]   | 1.70                     | 0.50              |
| 4:3:333:PRO:CG  | 4:7:104:LEU:N[1_554]   | 1.70                     | 0.50              |
| 4:4:26:ALA:N    | 4:8:124:PHE:N[1_554]   | 1.70                     | 0.50              |
| 4:2:79:TRP:CD1  | 4:7:247:VAL:C[1_554]   | 1.70                     | 0.50              |
| 4:5:109:PRO:N   | 4:V:195:GLU:CG[1_554]  | 1.70                     | 0.50              |
| 4:4:319:ALA:CA  | 4:8:296:ASN:ND2[1_554] | 1.70                     | 0.50              |
| 4:3:345:ILE:N   | 4:7:367:PRO:CA[1_554]  | 1.70                     | 0.50              |
| 4:4:264:PRO:CA  | 4:8:178:LEU:CD2[1_554] | 1.70                     | 0.50              |
| 4:3:215:LYS:CE  | 4:7:31:PHE:CG[1_554]   | 1.70                     | 0.50              |
| 4:3:301:GLY:N   | 4:7:107:GLU:CB[1_554]  | 1.70                     | 0.50              |
| 4:4:273:GLY:O   | 4:8:162:ASN:CA[1_554]  | 1.70                     | 0.50              |
| 4:5:24:ASP:CG   | 4:9:124:PHE:C[1_554]   | 1.70                     | 0.50              |
| 4:3:312:ARG:NH2 | 4:7:299:MET:CB[1_554]  | 1.70                     | 0.50              |
| 4:3:25:ASP:CB   | 4:7:124:PHE:N[1_554]   | 1.70                     | 0.50              |
| 4:5:157:ASP:CB  | 4:9:72:GLU:C[1_554]    | 1.70                     | 0.50              |
| 4:5:114:ALA:CB  | 4:V:250:ILE:O[1_554]   | 1.70                     | 0.50              |
| 4:4:267:ILE:CD1 | 4:8:180:LEU:CB[1_554]  | 1.70                     | 0.50              |
| 4:5:317:ILE:CA  | 4:9:150:GLY:CA[1_554]  | 1.70                     | 0.50              |
| 4:5:337:TYR:CZ  | 4:9:86:TRP:NE1[1_554]  | 1.70                     | 0.50              |
| 4:4:293:LEU:C   | 4:8:169:TYR:CG[1_554]  | 1.70                     | 0.50              |
| 4:5:219:VAL:CG2 | 4:9:301:GLY:CA[1_554]  | 1.70                     | 0.50              |
| 4:3:257:CYS:CA  | 4:7:303:THR:OG1[1_554] | 1.70                     | 0.50              |
| 4:2:172:PRO:O   | 4:7:188:TYR:CD1[1_554] | 1.70                     | 0.50              |
| 4:3:210:ARG:NH1 | 4:7:70:PRO:CD[1_554]   | 1.70                     | 0.50              |
| 4:4:243:PRO:CB  | 4:8:60:SER:O[1_554]    | 1.70                     | 0.50              |
| 4:5:328:LYS:N   | 4:9:148:THR:C[1_554]   | 1.70                     | 0.50              |
| 4:3:161:HIS:N   | 4:7:110:LEU:CD1[1_554] | 1.70                     | 0.50              |
| 4:5:106:THR:C   | 4:9:114:ALA:CB[1_554]  | 1.70                     | 0.50              |
| 4:3:210:ARG:O   | 4:7:15:GLY:O[1_554]    | 1.70                     | 0.50              |
| 4:5:274:ILE:CG1 | 4:9:161:HIS:C[1_554]   | 1.70                     | 0.50              |
| 4:5:286:ASP:N   | 4:V:270:GLU:OE2[1_554] | 1.70                     | 0.50              |
| 4:3:19:ALA:N    | 4:7:118:LYS:CE[1_554]  | 1.70                     | 0.50              |
| 4:5:11:ASP:OD1  | 4:9:115:ASN:OD1[1_554] | 1.70                     | 0.50              |
| 4:4:340:TRP:CZ2 | 4:8:121:GLN:OE1[1_554] | 1.70                     | 0.50              |
| 4:5:185:LEU:N   | 4:9:158:GLY:CA[1_554]  | 1.71                     | 0.49              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:30:VAL:C    | 4:7:79:TRP:C[1_554]    | 1.71                     | 0.49              |
| 4:4:16:LEU:CA   | 4:8:77:THR:O[1_554]    | 1.71                     | 0.49              |
| 4:3:339:VAL:CG1 | 4:7:114:ALA:CA[1_554]  | 1.71                     | 0.49              |
| 4:2:110:LEU:O   | 4:7:193:LEU:N[1_554]   | 1.71                     | 0.49              |
| 4:3:344:SER:O   | 4:7:367:PRO:CD[1_554]  | 1.71                     | 0.49              |
| 4:3:306:TYR:CA  | 4:7:11:ASP:OD2[1_554]  | 1.71                     | 0.49              |
| 4:5:341:ILE:CA  | 4:9:120:THR:CB[1_554]  | 1.71                     | 0.49              |
| 4:3:288:ASP:O   | 4:9:65:LEU:N[1_554]    | 1.71                     | 0.49              |
| 4:5:24:ASP:OD1  | 4:9:125:GLU:CA[1_554]  | 1.71                     | 0.49              |
| 4:5:253:GLU:OE1 | 4:9:213:LYS:O[1_554]   | 1.71                     | 0.49              |
| 4:5:114:ALA:O   | 4:V:237:GLU:CD[1_554]  | 1.71                     | 0.49              |
| 4:4:314:GLN:CG  | 4:8:143:TYR:N[1_554]   | 1.71                     | 0.49              |
| 4:3:196:ARG:CG  | 4:7:211:ASP:O[1_554]   | 1.71                     | 0.49              |
| 4:4:304:THR:N   | 4:8:137:GLN:OE1[1_554] | 1.71                     | 0.49              |
| 4:3:16:LEU:CD1  | 4:7:78:ASN:C[1_554]    | 1.71                     | 0.49              |
| 4:4:280:ASN:O   | 4:8:284:LYS:O[1_554]   | 1.71                     | 0.49              |
| 4:5:20:GLY:C    | 4:9:121:GLN:CD[1_554]  | 1.71                     | 0.49              |
| 4:4:345:ILE:CA  | 4:8:367:PRO:N[1_554]   | 1.71                     | 0.49              |
| 4:4:370:VAL:CA  | 4:9:231:ALA:CA[1_554]  | 1.71                     | 0.49              |
| 4:3:154:ASP:CB  | 4:7:111:ASN:CA[1_554]  | 1.71                     | 0.49              |
| 4:3:279:TYR:N   | 4:7:164:PRO:CG[1_554]  | 1.71                     | 0.49              |
| 4:4:316:GLU:CG  | 4:8:151:ILE:O[1_554]   | 1.71                     | 0.49              |
| 4:3:178:LEU:CG  | 4:7:177:ARG:CB[1_554]  | 1.71                     | 0.49              |
| 4:4:339:VAL:CA  | 4:8:116:ARG:C[1_554]   | 1.71                     | 0.49              |
| 4:3:257:CYS:N   | 4:7:303:THR:N[1_554]   | 1.71                     | 0.49              |
| 4:4:15:GLY:CA   | 4:8:77:THR:OG1[1_554]  | 1.71                     | 0.49              |
| 4:4:259:GLU:N   | 4:8:155:SER:O[1_554]   | 1.71                     | 0.49              |
| 4:2:371:HIS:CE1 | 4:7:252:ASN:C[1_554]   | 1.71                     | 0.49              |
| 4:5:367:PRO:O   | 4:V:230:ALA:C[1_554]   | 1.71                     | 0.49              |
| 4:3:279:TYR:O   | 4:7:285:CYS:SG[1_554]  | 1.71                     | 0.49              |
| 4:5:314:GLN:OE1 | 4:9:147:ARG:CA[1_554]  | 1.71                     | 0.49              |
| 4:5:259:GLU:CB  | 4:9:304:THR:CA[1_554]  | 1.71                     | 0.49              |
| 4:5:204:ALA:CA  | 4:9:62:ARG:CD[1_554]   | 1.71                     | 0.49              |
| 4:3:267:ILE:CA  | 4:7:180:LEU:CG[1_554]  | 1.71                     | 0.49              |
| 4:2:75:ILE:CA   | 4:7:198:TYR:CA[1_554]  | 1.71                     | 0.49              |
| 4:3:313:MET:CE  | 4:7:163:VAL:CG1[1_554] | 1.71                     | 0.49              |
| 4:3:266:PHE:CE1 | 4:7:261:LEU:CD1[1_554] | 1.71                     | 0.49              |
| 4:3:173:HIS:NE2 | 4:8:265:SER:CA[1_554]  | 1.71                     | 0.49              |
| 4:4:297:ASN:CG  | 4:8:170:ALA:CA[1_554]  | 1.71                     | 0.49              |
| 4:3:196:ARG:NE  | 4:7:211:ASP:OD1[1_554] | 1.71                     | 0.49              |
| 4:5:259:GLU:CA  | 4:9:304:THR:CG2[1_554] | 1.71                     | 0.49              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:110:LEU:CG  | 4:7:192:ILE:N[1_554]   | 1.71                     | 0.49              |
| 4:2:109:PRO:CG  | 4:7:195:GLU:OE2[1_554] | 1.71                     | 0.49              |
| 4:5:178:LEU:CB  | 4:9:177:ARG:CB[1_554]  | 1.71                     | 0.49              |
| 4:5:184:ASP:OD2 | 4:9:179:ASP:CB[1_554]  | 1.71                     | 0.49              |
| 4:3:357:ILE:CG1 | 4:8:231:ALA:O[1_554]   | 1.71                     | 0.49              |
| 4:2:76:ILE:C    | 4:7:198:TYR:CE1[1_554] | 1.71                     | 0.49              |
| 4:3:259:GLU:O   | 4:7:155:SER:CB[1_554]  | 1.71                     | 0.49              |
| 4:3:304:THR:CA  | 4:7:137:GLN:OE1[1_554] | 1.71                     | 0.49              |
| 4:3:188:TYR:O   | 4:7:182:GLY:C[1_554]   | 1.71                     | 0.49              |
| 4:2:115:ASN:N   | 4:7:250:ILE:C[1_554]   | 1.71                     | 0.49              |
| 4:3:372:ARG:CA  | 4:8:227:MET:N[1_554]   | 1.71                     | 0.49              |
| 4:4:278:THR:OG1 | 4:8:163:VAL:CG1[1_554] | 1.71                     | 0.49              |
| 4:3:257:CYS:N   | 4:7:303:THR:OG1[1_554] | 1.71                     | 0.49              |
| 4:5:215:LYS:CD  | 4:9:31:PHE:CA[1_554]   | 1.71                     | 0.49              |
| 4:3:215:LYS:CG  | 4:7:31:PHE:CA[1_554]   | 1.71                     | 0.49              |
| 4:4:274:ILE:CD1 | 4:8:161:HIS:CA[1_554]  | 1.71                     | 0.49              |
| 4:4:140:LEU:CA  | 4:8:371:HIS:CD2[1_554] | 1.71                     | 0.49              |
| 4:3:299:MET:CG  | 4:7:136:ILE:CB[1_554]  | 1.71                     | 0.49              |
| 4:4:18:LYS:CB   | 4:8:79:TRP:CE3[1_554]  | 1.71                     | 0.49              |
| 4:3:281:SER:O   | 4:7:173:HIS:CE1[1_554] | 1.71                     | 0.49              |
| 4:4:334:GLU:CA  | 4:8:105:LEU:CD1[1_554] | 1.71                     | 0.49              |
| 4:3:371:HIS:NE2 | 4:8:252:ASN:O[1_554]   | 1.71                     | 0.49              |
| 4:5:157:ASP:CG  | 4:9:72:GLU:C[1_554]    | 1.71                     | 0.49              |
| 4:3:311:ASP:OD1 | 4:7:144:ALA:CB[1_554]  | 1.71                     | 0.49              |
| 4:4:346:LEU:CB  | 4:8:368:SER:OG[1_554]  | 1.71                     | 0.49              |
| 4:4:18:LYS:C    | 4:8:118:LYS:CE[1_554]  | 1.71                     | 0.49              |
| 4:4:183:ARG:CD  | 4:8:72:GLU:OE2[1_554]  | 1.71                     | 0.49              |
| 4:2:76:ILE:O    | 4:7:198:TYR:CE1[1_554] | 1.71                     | 0.49              |
| 4:5:309:ILE:N   | 4:9:141:SER:OG[1_554]  | 1.71                     | 0.49              |
| 4:4:340:TRP:CZ3 | 4:8:121:GLN:N[1_554]   | 1.71                     | 0.49              |
| 4:5:294:TYR:CZ  | 4:9:289:ILE:CD1[1_554] | 1.71                     | 0.49              |
| 4:3:109:PRO:N   | 4:8:195:GLU:CB[1_554]  | 1.71                     | 0.49              |
| 4:3:326:LYS:C   | 4:7:167:GLU:CG[1_554]  | 1.71                     | 0.49              |
| 4:3:344:SER:CA  | 4:7:367:PRO:CD[1_554]  | 1.71                     | 0.49              |
| 4:4:27:PRO:CG   | 4:8:122:ILE:CB[1_554]  | 1.71                     | 0.49              |
| 4:4:315:LYS:CB  | 4:8:298:VAL:CG2[1_554] | 1.71                     | 0.49              |
| 4:5:372:ARG:CA  | 4:V:227:MET:CB[1_554]  | 1.71                     | 0.49              |
| 4:4:274:ILE:O   | 4:8:163:VAL:CA[1_554]  | 1.71                     | 0.49              |
| 4:1:288:ASP:O   | 4:7:39:ARG:CG[1_554]   | 1.71                     | 0.49              |
| 4:3:154:ASP:N   | 4:7:110:LEU:CA[1_554]  | 1.71                     | 0.49              |
| 4:4:157:ASP:OD1 | 4:8:71:ILE:C[1_554]    | 1.72                     | 0.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:240:TYR:CZ  | 4:8:56:ASP:OD2[1_554]  | 1.72                     | 0.48              |
| 4:2:292:ASP:OD2 | 4:8:40:HIS:CB[1_554]   | 1.72                     | 0.48              |
| 4:3:136:ILE:CB  | 4:7:113:LYS:NZ[1_554]  | 1.72                     | 0.48              |
| 4:5:166:TYR:CZ  | 4:W:40:HIS:N[1_554]    | 1.72                     | 0.48              |
| 4:5:298:VAL:O   | 4:9:136:ILE:CD1[1_554] | 1.72                     | 0.48              |
| 4:5:154:ASP:OD2 | 4:9:111:ASN:C[1_554]   | 1.72                     | 0.48              |
| 4:5:327:ILE:CG1 | 4:9:149:THR:C[1_554]   | 1.72                     | 0.48              |
| 4:4:311:ASP:CB  | 4:8:141:SER:O[1_554]   | 1.72                     | 0.48              |
| 4:5:341:ILE:C   | 4:9:120:THR:OG1[1_554] | 1.72                     | 0.48              |
| 4:3:116:ARG:N   | 4:8:196:ARG:CZ[1_554]  | 1.72                     | 0.48              |
| 4:5:321:ALA:CB  | 4:9:292:ASP:CB[1_554]  | 1.72                     | 0.48              |
| 4:3:325:MET:C   | 4:7:167:GLU:CG[1_554]  | 1.72                     | 0.48              |
| 4:5:32:PRO:O    | 4:9:78:ASN:OD1[1_554]  | 1.72                     | 0.48              |
| 4:4:335:ARG:NE  | 4:8:106:THR:CG2[1_554] | 1.72                     | 0.48              |
| 4:4:30:VAL:CA   | 4:8:80:ASP:N[1_554]    | 1.72                     | 0.48              |
| 4:5:223:PHE:CE1 | 4:9:304:THR:C[1_554]   | 1.72                     | 0.48              |
| 4:4:184:ASP:OD2 | 4:8:179:ASP:CB[1_554]  | 1.72                     | 0.48              |
| 4:4:227:MET:CG  | 4:8:306:TYR:C[1_554]   | 1.72                     | 0.48              |
| 4:3:284:LYS:C   | 4:8:268:GLY:C[1_554]   | 1.72                     | 0.48              |
| 4:4:113:LYS:C   | 4:9:251:GLY:C[1_554]   | 1.72                     | 0.48              |
| 4:5:270:GLU:C   | 4:9:272:ALA:N[1_554]   | 1.72                     | 0.48              |
| 4:5:326:LYS:CA  | 4:9:167:GLU:CD[1_554]  | 1.72                     | 0.48              |
| 4:3:284:LYS:O   | 4:8:269:MET:N[1_554]   | 1.72                     | 0.48              |
| 4:5:318:THR:C   | 4:9:296:ASN:ND2[1_554] | 1.72                     | 0.48              |
| 4:3:293:LEU:CG  | 4:7:169:TYR:OH[1_554]  | 1.72                     | 0.48              |
| 4:3:226:GLU:CD  | 4:7:333:PRO:C[1_554]   | 1.72                     | 0.48              |
| 4:4:340:TRP:CH2 | 4:8:121:GLN:CA[1_554]  | 1.72                     | 0.48              |
| 4:2:173:HIS:CA  | 4:7:267:ILE:CA[1_554]  | 1.72                     | 0.48              |
| 4:4:195:GLU:CB  | 4:8:189:LEU:CG[1_554]  | 1.72                     | 0.48              |
| 4:3:220:ALA:CA  | 4:7:335:ARG:O[1_554]   | 1.72                     | 0.48              |
| 4:3:215:LYS:O   | 4:7:30:VAL:CG1[1_554]  | 1.72                     | 0.48              |
| 4:2:77:THR:CA   | 4:7:246:GLN:NE2[1_554] | 1.72                     | 0.48              |
| 4:4:180:LEU:CD2 | 4:8:178:LEU:CA[1_554]  | 1.72                     | 0.48              |
| 4:5:223:PHE:CD1 | 4:9:304:THR:C[1_554]   | 1.72                     | 0.48              |
| 4:4:349:LEU:CD2 | 4:8:365:ALA:CB[1_554]  | 1.72                     | 0.48              |
| 4:3:115:ASN:C   | 4:8:196:ARG:CZ[1_554]  | 1.72                     | 0.48              |
| 4:5:276:GLU:CB  | 4:9:278:THR:O[1_554]   | 1.72                     | 0.48              |
| 4:5:301:GLY:CA  | 4:9:107:GLU:C[1_554]   | 1.72                     | 0.48              |
| 4:3:24:ASP:N    | 4:7:125:GLU:CG[1_554]  | 1.72                     | 0.48              |
| 4:3:21:PHE:O    | 4:7:125:GLU:OE1[1_554] | 1.72                     | 0.48              |
| 4:5:278:THR:CG2 | 4:9:164:PRO:N[1_554]   | 1.72                     | 0.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:325:MET:CB  | 4:8:166:TYR:OH[1_554]  | 1.72                     | 0.48              |
| 4:5:205:GLU:OE2 | 4:9:203:THR:OG1[1_554] | 1.72                     | 0.48              |
| 4:5:27:PRO:CA   | 4:9:122:ILE:CA[1_554]  | 1.72                     | 0.48              |
| 4:4:319:ALA:CA  | 4:8:292:ASP:O[1_554]   | 1.72                     | 0.48              |
| 4:5:141:SER:OG  | 4:9:107:GLU:CD[1_554]  | 1.72                     | 0.48              |
| 4:2:117:GLU:CG  | 4:7:236:LEU:O[1_554]   | 1.72                     | 0.48              |
| 4:3:222:ASP:CB  | 4:7:332:PRO:CA[1_554]  | 1.72                     | 0.48              |
| 4:3:75:ILE:CD1  | 4:8:193:LEU:C[1_554]   | 1.72                     | 0.48              |
| 4:3:262:PHE:CE2 | 4:7:154:ASP:CA[1_554]  | 1.72                     | 0.48              |
| 4:3:345:ILE:N   | 4:7:366:GLY:C[1_554]   | 1.72                     | 0.48              |
| 4:5:263:GLN:CB  | 4:9:274:ILE:CB[1_554]  | 1.72                     | 0.48              |
| 4:5:113:LYS:N   | 4:V:253:GLU:CG[1_554]  | 1.72                     | 0.48              |
| 4:1:288:ASP:OD1 | 4:7:65:LEU:O[1_554]    | 1.72                     | 0.48              |
| 4:5:150:GLY:O   | 4:9:169:TYR:CD1[1_554] | 1.72                     | 0.48              |
| 4:4:117:GLU:CA  | 4:9:237:GLU:OE2[1_554] | 1.72                     | 0.48              |
| 4:5:278:THR:N   | 4:9:164:PRO:CG[1_554]  | 1.72                     | 0.48              |
| 4:5:296:ASN:N   | 4:9:168:GLY:C[1_554]   | 1.72                     | 0.48              |
| 4:3:174:ALA:N   | 4:8:267:ILE:CA[1_554]  | 1.72                     | 0.48              |
| 4:5:113:LYS:N   | 4:V:253:GLU:N[1_554]   | 1.72                     | 0.48              |
| 4:4:156:GLY:CA  | 4:8:74:GLY:C[1_554]    | 1.72                     | 0.48              |
| 4:3:177:ARG:NH2 | 4:8:194:THR:CG2[1_554] | 1.72                     | 0.48              |
| 4:4:11:ASP:OD2  | 4:8:115:ASN:CA[1_554]  | 1.72                     | 0.48              |
| 4:4:221:LEU:CA  | 4:8:332:PRO:CD[1_554]  | 1.72                     | 0.48              |
| 4:5:117:GLU:OE2 | 4:V:236:LEU:CG[1_554]  | 1.72                     | 0.48              |
| 4:3:115:ASN:N   | 4:8:250:ILE:C[1_554]   | 1.72                     | 0.48              |
| 4:3:316:GLU:CB  | 4:7:151:ILE:O[1_554]   | 1.72                     | 0.48              |
| 4:5:316:GLU:N   | 4:9:296:ASN:O[1_554]   | 1.72                     | 0.48              |
| 4:4:345:ILE:CG2 | 4:8:369:ILE:N[1_554]   | 1.72                     | 0.48              |
| 4:3:315:LYS:CD  | 4:7:147:ARG:CG[1_554]  | 1.72                     | 0.48              |
| 4:4:340:TRP:CD1 | 4:8:118:LYS:CB[1_554]  | 1.72                     | 0.48              |
| 4:4:27:PRO:CG   | 4:8:122:ILE:CG1[1_554] | 1.72                     | 0.48              |
| 4:5:340:TRP:C   | 4:9:116:ARG:O[1_554]   | 1.72                     | 0.48              |
| 4:3:332:PRO:CB  | 4:7:134:VAL:CA[1_554]  | 1.72                     | 0.48              |
| 4:4:210:ARG:CB  | 4:8:69:TYR:CD2[1_554]  | 1.72                     | 0.48              |
| 4:4:113:LYS:CE  | 4:9:254:ARG:CB[1_554]  | 1.72                     | 0.48              |
| 4:3:136:ILE:CA  | 4:7:113:LYS:NZ[1_554]  | 1.72                     | 0.48              |
| 4:4:214:GLU:O   | 4:8:17:VAL:N[1_554]    | 1.72                     | 0.48              |
| 4:4:270:GLU:C   | 4:8:272:ALA:CA[1_554]  | 1.72                     | 0.48              |
| 4:3:173:HIS:C   | 4:8:267:ILE:CB[1_554]  | 1.72                     | 0.48              |
| 4:3:196:ARG:CD  | 4:7:211:ASP:O[1_554]   | 1.72                     | 0.48              |
| 4:4:242:LEU:O   | 4:8:60:SER:CB[1_554]   | 1.72                     | 0.48              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:1:291:LYS:CB  | 4:7:64:ILE:CB[1_554]   | 1.72                     | 0.48              |
| 4:5:191:LYS:C   | 4:9:186:THR:O[1_554]   | 1.72                     | 0.48              |
| 4:3:294:TYR:CA  | 4:7:166:TYR:O[1_554]   | 1.72                     | 0.48              |
| 4:4:331:ALA:CB  | 4:8:140:LEU:CG[1_554]  | 1.72                     | 0.48              |
| 4:4:274:ILE:CA  | 4:8:162:ASN:C[1_554]   | 1.72                     | 0.48              |
| 4:4:215:LYS:CB  | 4:8:30:VAL:C[1_554]    | 1.72                     | 0.48              |
| 4:3:340:TRP:CZ2 | 4:7:121:GLN:OE1[1_554] | 1.72                     | 0.48              |
| 4:3:339:VAL:O   | 4:7:117:GLU:N[1_554]   | 1.72                     | 0.48              |
| 4:2:286:ASP:N   | 4:7:270:GLU:CD[1_554]  | 1.72                     | 0.48              |
| 4:5:151:ILE:CG1 | 4:9:170:ALA:C[1_554]   | 1.72                     | 0.48              |
| 4:4:253:GLU:CB  | 4:8:214:GLU:CG[1_554]  | 1.72                     | 0.48              |
| 4:4:273:GLY:N   | 4:8:162:ASN:CG[1_554]  | 1.72                     | 0.48              |
| 4:5:17:VAL:N    | 4:9:79:TRP:N[1_554]    | 1.72                     | 0.48              |
| 4:2:175:ILE:CG1 | 4:7:191:LYS:NZ[1_554]  | 1.72                     | 0.48              |
| 4:3:317:ILE:CB  | 4:7:165:ILE:N[1_554]   | 1.72                     | 0.48              |
| 4:5:24:ASP:CB   | 4:9:124:PHE:O[1_554]   | 1.73                     | 0.47              |
| 4:3:277:THR:CB  | 4:7:175:ILE:CA[1_554]  | 1.73                     | 0.47              |
| 4:4:242:LEU:C   | 4:8:60:SER:CB[1_554]   | 1.73                     | 0.47              |
| 4:5:367:PRO:CD  | 4:V:233:SER:C[1_554]   | 1.73                     | 0.47              |
| 4:3:258:PRO:CA  | 4:7:156:GLY:CA[1_554]  | 1.73                     | 0.47              |
| 4:4:112:PRO:CB  | 4:9:193:LEU:CD1[1_554] | 1.73                     | 0.47              |
| 4:3:215:LYS:CG  | 4:7:31:PHE:C[1_554]    | 1.73                     | 0.47              |
| 4:5:29:ALA:CB   | 4:9:83:GLU:OE1[1_554]  | 1.73                     | 0.47              |
| 4:3:188:TYR:C   | 4:7:183:ARG:C[1_554]   | 1.73                     | 0.47              |
| 4:5:294:TYR:CA  | 4:9:166:TYR:CB[1_554]  | 1.73                     | 0.47              |
| 4:3:191:LYS:O   | 4:7:186:THR:CA[1_554]  | 1.73                     | 0.47              |
| 4:5:198:TYR:CD2 | 4:9:208:ILE:CA[1_554]  | 1.73                     | 0.47              |
| 4:3:195:GLU:OE2 | 4:7:257:CYS:SG[1_554]  | 1.73                     | 0.47              |
| 4:5:262:PHE:CE1 | 4:9:153:LEU:O[1_554]   | 1.73                     | 0.47              |
| 4:5:265:SER:OG  | 4:9:261:LEU:O[1_554]   | 1.73                     | 0.47              |
| 4:5:317:ILE:C   | 4:9:150:GLY:CA[1_554]  | 1.73                     | 0.47              |
| 4:3:259:GLU:CA  | 4:7:304:THR:CG2[1_554] | 1.73                     | 0.47              |
| 4:3:142:LEU:O   | 4:7:372:ARG:N[1_554]   | 1.73                     | 0.47              |
| 4:5:218:TYR:CB  | 4:9:336:LYS:CG[1_554]  | 1.73                     | 0.47              |
| 4:4:188:TYR:CA  | 4:8:183:ARG:N[1_554]   | 1.73                     | 0.47              |
| 4:3:184:ASP:CB  | 4:7:73:HIS:CE1[1_554]  | 1.73                     | 0.47              |
| 4:3:279:TYR:CE2 | 4:7:285:CYS:CB[1_554]  | 1.73                     | 0.47              |
| 4:4:114:ALA:CB  | 4:9:250:ILE:CA[1_554]  | 1.73                     | 0.47              |
| 4:5:214:GLU:OE1 | 4:9:33:SER:CA[1_554]   | 1.73                     | 0.47              |
| 4:3:154:ASP:OD2 | 4:7:111:ASN:CA[1_554]  | 1.73                     | 0.47              |
| 4:5:180:LEU:CD2 | 4:9:178:LEU:C[1_554]   | 1.73                     | 0.47              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:183:ARG:N   | 4:7:73:HIS:N[1_554]    | 1.73                     | 0.47              |
| 4:5:315:LYS:CE  | 4:9:147:ARG:NH1[1_554] | 1.73                     | 0.47              |
| 4:5:30:VAL:N    | 4:9:79:TRP:O[1_554]    | 1.73                     | 0.47              |
| 4:5:173:HIS:ND1 | 4:V:267:ILE:N[1_554]   | 1.73                     | 0.47              |
| 4:4:319:ALA:N   | 4:8:296:ASN:CB[1_554]  | 1.73                     | 0.47              |
| 4:4:196:ARG:CA  | 4:8:212:ILE:CB[1_554]  | 1.73                     | 0.47              |
| 4:4:198:TYR:C   | 4:8:206:ARG:C[1_554]   | 1.73                     | 0.47              |
| 4:5:318:THR:O   | 4:9:292:ASP:C[1_554]   | 1.73                     | 0.47              |
| 4:5:340:TRP:CD2 | 4:9:119:MET:C[1_554]   | 1.73                     | 0.47              |
| 4:2:108:ALA:N   | 4:7:195:GLU:O[1_554]   | 1.73                     | 0.47              |
| 4:4:113:LYS:C   | 4:9:252:ASN:N[1_554]   | 1.73                     | 0.47              |
| 4:2:326:LYS:CE  | 4:8:44:MET:C[1_554]    | 1.73                     | 0.47              |
| 4:5:154:ASP:CG  | 4:9:111:ASN:CA[1_554]  | 1.73                     | 0.47              |
| 4:5:56:ASP:OD1  | 4:9:81:ASP:OD1[1_554]  | 1.73                     | 0.47              |
| 4:5:139:VAL:C   | 4:9:371:HIS:CE1[1_554] | 1.73                     | 0.47              |
| 4:5:320:LEU:CD1 | 4:9:282:ILE:CD1[1_554] | 1.73                     | 0.47              |
| 4:3:280:ASN:ND2 | 4:7:281:SER:C[1_554]   | 1.73                     | 0.47              |
| 4:4:166:TYR:CG  | 4:V:40:HIS:CD2[1_554]  | 1.73                     | 0.47              |
| 4:3:214:GLU:OE2 | 4:7:33:SER:OG[1_554]   | 1.73                     | 0.47              |
| 4:5:196:ARG:CB  | 4:9:212:ILE:CB[1_554]  | 1.73                     | 0.47              |
| 4:4:196:ARG:C   | 4:8:212:ILE:CB[1_554]  | 1.73                     | 0.47              |
| 4:4:198:TYR:CD2 | 4:8:208:ILE:CA[1_554]  | 1.73                     | 0.47              |
| 4:5:24:ASP:CA   | 4:9:124:PHE:O[1_554]   | 1.73                     | 0.47              |
| 4:4:173:HIS:CE1 | 4:9:265:SER:CA[1_554]  | 1.73                     | 0.47              |
| 4:4:144:ALA:N   | 4:8:371:HIS:CA[1_554]  | 1.73                     | 0.47              |
| 4:4:346:LEU:CG  | 4:8:368:SER:OG[1_554]  | 1.73                     | 0.47              |
| 4:2:287:ILE:O   | 4:8:63:GLY:O[1_554]    | 1.73                     | 0.47              |
| 4:5:205:GLU:CB  | 4:9:62:ARG:NH2[1_554]  | 1.73                     | 0.47              |
| 4:5:59:GLN:NE2  | 4:9:68:LYS:CG[1_554]   | 1.73                     | 0.47              |
| 4:3:320:LEU:CD2 | 4:7:293:LEU:CB[1_554]  | 1.73                     | 0.47              |
| 4:5:266:PHE:CB  | 4:9:261:LEU:CB[1_554]  | 1.73                     | 0.47              |
| 4:2:117:GLU:CA  | 4:7:237:GLU:CG[1_554]  | 1.73                     | 0.47              |
| 4:1:326:LYS:CD  | 4:7:43:VAL:CA[1_554]   | 1.73                     | 0.47              |
| 4:3:257:CYS:C   | 4:7:156:GLY:O[1_554]   | 1.73                     | 0.47              |
| 4:3:117:GLU:OE2 | 4:8:236:LEU:O[1_554]   | 1.73                     | 0.47              |
| 4:3:316:GLU:CB  | 4:7:152:VAL:N[1_554]   | 1.73                     | 0.47              |
| 4:5:327:ILE:CA  | 4:9:149:THR:N[1_554]   | 1.73                     | 0.47              |
| 4:5:186:THR:O   | 4:9:183:ARG:CB[1_554]  | 1.73                     | 0.47              |
| 4:5:309:ILE:N   | 4:9:338:SER:CB[1_554]  | 1.73                     | 0.47              |
| 4:4:181:ALA:O   | 4:8:158:GLY:C[1_554]   | 1.73                     | 0.47              |
| 4:5:24:ASP:CB   | 4:9:124:PHE:CA[1_554]  | 1.73                     | 0.47              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:337:TYR:CD1 | 4:9:86:TRP:CH2[1_554]  | 1.73                     | 0.47              |
| 4:3:117:GLU:CD  | 4:8:236:LEU:C[1_554]   | 1.73                     | 0.47              |
| 4:5:25:ASP:C    | 4:9:123:MET:CB[1_554]  | 1.73                     | 0.47              |
| 4:3:265:SER:O   | 4:7:260:THR:O[1_554]   | 1.73                     | 0.47              |
| 4:4:340:TRP:N   | 4:8:118:LYS:N[1_554]   | 1.73                     | 0.47              |
| 4:3:208:ILE:CG2 | 4:7:59:GLN:CG[1_554]   | 1.73                     | 0.47              |
| 4:4:272:ALA:O   | 4:8:277:THR:CG2[1_554] | 1.73                     | 0.47              |
| 4:2:368:SER:C   | 4:7:236:LEU:CB[1_554]  | 1.73                     | 0.47              |
| 4:5:161:HIS:C   | 4:9:110:LEU:CD2[1_554] | 1.73                     | 0.47              |
| 4:3:255:PHE:O   | 4:7:303:THR:N[1_554]   | 1.73                     | 0.47              |
| 4:3:227:MET:CE  | 4:7:306:TYR:C[1_554]   | 1.73                     | 0.47              |
| 4:3:258:PRO:N   | 4:7:155:SER:O[1_554]   | 1.73                     | 0.47              |
| 4:4:304:THR:CB  | 4:8:137:GLN:CD[1_554]  | 1.73                     | 0.47              |
| 4:4:153:LEU:C   | 4:8:109:PRO:CA[1_554]  | 1.73                     | 0.47              |
| 4:5:336:LYS:CD  | 4:9:12:ASN:ND2[1_554]  | 1.73                     | 0.47              |
| 4:3:72:GLU:O    | 4:8:198:TYR:O[1_554]   | 1.73                     | 0.47              |
| 4:3:188:TYR:C   | 4:7:182:GLY:O[1_554]   | 1.73                     | 0.47              |
| 4:3:253:GLU:CB  | 4:7:214:GLU:CG[1_554]  | 1.73                     | 0.47              |
| 4:5:214:GLU:CD  | 4:9:33:SER:OG[1_554]   | 1.73                     | 0.47              |
| 4:5:221:LEU:CG  | 4:9:332:PRO:CA[1_554]  | 1.73                     | 0.47              |
| 4:5:341:ILE:O   | 4:9:370:VAL:CG1[1_554] | 1.73                     | 0.47              |
| 4:4:335:ARG:CZ  | 4:8:106:THR:CB[1_554]  | 1.73                     | 0.47              |
| 4:4:300:SER:O   | 4:8:108:ALA:O[1_554]   | 1.73                     | 0.47              |
| 4:3:210:ARG:CD  | 4:7:69:TYR:CG[1_554]   | 1.73                     | 0.47              |
| 4:2:173:HIS:O   | 4:7:267:ILE:C[1_554]   | 1.73                     | 0.47              |
| 4:5:112:PRO:CG  | 4:V:193:LEU:CD1[1_554] | 1.73                     | 0.47              |
| 4:5:334:GLU:CG  | 4:9:103:THR:O[1_554]   | 1.73                     | 0.47              |
| 4:3:144:ALA:N   | 4:7:370:VAL:C[1_554]   | 1.73                     | 0.47              |
| 4:4:327:ILE:CG2 | 4:8:148:THR:CA[1_554]  | 1.73                     | 0.47              |
| 4:3:191:LYS:CA  | 4:7:186:THR:CB[1_554]  | 1.73                     | 0.47              |
| 4:5:196:ARG:CG  | 4:9:211:ASP:C[1_554]   | 1.73                     | 0.47              |
| 4:4:191:LYS:CE  | 4:8:185:LEU:C[1_554]   | 1.73                     | 0.47              |
| 4:2:288:ASP:CB  | 4:8:65:LEU:O[1_554]    | 1.74                     | 0.46              |
| 4:5:346:LEU:CB  | 4:9:369:ILE:N[1_554]   | 1.74                     | 0.46              |
| 4:4:205:GLU:N   | 4:8:62:ARG:CG[1_554]   | 1.74                     | 0.46              |
| 4:4:161:HIS:C   | 4:8:110:LEU:CB[1_554]  | 1.74                     | 0.46              |
| 4:5:372:ARG:CA  | 4:V:227:MET:CA[1_554]  | 1.74                     | 0.46              |
| 4:4:25:ASP:CB   | 4:8:124:PHE:N[1_554]   | 1.74                     | 0.46              |
| 4:3:311:ASP:O   | 4:7:141:SER:O[1_554]   | 1.74                     | 0.46              |
| 4:3:30:VAL:CA   | 4:7:79:TRP:O[1_554]    | 1.74                     | 0.46              |
| 4:5:269:MET:CB  | 4:9:178:LEU:CD1[1_554] | 1.74                     | 0.46              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:198:TYR:CD1 | 4:9:208:ILE:CG2[1_554] | 1.74                     | 0.46              |
| 4:5:157:ASP:OD2 | 4:9:72:GLU:CG[1_554]   | 1.74                     | 0.46              |
| 4:3:26:ALA:N    | 4:7:121:GLN:C[1_554]   | 1.74                     | 0.46              |
| 4:5:369:ILE:CG2 | 4:V:232:SER:C[1_554]   | 1.74                     | 0.46              |
| 4:5:267:ILE:CG1 | 4:9:180:LEU:CD1[1_554] | 1.74                     | 0.46              |
| 4:3:74:GLY:C    | 4:8:198:TYR:N[1_554]   | 1.74                     | 0.46              |
| 4:3:341:ILE:CA  | 4:7:117:GLU:O[1_554]   | 1.74                     | 0.46              |
| 4:4:335:ARG:N   | 4:8:105:LEU:CB[1_554]  | 1.74                     | 0.46              |
| 4:3:113:LYS:CE  | 4:8:254:ARG:CG[1_554]  | 1.74                     | 0.46              |
| 4:5:253:GLU:CG  | 4:9:214:GLU:CA[1_554]  | 1.74                     | 0.46              |
| 4:5:178:LEU:CG  | 4:9:177:ARG:O[1_554]   | 1.74                     | 0.46              |
| 4:5:153:LEU:CG  | 4:9:109:PRO:CG[1_554]  | 1.74                     | 0.46              |
| 4:5:218:TYR:O   | 4:9:302:GLY:N[1_554]   | 1.74                     | 0.46              |
| 4:5:143:TYR:CG  | 4:9:372:ARG:N[1_554]   | 1.74                     | 0.46              |
| 4:3:218:TYR:CG  | 4:7:337:TYR:CE1[1_554] | 1.74                     | 0.46              |
| 4:3:250:ILE:CG1 | 4:7:210:ARG:CZ[1_554]  | 1.74                     | 0.46              |
| 4:4:293:LEU:CA  | 4:8:169:TYR:CG[1_554]  | 1.74                     | 0.46              |
| 4:4:258:PRO:O   | 4:8:155:SER:C[1_554]   | 1.74                     | 0.46              |
| 4:4:207:GLU:OE2 | 4:8:67:LEU:O[1_554]    | 1.74                     | 0.46              |
| 4:3:280:ASN:CA  | 4:7:174:ALA:CB[1_554]  | 1.74                     | 0.46              |
| 4:2:173:HIS:N   | 4:7:266:PHE:C[1_554]   | 1.74                     | 0.46              |
| 4:5:307:PRO:O   | 4:9:335:ARG:O[1_554]   | 1.74                     | 0.46              |
| 4:4:188:TYR:CE1 | 4:8:185:LEU:CD1[1_554] | 1.74                     | 0.46              |
| 4:3:281:SER:C   | 4:7:173:HIS:CE1[1_554] | 1.74                     | 0.46              |
| 4:3:243:PRO:CA  | 4:7:60:SER:CB[1_554]   | 1.74                     | 0.46              |
| 4:3:333:PRO:CD  | 4:7:104:LEU:CA[1_554]  | 1.74                     | 0.46              |
| 4:5:188:TYR:CD1 | 4:9:185:LEU:CB[1_554]  | 1.74                     | 0.46              |
| 4:3:210:ARG:CZ  | 4:7:33:SER:O[1_554]    | 1.74                     | 0.46              |
| 4:5:320:LEU:CA  | 4:9:293:LEU:CA[1_554]  | 1.74                     | 0.46              |
| 4:5:256:ARG:CB  | 4:9:306:TYR:CE1[1_554] | 1.74                     | 0.46              |
| 4:4:340:TRP:CA  | 4:8:118:LYS:CA[1_554]  | 1.74                     | 0.46              |
| 4:4:205:GLU:OE2 | 4:8:203:THR:OG1[1_554] | 1.74                     | 0.46              |
| 4:5:213:LYS:CD  | 4:9:157:ASP:CG[1_554]  | 1.74                     | 0.46              |
| 4:5:308:GLY:N   | 4:9:338:SER:C[1_554]   | 1.74                     | 0.46              |
| 4:2:111:ASN:CG  | 4:7:196:ARG:CB[1_554]  | 1.74                     | 0.46              |
| 4:4:314:GLN:O   | 4:8:142:LEU:CG[1_554]  | 1.74                     | 0.46              |
| 4:2:369:ILE:CB  | 4:7:234:SER:OG[1_554]  | 1.74                     | 0.46              |
| 4:5:205:GLU:OE2 | 4:9:203:THR:CB[1_554]  | 1.74                     | 0.46              |
| 4:5:11:ASP:N    | 4:9:118:LYS:CB[1_554]  | 1.74                     | 0.46              |
| 4:4:215:LYS:CA  | 4:8:31:PHE:N[1_554]    | 1.74                     | 0.46              |
| 4:3:282:ILE:CA  | 4:7:173:HIS:NE2[1_554] | 1.74                     | 0.46              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:329:ILE:CG2 | 4:8:139:VAL:CG1[1_554] | 1.74                     | 0.46              |
| 4:3:210:ARG:N   | 4:7:69:TYR:OH[1_554]   | 1.74                     | 0.46              |
| 4:3:156:GLY:O   | 4:7:74:GLY:N[1_554]    | 1.74                     | 0.46              |
| 4:3:337:TYR:N   | 4:7:119:MET:CB[1_554]  | 1.74                     | 0.46              |
| 4:5:154:ASP:O   | 4:9:110:LEU:N[1_554]   | 1.74                     | 0.46              |
| 4:5:27:PRO:O    | 4:9:122:ILE:CG2[1_554] | 1.74                     | 0.46              |
| 4:5:137:GLN:OE1 | 4:9:112:PRO:N[1_554]   | 1.74                     | 0.46              |
| 4:4:27:PRO:N    | 4:8:122:ILE:CG1[1_554] | 1.74                     | 0.46              |
| 4:3:24:ASP:CA   | 4:7:125:GLU:CB[1_554]  | 1.74                     | 0.46              |
| 4:5:201:VAL:CG2 | 4:9:203:THR:N[1_554]   | 1.74                     | 0.46              |
| 4:4:276:GLU:OE2 | 4:8:278:THR:O[1_554]   | 1.74                     | 0.46              |
| 4:4:310:ALA:CB  | 4:8:140:LEU:N[1_554]   | 1.74                     | 0.46              |
| 4:5:280:ASN:OD1 | 4:9:281:SER:C[1_554]   | 1.74                     | 0.46              |
| 4:5:317:ILE:CG2 | 4:9:150:GLY:C[1_554]   | 1.74                     | 0.46              |
| 4:5:265:SER:CB  | 4:9:261:LEU:O[1_554]   | 1.74                     | 0.46              |
| 4:3:31:PHE:CA   | 4:7:78:ASN:CG[1_554]   | 1.74                     | 0.46              |
| 4:4:338:SER:CB  | 4:8:116:ARG:CG[1_554]  | 1.74                     | 0.46              |
| 4:3:193:LEU:CG  | 4:7:210:ARG:CG[1_554]  | 1.74                     | 0.46              |
| 4:3:178:LEU:CB  | 4:7:177:ARG:N[1_554]   | 1.74                     | 0.46              |
| 4:3:209:VAL:CG1 | 4:7:69:TYR:OH[1_554]   | 1.74                     | 0.46              |
| 4:4:310:ALA:C   | 4:8:142:LEU:N[1_554]   | 1.74                     | 0.46              |
| 4:5:20:GLY:N    | 4:9:121:GLN:CD[1_554]  | 1.74                     | 0.46              |
| 4:3:281:SER:CA  | 4:7:173:HIS:CD2[1_554] | 1.74                     | 0.46              |
| 4:2:75:ILE:CA   | 4:7:198:TYR:N[1_554]   | 1.74                     | 0.46              |
| 4:5:348:SER:OG  | 4:9:362:TYR:CA[1_554]  | 1.74                     | 0.46              |
| 4:4:291:LYS:CG  | 4:V:64:ILE:CG1[1_554]  | 1.74                     | 0.46              |
| 4:5:213:LYS:NZ  | 4:9:14:SER:CB[1_554]   | 1.75                     | 0.45              |
| 4:3:18:LYS:C    | 4:7:118:LYS:CE[1_554]  | 1.75                     | 0.45              |
| 4:5:24:ASP:C    | 4:9:124:PHE:N[1_554]   | 1.75                     | 0.45              |
| 4:5:195:GLU:C   | 4:9:189:LEU:CD2[1_554] | 1.75                     | 0.45              |
| 4:2:110:LEU:C   | 4:7:192:ILE:CA[1_554]  | 1.75                     | 0.45              |
| 4:4:282:ILE:CD1 | 4:8:171:LEU:CD2[1_554] | 1.75                     | 0.45              |
| 4:4:316:GLU:O   | 4:8:296:ASN:O[1_554]   | 1.75                     | 0.45              |
| 1:D:637:LYS:NZ  | 4:5:311:ASP:C[1_556]   | 1.75                     | 0.45              |
| 4:3:144:ALA:CB  | 4:7:371:HIS:N[1_554]   | 1.75                     | 0.45              |
| 4:3:161:HIS:CB  | 4:7:110:LEU:CB[1_554]  | 1.75                     | 0.45              |
| 4:4:259:GLU:CB  | 4:8:304:THR:CB[1_554]  | 1.75                     | 0.45              |
| 4:4:255:PHE:CG  | 4:8:305:MET:CB[1_554]  | 1.75                     | 0.45              |
| 4:3:184:ASP:OD2 | 4:7:179:ASP:CB[1_554]  | 1.75                     | 0.45              |
| 4:4:172:PRO:CA  | 4:9:266:PHE:O[1_554]   | 1.75                     | 0.45              |
| 4:5:56:ASP:OD1  | 4:9:80:ASP:OD1[1_554]  | 1.75                     | 0.45              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:115:ASN:O   | 4:7:237:GLU:OE1[1_554] | 1.75                     | 0.45              |
| 4:3:268:GLY:N   | 4:7:180:LEU:CD2[1_554] | 1.75                     | 0.45              |
| 4:5:333:PRO:CD  | 4:9:104:LEU:CB[1_554]  | 1.75                     | 0.45              |
| 4:3:291:LYS:NZ  | 4:9:64:ILE:O[1_554]    | 1.75                     | 0.45              |
| 4:4:294:TYR:CD2 | 4:8:166:TYR:CB[1_554]  | 1.75                     | 0.45              |
| 4:3:300:SER:N   | 4:7:107:GLU:CD[1_554]  | 1.75                     | 0.45              |
| 4:2:110:LEU:CD1 | 4:7:191:LYS:CB[1_554]  | 1.75                     | 0.45              |
| 4:4:279:TYR:CE1 | 4:8:293:LEU:CD2[1_554] | 1.75                     | 0.45              |
| 4:5:269:MET:N   | 4:9:264:PRO:CB[1_554]  | 1.75                     | 0.45              |
| 4:4:213:LYS:CE  | 4:8:14:SER:CA[1_554]   | 1.75                     | 0.45              |
| 4:4:59:GLN:CD   | 4:8:68:LYS:CG[1_554]   | 1.75                     | 0.45              |
| 4:5:199:SER:C   | 4:9:206:ARG:N[1_554]   | 1.75                     | 0.45              |
| 4:5:200:PHE:CE1 | 4:9:207:GLU:CA[1_554]  | 1.75                     | 0.45              |
| 4:5:327:ILE:C   | 4:9:148:THR:CA[1_554]  | 1.75                     | 0.45              |
| 4:3:336:LYS:C   | 4:7:119:MET:SD[1_554]  | 1.75                     | 0.45              |
| 4:5:267:ILE:N   | 4:9:180:LEU:CD1[1_554] | 1.75                     | 0.45              |
| 4:3:254:ARG:NE  | 4:7:337:TYR:OH[1_554]  | 1.75                     | 0.45              |
| 4:4:370:VAL:N   | 4:9:230:ALA:C[1_554]   | 1.75                     | 0.45              |
| 4:5:253:GLU:OE1 | 4:9:214:GLU:CA[1_554]  | 1.75                     | 0.45              |
| 4:5:196:ARG:CD  | 4:9:211:ASP:O[1_554]   | 1.75                     | 0.45              |
| 4:3:143:TYR:O   | 4:7:369:ILE:O[1_554]   | 1.75                     | 0.45              |
| 4:3:264:PRO:CA  | 4:7:178:LEU:CD2[1_554] | 1.75                     | 0.45              |
| 4:5:180:LEU:CA  | 4:9:179:ASP:OD1[1_554] | 1.75                     | 0.45              |
| 4:4:260:THR:CB  | 4:8:155:SER:OG[1_554]  | 1.75                     | 0.45              |
| 4:2:366:GLY:C   | 4:7:235:SER:N[1_554]   | 1.75                     | 0.45              |
| 4:5:243:PRO:CB  | 4:9:60:SER:O[1_554]    | 1.75                     | 0.45              |
| 4:4:79:TRP:CZ2  | 4:9:249:THR:CG2[1_554] | 1.75                     | 0.45              |
| 4:5:17:VAL:CG1  | 4:9:79:TRP:CD1[1_554]  | 1.75                     | 0.45              |
| 4:5:294:TYR:OH  | 4:9:289:ILE:CB[1_554]  | 1.75                     | 0.45              |
| 4:3:334:GLU:CB  | 4:7:132:MET:CE[1_554]  | 1.75                     | 0.45              |
| 4:4:255:PHE:O   | 4:8:302:GLY:O[1_554]   | 1.75                     | 0.45              |
| 4:4:261:LEU:CB  | 4:8:154:ASP:C[1_554]   | 1.75                     | 0.45              |
| 4:4:332:PRO:C   | 4:8:105:LEU:O[1_554]   | 1.75                     | 0.45              |
| 4:4:214:GLU:CA  | 4:8:16:LEU:O[1_554]    | 1.75                     | 0.45              |
| 4:3:218:TYR:CD2 | 4:7:337:TYR:CD2[1_554] | 1.75                     | 0.45              |
| 4:4:181:ALA:CA  | 4:8:159:VAL:CG1[1_554] | 1.75                     | 0.45              |
| 4:3:370:VAL:CG2 | 4:8:230:ALA:O[1_554]   | 1.75                     | 0.45              |
| 4:3:342:GLY:O   | 4:7:368:SER:N[1_554]   | 1.75                     | 0.45              |
| 4:4:289:ILE:N   | 4:V:63:GLY:C[1_554]    | 1.75                     | 0.45              |
| 4:5:346:LEU:O   | 4:9:365:ALA:C[1_554]   | 1.75                     | 0.45              |
| 4:5:339:VAL:CA  | 4:9:116:ARG:CG[1_554]  | 1.75                     | 0.45              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:188:TYR:CA  | 4:9:183:ARG:C[1_554]   | 1.75                     | 0.45              |
| 4:5:335:ARG:CA  | 4:9:105:LEU:O[1_554]   | 1.75                     | 0.45              |
| 4:4:30:VAL:CB   | 4:8:79:TRP:C[1_554]    | 1.75                     | 0.45              |
| 4:3:288:ASP:OD1 | 4:9:65:LEU:O[1_554]    | 1.75                     | 0.45              |
| 4:5:327:ILE:CB  | 4:9:149:THR:CB[1_554]  | 1.75                     | 0.45              |
| 4:3:333:PRO:CB  | 4:7:105:LEU:N[1_554]   | 1.75                     | 0.45              |
| 4:2:114:ALA:O   | 4:7:238:LYS:O[1_554]   | 1.75                     | 0.45              |
| 4:5:329:ILE:CG1 | 4:9:142:LEU:CB[1_554]  | 1.75                     | 0.45              |
| 4:3:367:PRO:CD  | 4:8:235:SER:CB[1_554]  | 1.75                     | 0.45              |
| 4:3:320:LEU:N   | 4:7:293:LEU:N[1_554]   | 1.75                     | 0.45              |
| 4:5:293:LEU:CA  | 4:9:169:TYR:CD2[1_554] | 1.75                     | 0.45              |
| 4:5:154:ASP:CA  | 4:9:108:ALA:C[1_554]   | 1.75                     | 0.45              |
| 4:3:310:ALA:O   | 4:7:142:LEU:N[1_554]   | 1.75                     | 0.45              |
| 4:3:214:GLU:O   | 4:7:17:VAL:CA[1_554]   | 1.75                     | 0.45              |
| 4:5:184:ASP:OD1 | 4:9:73:HIS:ND1[1_554]  | 1.75                     | 0.45              |
| 4:5:260:THR:CG2 | 4:9:180:LEU:O[1_554]   | 1.75                     | 0.45              |
| 4:3:332:PRO:CG  | 4:7:134:VAL:C[1_554]   | 1.75                     | 0.45              |
| 4:5:72:GLU:O    | 4:V:198:TYR:O[1_554]   | 1.75                     | 0.45              |
| 4:3:291:LYS:CD  | 4:9:64:ILE:CD1[1_554]  | 1.75                     | 0.45              |
| 4:3:318:THR:N   | 4:7:149:THR:O[1_554]   | 1.75                     | 0.45              |
| 4:3:188:TYR:CG  | 4:7:182:GLY:N[1_554]   | 1.75                     | 0.45              |
| 4:5:17:VAL:O    | 4:9:79:TRP:CB[1_554]   | 1.75                     | 0.45              |
| 4:5:243:PRO:CG  | 4:9:59:GLN:O[1_554]    | 1.75                     | 0.45              |
| 4:3:223:PHE:CD1 | 4:7:304:THR:OG1[1_554] | 1.75                     | 0.45              |
| 4:3:335:ARG:CG  | 4:7:107:GLU:N[1_554]   | 1.75                     | 0.45              |
| 4:3:314:GLN:C   | 4:7:142:LEU:CD1[1_554] | 1.75                     | 0.45              |
| 4:5:369:ILE:CB  | 4:V:232:SER:N[1_554]   | 1.75                     | 0.45              |
| 4:4:334:GLU:OE2 | 4:8:133:TYR:C[1_554]   | 1.75                     | 0.45              |
| 4:4:280:ASN:CG  | 4:8:281:SER:C[1_554]   | 1.75                     | 0.45              |
| 4:4:309:ILE:N   | 4:8:141:SER:OG[1_554]  | 1.75                     | 0.45              |
| 4:4:227:MET:SD  | 4:8:305:MET:C[1_554]   | 1.75                     | 0.45              |
| 4:4:344:SER:C   | 4:8:367:PRO:CG[1_554]  | 1.75                     | 0.45              |
| 4:1:292:ASP:OD2 | 4:7:40:HIS:CA[1_554]   | 1.75                     | 0.45              |
| 4:5:315:LYS:N   | 4:9:298:VAL:CG2[1_554] | 1.75                     | 0.45              |
| 4:5:255:PHE:CG  | 4:9:305:MET:CG[1_554]  | 1.76                     | 0.44              |
| 4:3:226:GLU:CB  | 4:7:335:ARG:NH1[1_554] | 1.76                     | 0.44              |
| 4:4:293:LEU:CG  | 4:8:169:TYR:CZ[1_554]  | 1.76                     | 0.44              |
| 4:3:196:ARG:CB  | 4:7:211:ASP:C[1_554]   | 1.76                     | 0.44              |
| 4:3:137:GLN:OE1 | 4:7:112:PRO:CG[1_554]  | 1.76                     | 0.44              |
| 4:3:220:ALA:C   | 4:7:335:ARG:CB[1_554]  | 1.76                     | 0.44              |
| 4:4:23:GLY:O    | 4:8:362:TYR:CE2[1_554] | 1.76                     | 0.44              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:319:ALA:C   | 4:9:294:TYR:N[1_554]   | 1.76                     | 0.44              |
| 4:3:344:SER:N   | 4:7:367:PRO:CB[1_554]  | 1.76                     | 0.44              |
| 4:4:75:ILE:CB   | 4:9:198:TYR:CA[1_554]  | 1.76                     | 0.44              |
| 4:4:32:PRO:N    | 4:8:78:ASN:CB[1_554]   | 1.76                     | 0.44              |
| 4:3:370:VAL:C   | 4:8:230:ALA:O[1_554]   | 1.76                     | 0.44              |
| 4:4:113:LYS:CB  | 4:9:254:ARG:N[1_554]   | 1.76                     | 0.44              |
| 4:4:110:LEU:CD2 | 4:9:191:LYS:CE[1_554]  | 1.76                     | 0.44              |
| 4:5:327:ILE:N   | 4:9:149:THR:OG1[1_554] | 1.76                     | 0.44              |
| 4:3:336:LYS:CD  | 4:7:86:TRP:CE2[1_554]  | 1.76                     | 0.44              |
| 4:3:334:GLU:N   | 4:7:105:LEU:CB[1_554]  | 1.76                     | 0.44              |
| 4:5:199:SER:N   | 4:9:206:ARG:N[1_554]   | 1.76                     | 0.44              |
| 4:4:317:ILE:CG2 | 4:8:165:ILE:N[1_554]   | 1.76                     | 0.44              |
| 4:5:180:LEU:CD2 | 4:9:178:LEU:CA[1_554]  | 1.76                     | 0.44              |
| 4:5:154:ASP:CA  | 4:9:109:PRO:N[1_554]   | 1.76                     | 0.44              |
| 4:4:227:MET:SD  | 4:8:306:TYR:C[1_554]   | 1.76                     | 0.44              |
| 4:3:156:GLY:O   | 4:7:73:HIS:C[1_554]    | 1.76                     | 0.44              |
| 4:5:344:SER:C   | 4:9:362:TYR:CE1[1_554] | 1.76                     | 0.44              |
| 4:4:259:GLU:CD  | 4:8:304:THR:CA[1_554]  | 1.76                     | 0.44              |
| 4:5:276:GLU:OE1 | 4:9:279:TYR:CA[1_554]  | 1.76                     | 0.44              |
| 4:5:32:PRO:N    | 4:9:78:ASN:CB[1_554]   | 1.76                     | 0.44              |
| 4:4:151:ILE:N   | 4:8:169:TYR:CE1[1_554] | 1.76                     | 0.44              |
| 4:4:333:PRO:CB  | 4:8:104:LEU:CB[1_554]  | 1.76                     | 0.44              |
| 4:4:305:MET:CB  | 4:8:12:ASN:N[1_554]    | 1.76                     | 0.44              |
| 4:5:211:ASP:OD2 | 4:9:32:PRO:N[1_554]    | 1.76                     | 0.44              |
| 4:4:194:THR:N   | 4:8:209:VAL:CG1[1_554] | 1.76                     | 0.44              |
| 4:3:271:SER:O   | 4:7:277:THR:CB[1_554]  | 1.76                     | 0.44              |
| 4:5:300:SER:CB  | 4:9:107:GLU:CD[1_554]  | 1.76                     | 0.44              |
| 4:4:11:ASP:OD1  | 4:8:115:ASN:OD1[1_554] | 1.76                     | 0.44              |
| 4:4:327:ILE:CD1 | 4:8:149:THR:CB[1_554]  | 1.76                     | 0.44              |
| 4:3:315:LYS:C   | 4:7:142:LEU:CD1[1_554] | 1.76                     | 0.44              |
| 4:4:173:HIS:CG  | 4:9:264:PRO:O[1_554]   | 1.76                     | 0.44              |
| 4:4:332:PRO:N   | 4:8:135:ALA:CA[1_554]  | 1.76                     | 0.44              |
| 4:4:211:ASP:OD1 | 4:8:32:PRO:CD[1_554]   | 1.76                     | 0.44              |
| 4:4:155:SER:CB  | 4:8:108:ALA:CB[1_554]  | 1.76                     | 0.44              |
| 4:4:162:ASN:CB  | 4:8:172:PRO:O[1_554]   | 1.76                     | 0.44              |
| 4:3:212:ILE:O   | 4:7:16:LEU:CG[1_554]   | 1.76                     | 0.44              |
| 4:3:303:THR:O   | 4:7:137:GLN:OE1[1_554] | 1.76                     | 0.44              |
| 4:5:326:LYS:C   | 4:9:167:GLU:CD[1_554]  | 1.76                     | 0.44              |
| 4:4:31:PHE:CB   | 4:8:80:ASP:CB[1_554]   | 1.76                     | 0.44              |
| 4:4:18:LYS:CA   | 4:8:79:TRP:CG[1_554]   | 1.76                     | 0.44              |
| 4:3:325:MET:C   | 4:7:167:GLU:OE2[1_554] | 1.76                     | 0.44              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:62:ARG:CZ   | 4:9:67:LEU:O[1_554]    | 1.76                     | 0.44              |
| 4:4:272:ALA:CA  | 4:8:277:THR:CB[1_554]  | 1.76                     | 0.44              |
| 4:4:272:ALA:N   | 4:8:277:THR:OG1[1_554] | 1.76                     | 0.44              |
| 4:3:299:MET:N   | 4:7:136:ILE:CD1[1_554] | 1.76                     | 0.44              |
| 4:3:293:LEU:CG  | 4:7:169:TYR:CZ[1_554]  | 1.76                     | 0.44              |
| 4:4:255:PHE:C   | 4:8:302:GLY:CA[1_554]  | 1.76                     | 0.44              |
| 4:4:181:ALA:N   | 4:8:159:VAL:CG1[1_554] | 1.76                     | 0.44              |
| 4:3:213:LYS:CD  | 4:7:14:SER:C[1_554]    | 1.76                     | 0.44              |
| 4:3:372:ARG:CG  | 4:8:227:MET:C[1_554]   | 1.76                     | 0.44              |
| 4:3:15:GLY:N    | 4:7:77:THR:CG2[1_554]  | 1.76                     | 0.44              |
| 4:4:144:ALA:C   | 4:8:370:VAL:C[1_554]   | 1.76                     | 0.44              |
| 4:3:211:ASP:CA  | 4:7:32:PRO:CA[1_554]   | 1.76                     | 0.44              |
| 4:4:309:ILE:CD1 | 4:8:154:ASP:OD2[1_554] | 1.76                     | 0.44              |
| 4:3:214:GLU:N   | 4:7:15:GLY:O[1_554]    | 1.76                     | 0.44              |
| 4:4:195:GLU:OE2 | 4:8:257:CYS:SG[1_554]  | 1.76                     | 0.44              |
| 4:2:368:SER:N   | 4:7:236:LEU:CB[1_554]  | 1.76                     | 0.44              |
| 4:4:196:ARG:C   | 4:8:212:ILE:CG1[1_554] | 1.76                     | 0.44              |
| 4:4:308:GLY:CA  | 4:8:338:SER:O[1_554]   | 1.76                     | 0.44              |
| 4:4:261:LEU:C   | 4:8:154:ASP:O[1_554]   | 1.76                     | 0.44              |
| 4:5:305:MET:CA  | 4:9:11:ASP:OD2[1_554]  | 1.76                     | 0.44              |
| 4:4:110:LEU:CG  | 4:9:191:LYS:CD[1_554]  | 1.76                     | 0.44              |
| 4:5:283:MET:CG  | 4:9:285:CYS:O[1_554]   | 1.76                     | 0.44              |
| 4:4:178:LEU:CB  | 4:8:177:ARG:CA[1_554]  | 1.76                     | 0.44              |
| 4:3:145:SER:CB  | 4:7:372:ARG:NH2[1_554] | 1.76                     | 0.44              |
| 4:2:77:THR:O    | 4:7:246:GLN:CD[1_554]  | 1.76                     | 0.44              |
| 4:5:30:VAL:CG1  | 4:9:82:MET:CG[1_554]   | 1.76                     | 0.44              |
| 4:5:208:ILE:CD1 | 4:9:59:GLN:CG[1_554]   | 1.76                     | 0.44              |
| 4:4:113:LYS:C   | 4:9:251:GLY:N[1_554]   | 1.76                     | 0.44              |
| 4:5:327:ILE:CD1 | 4:9:149:THR:OG1[1_554] | 1.76                     | 0.44              |
| 4:3:270:GLU:N   | 4:7:272:ALA:C[1_554]   | 1.76                     | 0.44              |
| 4:3:157:ASP:CA  | 4:7:72:GLU:C[1_554]    | 1.76                     | 0.44              |
| 4:4:266:PHE:CG  | 4:8:261:LEU:CD2[1_554] | 1.76                     | 0.44              |
| 4:3:110:LEU:CA  | 4:8:192:ILE:CG2[1_554] | 1.76                     | 0.44              |
| 4:5:317:ILE:CG2 | 4:9:151:ILE:CA[1_554]  | 1.76                     | 0.44              |
| 4:5:335:ARG:O   | 4:9:107:GLU:N[1_554]   | 1.76                     | 0.44              |
| 4:5:255:PHE:CE1 | 4:9:306:TYR:N[1_554]   | 1.76                     | 0.44              |
| 4:5:319:ALA:N   | 4:9:292:ASP:O[1_554]   | 1.76                     | 0.44              |
| 4:3:218:TYR:C   | 4:7:336:LYS:O[1_554]   | 1.76                     | 0.44              |
| 4:3:280:ASN:OD1 | 4:7:281:SER:C[1_554]   | 1.76                     | 0.44              |
| 4:5:300:SER:N   | 4:9:136:ILE:CA[1_554]  | 1.76                     | 0.44              |
| 4:4:15:GLY:N    | 4:8:77:THR:CG2[1_554]  | 1.76                     | 0.44              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:334:GLU:O   | 4:7:119:MET:CE[1_554]  | 1.76                     | 0.44              |
| 4:3:259:GLU:CB  | 4:7:304:THR:CA[1_554]  | 1.76                     | 0.44              |
| 4:5:218:TYR:CZ  | 4:9:337:TYR:CD2[1_554] | 1.76                     | 0.44              |
| 4:5:157:ASP:OD2 | 4:9:72:GLU:N[1_554]    | 1.76                     | 0.44              |
| 4:5:279:TYR:OH  | 4:9:290:ARG:CB[1_554]  | 1.76                     | 0.44              |
| 4:5:188:TYR:N   | 4:9:183:ARG:CA[1_554]  | 1.76                     | 0.44              |
| 4:5:164:PRO:CB  | 4:9:172:PRO:CG[1_554]  | 1.76                     | 0.44              |
| 4:4:142:LEU:O   | 4:8:372:ARG:CG[1_554]  | 1.76                     | 0.44              |
| 4:5:295:ALA:N   | 4:9:167:GLU:C[1_554]   | 1.76                     | 0.44              |
| 4:5:193:LEU:CD1 | 4:9:211:ASP:N[1_554]   | 1.76                     | 0.44              |
| 4:5:293:LEU:O   | 4:9:169:TYR:O[1_554]   | 1.76                     | 0.44              |
| 4:5:265:SER:N   | 4:9:261:LEU:O[1_554]   | 1.76                     | 0.44              |
| 4:5:155:SER:O   | 4:9:108:ALA:CB[1_554]  | 1.76                     | 0.44              |
| 4:3:318:THR:N   | 4:7:150:GLY:CA[1_554]  | 1.76                     | 0.44              |
| 4:5:275:HIS:N   | 4:9:162:ASN:CA[1_554]  | 1.76                     | 0.44              |
| 4:3:275:HIS:N   | 4:7:162:ASN:CA[1_554]  | 1.76                     | 0.44              |
| 4:3:306:TYR:O   | 4:7:339:VAL:CB[1_554]  | 1.76                     | 0.44              |
| 4:3:325:MET:CB  | 4:7:166:TYR:OH[1_554]  | 1.76                     | 0.44              |
| 4:5:62:ARG:NH1  | 4:9:67:LEU:CA[1_554]   | 1.76                     | 0.44              |
| 4:4:278:THR:CB  | 4:8:164:PRO:CD[1_554]  | 1.76                     | 0.44              |
| 4:3:262:PHE:CD1 | 4:7:153:LEU:CA[1_554]  | 1.76                     | 0.44              |
| 4:4:276:GLU:O   | 4:8:281:SER:OG[1_554]  | 1.76                     | 0.44              |
| 4:5:24:ASP:C    | 4:9:124:PHE:CG[1_554]  | 1.76                     | 0.44              |
| 4:5:276:GLU:OE2 | 4:9:278:THR:CA[1_554]  | 1.76                     | 0.44              |
| 4:3:281:SER:N   | 4:7:174:ALA:N[1_554]   | 1.76                     | 0.44              |
| 4:4:19:ALA:N    | 4:8:118:LYS:CE[1_554]  | 1.76                     | 0.44              |
| 4:5:302:GLY:O   | 4:9:12:ASN:O[1_554]    | 1.77                     | 0.43              |
| 4:3:32:PRO:N    | 4:7:78:ASN:ND2[1_554]  | 1.77                     | 0.43              |
| 4:5:31:PHE:N    | 4:9:79:TRP:C[1_554]    | 1.77                     | 0.43              |
| 4:5:196:ARG:NE  | 4:9:211:ASP:C[1_554]   | 1.77                     | 0.43              |
| 4:3:341:ILE:CD1 | 4:7:120:THR:N[1_554]   | 1.77                     | 0.43              |
| 4:5:192:ILE:N   | 4:9:186:THR:N[1_554]   | 1.77                     | 0.43              |
| 4:4:150:GLY:C   | 4:8:169:TYR:CE1[1_554] | 1.77                     | 0.43              |
| 4:3:240:TYR:OH  | 4:7:56:ASP:CA[1_554]   | 1.77                     | 0.43              |
| 4:3:277:THR:CA  | 4:7:174:ALA:C[1_554]   | 1.77                     | 0.43              |
| 4:3:204:ALA:CB  | 4:7:63:GLY:N[1_554]    | 1.77                     | 0.43              |
| 4:5:334:GLU:C   | 4:9:105:LEU:N[1_554]   | 1.77                     | 0.43              |
| 4:5:212:ILE:O   | 4:9:16:LEU:CD2[1_554]  | 1.77                     | 0.43              |
| 4:5:371:HIS:ND1 | 4:V:252:ASN:CB[1_554]  | 1.77                     | 0.43              |
| 4:3:309:ILE:N   | 4:7:339:VAL:CB[1_554]  | 1.77                     | 0.43              |
| 4:3:345:ILE:C   | 4:7:366:GLY:CA[1_554]  | 1.77                     | 0.43              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:211:ASP:OD1 | 4:8:32:PRO:CG[1_554]   | 1.77                     | 0.43              |
| 4:3:329:ILE:CG2 | 4:7:139:VAL:CG2[1_554] | 1.77                     | 0.43              |
| 4:5:346:LEU:CD2 | 4:9:368:SER:CA[1_554]  | 1.77                     | 0.43              |
| 4:5:196:ARG:CD  | 4:9:211:ASP:C[1_554]   | 1.77                     | 0.43              |
| 4:3:340:TRP:CD1 | 4:7:118:LYS:CG[1_554]  | 1.77                     | 0.43              |
| 4:5:262:PHE:CG  | 4:9:153:LEU:C[1_554]   | 1.77                     | 0.43              |
| 4:4:286:ASP:CG  | 4:9:270:GLU:OE1[1_554] | 1.77                     | 0.43              |
| 4:3:24:ASP:CB   | 4:7:125:GLU:OE1[1_554] | 1.77                     | 0.43              |
| 4:4:266:PHE:CA  | 4:8:261:LEU:CA[1_554]  | 1.77                     | 0.43              |
| 4:4:275:HIS:CB  | 4:8:152:VAL:N[1_554]   | 1.77                     | 0.43              |
| 4:4:304:THR:CB  | 4:8:107:GLU:O[1_554]   | 1.77                     | 0.43              |
| 1:A:553:MLY:CH1 | 4:4:328:LYS:NZ[1_556]  | 1.77                     | 0.43              |
| 1:D:637:LYS:CE  | 4:5:311:ASP:CA[1_556]  | 1.77                     | 0.43              |
| 4:5:295:ALA:N   | 4:9:167:GLU:CA[1_554]  | 1.77                     | 0.43              |
| 4:3:204:ALA:C   | 4:7:62:ARG:CD[1_554]   | 1.77                     | 0.43              |
| 4:3:372:ARG:CB  | 4:8:227:MET:C[1_554]   | 1.77                     | 0.43              |
| 4:5:346:LEU:C   | 4:9:366:GLY:O[1_554]   | 1.77                     | 0.43              |
| 4:5:21:PHE:CB   | 4:9:125:GLU:CG[1_554]  | 1.77                     | 0.43              |
| 4:4:112:PRO:CD  | 4:9:193:LEU:CD1[1_554] | 1.77                     | 0.43              |
| 4:5:316:GLU:CG  | 4:9:298:VAL:N[1_554]   | 1.77                     | 0.43              |
| 4:5:362:TYR:CE1 | 4:V:233:SER:O[1_554]   | 1.77                     | 0.43              |
| 4:5:322:PRO:CB  | 4:9:291:LYS:CE[1_554]  | 1.77                     | 0.43              |
| 4:3:199:SER:N   | 4:7:206:ARG:N[1_554]   | 1.77                     | 0.43              |
| 4:2:115:ASN:ND2 | 4:7:198:TYR:CE2[1_554] | 1.77                     | 0.43              |
| 4:5:187:ASP:N   | 4:9:183:ARG:CD[1_554]  | 1.77                     | 0.43              |
| 4:5:289:ILE:CA  | 4:W:63:GLY:C[1_554]    | 1.77                     | 0.43              |
| 4:3:275:HIS:ND1 | 4:7:152:VAL:O[1_554]   | 1.77                     | 0.43              |
| 4:3:276:GLU:CG  | 4:7:278:THR:O[1_554]   | 1.77                     | 0.43              |
| 4:4:345:ILE:CD1 | 4:8:369:ILE:CG2[1_554] | 1.77                     | 0.43              |
| 4:3:191:LYS:C   | 4:7:186:THR:C[1_554]   | 1.77                     | 0.43              |
| 4:3:143:TYR:CE2 | 4:7:368:SER:CA[1_554]  | 1.77                     | 0.43              |
| 4:5:262:PHE:CG  | 4:9:153:LEU:CA[1_554]  | 1.77                     | 0.43              |
| 4:3:313:MET:CG  | 4:7:138:ALA:CA[1_554]  | 1.77                     | 0.43              |
| 4:3:193:LEU:O   | 4:7:210:ARG:CA[1_554]  | 1.77                     | 0.43              |
| 4:3:253:GLU:OE2 | 4:7:214:GLU:CG[1_554]  | 1.77                     | 0.43              |
| 4:4:113:LYS:CA  | 4:9:253:GLU:N[1_554]   | 1.77                     | 0.43              |
| 4:3:204:ALA:O   | 4:7:62:ARG:CD[1_554]   | 1.77                     | 0.43              |
| 4:4:250:ILE:CG2 | 4:8:214:GLU:OE1[1_554] | 1.77                     | 0.43              |
| 4:5:267:ILE:CD1 | 4:9:180:LEU:N[1_554]   | 1.77                     | 0.43              |
| 4:3:217:CYS:O   | 4:7:18:LYS:CD[1_554]   | 1.77                     | 0.43              |
| 4:3:143:TYR:CE2 | 4:7:368:SER:C[1_554]   | 1.77                     | 0.43              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:28:ARG:CZ   | 4:9:125:GLU:O[1_554]   | 1.77                     | 0.43              |
| 4:5:272:ALA:CA  | 4:9:277:THR:CG2[1_554] | 1.77                     | 0.43              |
| 4:4:16:LEU:N    | 4:8:77:THR:N[1_554]    | 1.77                     | 0.43              |
| 4:5:21:PHE:CB   | 4:9:125:GLU:OE1[1_554] | 1.77                     | 0.43              |
| 4:3:372:ARG:C   | 4:8:226:GLU:C[1_554]   | 1.77                     | 0.43              |
| 4:4:191:LYS:O   | 4:8:186:THR:CA[1_554]  | 1.77                     | 0.43              |
| 4:4:196:ARG:CD  | 4:8:211:ASP:CA[1_554]  | 1.77                     | 0.43              |
| 4:5:320:LEU:CB  | 4:9:293:LEU:C[1_554]   | 1.77                     | 0.43              |
| 4:5:191:LYS:N   | 4:9:186:THR:CB[1_554]  | 1.77                     | 0.43              |
| 4:3:162:ASN:CG  | 4:7:175:ILE:CB[1_554]  | 1.77                     | 0.43              |
| 4:5:200:PHE:CA  | 4:9:206:ARG:CD[1_554]  | 1.77                     | 0.43              |
| 4:5:14:SER:C    | 4:9:77:THR:CB[1_554]   | 1.77                     | 0.43              |
| 4:4:337:TYR:CE2 | 4:8:86:TRP:CE3[1_554]  | 1.77                     | 0.43              |
| 4:4:199:SER:C   | 4:8:206:ARG:CG[1_554]  | 1.77                     | 0.43              |
| 4:4:115:ASN:OD1 | 4:9:249:THR:C[1_554]   | 1.77                     | 0.43              |
| 4:3:197:GLY:C   | 4:7:208:ILE:C[1_554]   | 1.77                     | 0.43              |
| 4:4:117:GLU:OE1 | 4:9:237:GLU:N[1_554]   | 1.77                     | 0.43              |
| 4:2:175:ILE:CD1 | 4:7:191:LYS:CE[1_554]  | 1.77                     | 0.43              |
| 4:4:114:ALA:CA  | 4:9:250:ILE:CA[1_554]  | 1.77                     | 0.43              |
| 4:5:299:MET:CA  | 4:9:136:ILE:CG2[1_554] | 1.77                     | 0.43              |
| 4:1:288:ASP:C   | 4:7:39:ARG:NE[1_554]   | 1.78                     | 0.42              |
| 4:5:31:PHE:C    | 4:9:78:ASN:CG[1_554]   | 1.78                     | 0.42              |
| 4:2:369:ILE:O   | 4:7:229:THR:O[1_554]   | 1.78                     | 0.42              |
| 4:5:335:ARG:N   | 4:9:105:LEU:CA[1_554]  | 1.78                     | 0.42              |
| 4:3:24:ASP:CB   | 4:7:125:GLU:CD[1_554]  | 1.78                     | 0.42              |
| 4:2:172:PRO:C   | 4:7:266:PHE:O[1_554]   | 1.78                     | 0.42              |
| 4:5:302:GLY:CA  | 4:9:12:ASN:O[1_554]    | 1.78                     | 0.42              |
| 4:5:327:ILE:O   | 4:9:148:THR:CA[1_554]  | 1.78                     | 0.42              |
| 4:5:76:ILE:O    | 4:V:198:TYR:CE1[1_554] | 1.78                     | 0.42              |
| 4:5:172:PRO:O   | 4:V:266:PHE:O[1_554]   | 1.78                     | 0.42              |
| 4:4:263:GLN:CB  | 4:8:274:ILE:CG1[1_554] | 1.78                     | 0.42              |
| 4:3:369:ILE:CG2 | 4:8:234:SER:N[1_554]   | 1.78                     | 0.42              |
| 4:1:291:LYS:CB  | 4:7:64:ILE:CD1[1_554]  | 1.78                     | 0.42              |
| 4:4:76:ILE:C    | 4:9:198:TYR:CE1[1_554] | 1.78                     | 0.42              |
| 4:3:345:ILE:C   | 4:7:366:GLY:C[1_554]   | 1.78                     | 0.42              |
| 4:3:337:TYR:O   | 4:7:116:ARG:O[1_554]   | 1.78                     | 0.42              |
| 4:3:266:PHE:CE2 | 4:7:303:THR:O[1_554]   | 1.78                     | 0.42              |
| 4:4:345:ILE:O   | 4:8:365:ALA:O[1_554]   | 1.78                     | 0.42              |
| 4:4:75:ILE:CA   | 4:9:197:GLY:O[1_554]   | 1.78                     | 0.42              |
| 4:1:286:ASP:O   | 4:7:39:ARG:NH2[1_554]  | 1.78                     | 0.42              |
| 4:3:181:ALA:CB  | 4:7:73:HIS:O[1_554]    | 1.78                     | 0.42              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:369:ILE:CB  | 4:V:232:SER:CA[1_554]  | 1.78                     | 0.42              |
| 4:5:24:ASP:CG   | 4:9:125:GLU:C[1_554]   | 1.78                     | 0.42              |
| 4:5:274:ILE:CA  | 4:9:162:ASN:C[1_554]   | 1.78                     | 0.42              |
| 4:5:293:LEU:CB  | 4:9:169:TYR:CD2[1_554] | 1.78                     | 0.42              |
| 4:3:18:LYS:CD   | 4:7:79:TRP:CG[1_554]   | 1.78                     | 0.42              |
| 4:4:372:ARG:C   | 4:9:226:GLU:C[1_554]   | 1.78                     | 0.42              |
| 4:4:299:MET:CB  | 4:8:136:ILE:N[1_554]   | 1.78                     | 0.42              |
| 4:4:294:TYR:O   | 4:8:166:TYR:O[1_554]   | 1.78                     | 0.42              |
| 4:3:199:SER:O   | 4:7:203:THR:O[1_554]   | 1.78                     | 0.42              |
| 4:4:110:LEU:O   | 4:9:192:ILE:O[1_554]   | 1.78                     | 0.42              |
| 4:4:271:SER:O   | 4:8:277:THR:CB[1_554]  | 1.78                     | 0.42              |
| 4:4:221:LEU:O   | 4:8:332:PRO:CB[1_554]  | 1.78                     | 0.42              |
| 4:5:30:VAL:C    | 4:9:79:TRP:O[1_554]    | 1.78                     | 0.42              |
| 4:4:243:PRO:CG  | 4:8:60:SER:CA[1_554]   | 1.78                     | 0.42              |
| 4:3:263:GLN:CD  | 4:7:153:LEU:CD2[1_554] | 1.78                     | 0.42              |
| 4:5:337:TYR:C   | 4:9:119:MET:CE[1_554]  | 1.78                     | 0.42              |
| 4:3:331:ALA:CA  | 4:7:135:ALA:C[1_554]   | 1.78                     | 0.42              |
| 4:5:260:THR:CA  | 4:9:155:SER:OG[1_554]  | 1.78                     | 0.42              |
| 4:4:262:PHE:CB  | 4:8:153:LEU:CA[1_554]  | 1.78                     | 0.42              |
| 4:5:207:GLU:OE1 | 4:9:67:LEU:CG[1_554]   | 1.78                     | 0.42              |
| 4:5:322:PRO:CB  | 4:9:288:ASP:O[1_554]   | 1.78                     | 0.42              |
| 4:3:303:THR:N   | 4:7:74:GLY:O[1_554]    | 1.78                     | 0.42              |
| 4:5:208:ILE:CB  | 4:9:59:GLN:NE2[1_554]  | 1.78                     | 0.42              |
| 4:5:30:VAL:O    | 4:9:80:ASP:C[1_554]    | 1.78                     | 0.42              |
| 4:5:320:LEU:CB  | 4:9:293:LEU:CA[1_554]  | 1.78                     | 0.42              |
| 4:5:185:LEU:CD1 | 4:9:181:ALA:CB[1_554]  | 1.78                     | 0.42              |
| 4:4:204:ALA:CB  | 4:8:63:GLY:N[1_554]    | 1.78                     | 0.42              |
| 4:5:267:ILE:CA  | 4:9:180:LEU:CD2[1_554] | 1.78                     | 0.42              |
| 4:3:208:ILE:C   | 4:7:59:GLN:NE2[1_554]  | 1.78                     | 0.42              |
| 4:5:337:TYR:CZ  | 4:9:86:TRP:CD2[1_554]  | 1.78                     | 0.42              |
| 4:3:153:LEU:CD2 | 4:7:109:PRO:CD[1_554]  | 1.78                     | 0.42              |
| 4:3:314:GLN:C   | 4:7:142:LEU:CB[1_554]  | 1.78                     | 0.42              |
| 4:5:294:TYR:CB  | 4:9:166:TYR:CD2[1_554] | 1.78                     | 0.42              |
| 4:4:343:GLY:O   | 4:8:367:PRO:CD[1_554]  | 1.78                     | 0.42              |
| 4:5:136:ILE:N   | 4:9:113:LYS:CD[1_554]  | 1.78                     | 0.42              |
| 4:3:266:PHE:CD1 | 4:7:261:LEU:CG[1_554]  | 1.78                     | 0.42              |
| 4:2:173:HIS:NE2 | 4:7:266:PHE:N[1_554]   | 1.78                     | 0.42              |
| 4:2:289:ILE:CG2 | 4:8:39:ARG:CZ[1_554]   | 1.78                     | 0.42              |
| 4:3:258:PRO:C   | 4:7:155:SER:CA[1_554]  | 1.78                     | 0.42              |
| 4:2:173:HIS:N   | 4:7:266:PHE:O[1_554]   | 1.78                     | 0.42              |
| 4:4:333:PRO:O   | 4:8:105:LEU:CB[1_554]  | 1.78                     | 0.42              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:341:ILE:CG1 | 4:8:120:THR:OG1[1_554] | 1.78                     | 0.42              |
| 4:5:24:ASP:O    | 4:9:124:PHE:CD2[1_554] | 1.78                     | 0.42              |
| 4:3:319:ALA:CA  | 4:7:296:ASN:CB[1_554]  | 1.78                     | 0.42              |
| 4:5:28:ARG:C    | 4:9:83:GLU:OE1[1_554]  | 1.78                     | 0.42              |
| 4:3:371:HIS:CA  | 4:8:230:ALA:CB[1_554]  | 1.78                     | 0.42              |
| 4:5:173:HIS:CG  | 4:V:264:PRO:O[1_554]   | 1.78                     | 0.42              |
| 4:5:340:TRP:C   | 4:9:120:THR:CB[1_554]  | 1.78                     | 0.42              |
| 4:4:257:CYS:N   | 4:8:303:THR:CA[1_554]  | 1.78                     | 0.42              |
| 4:4:341:ILE:CG2 | 4:8:120:THR:CB[1_554]  | 1.78                     | 0.42              |
| 4:5:299:MET:CG  | 4:9:138:ALA:N[1_554]   | 1.78                     | 0.42              |
| 4:3:136:ILE:O   | 4:7:113:LYS:CE[1_554]  | 1.78                     | 0.42              |
| 4:3:18:LYS:CD   | 4:7:79:TRP:NE1[1_554]  | 1.78                     | 0.42              |
| 4:5:75:ILE:CB   | 4:V:197:GLY:C[1_554]   | 1.78                     | 0.42              |
| 4:4:266:PHE:N   | 4:8:261:LEU:CB[1_554]  | 1.78                     | 0.42              |
| 4:3:333:PRO:O   | 4:7:105:LEU:CD2[1_554] | 1.78                     | 0.42              |
| 4:4:254:ARG:CZ  | 4:8:337:TYR:OH[1_554]  | 1.78                     | 0.42              |
| 4:4:300:SER:C   | 4:8:107:GLU:CG[1_554]  | 1.78                     | 0.42              |
| 4:5:214:GLU:N   | 4:9:16:LEU:CA[1_554]   | 1.78                     | 0.42              |
| 4:4:325:MET:CE  | 4:8:166:TYR:OH[1_554]  | 1.78                     | 0.42              |
| 4:4:188:TYR:CB  | 4:8:181:ALA:C[1_554]   | 1.78                     | 0.42              |
| 4:3:281:SER:CA  | 4:7:173:HIS:C[1_554]   | 1.78                     | 0.42              |
| 4:3:215:LYS:CB  | 4:7:31:PHE:O[1_554]    | 1.78                     | 0.42              |
| 4:4:140:LEU:N   | 4:8:371:HIS:ND1[1_554] | 1.78                     | 0.42              |
| 4:3:183:ARG:CB  | 4:7:72:GLU:OE2[1_554]  | 1.78                     | 0.42              |
| 4:3:274:ILE:O   | 4:7:163:VAL:CA[1_554]  | 1.78                     | 0.42              |
| 4:5:163:VAL:C   | 4:9:172:PRO:CB[1_554]  | 1.78                     | 0.42              |
| 4:5:240:TYR:OH  | 4:9:56:ASP:OD2[1_554]  | 1.78                     | 0.42              |
| 4:3:196:ARG:NE  | 4:7:211:ASP:CB[1_554]  | 1.78                     | 0.42              |
| 4:5:184:ASP:OD1 | 4:9:73:HIS:NE2[1_554]  | 1.78                     | 0.42              |
| 4:2:116:ARG:O   | 4:7:237:GLU:CG[1_554]  | 1.78                     | 0.42              |
| 4:5:144:ALA:C   | 4:9:372:ARG:NH2[1_554] | 1.79                     | 0.41              |
| 4:3:145:SER:CB  | 4:7:372:ARG:CZ[1_554]  | 1.79                     | 0.41              |
| 4:5:210:ARG:CG  | 4:9:69:TYR:CE2[1_554]  | 1.79                     | 0.41              |
| 4:3:266:PHE:CG  | 4:7:261:LEU:CD2[1_554] | 1.79                     | 0.41              |
| 4:2:291:LYS:CE  | 4:8:64:ILE:O[1_554]    | 1.79                     | 0.41              |
| 4:3:16:LEU:CB   | 4:7:77:THR:C[1_554]    | 1.79                     | 0.41              |
| 4:2:369:ILE:CG2 | 4:7:234:SER:N[1_554]   | 1.79                     | 0.41              |
| 4:4:219:VAL:C   | 4:8:335:ARG:C[1_554]   | 1.79                     | 0.41              |
| 4:3:195:GLU:CG  | 4:7:189:LEU:CB[1_554]  | 1.79                     | 0.41              |
| 4:3:79:TRP:CZ2  | 4:8:249:THR:CG2[1_554] | 1.79                     | 0.41              |
| 4:4:220:ALA:CA  | 4:8:335:ARG:C[1_554]   | 1.79                     | 0.41              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:372:ARG:C   | 4:7:255:PHE:CE2[1_554] | 1.79                     | 0.41              |
| 4:4:157:ASP:OD1 | 4:8:72:GLU:CB[1_554]   | 1.79                     | 0.41              |
| 4:4:136:ILE:N   | 4:8:113:LYS:CE[1_554]  | 1.79                     | 0.41              |
| 4:5:297:ASN:OD1 | 4:9:165:ILE:CB[1_554]  | 1.79                     | 0.41              |
| 4:3:279:TYR:CD2 | 4:7:285:CYS:SG[1_554]  | 1.79                     | 0.41              |
| 4:5:208:ILE:CG1 | 4:9:59:GLN:CB[1_554]   | 1.79                     | 0.41              |
| 4:5:367:PRO:CG  | 4:V:234:SER:O[1_554]   | 1.79                     | 0.41              |
| 4:4:113:LYS:O   | 4:9:251:GLY:N[1_554]   | 1.79                     | 0.41              |
| 4:3:114:ALA:N   | 4:8:250:ILE:O[1_554]   | 1.79                     | 0.41              |
| 4:2:111:ASN:OD1 | 4:7:196:ARG:CG[1_554]  | 1.79                     | 0.41              |
| 4:3:185:LEU:CB  | 4:7:157:ASP:C[1_554]   | 1.79                     | 0.41              |
| 4:3:111:ASN:C   | 4:8:253:GLU:CG[1_554]  | 1.79                     | 0.41              |
| 4:4:362:TYR:CE1 | 4:9:233:SER:O[1_554]   | 1.79                     | 0.41              |
| 4:4:314:GLN:CB  | 4:8:142:LEU:CA[1_554]  | 1.79                     | 0.41              |
| 4:4:227:MET:SD  | 4:8:306:TYR:N[1_554]   | 1.79                     | 0.41              |
| 4:3:214:GLU:OE1 | 4:7:33:SER:CA[1_554]   | 1.79                     | 0.41              |
| 4:3:370:VAL:CA  | 4:8:230:ALA:CA[1_554]  | 1.79                     | 0.41              |
| 4:4:196:ARG:CB  | 4:8:211:ASP:N[1_554]   | 1.79                     | 0.41              |
| 4:4:372:ARG:N   | 4:9:230:ALA:CB[1_554]  | 1.79                     | 0.41              |
| 4:4:281:SER:CA  | 4:8:173:HIS:CD2[1_554] | 1.79                     | 0.41              |
| 4:3:184:ASP:OD1 | 4:7:73:HIS:CD2[1_554]  | 1.79                     | 0.41              |
| 4:5:310:ALA:CA  | 4:9:141:SER:CB[1_554]  | 1.79                     | 0.41              |
| 4:5:214:GLU:CG  | 4:9:16:LEU:N[1_554]    | 1.79                     | 0.41              |
| 4:3:255:PHE:O   | 4:7:302:GLY:CA[1_554]  | 1.79                     | 0.41              |
| 1:A:553:MLY:CH2 | 4:4:326:LYS:NZ[1_556]  | 1.79                     | 0.41              |
| 4:5:11:ASP:OD2  | 4:9:115:ASN:CB[1_554]  | 1.79                     | 0.41              |
| 4:2:372:ARG:CG  | 4:7:227:MET:C[1_554]   | 1.79                     | 0.41              |
| 4:5:345:ILE:O   | 4:9:366:GLY:O[1_554]   | 1.79                     | 0.41              |
| 4:5:321:ALA:CA  | 4:9:292:ASP:CB[1_554]  | 1.79                     | 0.41              |
| 4:3:140:LEU:CD2 | 4:7:117:GLU:CD[1_554]  | 1.79                     | 0.41              |
| 4:3:368:SER:N   | 4:8:236:LEU:N[1_554]   | 1.79                     | 0.41              |
| 4:5:343:GLY:C   | 4:9:367:PRO:C[1_554]   | 1.79                     | 0.41              |
| 4:4:255:PHE:O   | 4:8:303:THR:N[1_554]   | 1.79                     | 0.41              |
| 4:3:141:SER:C   | 4:7:371:HIS:O[1_554]   | 1.79                     | 0.41              |
| 4:3:339:VAL:O   | 4:7:117:GLU:CA[1_554]  | 1.79                     | 0.41              |
| 4:5:11:ASP:OD2  | 4:9:115:ASN:CA[1_554]  | 1.79                     | 0.41              |
| 4:5:200:PHE:CA  | 4:9:206:ARG:CB[1_554]  | 1.79                     | 0.41              |
| 4:5:60:SER:OG   | 4:9:37:ARG:CG[1_554]   | 1.79                     | 0.41              |
| 4:4:139:VAL:N   | 4:8:113:LYS:CG[1_554]  | 1.79                     | 0.41              |
| 4:3:370:VAL:CA  | 4:8:231:ALA:N[1_554]   | 1.79                     | 0.41              |
| 4:3:197:GLY:C   | 4:7:208:ILE:CG2[1_554] | 1.79                     | 0.41              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:308:GLY:CA  | 4:7:339:VAL:CA[1_554]  | 1.79                     | 0.41              |
| 4:3:309:ILE:N   | 4:7:339:VAL:N[1_554]   | 1.79                     | 0.41              |
| 4:4:270:GLU:N   | 4:8:272:ALA:C[1_554]   | 1.79                     | 0.41              |
| 4:3:281:SER:O   | 4:7:173:HIS:ND1[1_554] | 1.79                     | 0.41              |
| 4:5:22:ALA:N    | 4:9:125:GLU:CD[1_554]  | 1.79                     | 0.41              |
| 4:3:253:GLU:OE2 | 4:7:214:GLU:OE1[1_554] | 1.79                     | 0.41              |
| 4:3:173:HIS:NE2 | 4:8:264:PRO:O[1_554]   | 1.79                     | 0.41              |
| 4:4:184:ASP:OD1 | 4:8:73:HIS:ND1[1_554]  | 1.79                     | 0.41              |
| 4:5:300:SER:O   | 4:9:108:ALA:C[1_554]   | 1.79                     | 0.41              |
| 4:5:267:ILE:CG1 | 4:9:180:LEU:CD2[1_554] | 1.79                     | 0.41              |
| 4:3:367:PRO:CB  | 4:8:234:SER:O[1_554]   | 1.79                     | 0.41              |
| 4:2:116:ARG:CA  | 4:7:237:GLU:OE2[1_554] | 1.79                     | 0.41              |
| 4:4:256:ARG:CA  | 4:8:302:GLY:O[1_554]   | 1.79                     | 0.41              |
| 4:4:288:ASP:O   | 4:V:65:LEU:N[1_554]    | 1.79                     | 0.41              |
| 4:2:368:SER:CA  | 4:7:236:LEU:CA[1_554]  | 1.79                     | 0.41              |
| 4:4:157:ASP:C   | 4:8:72:GLU:C[1_554]    | 1.79                     | 0.41              |
| 4:4:344:SER:O   | 4:8:367:PRO:CD[1_554]  | 1.79                     | 0.41              |
| 4:3:311:ASP:O   | 4:7:142:LEU:N[1_554]   | 1.79                     | 0.41              |
| 4:3:294:TYR:CD2 | 4:7:166:TYR:CG[1_554]  | 1.79                     | 0.41              |
| 4:5:24:ASP:N    | 4:9:124:PHE:CB[1_554]  | 1.79                     | 0.41              |
| 4:5:136:ILE:C   | 4:9:113:LYS:CA[1_554]  | 1.79                     | 0.41              |
| 4:5:273:GLY:C   | 4:9:162:ASN:ND2[1_554] | 1.79                     | 0.41              |
| 4:3:211:ASP:O   | 4:7:32:PRO:C[1_554]    | 1.79                     | 0.41              |
| 4:3:312:ARG:N   | 4:7:141:SER:CA[1_554]  | 1.79                     | 0.41              |
| 4:3:255:PHE:CD2 | 4:7:305:MET:CG[1_554]  | 1.79                     | 0.41              |
| 4:5:178:LEU:CD2 | 4:9:177:ARG:N[1_554]   | 1.79                     | 0.41              |
| 4:3:211:ASP:O   | 4:7:31:PHE:C[1_554]    | 1.79                     | 0.41              |
| 4:5:218:TYR:O   | 4:9:301:GLY:O[1_554]   | 1.79                     | 0.41              |
| 4:5:60:SER:CA   | 4:9:66:THR:OG1[1_554]  | 1.79                     | 0.41              |
| 4:5:207:GLU:OE2 | 4:9:68:LYS:N[1_554]    | 1.79                     | 0.41              |
| 4:4:193:LEU:O   | 4:8:210:ARG:CA[1_554]  | 1.79                     | 0.41              |
| 4:4:308:GLY:C   | 4:8:338:SER:C[1_554]   | 1.79                     | 0.41              |
| 4:4:156:GLY:C   | 4:8:74:GLY:C[1_554]    | 1.79                     | 0.41              |
| 4:3:214:GLU:O   | 4:7:16:LEU:O[1_554]    | 1.79                     | 0.41              |
| 4:4:117:GLU:CB  | 4:9:237:GLU:CG[1_554]  | 1.79                     | 0.41              |
| 4:3:178:LEU:CG  | 4:7:177:ARG:O[1_554]   | 1.80                     | 0.40              |
| 4:3:311:ASP:CB  | 4:7:141:SER:O[1_554]   | 1.80                     | 0.40              |
| 4:3:142:LEU:C   | 4:7:372:ARG:CB[1_554]  | 1.80                     | 0.40              |
| 4:3:253:GLU:OE1 | 4:7:214:GLU:CG[1_554]  | 1.80                     | 0.40              |
| 4:3:243:PRO:CD  | 4:7:60:SER:C[1_554]    | 1.80                     | 0.40              |
| 4:4:166:TYR:CG  | 4:V:40:HIS:CE1[1_554]  | 1.80                     | 0.40              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:336:LYS:CE  | 4:8:86:TRP:CD1[1_554]  | 1.80                     | 0.40              |
| 4:4:26:ALA:N    | 4:8:123:MET:N[1_554]   | 1.80                     | 0.40              |
| 4:3:315:LYS:CA  | 4:7:142:LEU:CD1[1_554] | 1.80                     | 0.40              |
| 4:4:266:PHE:CA  | 4:8:261:LEU:CB[1_554]  | 1.80                     | 0.40              |
| 4:4:316:GLU:CG  | 4:8:298:VAL:O[1_554]   | 1.80                     | 0.40              |
| 4:4:25:ASP:CB   | 4:8:124:PHE:CB[1_554]  | 1.80                     | 0.40              |
| 4:4:307:PRO:CB  | 4:8:340:TRP:CB[1_554]  | 1.80                     | 0.40              |
| 4:4:262:PHE:CB  | 4:8:153:LEU:C[1_554]   | 1.80                     | 0.40              |
| 4:5:299:MET:CB  | 4:9:137:GLN:N[1_554]   | 1.80                     | 0.40              |
| 4:4:223:PHE:CZ  | 4:8:301:GLY:O[1_554]   | 1.80                     | 0.40              |
| 4:5:280:ASN:OD1 | 4:9:280:ASN:C[1_554]   | 1.80                     | 0.40              |
| 4:3:227:MET:CE  | 4:7:306:TYR:CB[1_554]  | 1.80                     | 0.40              |
| 4:3:286:ASP:CB  | 4:8:270:GLU:CD[1_554]  | 1.80                     | 0.40              |
| 4:3:329:ILE:C   | 4:7:139:VAL:CG1[1_554] | 1.80                     | 0.40              |
| 4:3:117:GLU:CB  | 4:8:237:GLU:N[1_554]   | 1.80                     | 0.40              |
| 4:5:260:THR:N   | 4:9:155:SER:OG[1_554]  | 1.80                     | 0.40              |
| 4:5:348:SER:C   | 4:9:365:ALA:N[1_554]   | 1.80                     | 0.40              |
| 4:3:120:THR:CG2 | 4:8:233:SER:CB[1_554]  | 1.80                     | 0.40              |
| 4:5:331:ALA:CB  | 4:9:140:LEU:CA[1_554]  | 1.80                     | 0.40              |
| 4:3:118:LYS:CA  | 4:8:237:GLU:OE1[1_554] | 1.80                     | 0.40              |
| 4:3:112:PRO:CA  | 4:8:253:GLU:CG[1_554]  | 1.80                     | 0.40              |
| 4:3:222:ASP:CB  | 4:7:331:ALA:O[1_554]   | 1.80                     | 0.40              |
| 4:4:343:GLY:C   | 4:8:367:PRO:CG[1_554]  | 1.80                     | 0.40              |
| 4:5:109:PRO:CB  | 4:V:195:GLU:OE2[1_554] | 1.80                     | 0.40              |
| 4:3:299:MET:C   | 4:7:107:GLU:CG[1_554]  | 1.80                     | 0.40              |
| 4:3:286:ASP:CB  | 4:8:270:GLU:OE2[1_554] | 1.80                     | 0.40              |
| 4:3:24:ASP:O    | 4:7:362:TYR:OH[1_554]  | 1.80                     | 0.40              |
| 4:3:342:GLY:CA  | 4:7:367:PRO:O[1_554]   | 1.80                     | 0.40              |
| 4:4:56:ASP:CB   | 4:8:37:ARG:NH2[1_554]  | 1.80                     | 0.40              |
| 4:5:155:SER:N   | 4:9:109:PRO:N[1_554]   | 1.80                     | 0.40              |
| 4:5:166:TYR:CD2 | 4:W:40:HIS:CD2[1_554]  | 1.80                     | 0.40              |
| 4:3:198:TYR:CG  | 4:7:207:GLU:O[1_554]   | 1.80                     | 0.40              |
| 4:4:154:ASP:CA  | 4:8:110:LEU:N[1_554]   | 1.80                     | 0.40              |
| 4:5:143:TYR:CZ  | 4:9:369:ILE:O[1_554]   | 1.80                     | 0.40              |
| 4:3:115:ASN:CA  | 4:8:249:THR:C[1_554]   | 1.80                     | 0.40              |
| 4:4:317:ILE:N   | 4:8:150:GLY:O[1_554]   | 1.80                     | 0.40              |
| 4:2:172:PRO:CB  | 4:7:188:TYR:OH[1_554]  | 1.80                     | 0.40              |
| 4:5:10:CYS:CA   | 4:9:118:LYS:CD[1_554]  | 1.80                     | 0.40              |
| 4:4:367:PRO:CD  | 4:9:234:SER:O[1_554]   | 1.80                     | 0.40              |
| 4:4:211:ASP:OD1 | 4:8:32:PRO:N[1_554]    | 1.80                     | 0.40              |
| 1:A:411:GLU:OE2 | 4:4:225:ASN:O[1_556]   | 1.80                     | 0.40              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:118:LYS:N   | 4:9:237:GLU:CG[1_554]  | 1.80                     | 0.40              |
| 4:3:276:GLU:O   | 4:7:281:SER:OG[1_554]  | 1.80                     | 0.40              |
| 4:5:172:PRO:CG  | 4:V:266:PHE:CG[1_554]  | 1.80                     | 0.40              |
| 4:4:218:TYR:CD2 | 4:8:337:TYR:CG[1_554]  | 1.80                     | 0.40              |
| 4:4:276:GLU:C   | 4:8:281:SER:CB[1_554]  | 1.80                     | 0.40              |
| 4:5:274:ILE:CA  | 4:9:161:HIS:C[1_554]   | 1.80                     | 0.40              |
| 4:5:114:ALA:O   | 4:V:237:GLU:OE1[1_554] | 1.80                     | 0.40              |
| 4:4:276:GLU:OE1 | 4:8:278:THR:C[1_554]   | 1.80                     | 0.40              |
| 4:5:221:LEU:CD2 | 4:9:332:PRO:CG[1_554]  | 1.80                     | 0.40              |
| 4:3:327:ILE:CA  | 4:7:167:GLU:C[1_554]   | 1.80                     | 0.40              |
| 4:5:335:ARG:C   | 4:9:106:THR:N[1_554]   | 1.80                     | 0.40              |
| 4:4:258:PRO:CA  | 4:8:156:GLY:N[1_554]   | 1.80                     | 0.40              |
| 4:3:199:SER:CA  | 4:7:206:ARG:C[1_554]   | 1.80                     | 0.40              |
| 4:3:173:HIS:C   | 4:8:267:ILE:C[1_554]   | 1.80                     | 0.40              |
| 4:5:161:HIS:CB  | 4:9:110:LEU:CD1[1_554] | 1.80                     | 0.40              |
| 4:4:325:MET:CE  | 4:8:166:TYR:CZ[1_554]  | 1.80                     | 0.40              |
| 4:3:337:TYR:CG  | 4:7:119:MET:CB[1_554]  | 1.80                     | 0.40              |
| 4:4:139:VAL:C   | 4:8:371:HIS:CD2[1_554] | 1.80                     | 0.40              |
| 4:3:30:VAL:CG1  | 4:7:79:TRP:O[1_554]    | 1.80                     | 0.40              |
| 4:4:300:SER:OG  | 4:8:107:GLU:OE1[1_554] | 1.80                     | 0.40              |
| 4:5:279:TYR:O   | 4:9:285:CYS:CB[1_554]  | 1.80                     | 0.40              |
| 4:3:183:ARG:CZ  | 4:7:72:GLU:OE1[1_554]  | 1.80                     | 0.40              |
| 4:5:157:ASP:CG  | 4:9:72:GLU:CB[1_554]   | 1.80                     | 0.40              |
| 4:3:198:TYR:CD1 | 4:7:208:ILE:CA[1_554]  | 1.80                     | 0.40              |
| 4:4:178:LEU:CD1 | 4:8:177:ARG:C[1_554]   | 1.80                     | 0.40              |
| 4:4:166:TYR:CE1 | 4:V:40:HIS:CG[1_554]   | 1.80                     | 0.40              |
| 4:5:295:ALA:C   | 4:9:168:GLY:N[1_554]   | 1.80                     | 0.40              |
| 4:4:162:ASN:CG  | 4:8:175:ILE:CD1[1_554] | 1.80                     | 0.40              |
| 4:5:111:ASN:O   | 4:V:256:ARG:NH2[1_554] | 1.80                     | 0.40              |
| 4:5:258:PRO:O   | 4:9:155:SER:CA[1_554]  | 1.80                     | 0.40              |
| 4:4:314:GLN:CB  | 4:8:142:LEU:CB[1_554]  | 1.80                     | 0.40              |
| 4:3:109:PRO:N   | 4:8:195:GLU:CD[1_554]  | 1.80                     | 0.40              |
| 4:4:339:VAL:O   | 4:8:117:GLU:CB[1_554]  | 1.80                     | 0.40              |
| 4:2:372:ARG:O   | 4:7:255:PHE:CE2[1_554] | 1.80                     | 0.40              |
| 4:5:142:LEU:O   | 4:9:372:ARG:CZ[1_554]  | 1.80                     | 0.40              |
| 4:3:250:ILE:CG1 | 4:7:210:ARG:NH1[1_554] | 1.80                     | 0.40              |
| 4:3:370:VAL:CB  | 4:8:230:ALA:C[1_554]   | 1.80                     | 0.40              |
| 4:5:140:LEU:CD2 | 4:9:371:HIS:CG[1_554]  | 1.80                     | 0.40              |
| 4:3:328:LYS:CA  | 4:7:168:GLY:CA[1_554]  | 1.80                     | 0.40              |
| 4:3:16:LEU:CD1  | 4:7:78:ASN:N[1_554]    | 1.80                     | 0.40              |
| 4:3:372:ARG:C   | 4:8:255:PHE:CZ[1_554]  | 1.80                     | 0.40              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:117:GLU:CA  | 4:8:237:GLU:CD[1_554]  | 1.80                     | 0.40              |
| 4:3:215:LYS:CA  | 4:7:31:PHE:N[1_554]    | 1.80                     | 0.40              |
| 4:5:199:SER:C   | 4:9:206:ARG:C[1_554]   | 1.80                     | 0.40              |
| 4:3:180:LEU:C   | 4:7:179:ASP:OD1[1_554] | 1.80                     | 0.40              |
| 4:4:369:ILE:CA  | 4:9:229:THR:C[1_554]   | 1.80                     | 0.40              |
| 4:2:326:LYS:CD  | 4:8:45:VAL:N[1_554]    | 1.80                     | 0.40              |
| 4:4:137:GLN:O   | 4:8:113:LYS:N[1_554]   | 1.80                     | 0.40              |
| 4:5:110:LEU:O   | 4:V:192:ILE:CB[1_554]  | 1.81                     | 0.39              |
| 4:5:266:PHE:CD1 | 4:9:261:LEU:CG[1_554]  | 1.81                     | 0.39              |
| 4:5:299:MET:SD  | 4:9:138:ALA:N[1_554]   | 1.81                     | 0.39              |
| 4:4:262:PHE:CE2 | 4:8:153:LEU:O[1_554]   | 1.81                     | 0.39              |
| 4:4:344:SER:CA  | 4:8:367:PRO:CD[1_554]  | 1.81                     | 0.39              |
| 4:5:340:TRP:CG  | 4:9:119:MET:C[1_554]   | 1.81                     | 0.39              |
| 4:3:257:CYS:C   | 4:7:156:GLY:CA[1_554]  | 1.81                     | 0.39              |
| 4:4:159:VAL:N   | 4:8:177:ARG:NH2[1_554] | 1.81                     | 0.39              |
| 4:4:281:SER:CB  | 4:8:174:ALA:N[1_554]   | 1.81                     | 0.39              |
| 4:3:312:ARG:CZ  | 4:7:299:MET:CB[1_554]  | 1.81                     | 0.39              |
| 4:3:117:GLU:N   | 4:8:237:GLU:CD[1_554]  | 1.81                     | 0.39              |
| 4:4:340:TRP:N   | 4:8:116:ARG:C[1_554]   | 1.81                     | 0.39              |
| 4:4:314:GLN:CB  | 4:8:143:TYR:N[1_554]   | 1.81                     | 0.39              |
| 4:3:299:MET:SD  | 4:7:136:ILE:CG2[1_554] | 1.81                     | 0.39              |
| 4:3:281:SER:N   | 4:7:174:ALA:CB[1_554]  | 1.81                     | 0.39              |
| 4:4:181:ALA:CB  | 4:8:73:HIS:CB[1_554]   | 1.81                     | 0.39              |
| 4:5:113:LYS:O   | 4:V:252:ASN:N[1_554]   | 1.81                     | 0.39              |
| 4:4:166:TYR:CE2 | 4:V:39:ARG:O[1_554]    | 1.81                     | 0.39              |
| 4:3:220:ALA:CB  | 4:7:335:ARG:N[1_554]   | 1.81                     | 0.39              |
| 4:3:311:ASP:CG  | 4:7:144:ALA:CA[1_554]  | 1.81                     | 0.39              |
| 4:5:327:ILE:CA  | 4:9:148:THR:C[1_554]   | 1.81                     | 0.39              |
| 4:4:336:LYS:NZ  | 4:8:86:TRP:CE2[1_554]  | 1.81                     | 0.39              |
| 4:4:111:ASN:O   | 4:9:253:GLU:OE1[1_554] | 1.81                     | 0.39              |
| 4:2:113:LYS:O   | 4:7:250:ILE:C[1_554]   | 1.81                     | 0.39              |
| 4:4:319:ALA:O   | 4:8:293:LEU:C[1_554]   | 1.81                     | 0.39              |
| 4:4:16:LEU:C    | 4:8:77:THR:O[1_554]    | 1.81                     | 0.39              |
| 4:4:192:ILE:N   | 4:8:186:THR:N[1_554]   | 1.81                     | 0.39              |
| 4:5:243:PRO:CG  | 4:9:60:SER:N[1_554]    | 1.81                     | 0.39              |
| 4:5:108:ALA:C   | 4:V:195:GLU:CG[1_554]  | 1.81                     | 0.39              |
| 4:5:172:PRO:C   | 4:V:266:PHE:C[1_554]   | 1.81                     | 0.39              |
| 4:4:346:LEU:CD1 | 4:8:368:SER:OG[1_554]  | 1.81                     | 0.39              |
| 4:5:166:TYR:CA  | 4:W:40:HIS:CD2[1_554]  | 1.81                     | 0.39              |
| 4:3:334:GLU:N   | 4:7:105:LEU:CG[1_554]  | 1.81                     | 0.39              |
| 1:D:542:PHE:CD2 | 4:5:328:LYS:NZ[1_556]  | 1.81                     | 0.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:285:CYS:O   | 4:7:270:GLU:CG[1_554]  | 1.81                     | 0.39              |
| 4:3:327:ILE:CD1 | 4:7:167:GLU:N[1_554]   | 1.81                     | 0.39              |
| 4:5:208:ILE:N   | 4:9:59:GLN:CD[1_554]   | 1.81                     | 0.39              |
| 4:3:262:PHE:CG  | 4:7:153:LEU:CA[1_554]  | 1.81                     | 0.39              |
| 4:3:339:VAL:N   | 4:7:116:ARG:CB[1_554]  | 1.81                     | 0.39              |
| 4:5:268:GLY:O   | 4:9:264:PRO:CB[1_554]  | 1.81                     | 0.39              |
| 4:5:336:LYS:CG  | 4:9:12:ASN:CG[1_554]   | 1.81                     | 0.39              |
| 4:5:252:ASN:OD1 | 4:9:215:LYS:CA[1_554]  | 1.81                     | 0.39              |
| 4:4:370:VAL:CG1 | 4:9:233:SER:OG[1_554]  | 1.81                     | 0.39              |
| 4:3:75:ILE:N    | 4:8:198:TYR:CA[1_554]  | 1.81                     | 0.39              |
| 4:4:143:TYR:CA  | 4:8:371:HIS:C[1_554]   | 1.81                     | 0.39              |
| 4:3:154:ASP:OD1 | 4:7:111:ASN:CG[1_554]  | 1.81                     | 0.39              |
| 4:5:111:ASN:CA  | 4:V:192:ILE:O[1_554]   | 1.81                     | 0.39              |
| 4:4:308:GLY:C   | 4:8:338:SER:CB[1_554]  | 1.81                     | 0.39              |
| 4:4:30:VAL:N    | 4:8:79:TRP:O[1_554]    | 1.81                     | 0.39              |
| 4:5:255:PHE:CD1 | 4:9:305:MET:N[1_554]   | 1.81                     | 0.39              |
| 4:3:173:HIS:N   | 4:8:267:ILE:N[1_554]   | 1.81                     | 0.39              |
| 4:3:212:ILE:C   | 4:7:16:LEU:CD1[1_554]  | 1.81                     | 0.39              |
| 4:4:309:ILE:N   | 4:8:339:VAL:CA[1_554]  | 1.81                     | 0.39              |
| 4:5:317:ILE:CG1 | 4:9:150:GLY:CA[1_554]  | 1.81                     | 0.39              |
| 4:5:193:LEU:CB  | 4:9:210:ARG:CG[1_554]  | 1.81                     | 0.39              |
| 4:5:193:LEU:C   | 4:9:209:VAL:O[1_554]   | 1.81                     | 0.39              |
| 4:5:261:LEU:N   | 4:9:155:SER:CB[1_554]  | 1.81                     | 0.39              |
| 4:2:115:ASN:O   | 4:7:196:ARG:NH2[1_554] | 1.81                     | 0.39              |
| 4:3:333:PRO:CB  | 4:7:104:LEU:O[1_554]   | 1.81                     | 0.39              |
| 4:3:178:LEU:CD1 | 4:7:177:ARG:C[1_554]   | 1.81                     | 0.39              |
| 4:4:334:GLU:N   | 4:8:105:LEU:CB[1_554]  | 1.81                     | 0.39              |
| 4:5:270:GLU:N   | 4:9:272:ALA:O[1_554]   | 1.81                     | 0.39              |
| 4:3:279:TYR:N   | 4:7:164:PRO:CB[1_554]  | 1.81                     | 0.39              |
| 4:5:31:PHE:CB   | 4:9:80:ASP:N[1_554]    | 1.81                     | 0.39              |
| 4:3:305:MET:O   | 4:7:11:ASP:OD2[1_554]  | 1.81                     | 0.39              |
| 4:5:276:GLU:OE1 | 4:9:279:TYR:N[1_554]   | 1.81                     | 0.39              |
| 4:4:327:ILE:CG1 | 4:8:149:THR:CB[1_554]  | 1.81                     | 0.39              |
| 4:4:337:TYR:CB  | 4:8:119:MET:CG[1_554]  | 1.81                     | 0.39              |
| 4:2:172:PRO:CB  | 4:7:188:TYR:CZ[1_554]  | 1.81                     | 0.39              |
| 4:5:348:SER:CB  | 4:9:362:TYR:C[1_554]   | 1.81                     | 0.39              |
| 4:4:342:GLY:O   | 4:8:367:PRO:O[1_554]   | 1.81                     | 0.39              |
| 4:4:267:ILE:CA  | 4:8:180:LEU:CG[1_554]  | 1.81                     | 0.39              |
| 4:5:371:HIS:CG  | 4:V:230:ALA:CB[1_554]  | 1.81                     | 0.39              |
| 4:4:256:ARG:NH2 | 4:8:213:LYS:O[1_554]   | 1.81                     | 0.39              |
| 4:3:25:ASP:CA   | 4:7:124:PHE:CB[1_554]  | 1.81                     | 0.39              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:31:PHE:O    | 4:9:78:ASN:CB[1_554]   | 1.81                     | 0.39              |
| 4:4:215:LYS:CD  | 4:8:31:PHE:CG[1_554]   | 1.81                     | 0.39              |
| 4:3:337:TYR:N   | 4:7:119:MET:CE[1_554]  | 1.81                     | 0.39              |
| 4:3:343:GLY:N   | 4:7:117:GLU:CB[1_554]  | 1.81                     | 0.39              |
| 4:4:142:LEU:C   | 4:8:372:ARG:CA[1_554]  | 1.81                     | 0.39              |
| 4:4:31:PHE:N    | 4:8:79:TRP:C[1_554]    | 1.82                     | 0.38              |
| 4:3:113:LYS:C   | 4:8:251:GLY:N[1_554]   | 1.82                     | 0.38              |
| 4:4:335:ARG:CB  | 4:8:106:THR:C[1_554]   | 1.82                     | 0.38              |
| 4:4:297:ASN:CG  | 4:8:170:ALA:CB[1_554]  | 1.82                     | 0.38              |
| 4:4:342:GLY:C   | 4:8:367:PRO:C[1_554]   | 1.82                     | 0.38              |
| 4:4:328:LYS:O   | 4:8:168:GLY:C[1_554]   | 1.82                     | 0.38              |
| 4:5:141:SER:OG  | 4:9:116:ARG:NE[1_554]  | 1.82                     | 0.38              |
| 4:4:370:VAL:CG2 | 4:9:231:ALA:CA[1_554]  | 1.82                     | 0.38              |
| 4:4:211:ASP:C   | 4:8:32:PRO:N[1_554]    | 1.82                     | 0.38              |
| 4:4:288:ASP:C   | 4:V:64:ILE:CA[1_554]   | 1.82                     | 0.38              |
| 4:3:281:SER:CA  | 4:7:173:HIS:CG[1_554]  | 1.82                     | 0.38              |
| 4:4:156:GLY:O   | 4:8:74:GLY:C[1_554]    | 1.82                     | 0.38              |
| 4:4:75:ILE:N    | 4:9:197:GLY:CA[1_554]  | 1.82                     | 0.38              |
| 4:3:267:ILE:CD1 | 4:7:180:LEU:CB[1_554]  | 1.82                     | 0.38              |
| 4:2:173:HIS:CD2 | 4:7:267:ILE:N[1_554]   | 1.82                     | 0.38              |
| 4:4:286:ASP:CA  | 4:9:270:GLU:CG[1_554]  | 1.82                     | 0.38              |
| 4:4:145:SER:CB  | 4:8:372:ARG:NE[1_554]  | 1.82                     | 0.38              |
| 4:2:173:HIS:CE1 | 4:7:265:SER:C[1_554]   | 1.82                     | 0.38              |
| 4:3:142:LEU:CB  | 4:7:372:ARG:O[1_554]   | 1.82                     | 0.38              |
| 4:1:287:ILE:C   | 4:7:39:ARG:NH1[1_554]  | 1.82                     | 0.38              |
| 4:4:264:PRO:CA  | 4:8:274:ILE:CD1[1_554] | 1.82                     | 0.38              |
| 4:5:199:SER:N   | 4:9:206:ARG:CA[1_554]  | 1.82                     | 0.38              |
| 4:4:299:MET:CE  | 4:8:136:ILE:C[1_554]   | 1.82                     | 0.38              |
| 4:3:156:GLY:C   | 4:7:75:ILE:CA[1_554]   | 1.82                     | 0.38              |
| 4:5:198:TYR:CG  | 4:9:209:VAL:N[1_554]   | 1.82                     | 0.38              |
| 4:5:307:PRO:O   | 4:9:338:SER:N[1_554]   | 1.82                     | 0.38              |
| 4:4:277:THR:OG1 | 4:8:176:MET:N[1_554]   | 1.82                     | 0.38              |
| 4:5:194:THR:CB  | 4:9:190:MET:SD[1_554]  | 1.82                     | 0.38              |
| 4:3:338:SER:CA  | 4:7:116:ARG:CA[1_554]  | 1.82                     | 0.38              |
| 4:4:185:LEU:N   | 4:8:158:GLY:C[1_554]   | 1.82                     | 0.38              |
| 4:5:213:LYS:CG  | 4:9:157:ASP:CB[1_554]  | 1.82                     | 0.38              |
| 4:4:332:PRO:O   | 4:8:105:LEU:C[1_554]   | 1.82                     | 0.38              |
| 4:4:326:LYS:CE  | 4:V:45:VAL:CB[1_554]   | 1.82                     | 0.38              |
| 4:5:312:ARG:NH1 | 4:9:299:MET:SD[1_554]  | 1.82                     | 0.38              |
| 4:5:151:ILE:CG1 | 4:9:171:LEU:CA[1_554]  | 1.82                     | 0.38              |
| 4:5:75:ILE:N    | 4:V:197:GLY:CA[1_554]  | 1.82                     | 0.38              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:370:VAL:O   | 4:9:231:ALA:N[1_554]   | 1.82                     | 0.38              |
| 4:4:326:LYS:N   | 4:8:167:GLU:OE2[1_554] | 1.82                     | 0.38              |
| 4:5:317:ILE:N   | 4:9:296:ASN:O[1_554]   | 1.82                     | 0.38              |
| 4:4:269:MET:CA  | 4:8:271:SER:OG[1_554]  | 1.82                     | 0.38              |
| 4:4:345:ILE:O   | 4:8:366:GLY:C[1_554]   | 1.82                     | 0.38              |
| 4:4:326:LYS:CG  | 4:8:167:GLU:OE1[1_554] | 1.82                     | 0.38              |
| 4:3:207:GLU:CB  | 4:7:67:LEU:CD1[1_554]  | 1.82                     | 0.38              |
| 4:5:196:ARG:CZ  | 4:9:215:LYS:CG[1_554]  | 1.82                     | 0.38              |
| 4:4:283:MET:CB  | 4:8:285:CYS:O[1_554]   | 1.82                     | 0.38              |
| 4:3:256:ARG:CA  | 4:7:303:THR:N[1_554]   | 1.82                     | 0.38              |
| 4:5:19:ALA:C    | 4:9:122:ILE:CG1[1_554] | 1.82                     | 0.38              |
| 4:4:253:GLU:CG  | 4:8:214:GLU:CD[1_554]  | 1.82                     | 0.38              |
| 4:5:218:TYR:C   | 4:9:336:LYS:CA[1_554]  | 1.82                     | 0.38              |
| 4:5:221:LEU:CA  | 4:9:331:ALA:C[1_554]   | 1.82                     | 0.38              |
| 4:5:193:LEU:CA  | 4:9:210:ARG:N[1_554]   | 1.82                     | 0.38              |
| 4:3:190:MET:SD  | 4:7:206:ARG:NH2[1_554] | 1.82                     | 0.38              |
| 4:4:140:LEU:N   | 4:8:371:HIS:CD2[1_554] | 1.82                     | 0.38              |
| 4:5:145:SER:CB  | 4:9:372:ARG:CZ[1_554]  | 1.82                     | 0.38              |
| 4:3:153:LEU:CD1 | 4:7:109:PRO:CB[1_554]  | 1.82                     | 0.38              |
| 4:4:286:ASP:CB  | 4:9:270:GLU:OE2[1_554] | 1.82                     | 0.38              |
| 4:3:157:ASP:OD2 | 4:7:72:GLU:CG[1_554]   | 1.82                     | 0.38              |
| 4:3:314:GLN:CB  | 4:7:142:LEU:CB[1_554]  | 1.82                     | 0.38              |
| 4:3:211:ASP:N   | 4:7:34:ILE:CD1[1_554]  | 1.82                     | 0.38              |
| 4:4:153:LEU:O   | 4:8:108:ALA:O[1_554]   | 1.82                     | 0.38              |
| 4:5:281:SER:OG  | 4:9:172:PRO:C[1_554]   | 1.82                     | 0.38              |
| 4:4:327:ILE:CA  | 4:8:148:THR:O[1_554]   | 1.82                     | 0.38              |
| 4:5:25:ASP:N    | 4:9:124:PHE:N[1_554]   | 1.82                     | 0.38              |
| 4:3:255:PHE:CG  | 4:7:305:MET:SD[1_554]  | 1.82                     | 0.38              |
| 4:4:117:GLU:CA  | 4:9:237:GLU:CD[1_554]  | 1.82                     | 0.38              |
| 4:4:172:PRO:CG  | 4:9:266:PHE:CD2[1_554] | 1.82                     | 0.38              |
| 4:5:159:VAL:N   | 4:9:177:ARG:NH1[1_554] | 1.82                     | 0.38              |
| 4:2:357:ILE:CA  | 4:7:232:SER:C[1_554]   | 1.82                     | 0.38              |
| 4:4:255:PHE:CZ  | 4:8:305:MET:CB[1_554]  | 1.82                     | 0.38              |
| 4:3:74:GLY:O    | 4:8:197:GLY:C[1_554]   | 1.82                     | 0.38              |
| 4:4:332:PRO:CD  | 4:8:134:VAL:O[1_554]   | 1.82                     | 0.38              |
| 4:3:222:ASP:CG  | 4:7:331:ALA:C[1_554]   | 1.82                     | 0.38              |
| 4:4:291:LYS:NZ  | 4:V:64:ILE:CG1[1_554]  | 1.82                     | 0.38              |
| 4:4:274:ILE:CB  | 4:8:161:HIS:CB[1_554]  | 1.82                     | 0.38              |
| 4:4:222:ASP:CB  | 4:8:332:PRO:N[1_554]   | 1.82                     | 0.38              |
| 4:4:198:TYR:C   | 4:8:206:ARG:O[1_554]   | 1.82                     | 0.38              |
| 4:4:333:PRO:N   | 4:8:105:LEU:N[1_554]   | 1.82                     | 0.38              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:315:LYS:NZ  | 4:7:147:ARG:NH1[1_554] | 1.82                     | 0.38              |
| 4:4:368:SER:N   | 4:9:236:LEU:CD2[1_554] | 1.82                     | 0.38              |
| 4:3:219:VAL:O   | 4:7:338:SER:N[1_554]   | 1.82                     | 0.38              |
| 4:5:325:MET:CG  | 4:9:166:TYR:OH[1_554]  | 1.82                     | 0.38              |
| 4:5:213:LYS:NZ  | 4:9:15:GLY:N[1_554]    | 1.82                     | 0.38              |
| 4:4:199:SER:CB  | 4:8:206:ARG:CA[1_554]  | 1.82                     | 0.38              |
| 4:5:314:GLN:CD  | 4:9:147:ARG:CA[1_554]  | 1.82                     | 0.38              |
| 4:5:326:LYS:N   | 4:9:167:GLU:OE2[1_554] | 1.82                     | 0.38              |
| 4:4:344:SER:CA  | 4:8:367:PRO:CB[1_554]  | 1.82                     | 0.38              |
| 4:3:256:ARG:CA  | 4:7:302:GLY:C[1_554]   | 1.82                     | 0.38              |
| 4:3:184:ASP:CA  | 4:7:73:HIS:CE1[1_554]  | 1.82                     | 0.38              |
| 4:2:117:GLU:CG  | 4:7:237:GLU:CA[1_554]  | 1.82                     | 0.38              |
| 4:5:173:HIS:NE2 | 4:V:265:SER:C[1_554]   | 1.82                     | 0.38              |
| 4:5:218:TYR:CB  | 4:9:336:LYS:N[1_554]   | 1.82                     | 0.38              |
| 4:4:263:GLN:O   | 4:8:274:ILE:CD1[1_554] | 1.82                     | 0.38              |
| 4:4:17:VAL:C    | 4:8:79:TRP:CB[1_554]   | 1.82                     | 0.38              |
| 4:3:75:ILE:CG2  | 4:8:198:TYR:CB[1_554]  | 1.82                     | 0.38              |
| 4:5:331:ALA:C   | 4:9:140:LEU:CG[1_554]  | 1.82                     | 0.38              |
| 4:3:211:ASP:OD2 | 4:7:55:GLY:CA[1_554]   | 1.83                     | 0.37              |
| 4:2:110:LEU:C   | 4:7:192:ILE:O[1_554]   | 1.83                     | 0.37              |
| 4:3:210:ARG:CD  | 4:7:69:TYR:CA[1_554]   | 1.83                     | 0.37              |
| 4:3:293:LEU:CG  | 4:7:169:TYR:CE2[1_554] | 1.83                     | 0.37              |
| 4:3:75:ILE:CB   | 4:8:198:TYR:CA[1_554]  | 1.83                     | 0.37              |
| 4:5:347:ALA:C   | 4:9:366:GLY:N[1_554]   | 1.83                     | 0.37              |
| 4:3:188:TYR:CE2 | 4:7:182:GLY:CA[1_554]  | 1.83                     | 0.37              |
| 4:3:154:ASP:CA  | 4:7:110:LEU:C[1_554]   | 1.83                     | 0.37              |
| 4:3:305:MET:CA  | 4:7:106:THR:OG1[1_554] | 1.83                     | 0.37              |
| 4:4:243:PRO:CD  | 4:8:59:GLN:O[1_554]    | 1.83                     | 0.37              |
| 4:3:157:ASP:O   | 4:7:72:GLU:O[1_554]    | 1.83                     | 0.37              |
| 4:4:366:GLY:O   | 4:9:234:SER:OG[1_554]  | 1.83                     | 0.37              |
| 4:3:213:LYS:CA  | 4:7:16:LEU:N[1_554]    | 1.83                     | 0.37              |
| 4:4:215:LYS:CG  | 4:8:31:PHE:CG[1_554]   | 1.83                     | 0.37              |
| 4:3:141:SER:OG  | 4:7:116:ARG:CB[1_554]  | 1.83                     | 0.37              |
| 4:5:159:VAL:CA  | 4:9:177:ARG:NH2[1_554] | 1.83                     | 0.37              |
| 4:2:110:LEU:C   | 4:7:193:LEU:N[1_554]   | 1.83                     | 0.37              |
| 4:3:115:ASN:ND2 | 4:8:198:TYR:CZ[1_554]  | 1.83                     | 0.37              |
| 4:5:337:TYR:CE1 | 4:9:86:TRP:CE2[1_554]  | 1.83                     | 0.37              |
| 4:5:113:LYS:CE  | 4:V:252:ASN:O[1_554]   | 1.83                     | 0.37              |
| 4:2:114:ALA:N   | 4:7:250:ILE:CB[1_554]  | 1.83                     | 0.37              |
| 4:3:192:ILE:CA  | 4:7:186:THR:OG1[1_554] | 1.83                     | 0.37              |
| 4:4:178:LEU:CG  | 4:8:177:ARG:O[1_554]   | 1.83                     | 0.37              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:215:LYS:N   | 4:9:16:LEU:CB[1_554]   | 1.83                     | 0.37              |
| 4:4:193:LEU:CD1 | 4:8:210:ARG:NE[1_554]  | 1.83                     | 0.37              |
| 4:3:156:GLY:CA  | 4:7:75:ILE:CG1[1_554]  | 1.83                     | 0.37              |
| 4:4:371:HIS:CE1 | 4:9:252:ASN:O[1_554]   | 1.83                     | 0.37              |
| 4:4:297:ASN:N   | 4:8:168:GLY:O[1_554]   | 1.83                     | 0.37              |
| 4:4:173:HIS:ND1 | 4:9:267:ILE:N[1_554]   | 1.83                     | 0.37              |
| 4:4:188:TYR:C   | 4:8:183:ARG:C[1_554]   | 1.83                     | 0.37              |
| 4:4:310:ALA:O   | 4:8:141:SER:C[1_554]   | 1.83                     | 0.37              |
| 4:3:172:PRO:CB  | 4:8:188:TYR:OH[1_554]  | 1.83                     | 0.37              |
| 4:4:178:LEU:CD2 | 4:8:176:MET:C[1_554]   | 1.83                     | 0.37              |
| 4:4:369:ILE:O   | 4:9:229:THR:O[1_554]   | 1.83                     | 0.37              |
| 4:2:110:LEU:CA  | 4:7:192:ILE:C[1_554]   | 1.83                     | 0.37              |
| 4:5:220:ALA:O   | 4:9:335:ARG:CD[1_554]  | 1.83                     | 0.37              |
| 4:3:308:GLY:C   | 4:7:338:SER:C[1_554]   | 1.83                     | 0.37              |
| 4:4:313:MET:N   | 4:8:152:VAL:CG2[1_554] | 1.83                     | 0.37              |
| 4:5:320:LEU:N   | 4:9:292:ASP:O[1_554]   | 1.83                     | 0.37              |
| 4:4:257:CYS:O   | 4:8:156:GLY:O[1_554]   | 1.83                     | 0.37              |
| 4:5:259:GLU:OE2 | 4:9:309:ILE:CD1[1_554] | 1.83                     | 0.37              |
| 4:2:288:ASP:O   | 4:8:64:ILE:O[1_554]    | 1.83                     | 0.37              |
| 4:3:316:GLU:CG  | 4:7:151:ILE:O[1_554]   | 1.83                     | 0.37              |
| 4:5:277:THR:O   | 4:9:174:ALA:CA[1_554]  | 1.83                     | 0.37              |
| 4:5:305:MET:SD  | 4:9:11:ASP:CA[1_554]   | 1.83                     | 0.37              |
| 4:5:319:ALA:CA  | 4:9:295:ALA:C[1_554]   | 1.83                     | 0.37              |
| 4:4:343:GLY:N   | 4:8:117:GLU:CG[1_554]  | 1.83                     | 0.37              |
| 4:5:154:ASP:OD1 | 4:9:108:ALA:O[1_554]   | 1.83                     | 0.37              |
| 4:5:318:THR:CB  | 4:9:296:ASN:ND2[1_554] | 1.83                     | 0.37              |
| 4:4:329:ILE:CB  | 4:8:139:VAL:CG1[1_554] | 1.83                     | 0.37              |
| 4:3:173:HIS:O   | 4:8:267:ILE:CB[1_554]  | 1.83                     | 0.37              |
| 4:4:210:ARG:CG  | 4:8:69:TYR:CE2[1_554]  | 1.83                     | 0.37              |
| 4:5:110:LEU:CB  | 4:V:192:ILE:N[1_554]   | 1.83                     | 0.37              |
| 4:4:179:ASP:O   | 4:8:179:ASP:CG[1_554]  | 1.83                     | 0.37              |
| 4:4:314:GLN:CB  | 4:8:142:LEU:O[1_554]   | 1.83                     | 0.37              |
| 4:3:173:HIS:CG  | 4:8:264:PRO:O[1_554]   | 1.83                     | 0.37              |
| 4:4:178:LEU:CG  | 4:8:177:ARG:CB[1_554]  | 1.83                     | 0.37              |
| 4:5:62:ARG:NH1  | 4:9:67:LEU:C[1_554]    | 1.83                     | 0.37              |
| 4:3:114:ALA:CB  | 4:8:250:ILE:O[1_554]   | 1.83                     | 0.37              |
| 4:5:308:GLY:O   | 4:9:338:SER:OG[1_554]  | 1.83                     | 0.37              |
| 4:3:308:GLY:C   | 4:7:339:VAL:CA[1_554]  | 1.83                     | 0.37              |
| 4:4:154:ASP:OD1 | 4:8:111:ASN:CG[1_554]  | 1.83                     | 0.37              |
| 4:3:265:SER:O   | 4:7:261:LEU:N[1_554]   | 1.83                     | 0.37              |
| 4:5:288:ASP:CA  | 4:W:63:GLY:CA[1_554]   | 1.83                     | 0.37              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:15:GLY:C    | 4:9:77:THR:CA[1_554]   | 1.83                     | 0.37              |
| 4:3:307:PRO:C   | 4:7:340:TRP:N[1_554]   | 1.83                     | 0.37              |
| 4:5:181:ALA:CA  | 4:9:159:VAL:CB[1_554]  | 1.83                     | 0.37              |
| 4:3:215:LYS:CG  | 4:7:31:PHE:O[1_554]    | 1.83                     | 0.37              |
| 4:3:293:LEU:CA  | 4:7:169:TYR:CG[1_554]  | 1.83                     | 0.37              |
| 4:3:174:ALA:O   | 4:7:173:HIS:CA[1_554]  | 1.83                     | 0.37              |
| 4:4:213:LYS:CE  | 4:8:14:SER:O[1_554]    | 1.83                     | 0.37              |
| 4:3:208:ILE:CB  | 4:7:59:GLN:CD[1_554]   | 1.83                     | 0.37              |
| 4:4:326:LYS:CD  | 4:V:45:VAL:N[1_554]    | 1.83                     | 0.37              |
| 4:3:223:PHE:CZ  | 4:7:301:GLY:O[1_554]   | 1.83                     | 0.37              |
| 4:3:300:SER:CB  | 4:7:107:GLU:OE2[1_554] | 1.83                     | 0.37              |
| 4:5:294:TYR:CB  | 4:9:166:TYR:C[1_554]   | 1.83                     | 0.37              |
| 4:5:207:GLU:CG  | 4:9:67:LEU:CD1[1_554]  | 1.83                     | 0.37              |
| 4:2:175:ILE:CB  | 4:7:191:LYS:CE[1_554]  | 1.83                     | 0.37              |
| 4:4:222:ASP:N   | 4:8:331:ALA:CA[1_554]  | 1.83                     | 0.37              |
| 4:3:185:LEU:CD1 | 4:7:159:VAL:CA[1_554]  | 1.83                     | 0.37              |
| 4:3:115:ASN:CA  | 4:8:249:THR:O[1_554]   | 1.83                     | 0.37              |
| 4:3:344:SER:C   | 4:7:367:PRO:N[1_554]   | 1.83                     | 0.37              |
| 4:5:22:ALA:N    | 4:9:362:TYR:OH[1_554]  | 1.83                     | 0.37              |
| 4:5:339:VAL:N   | 4:9:116:ARG:CG[1_554]  | 1.83                     | 0.37              |
| 4:4:297:ASN:CG  | 4:8:170:ALA:N[1_554]   | 1.83                     | 0.37              |
| 4:5:193:LEU:CD1 | 4:9:210:ARG:CA[1_554]  | 1.83                     | 0.37              |
| 4:5:301:GLY:C   | 4:9:137:GLN:NE2[1_554] | 1.83                     | 0.37              |
| 4:4:188:TYR:O   | 4:8:182:GLY:C[1_554]   | 1.83                     | 0.37              |
| 4:5:272:ALA:CA  | 4:9:277:THR:OG1[1_554] | 1.83                     | 0.37              |
| 4:4:336:LYS:CD  | 4:8:86:TRP:NE1[1_554]  | 1.83                     | 0.37              |
| 4:3:262:PHE:CD2 | 4:7:154:ASP:N[1_554]   | 1.83                     | 0.37              |
| 4:4:343:GLY:N   | 4:8:117:GLU:CB[1_554]  | 1.83                     | 0.37              |
| 4:3:191:LYS:C   | 4:7:186:THR:CG2[1_554] | 1.83                     | 0.37              |
| 4:5:223:PHE:CD1 | 4:9:335:ARG:NE[1_554]  | 1.83                     | 0.37              |
| 4:5:307:PRO:CA  | 4:9:337:TYR:CA[1_554]  | 1.83                     | 0.37              |
| 4:4:219:VAL:CG1 | 4:8:300:SER:OG[1_554]  | 1.83                     | 0.37              |
| 4:4:205:GLU:N   | 4:8:62:ARG:NE[1_554]   | 1.83                     | 0.37              |
| 4:5:198:TYR:CG  | 4:9:208:ILE:O[1_554]   | 1.83                     | 0.37              |
| 4:3:77:THR:CG2  | 4:8:246:GLN:CD[1_554]  | 1.83                     | 0.37              |
| 4:3:273:GLY:O   | 4:7:162:ASN:CG[1_554]  | 1.83                     | 0.37              |
| 4:5:113:LYS:N   | 4:V:253:GLU:OE2[1_554] | 1.83                     | 0.37              |
| 4:5:318:THR:N   | 4:9:150:GLY:CA[1_554]  | 1.83                     | 0.37              |
| 4:4:214:GLU:CA  | 4:8:16:LEU:N[1_554]    | 1.83                     | 0.37              |
| 4:4:143:TYR:CG  | 4:8:368:SER:O[1_554]   | 1.83                     | 0.37              |
| 4:2:284:LYS:O   | 4:7:268:GLY:CA[1_554]  | 1.83                     | 0.37              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:357:ILE:CB  | 4:8:231:ALA:O[1_554]   | 1.83                     | 0.37              |
| 4:4:304:THR:CG2 | 4:8:108:ALA:CA[1_554]  | 1.83                     | 0.37              |
| 4:4:188:TYR:CA  | 4:8:183:ARG:CA[1_554]  | 1.83                     | 0.37              |
| 4:3:139:VAL:C   | 4:7:371:HIS:CE1[1_554] | 1.84                     | 0.36              |
| 4:3:207:GLU:CD  | 4:7:67:LEU:N[1_554]    | 1.84                     | 0.36              |
| 4:3:294:TYR:CD1 | 4:7:166:TYR:N[1_554]   | 1.84                     | 0.36              |
| 4:3:15:GLY:N    | 4:7:77:THR:CB[1_554]   | 1.84                     | 0.36              |
| 4:4:180:LEU:CB  | 4:8:178:LEU:O[1_554]   | 1.84                     | 0.36              |
| 4:4:198:TYR:CB  | 4:8:208:ILE:CA[1_554]  | 1.84                     | 0.36              |
| 4:5:260:THR:O   | 4:9:160:THR:CG2[1_554] | 1.84                     | 0.36              |
| 4:3:257:CYS:O   | 4:7:156:GLY:N[1_554]   | 1.84                     | 0.36              |
| 4:5:340:TRP:CD2 | 4:9:118:LYS:O[1_554]   | 1.84                     | 0.36              |
| 4:5:288:ASP:O   | 4:W:63:GLY:C[1_554]    | 1.84                     | 0.36              |
| 4:3:205:GLU:OE2 | 4:7:203:THR:OG1[1_554] | 1.84                     | 0.36              |
| 4:4:24:ASP:CG   | 4:8:125:GLU:CG[1_554]  | 1.84                     | 0.36              |
| 4:4:369:ILE:O   | 4:9:228:ALA:O[1_554]   | 1.84                     | 0.36              |
| 4:4:337:TYR:CD1 | 4:8:86:TRP:CH2[1_554]  | 1.84                     | 0.36              |
| 4:3:367:PRO:O   | 4:8:236:LEU:CG[1_554]  | 1.84                     | 0.36              |
| 4:5:195:GLU:CA  | 4:9:189:LEU:CD2[1_554] | 1.84                     | 0.36              |
| 4:5:372:ARG:C   | 4:V:227:MET:CG[1_554]  | 1.84                     | 0.36              |
| 4:4:27:PRO:O    | 4:8:122:ILE:CG2[1_554] | 1.84                     | 0.36              |
| 4:5:111:ASN:OD1 | 4:V:196:ARG:CG[1_554]  | 1.84                     | 0.36              |
| 4:3:255:PHE:O   | 4:7:301:GLY:C[1_554]   | 1.84                     | 0.36              |
| 4:5:336:LYS:N   | 4:9:106:THR:N[1_554]   | 1.84                     | 0.36              |
| 4:4:310:ALA:CA  | 4:8:140:LEU:CA[1_554]  | 1.84                     | 0.36              |
| 4:5:113:LYS:NZ  | 4:V:254:ARG:CB[1_554]  | 1.84                     | 0.36              |
| 4:5:221:LEU:CD1 | 4:9:332:PRO:CB[1_554]  | 1.84                     | 0.36              |
| 4:3:261:LEU:CA  | 4:7:160:THR:CA[1_554]  | 1.84                     | 0.36              |
| 4:4:312:ARG:CA  | 4:8:298:VAL:CG1[1_554] | 1.84                     | 0.36              |
| 4:3:276:GLU:OE2 | 4:7:279:TYR:N[1_554]   | 1.84                     | 0.36              |
| 4:2:110:LEU:CA  | 4:7:192:ILE:N[1_554]   | 1.84                     | 0.36              |
| 4:4:191:LYS:CA  | 4:8:186:THR:CB[1_554]  | 1.84                     | 0.36              |
| 4:4:312:ARG:N   | 4:8:141:SER:O[1_554]   | 1.84                     | 0.36              |
| 4:1:292:ASP:OD2 | 4:7:39:ARG:O[1_554]    | 1.84                     | 0.36              |
| 4:4:326:LYS:O   | 4:8:167:GLU:N[1_554]   | 1.84                     | 0.36              |
| 4:5:267:ILE:CA  | 4:9:180:LEU:CD1[1_554] | 1.84                     | 0.36              |
| 4:5:329:ILE:CG2 | 4:9:139:VAL:CA[1_554]  | 1.84                     | 0.36              |
| 4:4:198:TYR:CA  | 4:8:205:GLU:O[1_554]   | 1.84                     | 0.36              |
| 4:5:327:ILE:CG1 | 4:9:149:THR:CG2[1_554] | 1.84                     | 0.36              |
| 4:5:340:TRP:CE3 | 4:9:119:MET:C[1_554]   | 1.84                     | 0.36              |
| 4:5:320:LEU:N   | 4:9:293:LEU:N[1_554]   | 1.84                     | 0.36              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:319:ALA:O   | 4:7:293:LEU:C[1_554]   | 1.84                     | 0.36              |
| 4:3:196:ARG:O   | 4:7:208:ILE:O[1_554]   | 1.84                     | 0.36              |
| 4:5:249:THR:O   | 4:9:211:ASP:OD1[1_554] | 1.84                     | 0.36              |
| 4:4:340:TRP:N   | 4:8:117:GLU:N[1_554]   | 1.84                     | 0.36              |
| 4:3:260:THR:CB  | 4:7:155:SER:OG[1_554]  | 1.84                     | 0.36              |
| 4:3:75:ILE:CA   | 4:8:198:TYR:CA[1_554]  | 1.84                     | 0.36              |
| 4:4:316:GLU:OE1 | 4:8:297:ASN:CA[1_554]  | 1.84                     | 0.36              |
| 4:5:181:ALA:CB  | 4:9:73:HIS:O[1_554]    | 1.84                     | 0.36              |
| 4:3:341:ILE:N   | 4:7:117:GLU:CA[1_554]  | 1.84                     | 0.36              |
| 4:2:115:ASN:CG  | 4:7:249:THR:C[1_554]   | 1.84                     | 0.36              |
| 4:5:312:ARG:CB  | 4:9:299:MET:C[1_554]   | 1.84                     | 0.36              |
| 4:4:177:ARG:CZ  | 4:9:194:THR:CB[1_554]  | 1.84                     | 0.36              |
| 4:3:198:TYR:O   | 4:7:206:ARG:O[1_554]   | 1.84                     | 0.36              |
| 4:5:196:ARG:NH1 | 4:9:215:LYS:CA[1_554]  | 1.84                     | 0.36              |
| 4:3:285:CYS:O   | 4:8:270:GLU:CG[1_554]  | 1.84                     | 0.36              |
| 4:4:114:ALA:CB  | 4:9:250:ILE:CB[1_554]  | 1.84                     | 0.36              |
| 4:5:144:ALA:CB  | 4:9:370:VAL:CG2[1_554] | 1.84                     | 0.36              |
| 4:2:114:ALA:C   | 4:7:250:ILE:CA[1_554]  | 1.84                     | 0.36              |
| 4:5:269:MET:O   | 4:9:272:ALA:C[1_554]   | 1.84                     | 0.36              |
| 4:5:318:THR:CB  | 4:9:296:ASN:OD1[1_554] | 1.84                     | 0.36              |
| 4:4:143:TYR:CB  | 4:8:372:ARG:N[1_554]   | 1.84                     | 0.36              |
| 4:5:280:ASN:CB  | 4:9:281:SER:O[1_554]   | 1.84                     | 0.36              |
| 4:3:281:SER:CB  | 4:7:173:HIS:CA[1_554]  | 1.84                     | 0.36              |
| 4:5:319:ALA:N   | 4:9:296:ASN:ND2[1_554] | 1.84                     | 0.36              |
| 4:4:340:TRP:N   | 4:8:115:ASN:O[1_554]   | 1.84                     | 0.36              |
| 4:4:26:ALA:CA   | 4:8:122:ILE:CA[1_554]  | 1.84                     | 0.36              |
| 4:5:210:ARG:NH1 | 4:9:33:SER:C[1_554]    | 1.84                     | 0.36              |
| 4:3:362:TYR:CD1 | 4:8:233:SER:O[1_554]   | 1.84                     | 0.36              |
| 4:4:32:PRO:N    | 4:8:78:ASN:OD1[1_554]  | 1.84                     | 0.36              |
| 4:3:299:MET:CA  | 4:7:136:ILE:CB[1_554]  | 1.84                     | 0.36              |
| 4:4:25:ASP:O    | 4:8:120:THR:O[1_554]   | 1.84                     | 0.36              |
| 4:5:186:THR:CG2 | 4:9:183:ARG:NE[1_554]  | 1.84                     | 0.36              |
| 4:4:31:PHE:CA   | 4:8:78:ASN:CG[1_554]   | 1.84                     | 0.36              |
| 4:5:274:ILE:N   | 4:9:161:HIS:C[1_554]   | 1.84                     | 0.36              |
| 4:2:372:ARG:N   | 4:7:226:GLU:O[1_554]   | 1.84                     | 0.36              |
| 4:5:289:ILE:O   | 4:W:64:ILE:CG2[1_554]  | 1.84                     | 0.36              |
| 4:4:227:MET:CB  | 4:8:307:PRO:N[1_554]   | 1.84                     | 0.36              |
| 4:4:25:ASP:N    | 4:8:124:PHE:CB[1_554]  | 1.84                     | 0.36              |
| 4:2:173:HIS:NE2 | 4:7:265:SER:CA[1_554]  | 1.84                     | 0.36              |
| 4:3:275:HIS:CD2 | 4:7:151:ILE:CG1[1_554] | 1.84                     | 0.36              |
| 4:5:166:TYR:CB  | 4:W:40:HIS:CD2[1_554]  | 1.84                     | 0.36              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:338:SER:N   | 4:7:119:MET:CG[1_554]  | 1.84                     | 0.36              |
| 4:4:223:PHE:O   | 4:8:335:ARG:CZ[1_554]  | 1.84                     | 0.36              |
| 4:4:319:ALA:C   | 4:8:292:ASP:C[1_554]   | 1.84                     | 0.36              |
| 4:4:304:THR:OG1 | 4:8:107:GLU:C[1_554]   | 1.84                     | 0.36              |
| 4:5:214:GLU:CA  | 4:9:16:LEU:N[1_554]    | 1.84                     | 0.36              |
| 4:3:17:VAL:O    | 4:7:79:TRP:CD1[1_554]  | 1.84                     | 0.36              |
| 4:3:178:LEU:CD2 | 4:7:176:MET:C[1_554]   | 1.84                     | 0.36              |
| 4:3:195:GLU:O   | 4:7:212:ILE:CG2[1_554] | 1.84                     | 0.36              |
| 4:4:109:PRO:N   | 4:9:195:GLU:CD[1_554]  | 1.84                     | 0.36              |
| 4:4:305:MET:CB  | 4:8:11:ASP:OD1[1_554]  | 1.84                     | 0.36              |
| 4:5:179:ASP:C   | 4:9:179:ASP:OD1[1_554] | 1.84                     | 0.36              |
| 4:4:327:ILE:CG1 | 4:8:149:THR:N[1_554]   | 1.84                     | 0.36              |
| 4:3:26:ALA:CA   | 4:7:121:GLN:C[1_554]   | 1.84                     | 0.36              |
| 4:4:334:GLU:O   | 4:8:105:LEU:CD1[1_554] | 1.84                     | 0.36              |
| 4:5:184:ASP:N   | 4:9:73:HIS:CE1[1_554]  | 1.84                     | 0.36              |
| 4:3:16:LEU:CG   | 4:7:78:ASN:O[1_554]    | 1.84                     | 0.36              |
| 4:4:151:ILE:CG2 | 4:8:170:ALA:C[1_554]   | 1.84                     | 0.36              |
| 4:5:367:PRO:C   | 4:V:233:SER:CA[1_554]  | 1.84                     | 0.36              |
| 4:3:15:GLY:C    | 4:7:77:THR:C[1_554]    | 1.84                     | 0.36              |
| 4:4:306:TYR:C   | 4:8:11:ASP:OD2[1_554]  | 1.84                     | 0.36              |
| 4:3:195:GLU:N   | 4:7:209:VAL:CG2[1_554] | 1.84                     | 0.36              |
| 4:2:366:GLY:C   | 4:7:235:SER:C[1_554]   | 1.84                     | 0.36              |
| 4:3:275:HIS:CB  | 4:7:152:VAL:N[1_554]   | 1.84                     | 0.36              |
| 4:3:266:PHE:N   | 4:7:261:LEU:CB[1_554]  | 1.84                     | 0.36              |
| 4:4:211:ASP:CG  | 4:8:32:PRO:O[1_554]    | 1.84                     | 0.36              |
| 4:4:274:ILE:CB  | 4:8:161:HIS:C[1_554]   | 1.84                     | 0.36              |
| 4:3:223:PHE:CE2 | 4:7:300:SER:O[1_554]   | 1.85                     | 0.35              |
| 4:2:111:ASN:CA  | 4:7:192:ILE:O[1_554]   | 1.85                     | 0.35              |
| 4:4:140:LEU:CA  | 4:8:371:HIS:CE1[1_554] | 1.85                     | 0.35              |
| 4:5:106:THR:OG1 | 4:9:114:ALA:C[1_554]   | 1.85                     | 0.35              |
| 4:3:140:LEU:CA  | 4:7:371:HIS:CG[1_554]  | 1.85                     | 0.35              |
| 4:5:214:GLU:CB  | 4:9:17:VAL:N[1_554]    | 1.85                     | 0.35              |
| 4:5:117:GLU:CD  | 4:V:236:LEU:CG[1_554]  | 1.85                     | 0.35              |
| 4:4:346:LEU:N   | 4:8:368:SER:N[1_554]   | 1.85                     | 0.35              |
| 4:4:314:GLN:NE2 | 4:8:147:ARG:O[1_554]   | 1.85                     | 0.35              |
| 4:5:347:ALA:N   | 4:9:366:GLY:CA[1_554]  | 1.85                     | 0.35              |
| 4:5:223:PHE:CA  | 4:9:335:ARG:NH2[1_554] | 1.85                     | 0.35              |
| 4:3:211:ASP:C   | 4:7:32:PRO:C[1_554]    | 1.85                     | 0.35              |
| 4:3:111:ASN:ND2 | 4:8:196:ARG:CD[1_554]  | 1.85                     | 0.35              |
| 4:4:275:HIS:O   | 4:8:164:PRO:N[1_554]   | 1.85                     | 0.35              |
| 4:3:333:PRO:CG  | 4:7:103:THR:C[1_554]   | 1.85                     | 0.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:171:LEU:O   | 4:7:266:PHE:C[1_554]   | 1.85                     | 0.35              |
| 4:3:173:HIS:CA  | 4:8:267:ILE:N[1_554]   | 1.85                     | 0.35              |
| 4:4:223:PHE:CE1 | 4:8:301:GLY:O[1_554]   | 1.85                     | 0.35              |
| 4:4:111:ASN:N   | 4:9:192:ILE:C[1_554]   | 1.85                     | 0.35              |
| 4:5:274:ILE:C   | 4:9:162:ASN:CB[1_554]  | 1.85                     | 0.35              |
| 4:5:258:PRO:CD  | 4:9:302:GLY:C[1_554]   | 1.85                     | 0.35              |
| 4:5:267:ILE:O   | 4:9:180:LEU:CD2[1_554] | 1.85                     | 0.35              |
| 4:5:11:ASP:N    | 4:9:118:LYS:CG[1_554]  | 1.85                     | 0.35              |
| 4:2:370:VAL:O   | 4:7:230:ALA:C[1_554]   | 1.85                     | 0.35              |
| 4:3:270:GLU:C   | 4:7:272:ALA:CA[1_554]  | 1.85                     | 0.35              |
| 4:4:371:HIS:NE2 | 4:9:252:ASN:O[1_554]   | 1.85                     | 0.35              |
| 4:3:341:ILE:CG1 | 4:7:120:THR:C[1_554]   | 1.85                     | 0.35              |
| 4:3:243:PRO:C   | 4:7:60:SER:OG[1_554]   | 1.85                     | 0.35              |
| 4:3:180:LEU:C   | 4:7:159:VAL:CG1[1_554] | 1.85                     | 0.35              |
| 4:3:371:HIS:N   | 4:8:230:ALA:CB[1_554]  | 1.85                     | 0.35              |
| 4:3:293:LEU:O   | 4:7:169:TYR:CA[1_554]  | 1.85                     | 0.35              |
| 4:4:312:ARG:NE  | 4:8:299:MET:N[1_554]   | 1.85                     | 0.35              |
| 4:2:110:LEU:N   | 4:7:192:ILE:C[1_554]   | 1.85                     | 0.35              |
| 4:5:335:ARG:CB  | 4:9:106:THR:CB[1_554]  | 1.85                     | 0.35              |
| 4:2:367:PRO:CD  | 4:7:235:SER:CA[1_554]  | 1.85                     | 0.35              |
| 4:4:274:ILE:CG1 | 4:8:161:HIS:CG[1_554]  | 1.85                     | 0.35              |
| 4:5:196:ARG:CB  | 4:9:212:ILE:C[1_554]   | 1.85                     | 0.35              |
| 4:5:183:ARG:NH2 | 4:9:72:GLU:OE1[1_554]  | 1.85                     | 0.35              |
| 4:2:79:TRP:NE1  | 4:7:247:VAL:C[1_554]   | 1.85                     | 0.35              |
| 4:4:24:ASP:CA   | 4:8:125:GLU:CB[1_554]  | 1.85                     | 0.35              |
| 4:3:340:TRP:O   | 4:7:117:GLU:C[1_554]   | 1.85                     | 0.35              |
| 4:2:292:ASP:CG  | 4:8:40:HIS:CB[1_554]   | 1.85                     | 0.35              |
| 4:3:299:MET:CB  | 4:7:136:ILE:N[1_554]   | 1.85                     | 0.35              |
| 4:3:196:ARG:CD  | 4:7:211:ASP:OD1[1_554] | 1.85                     | 0.35              |
| 4:4:115:ASN:N   | 4:9:250:ILE:CA[1_554]  | 1.85                     | 0.35              |
| 4:5:162:ASN:ND2 | 4:9:175:ILE:CD1[1_554] | 1.85                     | 0.35              |
| 4:5:22:ALA:N    | 4:9:125:GLU:OE2[1_554] | 1.85                     | 0.35              |
| 4:3:294:TYR:CD2 | 4:7:166:TYR:CD2[1_554] | 1.85                     | 0.35              |
| 4:5:295:ALA:CB  | 4:9:167:GLU:CB[1_554]  | 1.85                     | 0.35              |
| 4:5:279:TYR:CA  | 4:9:285:CYS:SG[1_554]  | 1.85                     | 0.35              |
| 4:5:340:TRP:CG  | 4:9:120:THR:N[1_554]   | 1.85                     | 0.35              |
| 4:4:253:GLU:CD  | 4:8:214:GLU:CA[1_554]  | 1.85                     | 0.35              |
| 4:5:293:LEU:CG  | 4:9:169:TYR:CD2[1_554] | 1.85                     | 0.35              |
| 4:5:177:ARG:NH2 | 4:V:194:THR:CG2[1_554] | 1.85                     | 0.35              |
| 4:4:221:LEU:O   | 4:8:332:PRO:O[1_554]   | 1.85                     | 0.35              |
| 4:4:371:HIS:CA  | 4:9:230:ALA:CA[1_554]  | 1.85                     | 0.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:240:TYR:OH  | 4:7:56:ASP:N[1_554]    | 1.85                     | 0.35              |
| 4:3:113:LYS:CG  | 4:8:254:ARG:C[1_554]   | 1.85                     | 0.35              |
| 4:5:21:PHE:C    | 4:9:125:GLU:OE1[1_554] | 1.85                     | 0.35              |
| 4:4:214:GLU:C   | 4:8:16:LEU:CB[1_554]   | 1.85                     | 0.35              |
| 4:2:366:GLY:O   | 4:7:235:SER:N[1_554]   | 1.85                     | 0.35              |
| 4:5:289:ILE:N   | 4:W:63:GLY:CA[1_554]   | 1.85                     | 0.35              |
| 4:4:113:LYS:CG  | 4:9:253:GLU:C[1_554]   | 1.85                     | 0.35              |
| 4:5:188:TYR:CA  | 4:9:185:LEU:N[1_554]   | 1.85                     | 0.35              |
| 4:4:256:ARG:NH1 | 4:8:306:TYR:CD1[1_554] | 1.85                     | 0.35              |
| 4:3:318:THR:C   | 4:7:149:THR:O[1_554]   | 1.85                     | 0.35              |
| 4:3:187:ASP:C   | 4:7:183:ARG:CB[1_554]  | 1.85                     | 0.35              |
| 4:4:300:SER:C   | 4:8:108:ALA:N[1_554]   | 1.85                     | 0.35              |
| 4:3:31:PHE:N    | 4:7:78:ASN:OD1[1_554]  | 1.85                     | 0.35              |
| 4:3:319:ALA:CB  | 4:7:296:ASN:N[1_554]   | 1.85                     | 0.35              |
| 4:5:256:ARG:O   | 4:9:303:THR:O[1_554]   | 1.85                     | 0.35              |
| 4:2:366:GLY:C   | 4:7:235:SER:CA[1_554]  | 1.85                     | 0.35              |
| 4:5:223:PHE:CD2 | 4:9:304:THR:CB[1_554]  | 1.85                     | 0.35              |
| 4:5:299:MET:CE  | 4:9:138:ALA:C[1_554]   | 1.85                     | 0.35              |
| 4:4:208:ILE:CG1 | 4:8:59:GLN:CG[1_554]   | 1.85                     | 0.35              |
| 4:4:195:GLU:C   | 4:8:209:VAL:O[1_554]   | 1.85                     | 0.35              |
| 4:3:372:ARG:CD  | 4:8:227:MET:CB[1_554]  | 1.85                     | 0.35              |
| 4:2:149:THR:CG2 | 4:8:40:HIS:CD2[1_554]  | 1.85                     | 0.35              |
| 4:4:75:ILE:CG2  | 4:9:198:TYR:CB[1_554]  | 1.85                     | 0.35              |
| 4:3:115:ASN:ND2 | 4:8:198:TYR:OH[1_554]  | 1.85                     | 0.35              |
| 4:4:227:MET:CG  | 4:8:305:MET:O[1_554]   | 1.85                     | 0.35              |
| 4:5:156:GLY:O   | 4:9:73:HIS:O[1_554]    | 1.85                     | 0.35              |
| 4:4:270:GLU:CG  | 4:8:271:SER:O[1_554]   | 1.85                     | 0.35              |
| 4:4:227:MET:CG  | 4:8:307:PRO:N[1_554]   | 1.85                     | 0.35              |
| 4:4:334:GLU:N   | 4:8:105:LEU:CA[1_554]  | 1.85                     | 0.35              |
| 4:4:341:ILE:N   | 4:8:117:GLU:O[1_554]   | 1.85                     | 0.35              |
| 4:5:262:PHE:CB  | 4:9:153:LEU:CD1[1_554] | 1.85                     | 0.35              |
| 4:3:211:ASP:CA  | 4:7:32:PRO:CB[1_554]   | 1.85                     | 0.35              |
| 4:5:315:LYS:C   | 4:9:296:ASN:C[1_554]   | 1.85                     | 0.35              |
| 4:3:144:ALA:O   | 4:7:370:VAL:CG2[1_554] | 1.85                     | 0.35              |
| 4:3:220:ALA:O   | 4:7:299:MET:O[1_554]   | 1.85                     | 0.35              |
| 4:5:59:GLN:O    | 4:9:66:THR:CB[1_554]   | 1.85                     | 0.35              |
| 4:4:159:VAL:C   | 4:8:177:ARG:CZ[1_554]  | 1.85                     | 0.35              |
| 4:3:205:GLU:OE2 | 4:7:203:THR:CG2[1_554] | 1.85                     | 0.35              |
| 4:5:21:PHE:CA   | 4:9:125:GLU:CG[1_554]  | 1.85                     | 0.35              |
| 4:3:278:THR:O   | 4:7:171:LEU:O[1_554]   | 1.85                     | 0.35              |
| 4:4:340:TRP:CE2 | 4:8:121:GLN:CB[1_554]  | 1.85                     | 0.35              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:270:GLU:N   | 4:8:272:ALA:N[1_554]   | 1.85                     | 0.35              |
| 4:5:269:MET:N   | 4:9:264:PRO:CG[1_554]  | 1.85                     | 0.35              |
| 4:3:263:GLN:CB  | 4:7:274:ILE:CG1[1_554] | 1.85                     | 0.35              |
| 4:3:113:LYS:NZ  | 4:8:254:ARG:O[1_554]   | 1.85                     | 0.35              |
| 1:A:411:GLU:OE2 | 4:4:229:THR:OG1[1_556] | 1.85                     | 0.35              |
| 4:3:319:ALA:CA  | 4:7:296:ASN:ND2[1_554] | 1.86                     | 0.34              |
| 4:2:113:LYS:CD  | 4:7:254:ARG:O[1_554]   | 1.86                     | 0.34              |
| 4:4:142:LEU:C   | 4:8:371:HIS:O[1_554]   | 1.86                     | 0.34              |
| 4:3:201:VAL:CG2 | 4:7:203:THR:CA[1_554]  | 1.86                     | 0.34              |
| 4:5:215:LYS:N   | 4:9:16:LEU:CD1[1_554]  | 1.86                     | 0.34              |
| 4:5:18:LYS:N    | 4:9:79:TRP:CE2[1_554]  | 1.86                     | 0.34              |
| 4:4:243:PRO:CG  | 4:8:61:LYS:N[1_554]    | 1.86                     | 0.34              |
| 4:3:332:PRO:N   | 4:7:135:ALA:CA[1_554]  | 1.86                     | 0.34              |
| 4:4:211:ASP:CA  | 4:8:33:SER:N[1_554]    | 1.86                     | 0.34              |
| 4:5:155:SER:N   | 4:9:108:ALA:CA[1_554]  | 1.86                     | 0.34              |
| 4:4:207:GLU:CA  | 4:8:67:LEU:CD1[1_554]  | 1.86                     | 0.34              |
| 4:5:294:TYR:CD1 | 4:9:166:TYR:CB[1_554]  | 1.86                     | 0.34              |
| 4:5:140:LEU:C   | 4:9:116:ARG:CD[1_554]  | 1.86                     | 0.34              |
| 4:5:315:LYS:O   | 4:9:297:ASN:N[1_554]   | 1.86                     | 0.34              |
| 4:5:27:PRO:N    | 4:9:122:ILE:C[1_554]   | 1.86                     | 0.34              |
| 4:4:155:SER:O   | 4:8:108:ALA:CB[1_554]  | 1.86                     | 0.34              |
| 4:5:371:HIS:N   | 4:V:230:ALA:C[1_554]   | 1.86                     | 0.34              |
| 4:5:338:SER:OG  | 4:9:134:VAL:C[1_554]   | 1.86                     | 0.34              |
| 4:3:293:LEU:O   | 4:7:169:TYR:CD2[1_554] | 1.86                     | 0.34              |
| 4:4:205:GLU:CG  | 4:8:203:THR:OG1[1_554] | 1.86                     | 0.34              |
| 4:3:343:GLY:N   | 4:7:117:GLU:CG[1_554]  | 1.86                     | 0.34              |
| 4:5:257:CYS:N   | 4:9:303:THR:OG1[1_554] | 1.86                     | 0.34              |
| 4:3:308:GLY:O   | 4:7:338:SER:CB[1_554]  | 1.86                     | 0.34              |
| 4:3:18:LYS:CB   | 4:7:79:TRP:CD2[1_554]  | 1.86                     | 0.34              |
| 4:5:253:GLU:OE2 | 4:9:215:LYS:N[1_554]   | 1.86                     | 0.34              |
| 4:3:185:LEU:N   | 4:7:158:GLY:C[1_554]   | 1.86                     | 0.34              |
| 4:5:30:VAL:N    | 4:9:83:GLU:CB[1_554]   | 1.86                     | 0.34              |
| 4:4:327:ILE:N   | 4:8:167:GLU:CA[1_554]  | 1.86                     | 0.34              |
| 4:5:162:ASN:N   | 4:9:110:LEU:CG[1_554]  | 1.86                     | 0.34              |
| 4:3:300:SER:O   | 4:7:108:ALA:N[1_554]   | 1.86                     | 0.34              |
| 4:5:137:GLN:N   | 4:9:113:LYS:CB[1_554]  | 1.86                     | 0.34              |
| 4:5:260:THR:C   | 4:9:155:SER:OG[1_554]  | 1.86                     | 0.34              |
| 4:4:213:LYS:C   | 4:8:16:LEU:CB[1_554]   | 1.86                     | 0.34              |
| 4:3:193:LEU:CD1 | 4:7:210:ARG:CD[1_554]  | 1.86                     | 0.34              |
| 4:4:178:LEU:CD2 | 4:8:176:MET:O[1_554]   | 1.86                     | 0.34              |
| 4:4:145:SER:OG  | 4:8:372:ARG:NH2[1_554] | 1.86                     | 0.34              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:276:GLU:CA  | 4:9:151:ILE:CD1[1_554] | 1.86                     | 0.34              |
| 4:4:329:ILE:CG2 | 4:8:139:VAL:C[1_554]   | 1.86                     | 0.34              |
| 1:A:411:GLU:OE1 | 4:4:226:GLU:CD[1_556]  | 1.86                     | 0.34              |
| 4:2:109:PRO:O   | 4:7:192:ILE:CG2[1_554] | 1.86                     | 0.34              |
| 4:5:300:SER:CA  | 4:9:107:GLU:CG[1_554]  | 1.86                     | 0.34              |
| 4:5:367:PRO:CA  | 4:V:234:SER:N[1_554]   | 1.86                     | 0.34              |
| 4:2:372:ARG:CD  | 4:7:227:MET:C[1_554]   | 1.86                     | 0.34              |
| 4:2:290:ARG:C   | 4:8:64:ILE:CG2[1_554]  | 1.86                     | 0.34              |
| 4:2:357:ILE:CG1 | 4:7:231:ALA:C[1_554]   | 1.86                     | 0.34              |
| 4:5:198:TYR:CG  | 4:9:208:ILE:N[1_554]   | 1.86                     | 0.34              |
| 4:4:157:ASP:O   | 4:8:73:HIS:CB[1_554]   | 1.86                     | 0.34              |
| 4:3:180:LEU:CA  | 4:7:179:ASP:CG[1_554]  | 1.86                     | 0.34              |
| 4:4:312:ARG:O   | 4:8:298:VAL:CG1[1_554] | 1.86                     | 0.34              |
| 4:4:24:ASP:N    | 4:8:125:GLU:OE2[1_554] | 1.86                     | 0.34              |
| 4:4:180:LEU:CD1 | 4:8:178:LEU:O[1_554]   | 1.86                     | 0.34              |
| 4:3:144:ALA:N   | 4:7:371:HIS:C[1_554]   | 1.86                     | 0.34              |
| 4:3:299:MET:CG  | 4:7:136:ILE:C[1_554]   | 1.86                     | 0.34              |
| 4:5:280:ASN:ND2 | 4:9:281:SER:C[1_554]   | 1.86                     | 0.34              |
| 4:5:28:ARG:C    | 4:9:83:GLU:CD[1_554]   | 1.86                     | 0.34              |
| 4:3:327:ILE:C   | 4:7:167:GLU:C[1_554]   | 1.86                     | 0.34              |
| 4:5:277:THR:CG2 | 4:9:175:ILE:O[1_554]   | 1.86                     | 0.34              |
| 4:4:341:ILE:CB  | 4:8:120:THR:CA[1_554]  | 1.86                     | 0.34              |
| 4:3:269:MET:CB  | 4:7:178:LEU:CG[1_554]  | 1.86                     | 0.34              |
| 4:3:138:ALA:N   | 4:7:113:LYS:N[1_554]   | 1.86                     | 0.34              |
| 4:3:157:ASP:N   | 4:7:72:GLU:O[1_554]    | 1.86                     | 0.34              |
| 4:3:222:ASP:C   | 4:7:332:PRO:N[1_554]   | 1.86                     | 0.34              |
| 4:3:294:TYR:C   | 4:7:166:TYR:O[1_554]   | 1.86                     | 0.34              |
| 4:5:27:PRO:CB   | 4:9:122:ILE:CG2[1_554] | 1.86                     | 0.34              |
| 4:4:210:ARG:NH2 | 4:8:34:ILE:CA[1_554]   | 1.86                     | 0.34              |
| 4:4:337:TYR:OH  | 4:8:86:TRP:CD2[1_554]  | 1.86                     | 0.34              |
| 4:4:299:MET:CG  | 4:8:136:ILE:CA[1_554]  | 1.86                     | 0.34              |
| 4:4:157:ASP:CB  | 4:8:72:GLU:N[1_554]    | 1.86                     | 0.34              |
| 4:5:348:SER:CA  | 4:9:362:TYR:O[1_554]   | 1.86                     | 0.34              |
| 4:4:294:TYR:O   | 4:8:169:TYR:N[1_554]   | 1.86                     | 0.34              |
| 4:5:199:SER:CB  | 4:9:205:GLU:C[1_554]   | 1.86                     | 0.34              |
| 4:5:274:ILE:N   | 4:9:162:ASN:CB[1_554]  | 1.86                     | 0.34              |
| 4:3:280:ASN:O   | 4:7:284:LYS:O[1_554]   | 1.86                     | 0.34              |
| 4:3:144:ALA:CB  | 4:7:370:VAL:CG1[1_554] | 1.86                     | 0.34              |
| 4:5:31:PHE:O    | 4:9:79:TRP:N[1_554]    | 1.86                     | 0.34              |
| 4:4:256:ARG:O   | 4:8:303:THR:OG1[1_554] | 1.86                     | 0.34              |
| 4:4:300:SER:C   | 4:8:107:GLU:C[1_554]   | 1.86                     | 0.34              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:279:TYR:CG  | 4:9:293:LEU:CD2[1_554] | 1.86                     | 0.34              |
| 4:3:154:ASP:O   | 4:7:110:LEU:N[1_554]   | 1.86                     | 0.34              |
| 4:4:279:TYR:CA  | 4:8:164:PRO:CB[1_554]  | 1.86                     | 0.34              |
| 4:5:253:GLU:CD  | 4:9:214:GLU:CB[1_554]  | 1.86                     | 0.34              |
| 4:5:274:ILE:CD1 | 4:9:161:HIS:C[1_554]   | 1.86                     | 0.34              |
| 4:5:114:ALA:CA  | 4:V:250:ILE:C[1_554]   | 1.86                     | 0.34              |
| 4:4:282:ILE:CG2 | 4:8:171:LEU:CD2[1_554] | 1.86                     | 0.34              |
| 4:3:262:PHE:CA  | 4:7:153:LEU:CG[1_554]  | 1.86                     | 0.34              |
| 4:2:116:ARG:NE  | 4:7:252:ASN:OD1[1_554] | 1.86                     | 0.34              |
| 4:5:262:PHE:CG  | 4:9:153:LEU:O[1_554]   | 1.86                     | 0.34              |
| 4:3:299:MET:SD  | 4:7:136:ILE:C[1_554]   | 1.86                     | 0.34              |
| 4:4:276:GLU:OE2 | 4:8:278:THR:N[1_554]   | 1.86                     | 0.34              |
| 4:4:280:ASN:OD1 | 4:8:281:SER:O[1_554]   | 1.86                     | 0.34              |
| 4:4:144:ALA:O   | 4:8:370:VAL:CG2[1_554] | 1.86                     | 0.34              |
| 4:4:281:SER:C   | 4:8:173:HIS:CG[1_554]  | 1.86                     | 0.34              |
| 4:3:155:SER:O   | 4:7:74:GLY:O[1_554]    | 1.86                     | 0.34              |
| 4:5:266:PHE:CD1 | 4:9:261:LEU:CD1[1_554] | 1.86                     | 0.34              |
| 4:5:269:MET:SD  | 4:9:178:LEU:CD1[1_554] | 1.86                     | 0.34              |
| 4:5:140:LEU:CG  | 4:9:371:HIS:CG[1_554]  | 1.86                     | 0.34              |
| 4:2:177:ARG:NH2 | 4:7:194:THR:CG2[1_554] | 1.87                     | 0.33              |
| 4:3:16:LEU:CG   | 4:7:78:ASN:C[1_554]    | 1.87                     | 0.33              |
| 4:5:339:VAL:CG1 | 4:9:116:ARG:CA[1_554]  | 1.87                     | 0.33              |
| 4:5:282:ILE:CB  | 4:9:171:LEU:CD1[1_554] | 1.87                     | 0.33              |
| 4:5:266:PHE:N   | 4:9:261:LEU:O[1_554]   | 1.87                     | 0.33              |
| 4:4:340:TRP:CH2 | 4:8:121:GLN:CD[1_554]  | 1.87                     | 0.33              |
| 4:5:294:TYR:O   | 4:9:168:GLY:N[1_554]   | 1.87                     | 0.33              |
| 4:4:339:VAL:CG2 | 4:8:116:ARG:N[1_554]   | 1.87                     | 0.33              |
| 4:2:116:ARG:CA  | 4:7:196:ARG:NH2[1_554] | 1.87                     | 0.33              |
| 4:3:341:ILE:CB  | 4:7:120:THR:CG2[1_554] | 1.87                     | 0.33              |
| 4:4:141:SER:O   | 4:8:116:ARG:NH1[1_554] | 1.87                     | 0.33              |
| 4:5:304:THR:CA  | 4:9:137:GLN:CG[1_554]  | 1.87                     | 0.33              |
| 4:5:287:ILE:C   | 4:W:63:GLY:N[1_554]    | 1.87                     | 0.33              |
| 4:3:326:LYS:CD  | 4:9:44:MET:CA[1_554]   | 1.87                     | 0.33              |
| 4:3:157:ASP:O   | 4:7:72:GLU:C[1_554]    | 1.87                     | 0.33              |
| 4:3:274:ILE:O   | 4:7:163:VAL:N[1_554]   | 1.87                     | 0.33              |
| 4:5:198:TYR:CZ  | 4:9:208:ILE:CG1[1_554] | 1.87                     | 0.33              |
| 4:4:276:GLU:CA  | 4:8:151:ILE:CD1[1_554] | 1.87                     | 0.33              |
| 4:3:262:PHE:CE1 | 4:7:152:VAL:CG1[1_554] | 1.87                     | 0.33              |
| 4:5:199:SER:N   | 4:9:206:ARG:C[1_554]   | 1.87                     | 0.33              |
| 4:3:340:TRP:CG  | 4:7:118:LYS:CB[1_554]  | 1.87                     | 0.33              |
| 4:5:344:SER:CA  | 4:9:362:TYR:CE1[1_554] | 1.87                     | 0.33              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:113:LYS:N   | 4:V:253:GLU:OE1[1_554] | 1.87                     | 0.33              |
| 4:3:300:SER:N   | 4:7:107:GLU:OE2[1_554] | 1.87                     | 0.33              |
| 4:5:151:ILE:CG1 | 4:9:171:LEU:N[1_554]   | 1.87                     | 0.33              |
| 4:4:258:PRO:C   | 4:8:155:SER:CA[1_554]  | 1.87                     | 0.33              |
| 4:4:306:TYR:N   | 4:8:11:ASP:OD2[1_554]  | 1.87                     | 0.33              |
| 4:3:191:LYS:N   | 4:7:186:THR:CB[1_554]  | 1.87                     | 0.33              |
| 4:5:337:TYR:OH  | 4:9:86:TRP:CD1[1_554]  | 1.87                     | 0.33              |
| 4:2:173:HIS:CB  | 4:7:267:ILE:CG2[1_554] | 1.87                     | 0.33              |
| 4:4:265:SER:OG  | 4:8:274:ILE:CB[1_554]  | 1.87                     | 0.33              |
| 4:3:112:PRO:CB  | 4:8:193:LEU:CD1[1_554] | 1.87                     | 0.33              |
| 4:5:263:GLN:CB  | 4:9:274:ILE:CG1[1_554] | 1.87                     | 0.33              |
| 4:5:316:GLU:OE1 | 4:9:297:ASN:CA[1_554]  | 1.87                     | 0.33              |
| 4:5:163:VAL:CA  | 4:9:172:PRO:CB[1_554]  | 1.87                     | 0.33              |
| 4:5:369:ILE:CD1 | 4:V:232:SER:OG[1_554]  | 1.87                     | 0.33              |
| 4:3:113:LYS:CG  | 4:8:254:ARG:CB[1_554]  | 1.87                     | 0.33              |
| 4:5:369:ILE:CA  | 4:V:228:ALA:O[1_554]   | 1.87                     | 0.33              |
| 4:5:256:ARG:C   | 4:9:303:THR:O[1_554]   | 1.87                     | 0.33              |
| 4:5:157:ASP:CB  | 4:9:72:GLU:CA[1_554]   | 1.87                     | 0.33              |
| 4:5:281:SER:OG  | 4:9:174:ALA:N[1_554]   | 1.87                     | 0.33              |
| 4:3:259:GLU:CB  | 4:7:304:THR:CB[1_554]  | 1.87                     | 0.33              |
| 4:5:295:ALA:CA  | 4:9:168:GLY:N[1_554]   | 1.87                     | 0.33              |
| 4:5:23:GLY:N    | 4:9:362:TYR:CZ[1_554]  | 1.87                     | 0.33              |
| 4:1:291:LYS:CD  | 4:7:64:ILE:C[1_554]    | 1.87                     | 0.33              |
| 4:5:141:SER:OG  | 4:9:107:GLU:OE2[1_554] | 1.87                     | 0.33              |
| 4:5:288:ASP:N   | 4:W:63:GLY:N[1_554]    | 1.87                     | 0.33              |
| 4:3:199:SER:CB  | 4:7:206:ARG:CA[1_554]  | 1.87                     | 0.33              |
| 4:5:190:MET:CE  | 4:9:206:ARG:NH1[1_554] | 1.87                     | 0.33              |
| 4:5:301:GLY:N   | 4:9:107:GLU:O[1_554]   | 1.87                     | 0.33              |
| 4:5:179:ASP:O   | 4:9:179:ASP:CG[1_554]  | 1.87                     | 0.33              |
| 4:4:327:ILE:O   | 4:8:148:THR:CG2[1_554] | 1.87                     | 0.33              |
| 4:5:166:TYR:CD2 | 4:W:40:HIS:CE1[1_554]  | 1.87                     | 0.33              |
| 4:3:300:SER:O   | 4:7:108:ALA:O[1_554]   | 1.87                     | 0.33              |
| 4:1:291:LYS:NZ  | 4:7:39:ARG:N[1_554]    | 1.87                     | 0.33              |
| 4:3:154:ASP:CA  | 4:7:110:LEU:N[1_554]   | 1.87                     | 0.33              |
| 4:2:367:PRO:C   | 4:7:236:LEU:CB[1_554]  | 1.87                     | 0.33              |
| 4:3:284:LYS:CA  | 4:8:268:GLY:O[1_554]   | 1.87                     | 0.33              |
| 4:3:223:PHE:CB  | 4:7:335:ARG:CD[1_554]  | 1.87                     | 0.33              |
| 4:3:240:TYR:CG  | 4:7:56:ASP:OD2[1_554]  | 1.87                     | 0.33              |
| 4:4:210:ARG:CD  | 4:8:69:TYR:CG[1_554]   | 1.87                     | 0.33              |
| 4:4:331:ALA:O   | 4:8:135:ALA:CB[1_554]  | 1.87                     | 0.33              |
| 4:3:153:LEU:CA  | 4:7:109:PRO:C[1_554]   | 1.87                     | 0.33              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:259:GLU:OE1 | 4:8:305:MET:N[1_554]   | 1.87                     | 0.33              |
| 4:5:304:THR:CB  | 4:9:137:GLN:CD[1_554]  | 1.87                     | 0.33              |
| 4:4:144:ALA:CB  | 4:8:370:VAL:CG1[1_554] | 1.87                     | 0.33              |
| 4:5:31:PHE:C    | 4:9:78:ASN:O[1_554]    | 1.87                     | 0.33              |
| 4:3:164:PRO:CG  | 4:7:172:PRO:CG[1_554]  | 1.87                     | 0.33              |
| 4:3:221:LEU:O   | 4:7:332:PRO:CA[1_554]  | 1.87                     | 0.33              |
| 4:5:255:PHE:CD1 | 4:9:305:MET:O[1_554]   | 1.87                     | 0.33              |
| 4:5:213:LYS:NZ  | 4:9:14:SER:CA[1_554]   | 1.87                     | 0.33              |
| 4:5:333:PRO:C   | 4:9:104:LEU:C[1_554]   | 1.87                     | 0.33              |
| 4:3:193:LEU:CG  | 4:7:210:ARG:CB[1_554]  | 1.87                     | 0.33              |
| 4:3:279:TYR:CE1 | 4:7:293:LEU:CD2[1_554] | 1.87                     | 0.33              |
| 4:3:185:LEU:CG  | 4:7:158:GLY:N[1_554]   | 1.87                     | 0.33              |
| 4:5:265:SER:CB  | 4:9:262:PHE:CA[1_554]  | 1.87                     | 0.33              |
| 4:3:259:GLU:CD  | 4:7:304:THR:CB[1_554]  | 1.87                     | 0.33              |
| 4:4:294:TYR:CG  | 4:8:166:TYR:CA[1_554]  | 1.87                     | 0.33              |
| 4:5:161:HIS:N   | 4:9:110:LEU:CD1[1_554] | 1.87                     | 0.33              |
| 4:5:136:ILE:CB  | 4:9:113:LYS:CG[1_554]  | 1.87                     | 0.33              |
| 4:3:326:LYS:CD  | 4:9:44:MET:C[1_554]    | 1.87                     | 0.33              |
| 4:4:114:ALA:C   | 4:9:250:ILE:CA[1_554]  | 1.87                     | 0.33              |
| 4:3:205:GLU:N   | 4:7:62:ARG:CG[1_554]   | 1.87                     | 0.33              |
| 4:5:136:ILE:CA  | 4:9:113:LYS:CB[1_554]  | 1.87                     | 0.33              |
| 4:5:219:VAL:N   | 4:9:335:ARG:C[1_554]   | 1.87                     | 0.33              |
| 4:5:300:SER:C   | 4:9:107:GLU:CA[1_554]  | 1.87                     | 0.33              |
| 4:3:333:PRO:N   | 4:7:133:TYR:O[1_554]   | 1.87                     | 0.33              |
| 4:4:30:VAL:O    | 4:8:81:ASP:N[1_554]    | 1.87                     | 0.33              |
| 4:2:288:ASP:O   | 4:8:65:LEU:N[1_554]    | 1.88                     | 0.32              |
| 4:5:299:MET:C   | 4:9:136:ILE:C[1_554]   | 1.88                     | 0.32              |
| 4:4:198:TYR:CD2 | 4:8:207:GLU:O[1_554]   | 1.88                     | 0.32              |
| 4:4:278:THR:OG1 | 4:8:163:VAL:CA[1_554]  | 1.88                     | 0.32              |
| 4:3:191:LYS:O   | 4:7:186:THR:CB[1_554]  | 1.88                     | 0.32              |
| 4:5:333:PRO:CD  | 4:9:104:LEU:CD2[1_554] | 1.88                     | 0.32              |
| 4:5:340:TRP:CE3 | 4:9:119:MET:O[1_554]   | 1.88                     | 0.32              |
| 4:4:317:ILE:O   | 4:8:150:GLY:N[1_554]   | 1.88                     | 0.32              |
| 4:5:157:ASP:C   | 4:9:73:HIS:N[1_554]    | 1.88                     | 0.32              |
| 4:3:288:ASP:C   | 4:9:63:GLY:C[1_554]    | 1.88                     | 0.32              |
| 4:5:211:ASP:CG  | 4:9:32:PRO:CB[1_554]   | 1.88                     | 0.32              |
| 4:1:290:ARG:C   | 4:7:64:ILE:CG2[1_554]  | 1.88                     | 0.32              |
| 4:5:345:ILE:CD1 | 4:9:357:ILE:CG2[1_554] | 1.88                     | 0.32              |
| 4:3:311:ASP:N   | 4:7:141:SER:C[1_554]   | 1.88                     | 0.32              |
| 4:3:272:ALA:N   | 4:7:277:THR:OG1[1_554] | 1.88                     | 0.32              |
| 4:5:60:SER:CB   | 4:9:37:ARG:CG[1_554]   | 1.88                     | 0.32              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:266:PHE:O   | 4:7:185:LEU:CD1[1_554] | 1.88                     | 0.32              |
| 4:4:312:ARG:O   | 4:8:298:VAL:CB[1_554]  | 1.88                     | 0.32              |
| 4:3:280:ASN:OD1 | 4:7:281:SER:O[1_554]   | 1.88                     | 0.32              |
| 4:5:211:ASP:CG  | 4:9:32:PRO:CA[1_554]   | 1.88                     | 0.32              |
| 4:5:256:ARG:CD  | 4:9:306:TYR:CE1[1_554] | 1.88                     | 0.32              |
| 4:5:307:PRO:CB  | 4:9:337:TYR:O[1_554]   | 1.88                     | 0.32              |
| 4:4:283:MET:CB  | 4:8:285:CYS:CA[1_554]  | 1.88                     | 0.32              |
| 4:4:243:PRO:CD  | 4:8:59:GLN:C[1_554]    | 1.88                     | 0.32              |
| 4:2:367:PRO:N   | 4:7:236:LEU:N[1_554]   | 1.88                     | 0.32              |
| 4:4:345:ILE:CG2 | 4:8:369:ILE:CG2[1_554] | 1.88                     | 0.32              |
| 4:4:335:ARG:NH2 | 4:8:106:THR:CG2[1_554] | 1.88                     | 0.32              |
| 4:5:367:PRO:CA  | 4:V:233:SER:CB[1_554]  | 1.88                     | 0.32              |
| 4:4:156:GLY:O   | 4:8:73:HIS:O[1_554]    | 1.88                     | 0.32              |
| 4:4:155:SER:N   | 4:8:108:ALA:CB[1_554]  | 1.88                     | 0.32              |
| 4:2:357:ILE:CA  | 4:7:232:SER:O[1_554]   | 1.88                     | 0.32              |
| 4:3:77:THR:CB   | 4:8:246:GLN:OE1[1_554] | 1.88                     | 0.32              |
| 4:5:258:PRO:CD  | 4:9:302:GLY:N[1_554]   | 1.88                     | 0.32              |
| 4:4:183:ARG:N   | 4:8:73:HIS:N[1_554]    | 1.88                     | 0.32              |
| 4:5:199:SER:O   | 4:9:203:THR:O[1_554]   | 1.88                     | 0.32              |
| 4:3:198:TYR:N   | 4:7:208:ILE:C[1_554]   | 1.88                     | 0.32              |
| 4:3:345:ILE:N   | 4:7:367:PRO:CG[1_554]  | 1.88                     | 0.32              |
| 4:5:276:GLU:O   | 4:9:281:SER:OG[1_554]  | 1.88                     | 0.32              |
| 4:5:144:ALA:CA  | 4:9:370:VAL:O[1_554]   | 1.88                     | 0.32              |
| 4:5:192:ILE:C   | 4:9:213:LYS:CB[1_554]  | 1.88                     | 0.32              |
| 4:4:205:GLU:CA  | 4:8:62:ARG:CZ[1_554]   | 1.88                     | 0.32              |
| 4:4:340:TRP:C   | 4:8:117:GLU:CA[1_554]  | 1.88                     | 0.32              |
| 4:3:220:ALA:CB  | 4:7:335:ARG:CG[1_554]  | 1.88                     | 0.32              |
| 4:5:214:GLU:CG  | 4:9:16:LEU:CA[1_554]   | 1.88                     | 0.32              |
| 4:5:371:HIS:CB  | 4:V:230:ALA:CA[1_554]  | 1.88                     | 0.32              |
| 4:4:321:ALA:O   | 4:8:292:ASP:OD1[1_554] | 1.88                     | 0.32              |
| 4:5:276:GLU:CA  | 4:9:281:SER:CB[1_554]  | 1.88                     | 0.32              |
| 4:3:189:LEU:O   | 4:7:186:THR:OG1[1_554] | 1.88                     | 0.32              |
| 4:1:291:LYS:NZ  | 4:7:39:ARG:C[1_554]    | 1.88                     | 0.32              |
| 4:3:372:ARG:C   | 4:8:226:GLU:O[1_554]   | 1.88                     | 0.32              |
| 4:5:267:ILE:CB  | 4:9:180:LEU:CD2[1_554] | 1.88                     | 0.32              |
| 4:4:196:ARG:N   | 4:8:209:VAL:C[1_554]   | 1.88                     | 0.32              |
| 4:4:337:TYR:CG  | 4:8:119:MET:CB[1_554]  | 1.88                     | 0.32              |
| 4:5:142:LEU:C   | 4:9:372:ARG:CB[1_554]  | 1.88                     | 0.32              |
| 4:4:173:HIS:ND1 | 4:9:266:PHE:CA[1_554]  | 1.88                     | 0.32              |
| 4:4:327:ILE:CG2 | 4:8:149:THR:N[1_554]   | 1.88                     | 0.32              |
| 4:5:295:ALA:N   | 4:9:166:TYR:C[1_554]   | 1.88                     | 0.32              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:178:LEU:CD1 | 4:8:177:ARG:N[1_554]   | 1.88                     | 0.32              |
| 4:5:267:ILE:CD1 | 4:9:180:LEU:CG[1_554]  | 1.88                     | 0.32              |
| 4:4:316:GLU:CD  | 4:8:151:ILE:O[1_554]   | 1.88                     | 0.32              |
| 4:3:204:ALA:CB  | 4:7:62:ARG:CB[1_554]   | 1.88                     | 0.32              |
| 4:3:318:THR:CA  | 4:7:150:GLY:N[1_554]   | 1.88                     | 0.32              |
| 4:5:305:MET:CE  | 4:9:11:ASP:N[1_554]    | 1.88                     | 0.32              |
| 4:2:172:PRO:O   | 4:7:188:TYR:CE1[1_554] | 1.88                     | 0.32              |
| 4:5:18:LYS:CA   | 4:9:79:TRP:CD2[1_554]  | 1.88                     | 0.32              |
| 4:3:243:PRO:CG  | 4:7:59:GLN:C[1_554]    | 1.88                     | 0.32              |
| 4:5:160:THR:N   | 4:9:177:ARG:NH1[1_554] | 1.88                     | 0.32              |
| 4:5:339:VAL:CG2 | 4:9:111:ASN:ND2[1_554] | 1.88                     | 0.32              |
| 4:3:18:LYS:O    | 4:7:118:LYS:CE[1_554]  | 1.88                     | 0.32              |
| 4:3:147:ARG:O   | 4:7:372:ARG:C[1_554]   | 1.88                     | 0.32              |
| 4:3:189:LEU:N   | 4:7:182:GLY:C[1_554]   | 1.88                     | 0.32              |
| 4:3:313:MET:CA  | 4:7:138:ALA:O[1_554]   | 1.88                     | 0.32              |
| 4:3:159:VAL:C   | 4:7:177:ARG:CZ[1_554]  | 1.88                     | 0.32              |
| 4:4:281:SER:C   | 4:8:173:HIS:CE1[1_554] | 1.88                     | 0.32              |
| 4:3:319:ALA:C   | 4:7:292:ASP:C[1_554]   | 1.88                     | 0.32              |
| 4:4:157:ASP:N   | 4:8:72:GLU:O[1_554]    | 1.88                     | 0.32              |
| 4:5:316:GLU:OE1 | 4:9:297:ASN:OD1[1_554] | 1.88                     | 0.32              |
| 4:2:113:LYS:CE  | 4:7:254:ARG:CG[1_554]  | 1.88                     | 0.32              |
| 4:4:142:LEU:CA  | 4:8:371:HIS:O[1_554]   | 1.88                     | 0.32              |
| 4:5:157:ASP:CG  | 4:9:71:ILE:C[1_554]    | 1.88                     | 0.32              |
| 4:4:157:ASP:CB  | 4:8:72:GLU:O[1_554]    | 1.88                     | 0.32              |
| 4:3:326:LYS:CA  | 4:7:167:GLU:CB[1_554]  | 1.88                     | 0.32              |
| 4:5:113:LYS:O   | 4:V:252:ASN:OD1[1_554] | 1.88                     | 0.32              |
| 4:5:227:MET:O   | 4:9:307:PRO:CB[1_554]  | 1.88                     | 0.32              |
| 4:4:255:PHE:CE1 | 4:8:305:MET:C[1_554]   | 1.88                     | 0.32              |
| 4:3:15:GLY:O    | 4:7:77:THR:CG2[1_554]  | 1.88                     | 0.32              |
| 4:4:268:GLY:N   | 4:8:180:LEU:CD2[1_554] | 1.88                     | 0.32              |
| 4:5:211:ASP:CB  | 4:9:32:PRO:CD[1_554]   | 1.88                     | 0.32              |
| 4:3:141:SER:O   | 4:7:116:ARG:CD[1_554]  | 1.88                     | 0.32              |
| 4:3:194:THR:CA  | 4:7:209:VAL:CB[1_554]  | 1.88                     | 0.32              |
| 4:4:342:GLY:O   | 4:8:368:SER:CA[1_554]  | 1.88                     | 0.32              |
| 4:4:307:PRO:CA  | 4:8:340:TRP:N[1_554]   | 1.88                     | 0.32              |
| 4:3:216:LEU:N   | 4:7:30:VAL:CG1[1_554]  | 1.88                     | 0.32              |
| 4:2:113:LYS:CD  | 4:7:254:ARG:CA[1_554]  | 1.88                     | 0.32              |
| 4:4:305:MET:CG  | 4:8:12:ASN:N[1_554]    | 1.88                     | 0.32              |
| 4:4:76:ILE:O    | 4:9:198:TYR:CD1[1_554] | 1.88                     | 0.32              |
| 4:5:159:VAL:N   | 4:9:177:ARG:CZ[1_554]  | 1.88                     | 0.32              |
| 4:4:357:ILE:CG2 | 4:9:232:SER:C[1_554]   | 1.88                     | 0.32              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:191:LYS:CG  | 4:9:185:LEU:O[1_554]   | 1.88                     | 0.32              |
| 4:3:297:ASN:OD1 | 4:7:170:ALA:CB[1_554]  | 1.88                     | 0.32              |
| 4:5:312:ARG:CZ  | 4:9:299:MET:CB[1_554]  | 1.88                     | 0.32              |
| 4:3:305:MET:SD  | 4:7:12:ASN:ND2[1_554]  | 1.89                     | 0.31              |
| 4:3:269:MET:CA  | 4:7:271:SER:OG[1_554]  | 1.89                     | 0.31              |
| 4:3:275:HIS:O   | 4:7:164:PRO:CG[1_554]  | 1.89                     | 0.31              |
| 4:5:14:SER:O    | 4:9:77:THR:OG1[1_554]  | 1.89                     | 0.31              |
| 4:4:115:ASN:O   | 4:9:196:ARG:NH2[1_554] | 1.89                     | 0.31              |
| 4:3:117:GLU:CA  | 4:8:237:GLU:CB[1_554]  | 1.89                     | 0.31              |
| 4:2:75:ILE:O    | 4:7:198:TYR:CD1[1_554] | 1.89                     | 0.31              |
| 4:3:256:ARG:NH1 | 4:7:306:TYR:CD1[1_554] | 1.89                     | 0.31              |
| 4:3:192:ILE:N   | 4:7:186:THR:N[1_554]   | 1.89                     | 0.31              |
| 4:3:113:LYS:CB  | 4:8:254:ARG:CA[1_554]  | 1.89                     | 0.31              |
| 4:4:62:ARG:NH2  | 4:8:67:LEU:O[1_554]    | 1.89                     | 0.31              |
| 4:5:343:GLY:N   | 4:9:367:PRO:O[1_554]   | 1.89                     | 0.31              |
| 4:3:188:TYR:CB  | 4:7:181:ALA:C[1_554]   | 1.89                     | 0.31              |
| 4:3:337:TYR:OH  | 4:7:86:TRP:CE3[1_554]  | 1.89                     | 0.31              |
| 4:3:275:HIS:O   | 4:7:164:PRO:CA[1_554]  | 1.89                     | 0.31              |
| 4:5:314:GLN:NE2 | 4:9:147:ARG:CA[1_554]  | 1.89                     | 0.31              |
| 4:2:291:LYS:CD  | 4:8:64:ILE:CD1[1_554]  | 1.89                     | 0.31              |
| 4:5:279:TYR:CE2 | 4:9:282:ILE:O[1_554]   | 1.89                     | 0.31              |
| 4:4:253:GLU:OE2 | 4:8:214:GLU:CG[1_554]  | 1.89                     | 0.31              |
| 4:2:109:PRO:O   | 4:7:195:GLU:OE1[1_554] | 1.89                     | 0.31              |
| 4:3:224:GLU:N   | 4:7:331:ALA:CB[1_554]  | 1.89                     | 0.31              |
| 4:5:17:VAL:CB   | 4:9:79:TRP:CB[1_554]   | 1.89                     | 0.31              |
| 4:3:158:GLY:C   | 4:7:177:ARG:NH2[1_554] | 1.89                     | 0.31              |
| 4:3:340:TRP:CG  | 4:7:118:LYS:CD[1_554]  | 1.89                     | 0.31              |
| 4:3:282:ILE:CD1 | 4:7:171:LEU:CB[1_554]  | 1.89                     | 0.31              |
| 4:3:178:LEU:CD1 | 4:7:177:ARG:N[1_554]   | 1.89                     | 0.31              |
| 4:5:290:ARG:CD  | 4:9:286:ASP:CB[1_554]  | 1.89                     | 0.31              |
| 4:3:198:TYR:CB  | 4:7:207:GLU:CA[1_554]  | 1.89                     | 0.31              |
| 4:5:337:TYR:OH  | 4:9:86:TRP:CG[1_554]   | 1.89                     | 0.31              |
| 4:4:25:ASP:O    | 4:8:124:PHE:N[1_554]   | 1.89                     | 0.31              |
| 4:5:196:ARG:NH2 | 4:9:215:LYS:CD[1_554]  | 1.89                     | 0.31              |
| 4:4:140:LEU:O   | 4:8:371:HIS:CG[1_554]  | 1.89                     | 0.31              |
| 4:3:142:LEU:CG  | 4:7:372:ARG:O[1_554]   | 1.89                     | 0.31              |
| 4:2:112:PRO:CB  | 4:7:250:ILE:CG1[1_554] | 1.89                     | 0.31              |
| 4:4:151:ILE:CG1 | 4:8:172:PRO:N[1_554]   | 1.89                     | 0.31              |
| 4:4:223:PHE:CE1 | 4:8:304:THR:OG1[1_554] | 1.89                     | 0.31              |
| 4:5:333:PRO:O   | 4:9:104:LEU:O[1_554]   | 1.89                     | 0.31              |
| 4:3:370:VAL:CG1 | 4:8:233:SER:OG[1_554]  | 1.89                     | 0.31              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:181:ALA:O   | 4:8:158:GLY:O[1_554]   | 1.89                     | 0.31              |
| 4:4:30:VAL:CG2  | 4:8:79:TRP:O[1_554]    | 1.89                     | 0.31              |
| 4:5:290:ARG:CZ  | 4:9:286:ASP:CB[1_554]  | 1.89                     | 0.31              |
| 4:3:193:LEU:CD1 | 4:7:210:ARG:CZ[1_554]  | 1.89                     | 0.31              |
| 4:5:314:GLN:C   | 4:9:142:LEU:CD1[1_554] | 1.89                     | 0.31              |
| 4:3:274:ILE:CA  | 4:7:162:ASN:C[1_554]   | 1.89                     | 0.31              |
| 4:2:72:GLU:O    | 4:7:199:SER:CA[1_554]  | 1.89                     | 0.31              |
| 4:5:370:VAL:N   | 4:V:232:SER:N[1_554]   | 1.89                     | 0.31              |
| 4:3:110:LEU:CB  | 4:8:192:ILE:CB[1_554]  | 1.89                     | 0.31              |
| 4:3:137:GLN:C   | 4:7:113:LYS:CB[1_554]  | 1.89                     | 0.31              |
| 4:5:173:HIS:NE2 | 4:V:265:SER:CA[1_554]  | 1.89                     | 0.31              |
| 4:5:159:VAL:C   | 4:9:177:ARG:CZ[1_554]  | 1.89                     | 0.31              |
| 4:2:113:LYS:O   | 4:7:251:GLY:O[1_554]   | 1.89                     | 0.31              |
| 4:4:195:GLU:CA  | 4:8:189:LEU:CD2[1_554] | 1.89                     | 0.31              |
| 4:5:339:VAL:O   | 4:9:116:ARG:CA[1_554]  | 1.89                     | 0.31              |
| 4:3:140:LEU:CA  | 4:7:371:HIS:CD2[1_554] | 1.89                     | 0.31              |
| 4:3:314:GLN:N   | 4:7:142:LEU:CA[1_554]  | 1.89                     | 0.31              |
| 4:5:221:LEU:CG  | 4:9:332:PRO:N[1_554]   | 1.89                     | 0.31              |
| 4:4:303:THR:C   | 4:8:137:GLN:OE1[1_554] | 1.89                     | 0.31              |
| 4:3:338:SER:CA  | 4:7:116:ARG:O[1_554]   | 1.89                     | 0.31              |
| 4:4:31:PHE:C    | 4:8:78:ASN:CB[1_554]   | 1.89                     | 0.31              |
| 4:3:270:GLU:CG  | 4:7:271:SER:O[1_554]   | 1.89                     | 0.31              |
| 4:2:112:PRO:N   | 4:7:193:LEU:CD1[1_554] | 1.89                     | 0.31              |
| 4:4:140:LEU:O   | 4:8:371:HIS:ND1[1_554] | 1.89                     | 0.31              |
| 4:1:292:ASP:OD2 | 4:7:40:HIS:CB[1_554]   | 1.89                     | 0.31              |
| 4:3:304:THR:CG2 | 4:7:108:ALA:N[1_554]   | 1.89                     | 0.31              |
| 4:4:322:PRO:O   | 4:8:292:ASP:OD2[1_554] | 1.89                     | 0.31              |
| 4:5:140:LEU:CD1 | 4:9:117:GLU:CG[1_554]  | 1.89                     | 0.31              |
| 4:5:189:LEU:N   | 4:9:183:ARG:CA[1_554]  | 1.89                     | 0.31              |
| 4:4:220:ALA:N   | 4:8:335:ARG:CA[1_554]  | 1.89                     | 0.31              |
| 4:4:339:VAL:CG1 | 4:8:115:ASN:CA[1_554]  | 1.89                     | 0.31              |
| 4:4:337:TYR:CZ  | 4:8:86:TRP:CZ2[1_554]  | 1.89                     | 0.31              |
| 4:4:312:ARG:N   | 4:8:141:SER:C[1_554]   | 1.89                     | 0.31              |
| 4:4:106:THR:OG1 | 4:8:114:ALA:CB[1_554]  | 1.89                     | 0.31              |
| 4:3:266:PHE:N   | 4:7:261:LEU:CD2[1_554] | 1.89                     | 0.31              |
| 4:4:370:VAL:C   | 4:9:230:ALA:CB[1_554]  | 1.89                     | 0.31              |
| 4:5:313:MET:O   | 4:9:142:LEU:CD1[1_554] | 1.89                     | 0.31              |
| 4:3:211:ASP:OD2 | 4:7:32:PRO:O[1_554]    | 1.89                     | 0.31              |
| 4:4:314:GLN:CA  | 4:8:142:LEU:CD2[1_554] | 1.89                     | 0.31              |
| 4:5:293:LEU:CD1 | 4:9:169:TYR:CE2[1_554] | 1.89                     | 0.31              |
| 4:3:367:PRO:N   | 4:8:235:SER:C[1_554]   | 1.89                     | 0.31              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:140:LEU:C   | 4:7:371:HIS:CE1[1_554] | 1.89                     | 0.31              |
| 4:4:155:SER:O   | 4:8:74:GLY:O[1_554]    | 1.89                     | 0.31              |
| 4:3:144:ALA:O   | 4:7:370:VAL:C[1_554]   | 1.89                     | 0.31              |
| 4:5:263:GLN:CA  | 4:9:274:ILE:CG2[1_554] | 1.89                     | 0.31              |
| 4:3:218:TYR:CZ  | 4:7:337:TYR:CG[1_554]  | 1.89                     | 0.31              |
| 4:2:369:ILE:O   | 4:7:229:THR:CB[1_554]  | 1.89                     | 0.31              |
| 4:5:304:THR:OG1 | 4:9:137:GLN:CD[1_554]  | 1.89                     | 0.31              |
| 4:5:215:LYS:CE  | 4:9:31:PHE:CA[1_554]   | 1.89                     | 0.31              |
| 4:3:257:CYS:C   | 4:7:156:GLY:C[1_554]   | 1.89                     | 0.31              |
| 4:5:255:PHE:CE1 | 4:9:305:MET:CA[1_554]  | 1.89                     | 0.31              |
| 4:3:114:ALA:CB  | 4:8:238:LYS:O[1_554]   | 1.89                     | 0.31              |
| 4:4:370:VAL:CB  | 4:9:231:ALA:CA[1_554]  | 1.89                     | 0.31              |
| 4:4:250:ILE:CG2 | 4:8:214:GLU:OE2[1_554] | 1.89                     | 0.31              |
| 4:4:369:ILE:CG1 | 4:9:232:SER:OG[1_554]  | 1.89                     | 0.31              |
| 4:3:214:GLU:CA  | 4:7:16:LEU:O[1_554]    | 1.89                     | 0.31              |
| 4:4:109:PRO:CD  | 4:9:195:GLU:CG[1_554]  | 1.89                     | 0.31              |
| 4:5:341:ILE:N   | 4:9:120:THR:CB[1_554]  | 1.90                     | 0.30              |
| 4:4:259:GLU:OE1 | 4:8:304:THR:CA[1_554]  | 1.90                     | 0.30              |
| 4:4:139:VAL:O   | 4:8:371:HIS:CE1[1_554] | 1.90                     | 0.30              |
| 4:5:340:TRP:CE2 | 4:9:122:ILE:N[1_554]   | 1.90                     | 0.30              |
| 4:5:11:ASP:CG   | 4:9:115:ASN:CB[1_554]  | 1.90                     | 0.30              |
| 4:4:337:TYR:C   | 4:8:119:MET:SD[1_554]  | 1.90                     | 0.30              |
| 4:5:283:MET:CE  | 4:9:289:ILE:N[1_554]   | 1.90                     | 0.30              |
| 4:3:318:THR:CB  | 4:7:149:THR:C[1_554]   | 1.90                     | 0.30              |
| 4:5:212:ILE:CG2 | 4:9:210:ARG:NH1[1_554] | 1.90                     | 0.30              |
| 4:3:304:THR:CA  | 4:7:137:GLN:CG[1_554]  | 1.90                     | 0.30              |
| 4:4:325:MET:SD  | 4:8:166:TYR:OH[1_554]  | 1.90                     | 0.30              |
| 4:4:154:ASP:C   | 4:8:110:LEU:N[1_554]   | 1.90                     | 0.30              |
| 4:3:118:LYS:N   | 4:8:237:GLU:CG[1_554]  | 1.90                     | 0.30              |
| 4:4:113:LYS:NZ  | 4:9:254:ARG:CA[1_554]  | 1.90                     | 0.30              |
| 4:5:258:PRO:CB  | 4:9:301:GLY:CA[1_554]  | 1.90                     | 0.30              |
| 4:4:179:ASP:C   | 4:8:179:ASP:OD1[1_554] | 1.90                     | 0.30              |
| 4:5:346:LEU:C   | 4:9:365:ALA:O[1_554]   | 1.90                     | 0.30              |
| 1:A:637:LYS:CB  | 4:4:311:ASP:OD1[1_556] | 1.90                     | 0.30              |
| 4:5:283:MET:CB  | 4:9:285:CYS:CA[1_554]  | 1.90                     | 0.30              |
| 4:3:368:SER:N   | 4:8:236:LEU:CA[1_554]  | 1.90                     | 0.30              |
| 4:5:227:MET:SD  | 4:9:307:PRO:CD[1_554]  | 1.90                     | 0.30              |
| 4:3:311:ASP:O   | 4:7:141:SER:C[1_554]   | 1.90                     | 0.30              |
| 4:5:255:PHE:CZ  | 4:9:305:MET:C[1_554]   | 1.90                     | 0.30              |
| 4:5:154:ASP:CB  | 4:9:110:LEU:N[1_554]   | 1.90                     | 0.30              |
| 4:5:282:ILE:CG1 | 4:9:171:LEU:CB[1_554]  | 1.90                     | 0.30              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:261:LEU:O   | 4:7:161:HIS:C[1_554]   | 1.90                     | 0.30              |
| 4:4:319:ALA:CA  | 4:8:296:ASN:CB[1_554]  | 1.90                     | 0.30              |
| 4:4:294:TYR:CD1 | 4:8:166:TYR:N[1_554]   | 1.90                     | 0.30              |
| 4:3:337:TYR:CG  | 4:7:119:MET:CA[1_554]  | 1.90                     | 0.30              |
| 4:5:340:TRP:CB  | 4:9:119:MET:C[1_554]   | 1.90                     | 0.30              |
| 4:4:265:SER:O   | 4:8:260:THR:C[1_554]   | 1.90                     | 0.30              |
| 4:4:280:ASN:CA  | 4:8:174:ALA:CB[1_554]  | 1.90                     | 0.30              |
| 4:4:187:ASP:C   | 4:8:183:ARG:CB[1_554]  | 1.90                     | 0.30              |
| 4:2:113:LYS:CB  | 4:7:254:ARG:CG[1_554]  | 1.90                     | 0.30              |
| 4:3:276:GLU:OE1 | 4:7:278:THR:C[1_554]   | 1.90                     | 0.30              |
| 4:4:277:THR:C   | 4:8:174:ALA:O[1_554]   | 1.90                     | 0.30              |
| 4:3:334:GLU:C   | 4:7:105:LEU:CD1[1_554] | 1.90                     | 0.30              |
| 4:3:145:SER:CB  | 4:7:372:ARG:NE[1_554]  | 1.90                     | 0.30              |
| 4:5:326:LYS:NZ  | 4:W:45:VAL:CB[1_554]   | 1.90                     | 0.30              |
| 4:3:141:SER:O   | 4:7:371:HIS:O[1_554]   | 1.90                     | 0.30              |
| 4:5:177:ARG:CZ  | 4:V:194:THR:CB[1_554]  | 1.90                     | 0.30              |
| 4:4:240:TYR:CD2 | 4:8:56:ASP:OD2[1_554]  | 1.90                     | 0.30              |
| 4:4:154:ASP:CB  | 4:8:111:ASN:CA[1_554]  | 1.90                     | 0.30              |
| 4:4:32:PRO:CA   | 4:8:78:ASN:CB[1_554]   | 1.90                     | 0.30              |
| 4:4:216:LEU:CA  | 4:8:30:VAL:CG1[1_554]  | 1.90                     | 0.30              |
| 4:5:286:ASP:OD2 | 4:W:39:ARG:NH1[1_554]  | 1.90                     | 0.30              |
| 4:4:306:TYR:N   | 4:8:11:ASP:OD1[1_554]  | 1.90                     | 0.30              |
| 4:3:114:ALA:CA  | 4:8:250:ILE:CA[1_554]  | 1.90                     | 0.30              |
| 4:3:339:VAL:CA  | 4:7:117:GLU:N[1_554]   | 1.90                     | 0.30              |
| 4:4:223:PHE:CZ  | 4:8:304:THR:OG1[1_554] | 1.90                     | 0.30              |
| 4:3:24:ASP:N    | 4:7:125:GLU:OE1[1_554] | 1.90                     | 0.30              |
| 4:5:27:PRO:CA   | 4:9:122:ILE:C[1_554]   | 1.90                     | 0.30              |
| 4:5:257:CYS:N   | 4:9:303:THR:CB[1_554]  | 1.90                     | 0.30              |
| 4:3:108:ALA:C   | 4:8:195:GLU:CG[1_554]  | 1.90                     | 0.30              |
| 4:5:220:ALA:N   | 4:9:335:ARG:CD[1_554]  | 1.90                     | 0.30              |
| 4:5:204:ALA:O   | 4:9:62:ARG:CG[1_554]   | 1.90                     | 0.30              |
| 4:4:224:GLU:CB  | 4:8:310:ALA:CB[1_554]  | 1.90                     | 0.30              |
| 4:4:308:GLY:O   | 4:8:141:SER:OG[1_554]  | 1.90                     | 0.30              |
| 4:3:26:ALA:CA   | 4:7:123:MET:N[1_554]   | 1.90                     | 0.30              |
| 4:4:208:ILE:CB  | 4:8:59:GLN:CG[1_554]   | 1.90                     | 0.30              |
| 4:4:141:SER:C   | 4:8:116:ARG:CD[1_554]  | 1.90                     | 0.30              |
| 4:3:214:GLU:OE1 | 4:7:33:SER:CB[1_554]   | 1.90                     | 0.30              |
| 4:5:277:THR:C   | 4:9:174:ALA:C[1_554]   | 1.90                     | 0.30              |
| 4:3:207:GLU:CD  | 4:7:68:LYS:N[1_554]    | 1.90                     | 0.30              |
| 4:3:212:ILE:N   | 4:7:32:PRO:CA[1_554]   | 1.90                     | 0.30              |
| 4:2:114:ALA:N   | 4:7:250:ILE:O[1_554]   | 1.90                     | 0.30              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:340:TRP:CD2 | 4:8:121:GLN:CB[1_554]  | 1.90                     | 0.30              |
| 4:3:143:TYR:N   | 4:7:372:ARG:C[1_554]   | 1.90                     | 0.30              |
| 4:4:279:TYR:CB  | 4:8:164:PRO:CB[1_554]  | 1.90                     | 0.30              |
| 4:3:208:ILE:N   | 4:7:67:LEU:CD1[1_554]  | 1.90                     | 0.30              |
| 4:4:265:SER:O   | 4:8:261:LEU:N[1_554]   | 1.90                     | 0.30              |
| 4:5:270:GLU:CB  | 4:9:271:SER:C[1_554]   | 1.90                     | 0.30              |
| 4:4:18:LYS:N    | 4:8:79:TRP:NE1[1_554]  | 1.90                     | 0.30              |
| 4:4:215:LYS:CG  | 4:8:31:PHE:O[1_554]    | 1.90                     | 0.30              |
| 4:3:272:ALA:CA  | 4:7:277:THR:CB[1_554]  | 1.90                     | 0.30              |
| 4:4:291:LYS:CD  | 4:V:64:ILE:CD1[1_554]  | 1.90                     | 0.30              |
| 4:5:343:GLY:CA  | 4:9:367:PRO:O[1_554]   | 1.90                     | 0.30              |
| 4:3:157:ASP:CG  | 4:7:72:GLU:N[1_554]    | 1.90                     | 0.30              |
| 4:3:140:LEU:N   | 4:7:371:HIS:CE1[1_554] | 1.90                     | 0.30              |
| 4:1:292:ASP:OD2 | 4:7:40:HIS:N[1_554]    | 1.90                     | 0.30              |
| 4:5:319:ALA:N   | 4:9:296:ASN:N[1_554]   | 1.90                     | 0.30              |
| 4:5:173:HIS:N   | 4:V:267:ILE:CA[1_554]  | 1.90                     | 0.30              |
| 4:4:187:ASP:C   | 4:8:184:ASP:N[1_554]   | 1.90                     | 0.30              |
| 4:3:334:GLU:OE2 | 4:7:133:TYR:CA[1_554]  | 1.90                     | 0.30              |
| 4:3:210:ARG:CB  | 4:7:69:TYR:CZ[1_554]   | 1.90                     | 0.30              |
| 4:5:18:LYS:CD   | 4:9:79:TRP:CZ3[1_554]  | 1.90                     | 0.30              |
| 4:2:291:LYS:CA  | 4:8:64:ILE:CG2[1_554]  | 1.90                     | 0.30              |
| 4:4:262:PHE:CE1 | 4:8:152:VAL:CG1[1_554] | 1.90                     | 0.30              |
| 4:4:319:ALA:CB  | 4:8:296:ASN:CG[1_554]  | 1.90                     | 0.30              |
| 4:4:281:SER:CA  | 4:8:173:HIS:C[1_554]   | 1.90                     | 0.30              |
| 4:4:316:GLU:CA  | 4:8:151:ILE:O[1_554]   | 1.90                     | 0.30              |
| 4:4:339:VAL:CA  | 4:8:117:GLU:N[1_554]   | 1.90                     | 0.30              |
| 4:4:369:ILE:O   | 4:9:230:ALA:N[1_554]   | 1.90                     | 0.30              |
| 4:4:159:VAL:CA  | 4:8:177:ARG:NH2[1_554] | 1.91                     | 0.29              |
| 4:5:281:SER:CB  | 4:9:171:LEU:O[1_554]   | 1.91                     | 0.29              |
| 4:4:192:ILE:CG1 | 4:8:213:LYS:CD[1_554]  | 1.91                     | 0.29              |
| 4:3:338:SER:C   | 4:7:116:ARG:CB[1_554]  | 1.91                     | 0.29              |
| 4:3:285:CYS:C   | 4:8:270:GLU:OE2[1_554] | 1.91                     | 0.29              |
| 4:5:210:ARG:NH2 | 4:9:34:ILE:CA[1_554]   | 1.91                     | 0.29              |
| 4:2:357:ILE:CD1 | 4:7:232:SER:OG[1_554]  | 1.91                     | 0.29              |
| 4:4:331:ALA:CA  | 4:8:135:ALA:CA[1_554]  | 1.91                     | 0.29              |
| 4:3:345:ILE:CB  | 4:7:367:PRO:N[1_554]   | 1.91                     | 0.29              |
| 4:3:198:TYR:CB  | 4:7:207:GLU:O[1_554]   | 1.91                     | 0.29              |
| 4:4:157:ASP:O   | 4:8:73:HIS:N[1_554]    | 1.91                     | 0.29              |
| 4:5:290:ARG:CD  | 4:9:286:ASP:OD2[1_554] | 1.91                     | 0.29              |
| 4:4:305:MET:CE  | 4:8:10:CYS:C[1_554]    | 1.91                     | 0.29              |
| 4:4:144:ALA:C   | 4:8:370:VAL:CA[1_554]  | 1.91                     | 0.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:311:ASP:CA  | 4:9:141:SER:O[1_554]   | 1.91                     | 0.29              |
| 4:2:292:ASP:OD2 | 4:8:40:HIS:CA[1_554]   | 1.91                     | 0.29              |
| 4:5:316:GLU:CD  | 4:9:297:ASN:CG[1_554]  | 1.91                     | 0.29              |
| 4:3:15:GLY:C    | 4:7:77:THR:CA[1_554]   | 1.91                     | 0.29              |
| 4:5:136:ILE:CB  | 4:9:113:LYS:CD[1_554]  | 1.91                     | 0.29              |
| 4:4:214:GLU:CA  | 4:8:17:VAL:N[1_554]    | 1.91                     | 0.29              |
| 4:5:262:PHE:CE2 | 4:9:153:LEU:C[1_554]   | 1.91                     | 0.29              |
| 4:5:214:GLU:CA  | 4:9:16:LEU:C[1_554]    | 1.91                     | 0.29              |
| 4:5:20:GLY:O    | 4:9:121:GLN:CG[1_554]  | 1.91                     | 0.29              |
| 4:3:310:ALA:N   | 4:7:137:GLN:O[1_554]   | 1.91                     | 0.29              |
| 4:5:309:ILE:CG2 | 4:9:141:SER:OG[1_554]  | 1.91                     | 0.29              |
| 4:3:316:GLU:CG  | 4:7:152:VAL:CA[1_554]  | 1.91                     | 0.29              |
| 4:5:227:MET:CB  | 4:9:307:PRO:N[1_554]   | 1.91                     | 0.29              |
| 4:4:160:THR:OG1 | 4:8:161:HIS:NE2[1_554] | 1.91                     | 0.29              |
| 4:5:320:LEU:CA  | 4:9:293:LEU:N[1_554]   | 1.91                     | 0.29              |
| 4:5:110:LEU:CA  | 4:V:195:GLU:OE1[1_554] | 1.91                     | 0.29              |
| 4:5:312:ARG:O   | 4:9:298:VAL:CG1[1_554] | 1.91                     | 0.29              |
| 4:3:27:PRO:N    | 4:7:122:ILE:N[1_554]   | 1.91                     | 0.29              |
| 4:4:366:GLY:C   | 4:9:235:SER:N[1_554]   | 1.91                     | 0.29              |
| 4:4:281:SER:N   | 4:8:174:ALA:CA[1_554]  | 1.91                     | 0.29              |
| 4:3:207:GLU:CD  | 4:7:67:LEU:CB[1_554]   | 1.91                     | 0.29              |
| 4:4:240:TYR:OH  | 4:8:56:ASP:CA[1_554]   | 1.91                     | 0.29              |
| 4:4:369:ILE:N   | 4:9:229:THR:O[1_554]   | 1.91                     | 0.29              |
| 4:5:154:ASP:C   | 4:9:108:ALA:C[1_554]   | 1.91                     | 0.29              |
| 4:5:218:TYR:N   | 4:9:336:LYS:CB[1_554]  | 1.91                     | 0.29              |
| 4:4:314:GLN:O   | 4:8:142:LEU:CD2[1_554] | 1.91                     | 0.29              |
| 4:5:261:LEU:CA  | 4:9:160:THR:CG2[1_554] | 1.91                     | 0.29              |
| 4:4:16:LEU:N    | 4:8:77:THR:O[1_554]    | 1.91                     | 0.29              |
| 4:5:315:LYS:O   | 4:9:296:ASN:O[1_554]   | 1.91                     | 0.29              |
| 4:3:242:LEU:O   | 4:7:60:SER:OG[1_554]   | 1.91                     | 0.29              |
| 4:5:111:ASN:C   | 4:V:192:ILE:O[1_554]   | 1.91                     | 0.29              |
| 4:3:243:PRO:CG  | 4:7:60:SER:C[1_554]    | 1.91                     | 0.29              |
| 4:3:186:THR:CB  | 4:7:183:ARG:NH1[1_554] | 1.91                     | 0.29              |
| 4:3:154:ASP:OD1 | 4:7:111:ASN:C[1_554]   | 1.91                     | 0.29              |
| 4:2:113:LYS:CB  | 4:7:254:ARG:N[1_554]   | 1.91                     | 0.29              |
| 4:3:195:GLU:O   | 4:7:212:ILE:CB[1_554]  | 1.91                     | 0.29              |
| 4:4:199:SER:N   | 4:8:205:GLU:C[1_554]   | 1.91                     | 0.29              |
| 4:3:196:ARG:C   | 4:7:212:ILE:N[1_554]   | 1.91                     | 0.29              |
| 4:4:338:SER:OG  | 4:8:134:VAL:CG2[1_554] | 1.91                     | 0.29              |
| 4:4:222:ASP:C   | 4:8:331:ALA:CA[1_554]  | 1.91                     | 0.29              |
| 4:5:188:TYR:CB  | 4:9:181:ALA:C[1_554]   | 1.91                     | 0.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:290:ARG:NE  | 4:8:286:ASP:CB[1_554]  | 1.91                     | 0.29              |
| 4:4:76:ILE:O    | 4:9:198:TYR:CZ[1_554]  | 1.91                     | 0.29              |
| 4:5:218:TYR:CE1 | 4:9:337:TYR:CE1[1_554] | 1.91                     | 0.29              |
| 4:3:291:LYS:N   | 4:9:64:ILE:CG2[1_554]  | 1.91                     | 0.29              |
| 4:3:207:GLU:OE1 | 4:7:66:THR:C[1_554]    | 1.91                     | 0.29              |
| 4:3:215:LYS:O   | 4:7:30:VAL:CA[1_554]   | 1.91                     | 0.29              |
| 4:5:367:PRO:N   | 4:V:233:SER:O[1_554]   | 1.91                     | 0.29              |
| 4:5:15:GLY:CA   | 4:9:77:THR:OG1[1_554]  | 1.91                     | 0.29              |
| 4:4:190:MET:C   | 4:8:186:THR:CB[1_554]  | 1.91                     | 0.29              |
| 4:5:258:PRO:C   | 4:9:155:SER:O[1_554]   | 1.91                     | 0.29              |
| 4:3:286:ASP:CA  | 4:8:270:GLU:CG[1_554]  | 1.91                     | 0.29              |
| 4:4:136:ILE:O   | 4:8:113:LYS:CD[1_554]  | 1.91                     | 0.29              |
| 4:5:183:ARG:CZ  | 4:9:72:GLU:CD[1_554]   | 1.91                     | 0.29              |
| 4:5:243:PRO:CG  | 4:9:59:GLN:C[1_554]    | 1.91                     | 0.29              |
| 4:2:367:PRO:O   | 4:7:236:LEU:N[1_554]   | 1.91                     | 0.29              |
| 4:2:110:LEU:C   | 4:7:192:ILE:CB[1_554]  | 1.91                     | 0.29              |
| 4:5:367:PRO:N   | 4:V:234:SER:CA[1_554]  | 1.91                     | 0.29              |
| 4:4:141:SER:OG  | 4:8:116:ARG:CB[1_554]  | 1.91                     | 0.29              |
| 4:4:250:ILE:CG1 | 4:8:210:ARG:CZ[1_554]  | 1.91                     | 0.29              |
| 4:3:288:ASP:CA  | 4:9:62:ARG:O[1_554]    | 1.91                     | 0.29              |
| 4:4:318:THR:CG2 | 4:8:149:THR:O[1_554]   | 1.91                     | 0.29              |
| 4:3:173:HIS:CD2 | 4:8:267:ILE:N[1_554]   | 1.91                     | 0.29              |
| 4:5:28:ARG:O    | 4:9:83:GLU:OE1[1_554]  | 1.91                     | 0.29              |
| 4:3:345:ILE:CG2 | 4:7:369:ILE:N[1_554]   | 1.91                     | 0.29              |
| 4:2:326:LYS:CE  | 4:8:45:VAL:N[1_554]    | 1.91                     | 0.29              |
| 4:2:357:ILE:C   | 4:7:232:SER:O[1_554]   | 1.91                     | 0.29              |
| 4:3:309:ILE:C   | 4:7:137:GLN:O[1_554]   | 1.91                     | 0.29              |
| 4:5:151:ILE:CG2 | 4:9:169:TYR:O[1_554]   | 1.91                     | 0.29              |
| 4:4:30:VAL:O    | 4:8:80:ASP:O[1_554]    | 1.91                     | 0.29              |
| 4:4:16:LEU:CA   | 4:8:78:ASN:CA[1_554]   | 1.91                     | 0.29              |
| 4:5:187:ASP:OD1 | 4:9:183:ARG:CD[1_554]  | 1.91                     | 0.29              |
| 4:4:333:PRO:O   | 4:8:105:LEU:N[1_554]   | 1.91                     | 0.29              |
| 4:5:141:SER:C   | 4:9:116:ARG:NE[1_554]  | 1.91                     | 0.29              |
| 4:5:314:GLN:CG  | 4:9:142:LEU:C[1_554]   | 1.91                     | 0.29              |
| 4:4:273:GLY:N   | 4:8:277:THR:CG2[1_554] | 1.91                     | 0.29              |
| 4:5:281:SER:N   | 4:9:174:ALA:CA[1_554]  | 1.91                     | 0.29              |
| 4:4:272:ALA:CB  | 4:8:277:THR:O[1_554]   | 1.91                     | 0.29              |
| 4:4:333:PRO:CA  | 4:8:104:LEU:CA[1_554]  | 1.91                     | 0.29              |
| 4:5:270:GLU:CA  | 4:9:271:SER:C[1_554]   | 1.91                     | 0.29              |
| 4:4:280:ASN:CB  | 4:8:284:LYS:CB[1_554]  | 1.91                     | 0.29              |
| 4:3:264:PRO:CA  | 4:7:274:ILE:CD1[1_554] | 1.91                     | 0.29              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:172:PRO:CD  | 4:8:266:PHE:CB[1_554]  | 1.91                     | 0.29              |
| 4:4:218:TYR:CG  | 4:8:337:TYR:CD1[1_554] | 1.91                     | 0.29              |
| 4:4:141:SER:O   | 4:8:116:ARG:CD[1_554]  | 1.91                     | 0.29              |
| 4:5:281:SER:OG  | 4:9:173:HIS:C[1_554]   | 1.91                     | 0.29              |
| 4:2:367:PRO:N   | 4:7:235:SER:N[1_554]   | 1.91                     | 0.29              |
| 4:3:136:ILE:O   | 4:7:113:LYS:CB[1_554]  | 1.91                     | 0.29              |
| 4:4:155:SER:C   | 4:8:108:ALA:CB[1_554]  | 1.91                     | 0.29              |
| 4:4:265:SER:OG  | 4:8:261:LEU:O[1_554]   | 1.91                     | 0.29              |
| 4:3:366:GLY:C   | 4:8:234:SER:CB[1_554]  | 1.92                     | 0.28              |
| 4:4:370:VAL:C   | 4:9:230:ALA:O[1_554]   | 1.92                     | 0.28              |
| 4:5:109:PRO:O   | 4:V:195:GLU:OE2[1_554] | 1.92                     | 0.28              |
| 4:3:260:THR:CA  | 4:7:155:SER:CB[1_554]  | 1.92                     | 0.28              |
| 4:4:56:ASP:CG   | 4:8:37:ARG:NH2[1_554]  | 1.92                     | 0.28              |
| 4:5:75:ILE:CD1  | 4:V:195:GLU:C[1_554]   | 1.92                     | 0.28              |
| 4:3:256:ARG:NH2 | 4:7:213:LYS:CG[1_554]  | 1.92                     | 0.28              |
| 4:3:32:PRO:N    | 4:7:78:ASN:OD1[1_554]  | 1.92                     | 0.28              |
| 4:3:253:GLU:CD  | 4:7:214:GLU:CD[1_554]  | 1.92                     | 0.28              |
| 4:4:333:PRO:N   | 4:8:104:LEU:C[1_554]   | 1.92                     | 0.28              |
| 4:4:192:ILE:CB  | 4:8:213:LYS:CG[1_554]  | 1.92                     | 0.28              |
| 4:4:335:ARG:CG  | 4:8:106:THR:CB[1_554]  | 1.92                     | 0.28              |
| 4:5:110:LEU:CD2 | 4:V:191:LYS:NZ[1_554]  | 1.92                     | 0.28              |
| 4:5:190:MET:O   | 4:9:186:THR:CB[1_554]  | 1.92                     | 0.28              |
| 4:5:191:LYS:CB  | 4:9:188:TYR:N[1_554]   | 1.92                     | 0.28              |
| 4:3:255:PHE:O   | 4:7:302:GLY:N[1_554]   | 1.92                     | 0.28              |
| 4:5:151:ILE:CG2 | 4:9:169:TYR:C[1_554]   | 1.92                     | 0.28              |
| 4:3:25:ASP:C    | 4:7:124:PHE:N[1_554]   | 1.92                     | 0.28              |
| 4:4:30:VAL:C    | 4:8:79:TRP:O[1_554]    | 1.92                     | 0.28              |
| 4:4:256:ARG:C   | 4:8:303:THR:OG1[1_554] | 1.92                     | 0.28              |
| 4:4:116:ARG:CA  | 4:9:196:ARG:NH1[1_554] | 1.92                     | 0.28              |
| 4:4:281:SER:N   | 4:8:174:ALA:N[1_554]   | 1.92                     | 0.28              |
| 4:5:242:LEU:CD2 | 4:9:207:GLU:CD[1_554]  | 1.92                     | 0.28              |
| 4:5:304:THR:CA  | 4:9:137:GLN:CB[1_554]  | 1.92                     | 0.28              |
| 4:3:75:ILE:CA   | 4:8:197:GLY:O[1_554]   | 1.92                     | 0.28              |
| 4:3:210:ARG:CD  | 4:7:69:TYR:CD2[1_554]  | 1.92                     | 0.28              |
| 4:4:204:ALA:CB  | 4:8:62:ARG:O[1_554]    | 1.92                     | 0.28              |
| 4:3:262:PHE:CZ  | 4:7:154:ASP:CB[1_554]  | 1.92                     | 0.28              |
| 4:5:177:ARG:CZ  | 4:V:194:THR:OG1[1_554] | 1.92                     | 0.28              |
| 4:5:198:TYR:CA  | 4:9:205:GLU:O[1_554]   | 1.92                     | 0.28              |
| 4:5:24:ASP:CG   | 4:9:124:PHE:O[1_554]   | 1.92                     | 0.28              |
| 4:2:288:ASP:CA  | 4:8:39:ARG:NH1[1_554]  | 1.92                     | 0.28              |
| 4:3:262:PHE:CB  | 4:7:153:LEU:O[1_554]   | 1.92                     | 0.28              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:160:THR:CB  | 4:8:161:HIS:NE2[1_554] | 1.92                     | 0.28              |
| 4:3:294:TYR:C   | 4:7:169:TYR:N[1_554]   | 1.92                     | 0.28              |
| 4:5:186:THR:OG1 | 4:9:183:ARG:CZ[1_554]  | 1.92                     | 0.28              |
| 4:5:254:ARG:NE  | 4:9:336:LYS:NZ[1_554]  | 1.92                     | 0.28              |
| 4:5:259:GLU:N   | 4:9:304:THR:N[1_554]   | 1.92                     | 0.28              |
| 4:5:113:LYS:CA  | 4:V:252:ASN:C[1_554]   | 1.92                     | 0.28              |
| 4:5:268:GLY:N   | 4:9:264:PRO:CA[1_554]  | 1.92                     | 0.28              |
| 4:5:347:ALA:CA  | 4:9:366:GLY:C[1_554]   | 1.92                     | 0.28              |
| 4:3:196:ARG:CG  | 4:7:212:ILE:N[1_554]   | 1.92                     | 0.28              |
| 4:4:184:ASP:OD1 | 4:8:73:HIS:CD2[1_554]  | 1.92                     | 0.28              |
| 4:2:113:LYS:C   | 4:7:250:ILE:CG2[1_554] | 1.92                     | 0.28              |
| 4:5:151:ILE:CG2 | 4:9:170:ALA:CA[1_554]  | 1.92                     | 0.28              |
| 4:3:279:TYR:CG  | 4:7:285:CYS:SG[1_554]  | 1.92                     | 0.28              |
| 4:3:15:GLY:CA   | 4:7:77:THR:OG1[1_554]  | 1.92                     | 0.28              |
| 4:3:154:ASP:CB  | 4:7:110:LEU:O[1_554]   | 1.92                     | 0.28              |
| 4:5:207:GLU:CD  | 4:9:67:LEU:CG[1_554]   | 1.92                     | 0.28              |
| 4:5:336:LYS:CB  | 4:9:12:ASN:CG[1_554]   | 1.92                     | 0.28              |
| 4:5:316:GLU:CA  | 4:9:297:ASN:CA[1_554]  | 1.92                     | 0.28              |
| 4:5:178:LEU:CD2 | 4:9:176:MET:O[1_554]   | 1.92                     | 0.28              |
| 4:3:311:ASP:O   | 4:7:142:LEU:C[1_554]   | 1.92                     | 0.28              |
| 4:3:332:PRO:CG  | 4:7:134:VAL:N[1_554]   | 1.92                     | 0.28              |
| 4:2:172:PRO:CD  | 4:7:266:PHE:CD2[1_554] | 1.92                     | 0.28              |
| 4:5:220:ALA:CB  | 4:9:335:ARG:NH1[1_554] | 1.92                     | 0.28              |
| 4:3:345:ILE:CD1 | 4:7:369:ILE:CG2[1_554] | 1.92                     | 0.28              |
| 4:5:313:MET:CB  | 4:9:152:VAL:CB[1_554]  | 1.92                     | 0.28              |
| 4:3:115:ASN:O   | 4:8:237:GLU:OE1[1_554] | 1.92                     | 0.28              |
| 4:2:117:GLU:CB  | 4:7:237:GLU:N[1_554]   | 1.92                     | 0.28              |
| 4:5:199:SER:CA  | 4:9:205:GLU:C[1_554]   | 1.92                     | 0.28              |
| 4:1:291:LYS:NZ  | 4:7:39:ARG:CA[1_554]   | 1.92                     | 0.28              |
| 4:4:31:PHE:O    | 4:8:78:ASN:CA[1_554]   | 1.92                     | 0.28              |
| 4:5:151:ILE:CD1 | 4:9:171:LEU:CB[1_554]  | 1.92                     | 0.28              |
| 4:4:294:TYR:O   | 4:8:167:GLU:C[1_554]   | 1.92                     | 0.28              |
| 4:5:198:TYR:CG  | 4:9:208:ILE:CB[1_554]  | 1.92                     | 0.28              |
| 4:4:262:PHE:CE2 | 4:8:154:ASP:CA[1_554]  | 1.92                     | 0.28              |
| 4:4:335:ARG:CB  | 4:8:106:THR:CA[1_554]  | 1.92                     | 0.28              |
| 4:3:137:GLN:CB  | 4:7:112:PRO:C[1_554]   | 1.92                     | 0.28              |
| 4:5:243:PRO:CB  | 4:9:60:SER:CB[1_554]   | 1.92                     | 0.28              |
| 4:4:207:GLU:O   | 4:8:34:ILE:CD1[1_554]  | 1.92                     | 0.28              |
| 4:3:291:LYS:NZ  | 4:9:64:ILE:CB[1_554]   | 1.92                     | 0.28              |
| 4:4:210:ARG:CB  | 4:8:69:TYR:CZ[1_554]   | 1.92                     | 0.28              |
| 4:3:337:TYR:CB  | 4:7:119:MET:C[1_554]   | 1.92                     | 0.28              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:113:LYS:O   | 4:7:250:ILE:O[1_554]   | 1.92                     | 0.28              |
| 4:3:179:ASP:O   | 4:7:179:ASP:CG[1_554]  | 1.92                     | 0.28              |
| 4:4:319:ALA:O   | 4:8:295:ALA:N[1_554]   | 1.92                     | 0.28              |
| 4:2:115:ASN:N   | 4:7:249:THR:C[1_554]   | 1.92                     | 0.28              |
| 4:5:28:ARG:CA   | 4:9:126:THR:CB[1_554]  | 1.92                     | 0.28              |
| 4:4:340:TRP:CA  | 4:8:117:GLU:O[1_554]   | 1.92                     | 0.28              |
| 4:5:161:HIS:CG  | 4:9:110:LEU:CB[1_554]  | 1.92                     | 0.28              |
| 4:5:315:LYS:C   | 4:9:296:ASN:O[1_554]   | 1.92                     | 0.28              |
| 4:5:330:ILE:O   | 4:9:139:VAL:CG1[1_554] | 1.92                     | 0.28              |
| 4:5:151:ILE:CG2 | 4:9:170:ALA:N[1_554]   | 1.92                     | 0.28              |
| 4:4:306:TYR:CA  | 4:8:11:ASP:OD2[1_554]  | 1.92                     | 0.28              |
| 4:4:328:LYS:CA  | 4:8:168:GLY:CA[1_554]  | 1.92                     | 0.28              |
| 4:3:137:GLN:CB  | 4:7:112:PRO:CA[1_554]  | 1.92                     | 0.28              |
| 4:3:329:ILE:CB  | 4:7:139:VAL:CB[1_554]  | 1.92                     | 0.28              |
| 4:4:268:GLY:C   | 4:8:264:PRO:CG[1_554]  | 1.92                     | 0.28              |
| 4:5:317:ILE:CG2 | 4:9:151:ILE:N[1_554]   | 1.92                     | 0.28              |
| 4:3:187:ASP:N   | 4:7:183:ARG:CB[1_554]  | 1.92                     | 0.28              |
| 4:3:280:ASN:CG  | 4:7:281:SER:C[1_554]   | 1.92                     | 0.28              |
| 4:5:320:LEU:N   | 4:9:292:ASP:C[1_554]   | 1.92                     | 0.28              |
| 4:5:23:GLY:CA   | 4:9:362:TYR:CE2[1_554] | 1.92                     | 0.28              |
| 4:5:302:GLY:C   | 4:9:12:ASN:O[1_554]    | 1.92                     | 0.28              |
| 4:3:294:TYR:CG  | 4:7:166:TYR:CG[1_554]  | 1.92                     | 0.28              |
| 4:5:9:VAL:CG1   | 4:9:117:GLU:O[1_554]   | 1.92                     | 0.28              |
| 4:3:182:GLY:N   | 4:7:74:GLY:N[1_554]    | 1.92                     | 0.28              |
| 4:4:118:LYS:CB  | 4:9:249:THR:OG1[1_554] | 1.92                     | 0.28              |
| 4:5:276:GLU:O   | 4:9:281:SER:C[1_554]   | 1.92                     | 0.28              |
| 4:3:215:LYS:O   | 4:7:17:VAL:O[1_554]    | 1.92                     | 0.28              |
| 4:3:215:LYS:CD  | 4:7:31:PHE:CA[1_554]   | 1.92                     | 0.28              |
| 4:3:143:TYR:CD2 | 4:7:368:SER:C[1_554]   | 1.93                     | 0.27              |
| 4:5:214:GLU:O   | 4:9:16:LEU:CB[1_554]   | 1.93                     | 0.27              |
| 4:5:26:ALA:CB   | 4:9:123:MET:CG[1_554]  | 1.93                     | 0.27              |
| 4:4:279:TYR:CG  | 4:8:293:LEU:CD2[1_554] | 1.93                     | 0.27              |
| 4:4:320:LEU:CA  | 4:8:293:LEU:C[1_554]   | 1.93                     | 0.27              |
| 4:3:18:LYS:CG   | 4:7:79:TRP:CZ3[1_554]  | 1.93                     | 0.27              |
| 4:4:310:ALA:N   | 4:8:141:SER:CA[1_554]  | 1.93                     | 0.27              |
| 4:4:117:GLU:C   | 4:9:237:GLU:OE2[1_554] | 1.93                     | 0.27              |
| 4:5:305:MET:CB  | 4:9:11:ASP:OD2[1_554]  | 1.93                     | 0.27              |
| 4:5:143:TYR:CE2 | 4:9:369:ILE:CA[1_554]  | 1.93                     | 0.27              |
| 4:4:256:ARG:CZ  | 4:8:306:TYR:CE1[1_554] | 1.93                     | 0.27              |
| 4:3:154:ASP:CG  | 4:7:111:ASN:O[1_554]   | 1.93                     | 0.27              |
| 4:3:198:TYR:O   | 4:7:205:GLU:O[1_554]   | 1.93                     | 0.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:314:GLN:CG  | 4:7:143:TYR:N[1_554]   | 1.93                     | 0.27              |
| 4:4:186:THR:CA  | 4:8:157:ASP:OD2[1_554] | 1.93                     | 0.27              |
| 4:3:227:MET:CG  | 4:7:305:MET:C[1_554]   | 1.93                     | 0.27              |
| 4:5:340:TRP:CB  | 4:9:120:THR:N[1_554]   | 1.93                     | 0.27              |
| 4:3:255:PHE:CE2 | 4:7:305:MET:SD[1_554]  | 1.93                     | 0.27              |
| 4:5:327:ILE:CG2 | 4:9:149:THR:C[1_554]   | 1.93                     | 0.27              |
| 4:3:169:TYR:OH  | 4:8:266:PHE:CZ[1_554]  | 1.93                     | 0.27              |
| 4:2:110:LEU:CA  | 4:7:192:ILE:CG1[1_554] | 1.93                     | 0.27              |
| 4:3:173:HIS:CB  | 4:8:267:ILE:CA[1_554]  | 1.93                     | 0.27              |
| 4:2:113:LYS:CA  | 4:7:250:ILE:CG2[1_554] | 1.93                     | 0.27              |
| 4:5:31:PHE:O    | 4:9:78:ASN:CG[1_554]   | 1.93                     | 0.27              |
| 4:4:345:ILE:CG2 | 4:8:366:GLY:O[1_554]   | 1.93                     | 0.27              |
| 4:5:258:PRO:C   | 4:9:155:SER:CB[1_554]  | 1.93                     | 0.27              |
| 4:4:319:ALA:CB  | 4:8:295:ALA:C[1_554]   | 1.93                     | 0.27              |
| 4:3:109:PRO:CG  | 4:8:195:GLU:OE2[1_554] | 1.93                     | 0.27              |
| 4:4:141:SER:C   | 4:8:371:HIS:O[1_554]   | 1.93                     | 0.27              |
| 4:5:59:GLN:CB   | 4:9:68:LYS:NZ[1_554]   | 1.93                     | 0.27              |
| 4:3:291:LYS:CE  | 4:9:64:ILE:CG1[1_554]  | 1.93                     | 0.27              |
| 4:5:32:PRO:CA   | 4:9:78:ASN:CG[1_554]   | 1.93                     | 0.27              |
| 4:4:227:MET:CG  | 4:8:306:TYR:O[1_554]   | 1.93                     | 0.27              |
| 4:4:198:TYR:O   | 4:8:205:GLU:O[1_554]   | 1.93                     | 0.27              |
| 4:3:27:PRO:CD   | 4:7:122:ILE:CD1[1_554] | 1.93                     | 0.27              |
| 4:2:114:ALA:C   | 4:7:238:LYS:O[1_554]   | 1.93                     | 0.27              |
| 4:5:118:LYS:N   | 4:V:237:GLU:OE2[1_554] | 1.93                     | 0.27              |
| 4:3:294:TYR:O   | 4:7:168:GLY:N[1_554]   | 1.93                     | 0.27              |
| 4:5:266:PHE:CA  | 4:9:261:LEU:CB[1_554]  | 1.93                     | 0.27              |
| 4:4:267:ILE:CA  | 4:8:180:LEU:CD2[1_554] | 1.93                     | 0.27              |
| 4:5:196:ARG:CB  | 4:9:213:LYS:N[1_554]   | 1.93                     | 0.27              |
| 4:1:291:LYS:N   | 4:7:64:ILE:CB[1_554]   | 1.93                     | 0.27              |
| 4:4:204:ALA:CA  | 4:8:62:ARG:CA[1_554]   | 1.93                     | 0.27              |
| 4:2:116:ARG:CD  | 4:7:252:ASN:ND2[1_554] | 1.93                     | 0.27              |
| 4:3:207:GLU:CG  | 4:7:67:LEU:C[1_554]    | 1.93                     | 0.27              |
| 4:3:372:ARG:N   | 4:8:230:ALA:CB[1_554]  | 1.93                     | 0.27              |
| 4:3:113:LYS:CD  | 4:8:254:ARG:CA[1_554]  | 1.93                     | 0.27              |
| 4:5:348:SER:CA  | 4:9:366:GLY:N[1_554]   | 1.93                     | 0.27              |
| 4:3:180:LEU:CD1 | 4:7:178:LEU:O[1_554]   | 1.93                     | 0.27              |
| 4:4:371:HIS:CD2 | 4:9:255:PHE:CE2[1_554] | 1.93                     | 0.27              |
| 4:5:173:HIS:NE2 | 4:V:265:SER:O[1_554]   | 1.93                     | 0.27              |
| 4:5:310:ALA:CB  | 4:9:141:SER:C[1_554]   | 1.93                     | 0.27              |
| 4:4:258:PRO:CD  | 4:8:302:GLY:N[1_554]   | 1.93                     | 0.27              |
| 4:3:253:GLU:OE2 | 4:7:214:GLU:CD[1_554]  | 1.93                     | 0.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:16:LEU:CG   | 4:8:78:ASN:O[1_554]    | 1.93                     | 0.27              |
| 4:3:73:HIS:CG   | 4:8:199:SER:OG[1_554]  | 1.93                     | 0.27              |
| 4:3:261:LEU:C   | 4:7:161:HIS:N[1_554]   | 1.93                     | 0.27              |
| 4:3:196:ARG:CG  | 4:7:211:ASP:N[1_554]   | 1.93                     | 0.27              |
| 4:3:310:ALA:CB  | 4:7:140:LEU:C[1_554]   | 1.93                     | 0.27              |
| 4:5:261:LEU:O   | 4:9:161:HIS:O[1_554]   | 1.93                     | 0.27              |
| 4:5:311:ASP:C   | 4:9:298:VAL:CG1[1_554] | 1.93                     | 0.27              |
| 4:3:268:GLY:C   | 4:7:264:PRO:CG[1_554]  | 1.93                     | 0.27              |
| 4:4:243:PRO:C   | 4:8:60:SER:OG[1_554]   | 1.93                     | 0.27              |
| 4:4:197:GLY:O   | 4:8:208:ILE:CB[1_554]  | 1.93                     | 0.27              |
| 4:5:161:HIS:CA  | 4:9:110:LEU:CB[1_554]  | 1.93                     | 0.27              |
| 4:4:172:PRO:O   | 4:9:266:PHE:O[1_554]   | 1.93                     | 0.27              |
| 4:4:314:GLN:OE1 | 4:8:148:THR:N[1_554]   | 1.93                     | 0.27              |
| 4:4:270:GLU:CB  | 4:8:271:SER:C[1_554]   | 1.93                     | 0.27              |
| 4:3:304:THR:CB  | 4:7:137:GLN:NE2[1_554] | 1.93                     | 0.27              |
| 4:3:75:ILE:C    | 4:8:197:GLY:C[1_554]   | 1.93                     | 0.27              |
| 4:4:18:LYS:CE   | 4:8:79:TRP:NE1[1_554]  | 1.93                     | 0.27              |
| 4:5:162:ASN:CG  | 4:9:175:ILE:CD1[1_554] | 1.93                     | 0.27              |
| 4:4:289:ILE:CA  | 4:V:63:GLY:O[1_554]    | 1.93                     | 0.27              |
| 4:4:219:VAL:CA  | 4:8:301:GLY:N[1_554]   | 1.93                     | 0.27              |
| 4:4:184:ASP:O   | 4:8:184:ASP:OD1[1_554] | 1.93                     | 0.27              |
| 4:4:334:GLU:CB  | 4:8:105:LEU:CD1[1_554] | 1.93                     | 0.27              |
| 4:4:113:LYS:CB  | 4:9:252:ASN:C[1_554]   | 1.93                     | 0.27              |
| 4:3:110:LEU:CA  | 4:8:192:ILE:N[1_554]   | 1.93                     | 0.27              |
| 4:3:274:ILE:C   | 4:7:162:ASN:CA[1_554]  | 1.93                     | 0.27              |
| 4:5:319:ALA:C   | 4:9:294:TYR:C[1_554]   | 1.93                     | 0.27              |
| 4:5:316:GLU:O   | 4:9:296:ASN:O[1_554]   | 1.93                     | 0.27              |
| 4:5:315:LYS:CG  | 4:9:147:ARG:CZ[1_554]  | 1.93                     | 0.27              |
| 4:4:137:GLN:CG  | 4:8:112:PRO:CB[1_554]  | 1.93                     | 0.27              |
| 4:4:196:ARG:NE  | 4:8:211:ASP:O[1_554]   | 1.93                     | 0.27              |
| 4:3:256:ARG:NH2 | 4:7:213:LYS:C[1_554]   | 1.93                     | 0.27              |
| 4:5:349:LEU:CA  | 4:9:364:GLU:C[1_554]   | 1.93                     | 0.27              |
| 4:4:137:GLN:CA  | 4:8:112:PRO:C[1_554]   | 1.93                     | 0.27              |
| 4:5:196:ARG:NH1 | 4:9:215:LYS:N[1_554]   | 1.93                     | 0.27              |
| 4:4:184:ASP:CB  | 4:8:73:HIS:CE1[1_554]  | 1.93                     | 0.27              |
| 4:5:314:GLN:NE2 | 4:9:148:THR:N[1_554]   | 1.93                     | 0.27              |
| 4:4:336:LYS:C   | 4:8:119:MET:SD[1_554]  | 1.93                     | 0.27              |
| 4:3:341:ILE:CB  | 4:7:120:THR:CA[1_554]  | 1.93                     | 0.27              |
| 4:4:151:ILE:CG1 | 4:8:170:ALA:O[1_554]   | 1.93                     | 0.27              |
| 4:2:114:ALA:CB  | 4:7:238:LYS:O[1_554]   | 1.93                     | 0.27              |
| 4:4:317:ILE:CA  | 4:8:150:GLY:N[1_554]   | 1.93                     | 0.27              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:136:ILE:O   | 4:9:113:LYS:CA[1_554]  | 1.93                     | 0.27              |
| 4:4:261:LEU:N   | 4:8:155:SER:CA[1_554]  | 1.93                     | 0.27              |
| 4:3:304:THR:OG1 | 4:7:107:GLU:CA[1_554]  | 1.93                     | 0.27              |
| 4:5:59:GLN:CD   | 4:9:68:LYS:CB[1_554]   | 1.93                     | 0.27              |
| 4:5:110:LEU:N   | 4:V:195:GLU:CG[1_554]  | 1.93                     | 0.27              |
| 4:3:311:ASP:CA  | 4:7:140:LEU:O[1_554]   | 1.93                     | 0.27              |
| 4:4:250:ILE:CG1 | 4:8:210:ARG:NH1[1_554] | 1.93                     | 0.27              |
| 4:5:256:ARG:CB  | 4:9:306:TYR:CE2[1_554] | 1.93                     | 0.27              |
| 4:5:262:PHE:N   | 4:9:153:LEU:CG[1_554]  | 1.93                     | 0.27              |
| 4:3:261:LEU:O   | 4:7:161:HIS:CA[1_554]  | 1.93                     | 0.27              |
| 4:3:276:GLU:OE2 | 4:7:278:THR:N[1_554]   | 1.93                     | 0.27              |
| 4:5:198:TYR:CB  | 4:9:208:ILE:N[1_554]   | 1.93                     | 0.27              |
| 4:4:305:MET:CE  | 4:8:11:ASP:CA[1_554]   | 1.93                     | 0.27              |
| 4:3:187:ASP:C   | 4:7:183:ARG:CG[1_554]  | 1.93                     | 0.27              |
| 4:3:340:TRP:N   | 4:7:117:GLU:C[1_554]   | 1.93                     | 0.27              |
| 4:5:31:PHE:CB   | 4:9:80:ASP:CB[1_554]   | 1.93                     | 0.27              |
| 4:5:17:VAL:CB   | 4:9:79:TRP:CG[1_554]   | 1.93                     | 0.27              |
| 4:5:321:ALA:C   | 4:9:292:ASP:CA[1_554]  | 1.93                     | 0.27              |
| 4:5:24:ASP:O    | 4:9:124:PHE:CA[1_554]  | 1.93                     | 0.27              |
| 4:2:173:HIS:NE2 | 4:7:264:PRO:C[1_554]   | 1.93                     | 0.27              |
| 4:5:253:GLU:CG  | 4:9:214:GLU:CG[1_554]  | 1.93                     | 0.27              |
| 4:4:218:TYR:CD2 | 4:8:337:TYR:CD2[1_554] | 1.93                     | 0.27              |
| 4:5:207:GLU:O   | 4:9:34:ILE:CD1[1_554]  | 1.93                     | 0.27              |
| 4:4:188:TYR:CG  | 4:8:182:GLY:N[1_554]   | 1.93                     | 0.27              |
| 4:5:113:LYS:O   | 4:V:252:ASN:CB[1_554]  | 1.93                     | 0.27              |
| 4:5:254:ARG:CZ  | 4:9:336:LYS:CE[1_554]  | 1.93                     | 0.27              |
| 4:3:25:ASP:CA   | 4:7:124:PHE:CA[1_554]  | 1.93                     | 0.27              |
| 4:4:199:SER:N   | 4:8:205:GLU:O[1_554]   | 1.94                     | 0.26              |
| 4:5:319:ALA:C   | 4:9:293:LEU:C[1_554]   | 1.94                     | 0.26              |
| 4:3:154:ASP:CG  | 4:7:111:ASN:CB[1_554]  | 1.94                     | 0.26              |
| 4:4:218:TYR:C   | 4:8:336:LYS:O[1_554]   | 1.94                     | 0.26              |
| 4:5:265:SER:O   | 4:9:260:THR:C[1_554]   | 1.94                     | 0.26              |
| 4:5:276:GLU:CD  | 4:9:279:TYR:CA[1_554]  | 1.94                     | 0.26              |
| 4:4:327:ILE:O   | 4:8:148:THR:CB[1_554]  | 1.94                     | 0.26              |
| 4:4:178:LEU:O   | 4:8:177:ARG:NE[1_554]  | 1.94                     | 0.26              |
| 4:3:266:PHE:CA  | 4:7:261:LEU:CB[1_554]  | 1.94                     | 0.26              |
| 4:4:213:LYS:CG  | 4:8:15:GLY:CA[1_554]   | 1.94                     | 0.26              |
| 4:3:109:PRO:CG  | 4:8:195:GLU:CG[1_554]  | 1.94                     | 0.26              |
| 4:3:340:TRP:C   | 4:7:117:GLU:CA[1_554]  | 1.94                     | 0.26              |
| 4:5:25:ASP:O    | 4:9:123:MET:CB[1_554]  | 1.94                     | 0.26              |
| 4:4:113:LYS:CD  | 4:9:254:ARG:C[1_554]   | 1.94                     | 0.26              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:108:ALA:CB  | 4:8:196:ARG:N[1_554]   | 1.94                     | 0.26              |
| 4:4:212:ILE:N   | 4:8:32:PRO:CB[1_554]   | 1.94                     | 0.26              |
| 4:3:151:ILE:CG1 | 4:7:172:PRO:N[1_554]   | 1.94                     | 0.26              |
| 4:3:281:SER:CB  | 4:7:174:ALA:N[1_554]   | 1.94                     | 0.26              |
| 4:5:250:ILE:CD1 | 4:9:210:ARG:NH2[1_554] | 1.94                     | 0.26              |
| 4:5:143:TYR:CD2 | 4:9:369:ILE:O[1_554]   | 1.94                     | 0.26              |
| 4:3:264:PRO:C   | 4:7:178:LEU:CD2[1_554] | 1.94                     | 0.26              |
| 4:3:166:TYR:CE1 | 4:9:40:HIS:CE1[1_554]  | 1.94                     | 0.26              |
| 4:3:153:LEU:N   | 4:7:109:PRO:O[1_554]   | 1.94                     | 0.26              |
| 4:5:277:THR:OG1 | 4:9:176:MET:CB[1_554]  | 1.94                     | 0.26              |
| 4:5:227:MET:CG  | 4:9:307:PRO:O[1_554]   | 1.94                     | 0.26              |
| 4:3:279:TYR:CD2 | 4:7:285:CYS:CB[1_554]  | 1.94                     | 0.26              |
| 4:3:111:ASN:O   | 4:8:253:GLU:CD[1_554]  | 1.94                     | 0.26              |
| 4:4:166:TYR:CE1 | 4:V:40:HIS:CE1[1_554]  | 1.94                     | 0.26              |
| 4:5:370:VAL:C   | 4:V:231:ALA:CA[1_554]  | 1.94                     | 0.26              |
| 4:5:270:GLU:O   | 4:9:272:ALA:CA[1_554]  | 1.94                     | 0.26              |
| 4:3:317:ILE:CA  | 4:7:150:GLY:CA[1_554]  | 1.94                     | 0.26              |
| 4:5:340:TRP:CH2 | 4:9:120:THR:O[1_554]   | 1.94                     | 0.26              |
| 4:4:143:TYR:CE2 | 4:8:369:ILE:N[1_554]   | 1.94                     | 0.26              |
| 4:3:262:PHE:CD1 | 4:7:153:LEU:N[1_554]   | 1.94                     | 0.26              |
| 4:5:278:THR:CA  | 4:9:164:PRO:N[1_554]   | 1.94                     | 0.26              |
| 4:4:162:ASN:OD1 | 4:8:175:ILE:CG2[1_554] | 1.94                     | 0.26              |
| 4:3:113:LYS:C   | 4:8:251:GLY:C[1_554]   | 1.94                     | 0.26              |
| 4:5:154:ASP:CB  | 4:9:109:PRO:C[1_554]   | 1.94                     | 0.26              |
| 4:3:309:ILE:CA  | 4:7:141:SER:OG[1_554]  | 1.94                     | 0.26              |
| 4:5:9:VAL:O     | 4:9:118:LYS:CD[1_554]  | 1.94                     | 0.26              |
| 4:3:314:GLN:CA  | 4:7:142:LEU:CD2[1_554] | 1.94                     | 0.26              |
| 4:3:112:PRO:CG  | 4:8:193:LEU:CD2[1_554] | 1.94                     | 0.26              |
| 4:4:338:SER:C   | 4:8:116:ARG:CG[1_554]  | 1.94                     | 0.26              |
| 4:3:159:VAL:N   | 4:7:177:ARG:NH2[1_554] | 1.94                     | 0.26              |
| 4:5:332:PRO:O   | 4:9:104:LEU:CD2[1_554] | 1.94                     | 0.26              |
| 4:5:289:ILE:CG2 | 4:W:39:ARG:NH1[1_554]  | 1.94                     | 0.26              |
| 4:3:276:GLU:CA  | 4:7:281:SER:OG[1_554]  | 1.94                     | 0.26              |
| 4:4:17:VAL:O    | 4:8:79:TRP:N[1_554]    | 1.94                     | 0.26              |
| 4:3:110:LEU:CG  | 4:8:192:ILE:N[1_554]   | 1.94                     | 0.26              |
| 4:4:309:ILE:CA  | 4:8:339:VAL:CG2[1_554] | 1.94                     | 0.26              |
| 1:D:542:PHE:CE1 | 4:5:328:LYS:NZ[1_556]  | 1.94                     | 0.26              |
| 4:4:327:ILE:CA  | 4:8:167:GLU:CA[1_554]  | 1.94                     | 0.26              |
| 4:3:17:VAL:O    | 4:7:79:TRP:CG[1_554]   | 1.94                     | 0.26              |
| 4:5:211:ASP:OD1 | 4:9:32:PRO:CG[1_554]   | 1.94                     | 0.26              |
| 4:5:265:SER:C   | 4:9:261:LEU:CA[1_554]  | 1.94                     | 0.26              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:310:ALA:N   | 4:9:141:SER:N[1_554]   | 1.94                     | 0.26              |
| 4:5:190:MET:CG  | 4:9:187:ASP:OD1[1_554] | 1.94                     | 0.26              |
| 4:4:357:ILE:CG1 | 4:9:232:SER:N[1_554]   | 1.94                     | 0.26              |
| 4:3:257:CYS:CA  | 4:7:156:GLY:O[1_554]   | 1.94                     | 0.26              |
| 4:4:154:ASP:CA  | 4:8:108:ALA:O[1_554]   | 1.94                     | 0.26              |
| 4:4:27:PRO:C    | 4:8:122:ILE:CG1[1_554] | 1.94                     | 0.26              |
| 4:2:287:ILE:C   | 4:8:63:GLY:O[1_554]    | 1.94                     | 0.26              |
| 4:4:263:GLN:N   | 4:8:153:LEU:CD1[1_554] | 1.94                     | 0.26              |
| 4:5:370:VAL:C   | 4:V:231:ALA:N[1_554]   | 1.94                     | 0.26              |
| 4:3:180:LEU:CB  | 4:7:179:ASP:CA[1_554]  | 1.94                     | 0.26              |
| 4:5:280:ASN:O   | 4:9:284:LYS:C[1_554]   | 1.94                     | 0.26              |
| 4:4:281:SER:CB  | 4:8:171:LEU:O[1_554]   | 1.94                     | 0.26              |
| 4:5:291:LYS:CE  | 4:W:64:ILE:CG1[1_554]  | 1.94                     | 0.26              |
| 4:3:292:ASP:N   | 4:9:64:ILE:CG2[1_554]  | 1.94                     | 0.26              |
| 4:5:314:GLN:CB  | 4:9:142:LEU:O[1_554]   | 1.94                     | 0.26              |
| 4:4:308:GLY:N   | 4:8:339:VAL:CA[1_554]  | 1.94                     | 0.26              |
| 4:4:110:LEU:CG  | 4:9:191:LYS:CG[1_554]  | 1.94                     | 0.26              |
| 4:3:223:PHE:CZ  | 4:7:300:SER:C[1_554]   | 1.94                     | 0.26              |
| 4:5:313:MET:CG  | 4:9:152:VAL:CG1[1_554] | 1.94                     | 0.26              |
| 4:2:175:ILE:CG2 | 4:7:191:LYS:CE[1_554]  | 1.94                     | 0.26              |
| 4:4:338:SER:C   | 4:8:116:ARG:CB[1_554]  | 1.94                     | 0.26              |
| 4:2:113:LYS:CD  | 4:7:255:PHE:N[1_554]   | 1.94                     | 0.26              |
| 4:2:370:VAL:CA  | 4:7:230:ALA:CA[1_554]  | 1.94                     | 0.26              |
| 4:2:173:HIS:N   | 4:7:267:ILE:CG2[1_554] | 1.94                     | 0.26              |
| 4:3:293:LEU:CA  | 4:7:169:TYR:CE2[1_554] | 1.94                     | 0.26              |
| 4:2:112:PRO:O   | 4:7:250:ILE:CG2[1_554] | 1.94                     | 0.26              |
| 4:5:210:ARG:NH1 | 4:9:33:SER:CA[1_554]   | 1.94                     | 0.26              |
| 4:3:272:ALA:O   | 4:7:277:THR:CG2[1_554] | 1.94                     | 0.26              |
| 4:2:166:TYR:CD1 | 4:8:40:HIS:CD2[1_554]  | 1.94                     | 0.26              |
| 4:5:143:TYR:CB  | 4:9:372:ARG:CB[1_554]  | 1.94                     | 0.26              |
| 4:4:145:SER:OG  | 4:8:372:ARG:CD[1_554]  | 1.94                     | 0.26              |
| 4:4:277:THR:CB  | 4:8:175:ILE:CA[1_554]  | 1.94                     | 0.26              |
| 4:5:261:LEU:CD2 | 4:9:160:THR:CA[1_554]  | 1.94                     | 0.26              |
| 4:5:18:LYS:CE   | 4:9:79:TRP:CZ3[1_554]  | 1.94                     | 0.26              |
| 4:5:14:SER:CA   | 4:9:77:THR:OG1[1_554]  | 1.94                     | 0.26              |
| 4:3:178:LEU:O   | 4:7:177:ARG:NE[1_554]  | 1.94                     | 0.26              |
| 4:4:16:LEU:N    | 4:8:77:THR:CB[1_554]   | 1.94                     | 0.26              |
| 4:4:331:ALA:N   | 4:8:135:ALA:CB[1_554]  | 1.94                     | 0.26              |
| 4:3:317:ILE:C   | 4:7:149:THR:C[1_554]   | 1.94                     | 0.26              |
| 4:4:25:ASP:C    | 4:8:123:MET:C[1_554]   | 1.94                     | 0.26              |
| 4:5:20:GLY:N    | 4:9:121:GLN:NE2[1_554] | 1.94                     | 0.26              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:357:ILE:CG1 | 4:9:231:ALA:O[1_554]   | 1.94                     | 0.26              |
| 4:5:334:GLU:C   | 4:9:105:LEU:O[1_554]   | 1.94                     | 0.26              |
| 4:4:218:TYR:OH  | 4:8:337:TYR:CE2[1_554] | 1.94                     | 0.26              |
| 4:4:285:CYS:O   | 4:9:270:GLU:CG[1_554]  | 1.94                     | 0.26              |
| 4:5:145:SER:CB  | 4:9:133:TYR:OH[1_554]  | 1.94                     | 0.26              |
| 4:5:177:ARG:CZ  | 4:V:194:THR:CG2[1_554] | 1.94                     | 0.26              |
| 4:3:298:VAL:O   | 4:7:136:ILE:CG1[1_554] | 1.94                     | 0.26              |
| 4:5:280:ASN:ND2 | 4:9:284:LYS:N[1_554]   | 1.94                     | 0.26              |
| 4:5:214:GLU:CG  | 4:9:16:LEU:C[1_554]    | 1.94                     | 0.26              |
| 4:4:118:LYS:N   | 4:9:237:GLU:OE2[1_554] | 1.94                     | 0.26              |
| 4:5:277:THR:CB  | 4:9:176:MET:N[1_554]   | 1.94                     | 0.26              |
| 4:5:319:ALA:CA  | 4:9:295:ALA:CA[1_554]  | 1.94                     | 0.26              |
| 4:3:336:LYS:CE  | 4:7:86:TRP:CD2[1_554]  | 1.94                     | 0.26              |
| 4:3:321:ALA:C   | 4:7:292:ASP:CB[1_554]  | 1.94                     | 0.26              |
| 4:2:117:GLU:O   | 4:7:237:GLU:CG[1_554]  | 1.95                     | 0.25              |
| 4:4:226:GLU:CG  | 4:8:305:MET:CE[1_554]  | 1.95                     | 0.25              |
| 4:4:222:ASP:C   | 4:8:331:ALA:CB[1_554]  | 1.95                     | 0.25              |
| 4:3:369:ILE:CA  | 4:8:229:THR:O[1_554]   | 1.95                     | 0.25              |
| 4:3:113:LYS:CE  | 4:8:254:ARG:CB[1_554]  | 1.95                     | 0.25              |
| 4:4:294:TYR:CE2 | 4:8:166:TYR:CG[1_554]  | 1.95                     | 0.25              |
| 4:3:181:ALA:O   | 4:7:73:HIS:ND1[1_554]  | 1.95                     | 0.25              |
| 4:2:115:ASN:CA  | 4:7:250:ILE:CA[1_554]  | 1.95                     | 0.25              |
| 4:5:288:ASP:N   | 4:W:62:ARG:O[1_554]    | 1.95                     | 0.25              |
| 4:4:357:ILE:CB  | 4:9:231:ALA:O[1_554]   | 1.95                     | 0.25              |
| 4:4:339:VAL:CA  | 4:8:116:ARG:CB[1_554]  | 1.95                     | 0.25              |
| 4:5:257:CYS:CA  | 4:9:303:THR:CA[1_554]  | 1.95                     | 0.25              |
| 4:5:253:GLU:CD  | 4:9:214:GLU:C[1_554]   | 1.95                     | 0.25              |
| 4:4:195:GLU:CB  | 4:8:189:LEU:CB[1_554]  | 1.95                     | 0.25              |
| 4:4:24:ASP:C    | 4:8:125:GLU:N[1_554]   | 1.95                     | 0.25              |
| 4:4:60:SER:CA   | 4:8:66:THR:OG1[1_554]  | 1.95                     | 0.25              |
| 4:2:289:ILE:CG2 | 4:8:39:ARG:NH2[1_554]  | 1.95                     | 0.25              |
| 4:4:210:ARG:N   | 4:8:69:TYR:OH[1_554]   | 1.95                     | 0.25              |
| 4:4:156:GLY:C   | 4:8:75:ILE:CA[1_554]   | 1.95                     | 0.25              |
| 4:5:221:LEU:CA  | 4:9:331:ALA:CA[1_554]  | 1.95                     | 0.25              |
| 4:4:153:LEU:CG  | 4:8:109:PRO:CA[1_554]  | 1.95                     | 0.25              |
| 4:4:300:SER:C   | 4:8:107:GLU:CA[1_554]  | 1.95                     | 0.25              |
| 4:4:185:LEU:CG  | 4:8:159:VAL:N[1_554]   | 1.95                     | 0.25              |
| 4:5:259:GLU:OE1 | 4:9:309:ILE:CD1[1_554] | 1.95                     | 0.25              |
| 4:3:56:ASP:OD1  | 4:7:80:ASP:OD1[1_554]  | 1.95                     | 0.25              |
| 4:2:111:ASN:OD1 | 4:7:196:ARG:CB[1_554]  | 1.95                     | 0.25              |
| 4:3:262:PHE:O   | 4:7:153:LEU:CG[1_554]  | 1.95                     | 0.25              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:181:ALA:C   | 4:8:73:HIS:CA[1_554]   | 1.95                     | 0.25              |
| 4:4:270:GLU:N   | 4:8:271:SER:C[1_554]   | 1.95                     | 0.25              |
| 4:3:23:GLY:CA   | 4:7:125:GLU:OE2[1_554] | 1.95                     | 0.25              |
| 4:3:307:PRO:CA  | 4:7:340:TRP:N[1_554]   | 1.95                     | 0.25              |
| 4:4:113:LYS:CE  | 4:9:254:ARG:C[1_554]   | 1.95                     | 0.25              |
| 4:3:310:ALA:CB  | 4:7:140:LEU:CG[1_554]  | 1.95                     | 0.25              |
| 4:3:223:PHE:CZ  | 4:7:301:GLY:CA[1_554]  | 1.95                     | 0.25              |
| 4:5:349:LEU:CA  | 4:9:365:ALA:CB[1_554]  | 1.95                     | 0.25              |
| 4:3:310:ALA:C   | 4:7:140:LEU:O[1_554]   | 1.95                     | 0.25              |
| 4:1:288:ASP:CB  | 4:7:39:ARG:CD[1_554]   | 1.95                     | 0.25              |
| 4:3:116:ARG:N   | 4:8:196:ARG:NH1[1_554] | 1.95                     | 0.25              |
| 4:3:207:GLU:OE1 | 4:7:66:THR:O[1_554]    | 1.95                     | 0.25              |
| 4:3:18:LYS:CA   | 4:7:79:TRP:CG[1_554]   | 1.95                     | 0.25              |
| 4:5:326:LYS:CG  | 4:9:167:GLU:CD[1_554]  | 1.95                     | 0.25              |
| 4:3:338:SER:CB  | 4:7:116:ARG:CB[1_554]  | 1.95                     | 0.25              |
| 4:3:117:GLU:OE1 | 4:8:236:LEU:C[1_554]   | 1.95                     | 0.25              |
| 4:4:109:PRO:CB  | 4:9:195:GLU:CG[1_554]  | 1.95                     | 0.25              |
| 4:5:178:LEU:CD2 | 4:9:176:MET:C[1_554]   | 1.95                     | 0.25              |
| 4:2:367:PRO:CD  | 4:7:235:SER:CB[1_554]  | 1.95                     | 0.25              |
| 4:5:199:SER:CA  | 4:9:206:ARG:C[1_554]   | 1.95                     | 0.25              |
| 4:5:315:LYS:CG  | 4:9:147:ARG:NH1[1_554] | 1.95                     | 0.25              |
| 4:4:370:VAL:CB  | 4:9:231:ALA:C[1_554]   | 1.95                     | 0.25              |
| 4:5:140:LEU:CB  | 4:9:371:HIS:CG[1_554]  | 1.95                     | 0.25              |
| 4:4:333:PRO:CG  | 4:8:104:LEU:C[1_554]   | 1.95                     | 0.25              |
| 4:3:333:PRO:CD  | 4:7:133:TYR:O[1_554]   | 1.95                     | 0.25              |
| 4:3:166:TYR:CD1 | 4:9:40:HIS:ND1[1_554]  | 1.95                     | 0.25              |
| 4:3:198:TYR:CA  | 4:7:205:GLU:O[1_554]   | 1.95                     | 0.25              |
| 4:5:214:GLU:CB  | 4:9:16:LEU:N[1_554]    | 1.95                     | 0.25              |
| 4:3:267:ILE:CG1 | 4:7:180:LEU:CA[1_554]  | 1.95                     | 0.25              |
| 4:5:278:THR:C   | 4:9:164:PRO:CD[1_554]  | 1.95                     | 0.25              |
| 4:3:306:TYR:O   | 4:7:339:VAL:CG1[1_554] | 1.95                     | 0.25              |
| 4:4:25:ASP:C    | 4:8:120:THR:O[1_554]   | 1.95                     | 0.25              |
| 4:5:272:ALA:CB  | 4:9:277:THR:O[1_554]   | 1.95                     | 0.25              |
| 4:3:178:LEU:O   | 4:7:177:ARG:CG[1_554]  | 1.95                     | 0.25              |
| 4:5:211:ASP:OD2 | 4:9:32:PRO:CG[1_554]   | 1.95                     | 0.25              |
| 4:5:137:GLN:OE1 | 4:9:112:PRO:CA[1_554]  | 1.95                     | 0.25              |
| 4:5:310:ALA:C   | 4:9:141:SER:CA[1_554]  | 1.95                     | 0.25              |
| 4:5:186:THR:CA  | 4:9:183:ARG:NE[1_554]  | 1.95                     | 0.25              |
| 4:5:222:ASP:CA  | 4:9:331:ALA:CA[1_554]  | 1.95                     | 0.25              |
| 4:3:337:TYR:CE2 | 4:7:86:TRP:CE3[1_554]  | 1.95                     | 0.25              |
| 4:5:15:GLY:C    | 4:9:77:THR:N[1_554]    | 1.95                     | 0.25              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:289:ILE:CG2 | 4:V:39:ARG:NE[1_554]   | 1.95                     | 0.25              |
| 4:2:75:ILE:CB   | 4:7:198:TYR:CD2[1_554] | 1.95                     | 0.25              |
| 4:3:200:PHE:CD2 | 4:7:206:ARG:NE[1_554]  | 1.95                     | 0.25              |
| 4:4:299:MET:N   | 4:8:136:ILE:CD1[1_554] | 1.95                     | 0.25              |
| 4:3:294:TYR:CD2 | 4:7:166:TYR:CB[1_554]  | 1.95                     | 0.25              |
| 4:3:211:ASP:OD2 | 4:7:55:GLY:N[1_554]    | 1.95                     | 0.25              |
| 4:3:299:MET:CB  | 4:7:136:ILE:C[1_554]   | 1.95                     | 0.25              |
| 4:4:256:ARG:NH2 | 4:8:213:LYS:C[1_554]   | 1.95                     | 0.25              |
| 4:3:275:HIS:O   | 4:7:164:PRO:CD[1_554]  | 1.95                     | 0.25              |
| 4:3:112:PRO:N   | 4:8:253:GLU:CG[1_554]  | 1.95                     | 0.25              |
| 4:5:258:PRO:CD  | 4:9:302:GLY:CA[1_554]  | 1.95                     | 0.25              |
| 4:3:187:ASP:CA  | 4:7:183:ARG:CD[1_554]  | 1.95                     | 0.25              |
| 4:5:192:ILE:CG1 | 4:9:213:LYS:NZ[1_554]  | 1.95                     | 0.25              |
| 4:5:31:PHE:CD2  | 4:9:78:ASN:OD1[1_554]  | 1.95                     | 0.25              |
| 4:5:260:THR:C   | 4:9:160:THR:OG1[1_554] | 1.95                     | 0.25              |
| 4:3:114:ALA:C   | 4:8:251:GLY:N[1_554]   | 1.95                     | 0.25              |
| 4:3:18:LYS:CD   | 4:7:79:TRP:CZ2[1_554]  | 1.95                     | 0.25              |
| 4:5:207:GLU:CD  | 4:9:67:LEU:CD2[1_554]  | 1.95                     | 0.25              |
| 4:4:299:MET:CG  | 4:8:136:ILE:CB[1_554]  | 1.95                     | 0.25              |
| 4:5:255:PHE:N   | 4:9:302:GLY:O[1_554]   | 1.95                     | 0.25              |
| 4:4:270:GLU:C   | 4:8:272:ALA:C[1_554]   | 1.95                     | 0.25              |
| 4:2:117:GLU:CB  | 4:7:238:LYS:N[1_554]   | 1.95                     | 0.25              |
| 4:4:258:PRO:N   | 4:8:156:GLY:CA[1_554]  | 1.95                     | 0.25              |
| 4:4:276:GLU:CD  | 4:8:278:THR:CA[1_554]  | 1.95                     | 0.25              |
| 4:3:283:MET:CE  | 4:7:289:ILE:CG2[1_554] | 1.95                     | 0.25              |
| 4:2:287:ILE:N   | 4:7:270:GLU:CD[1_554]  | 1.95                     | 0.25              |
| 4:5:255:PHE:CA  | 4:9:305:MET:CG[1_554]  | 1.96                     | 0.24              |
| 4:2:119:MET:N   | 4:7:237:GLU:OE1[1_554] | 1.96                     | 0.24              |
| 4:4:286:ASP:C   | 4:9:270:GLU:CD[1_554]  | 1.96                     | 0.24              |
| 4:4:339:VAL:CB  | 4:8:115:ASN:CA[1_554]  | 1.96                     | 0.24              |
| 4:4:277:THR:CA  | 4:8:174:ALA:C[1_554]   | 1.96                     | 0.24              |
| 4:4:344:SER:CB  | 4:8:362:TYR:OH[1_554]  | 1.96                     | 0.24              |
| 4:2:287:ILE:C   | 4:8:63:GLY:CA[1_554]   | 1.96                     | 0.24              |
| 4:3:367:PRO:N   | 4:8:234:SER:O[1_554]   | 1.96                     | 0.24              |
| 4:4:340:TRP:C   | 4:8:118:LYS:N[1_554]   | 1.96                     | 0.24              |
| 4:5:177:ARG:NH1 | 4:V:194:THR:CG2[1_554] | 1.96                     | 0.24              |
| 4:3:283:MET:CG  | 4:7:286:ASP:C[1_554]   | 1.96                     | 0.24              |
| 4:3:275:HIS:CA  | 4:7:163:VAL:C[1_554]   | 1.96                     | 0.24              |
| 4:4:335:ARG:CG  | 4:8:107:GLU:N[1_554]   | 1.96                     | 0.24              |
| 4:4:115:ASN:ND2 | 4:9:198:TYR:CZ[1_554]  | 1.96                     | 0.24              |
| 4:3:178:LEU:CB  | 4:7:177:ARG:CA[1_554]  | 1.96                     | 0.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:116:ARG:CB  | 4:8:252:ASN:CG[1_554]  | 1.96                     | 0.24              |
| 4:4:278:THR:CG2 | 4:8:164:PRO:C[1_554]   | 1.96                     | 0.24              |
| 4:4:192:ILE:CD1 | 4:8:213:LYS:CE[1_554]  | 1.96                     | 0.24              |
| 4:3:196:ARG:CA  | 4:7:209:VAL:O[1_554]   | 1.96                     | 0.24              |
| 4:3:280:ASN:CB  | 4:7:284:LYS:CB[1_554]  | 1.96                     | 0.24              |
| 4:3:198:TYR:C   | 4:7:206:ARG:CA[1_554]  | 1.96                     | 0.24              |
| 4:5:61:LYS:N    | 4:9:66:THR:OG1[1_554]  | 1.96                     | 0.24              |
| 4:1:289:ILE:O   | 4:7:40:HIS:ND1[1_554]  | 1.96                     | 0.24              |
| 4:4:193:LEU:CD1 | 4:8:210:ARG:CG[1_554]  | 1.96                     | 0.24              |
| 4:4:333:PRO:C   | 4:8:105:LEU:CB[1_554]  | 1.96                     | 0.24              |
| 4:5:296:ASN:N   | 4:9:168:GLY:CA[1_554]  | 1.96                     | 0.24              |
| 4:3:172:PRO:CA  | 4:8:266:PHE:O[1_554]   | 1.96                     | 0.24              |
| 4:5:16:LEU:O    | 4:9:76:ILE:O[1_554]    | 1.96                     | 0.24              |
| 4:4:330:ILE:CG2 | 4:8:133:TYR:OH[1_554]  | 1.96                     | 0.24              |
| 4:3:313:MET:C   | 4:7:142:LEU:CB[1_554]  | 1.96                     | 0.24              |
| 4:4:196:ARG:CD  | 4:8:211:ASP:OD1[1_554] | 1.96                     | 0.24              |
| 4:4:211:ASP:CB  | 4:8:32:PRO:CA[1_554]   | 1.96                     | 0.24              |
| 4:4:326:LYS:C   | 4:8:167:GLU:OE1[1_554] | 1.96                     | 0.24              |
| 4:3:299:MET:CG  | 4:7:137:GLN:N[1_554]   | 1.96                     | 0.24              |
| 4:5:337:TYR:OH  | 4:9:86:TRP:CZ2[1_554]  | 1.96                     | 0.24              |
| 4:4:174:ALA:N   | 4:9:267:ILE:CA[1_554]  | 1.96                     | 0.24              |
| 4:3:338:SER:C   | 4:7:117:GLU:N[1_554]   | 1.96                     | 0.24              |
| 4:4:341:ILE:CA  | 4:8:120:THR:OG1[1_554] | 1.96                     | 0.24              |
| 4:5:162:ASN:CA  | 4:9:175:ILE:CD1[1_554] | 1.96                     | 0.24              |
| 4:3:201:VAL:CG2 | 4:7:203:THR:CB[1_554]  | 1.96                     | 0.24              |
| 4:5:220:ALA:CB  | 4:9:335:ARG:NE[1_554]  | 1.96                     | 0.24              |
| 4:4:18:LYS:CA   | 4:8:79:TRP:CD2[1_554]  | 1.96                     | 0.24              |
| 4:5:283:MET:N   | 4:9:285:CYS:CA[1_554]  | 1.96                     | 0.24              |
| 4:4:321:ALA:N   | 4:8:293:LEU:N[1_554]   | 1.96                     | 0.24              |
| 4:3:173:HIS:CB  | 4:8:267:ILE:CG2[1_554] | 1.96                     | 0.24              |
| 4:5:223:PHE:CE1 | 4:9:304:THR:O[1_554]   | 1.96                     | 0.24              |
| 4:4:115:ASN:C   | 4:9:196:ARG:NH1[1_554] | 1.96                     | 0.24              |
| 4:3:143:TYR:C   | 4:7:371:HIS:N[1_554]   | 1.96                     | 0.24              |
| 4:4:269:MET:CB  | 4:8:178:LEU:CG[1_554]  | 1.96                     | 0.24              |
| 4:4:262:PHE:CD1 | 4:8:153:LEU:O[1_554]   | 1.96                     | 0.24              |
| 4:5:142:LEU:C   | 4:9:372:ARG:NE[1_554]  | 1.96                     | 0.24              |
| 4:4:188:TYR:CD1 | 4:8:185:LEU:CB[1_554]  | 1.96                     | 0.24              |
| 4:3:288:ASP:C   | 4:9:64:ILE:CA[1_554]   | 1.96                     | 0.24              |
| 4:3:309:ILE:CG2 | 4:7:339:VAL:CG1[1_554] | 1.96                     | 0.24              |
| 4:3:137:GLN:CD  | 4:7:112:PRO:CB[1_554]  | 1.96                     | 0.24              |
| 4:5:110:LEU:CB  | 4:V:192:ILE:CA[1_554]  | 1.96                     | 0.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:166:TYR:CD1 | 4:8:40:HIS:CE1[1_554]  | 1.96                     | 0.24              |
| 4:2:77:THR:CA   | 4:7:246:GLN:OE1[1_554] | 1.96                     | 0.24              |
| 4:2:114:ALA:O   | 4:7:238:LYS:C[1_554]   | 1.96                     | 0.24              |
| 4:3:186:THR:C   | 4:7:183:ARG:CB[1_554]  | 1.96                     | 0.24              |
| 4:3:137:GLN:O   | 4:7:113:LYS:C[1_554]   | 1.96                     | 0.24              |
| 4:3:196:ARG:NH1 | 4:7:215:LYS:CG[1_554]  | 1.96                     | 0.24              |
| 4:4:205:GLU:O   | 4:8:59:GLN:OE1[1_554]  | 1.96                     | 0.24              |
| 4:4:313:MET:C   | 4:8:142:LEU:CB[1_554]  | 1.96                     | 0.24              |
| 4:5:189:LEU:CA  | 4:9:182:GLY:C[1_554]   | 1.96                     | 0.24              |
| 4:3:270:GLU:N   | 4:7:272:ALA:N[1_554]   | 1.96                     | 0.24              |
| 4:3:73:HIS:O    | 4:8:198:TYR:O[1_554]   | 1.96                     | 0.24              |
| 4:4:210:ARG:NH2 | 4:8:33:SER:O[1_554]    | 1.96                     | 0.24              |
| 4:5:340:TRP:CH2 | 4:9:121:GLN:N[1_554]   | 1.96                     | 0.24              |
| 4:3:161:HIS:O   | 4:7:110:LEU:CD2[1_554] | 1.96                     | 0.24              |
| 4:3:18:LYS:CG   | 4:7:79:TRP:CG[1_554]   | 1.96                     | 0.24              |
| 4:4:18:LYS:CE   | 4:8:79:TRP:CH2[1_554]  | 1.96                     | 0.24              |
| 4:4:17:VAL:O    | 4:8:79:TRP:CD1[1_554]  | 1.96                     | 0.24              |
| 4:5:253:GLU:CG  | 4:9:214:GLU:CB[1_554]  | 1.96                     | 0.24              |
| 4:5:196:ARG:CZ  | 4:9:215:LYS:CB[1_554]  | 1.96                     | 0.24              |
| 4:5:140:LEU:CG  | 4:9:371:HIS:ND1[1_554] | 1.96                     | 0.24              |
| 4:3:144:ALA:CB  | 4:7:370:VAL:C[1_554]   | 1.96                     | 0.24              |
| 4:5:115:ASN:CB  | 4:V:196:ARG:NH1[1_554] | 1.96                     | 0.24              |
| 4:5:340:TRP:CZ2 | 4:9:121:GLN:N[1_554]   | 1.96                     | 0.24              |
| 4:4:193:LEU:C   | 4:8:209:VAL:C[1_554]   | 1.96                     | 0.24              |
| 4:4:183:ARG:O   | 4:8:183:ARG:NH1[1_554] | 1.96                     | 0.24              |
| 4:3:283:MET:CB  | 4:7:285:CYS:CA[1_554]  | 1.96                     | 0.24              |
| 4:3:261:LEU:N   | 4:7:155:SER:CA[1_554]  | 1.96                     | 0.24              |
| 4:4:208:ILE:C   | 4:8:59:GLN:NE2[1_554]  | 1.96                     | 0.24              |
| 4:3:326:LYS:CB  | 4:7:167:GLU:OE1[1_554] | 1.96                     | 0.24              |
| 4:5:11:ASP:CB   | 4:9:118:LYS:CB[1_554]  | 1.96                     | 0.24              |
| 4:4:112:PRO:N   | 4:9:253:GLU:CG[1_554]  | 1.96                     | 0.24              |
| 4:2:370:VAL:CA  | 4:7:230:ALA:O[1_554]   | 1.96                     | 0.24              |
| 4:4:117:GLU:CD  | 4:9:236:LEU:C[1_554]   | 1.96                     | 0.24              |
| 4:4:180:LEU:CD2 | 4:8:178:LEU:CB[1_554]  | 1.96                     | 0.24              |
| 4:2:110:LEU:CB  | 4:7:192:ILE:CB[1_554]  | 1.96                     | 0.24              |
| 4:3:200:PHE:N   | 4:7:206:ARG:CD[1_554]  | 1.96                     | 0.24              |
| 4:3:281:SER:N   | 4:7:174:ALA:CA[1_554]  | 1.96                     | 0.24              |
| 4:3:113:LYS:CG  | 4:8:255:PHE:N[1_554]   | 1.96                     | 0.24              |
| 4:2:367:PRO:O   | 4:7:236:LEU:CA[1_554]  | 1.96                     | 0.24              |
| 4:5:249:THR:CG2 | 4:9:211:ASP:OD1[1_554] | 1.96                     | 0.24              |
| 4:4:187:ASP:C   | 4:8:183:ARG:CA[1_554]  | 1.96                     | 0.24              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:139:VAL:CA  | 4:7:113:LYS:CG[1_554]  | 1.96                     | 0.24              |
| 4:3:305:MET:N   | 4:7:137:GLN:NE2[1_554] | 1.96                     | 0.24              |
| 4:5:340:TRP:CE2 | 4:9:121:GLN:N[1_554]   | 1.96                     | 0.24              |
| 4:5:15:GLY:O    | 4:9:78:ASN:N[1_554]    | 1.96                     | 0.24              |
| 4:5:205:GLU:C   | 4:9:62:ARG:NE[1_554]   | 1.96                     | 0.24              |
| 4:3:117:GLU:C   | 4:8:237:GLU:OE1[1_554] | 1.96                     | 0.24              |
| 4:5:114:ALA:N   | 4:V:252:ASN:N[1_554]   | 1.96                     | 0.24              |
| 4:5:312:ARG:CB  | 4:9:299:MET:O[1_554]   | 1.96                     | 0.24              |
| 4:5:319:ALA:CB  | 4:9:295:ALA:N[1_554]   | 1.96                     | 0.24              |
| 4:5:307:PRO:CA  | 4:9:338:SER:N[1_554]   | 1.96                     | 0.24              |
| 4:5:263:GLN:C   | 4:9:274:ILE:CB[1_554]  | 1.96                     | 0.24              |
| 4:4:172:PRO:C   | 4:9:266:PHE:C[1_554]   | 1.96                     | 0.24              |
| 4:3:223:PHE:O   | 4:7:335:ARG:NE[1_554]  | 1.96                     | 0.24              |
| 4:5:28:ARG:NE   | 4:9:126:THR:CB[1_554]  | 1.96                     | 0.24              |
| 4:3:188:TYR:CE1 | 4:7:185:LEU:CD1[1_554] | 1.96                     | 0.24              |
| 4:3:300:SER:OG  | 4:7:107:GLU:CD[1_554]  | 1.96                     | 0.24              |
| 4:5:289:ILE:CA  | 4:W:64:ILE:N[1_554]    | 1.96                     | 0.24              |
| 4:4:109:PRO:C   | 4:9:195:GLU:OE2[1_554] | 1.97                     | 0.23              |
| 4:4:281:SER:O   | 4:8:173:HIS:ND1[1_554] | 1.97                     | 0.23              |
| 4:4:283:MET:CE  | 4:8:289:ILE:CG1[1_554] | 1.97                     | 0.23              |
| 4:3:340:TRP:CE3 | 4:7:121:GLN:CA[1_554]  | 1.97                     | 0.23              |
| 4:4:72:GLU:O    | 4:9:199:SER:N[1_554]   | 1.97                     | 0.23              |
| 4:5:196:ARG:CA  | 4:9:212:ILE:CA[1_554]  | 1.97                     | 0.23              |
| 4:2:173:HIS:ND1 | 4:7:266:PHE:N[1_554]   | 1.97                     | 0.23              |
| 4:3:117:GLU:CG  | 4:8:237:GLU:N[1_554]   | 1.97                     | 0.23              |
| 4:5:340:TRP:C   | 4:9:120:THR:N[1_554]   | 1.97                     | 0.23              |
| 4:2:169:TYR:CZ  | 4:7:266:PHE:CZ[1_554]  | 1.97                     | 0.23              |
| 4:4:56:ASP:OD2  | 4:8:37:ARG:NH1[1_554]  | 1.97                     | 0.23              |
| 4:2:370:VAL:CG1 | 4:7:236:LEU:CD2[1_554] | 1.97                     | 0.23              |
| 4:3:25:ASP:CA   | 4:7:125:GLU:N[1_554]   | 1.97                     | 0.23              |
| 4:5:326:LYS:O   | 4:9:167:GLU:CD[1_554]  | 1.97                     | 0.23              |
| 4:3:141:SER:CA  | 4:7:371:HIS:ND1[1_554] | 1.97                     | 0.23              |
| 4:4:369:ILE:CG2 | 4:9:233:SER:N[1_554]   | 1.97                     | 0.23              |
| 4:5:26:ALA:O    | 4:9:123:MET:C[1_554]   | 1.97                     | 0.23              |
| 4:4:332:PRO:CG  | 4:8:134:VAL:C[1_554]   | 1.97                     | 0.23              |
| 4:2:108:ALA:CA  | 4:7:196:ARG:N[1_554]   | 1.97                     | 0.23              |
| 4:5:366:GLY:O   | 4:V:233:SER:N[1_554]   | 1.97                     | 0.23              |
| 4:4:310:ALA:C   | 4:8:140:LEU:O[1_554]   | 1.97                     | 0.23              |
| 4:4:215:LYS:CE  | 4:8:31:PHE:CD2[1_554]  | 1.97                     | 0.23              |
| 4:5:256:ARG:C   | 4:9:303:THR:C[1_554]   | 1.97                     | 0.23              |
| 1:A:410:ASN:OD1 | 4:4:226:GLU:OE2[1_556] | 1.97                     | 0.23              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:112:PRO:CD  | 4:V:192:ILE:O[1_554]   | 1.97                     | 0.23              |
| 4:4:117:GLU:OE1 | 4:9:237:GLU:CA[1_554]  | 1.97                     | 0.23              |
| 4:5:174:ALA:O   | 4:9:173:HIS:N[1_554]   | 1.97                     | 0.23              |
| 4:4:346:LEU:N   | 4:8:366:GLY:C[1_554]   | 1.97                     | 0.23              |
| 4:5:106:THR:CB  | 4:9:114:ALA:N[1_554]   | 1.97                     | 0.23              |
| 4:4:259:GLU:OE2 | 4:8:304:THR:O[1_554]   | 1.97                     | 0.23              |
| 4:3:193:LEU:CD1 | 4:7:210:ARG:CG[1_554]  | 1.97                     | 0.23              |
| 4:5:276:GLU:OE2 | 4:9:278:THR:N[1_554]   | 1.97                     | 0.23              |
| 4:5:115:ASN:C   | 4:V:196:ARG:CZ[1_554]  | 1.97                     | 0.23              |
| 4:5:368:SER:CA  | 4:V:229:THR:C[1_554]   | 1.97                     | 0.23              |
| 4:1:292:ASP:OD2 | 4:7:39:ARG:C[1_554]    | 1.97                     | 0.23              |
| 4:5:280:ASN:N   | 4:9:281:SER:O[1_554]   | 1.97                     | 0.23              |
| 4:5:367:PRO:C   | 4:V:230:ALA:O[1_554]   | 1.97                     | 0.23              |
| 4:5:184:ASP:CG  | 4:9:73:HIS:CE1[1_554]  | 1.97                     | 0.23              |
| 4:5:75:ILE:CD1  | 4:V:194:THR:C[1_554]   | 1.97                     | 0.23              |
| 4:3:196:ARG:CA  | 4:7:212:ILE:CA[1_554]  | 1.97                     | 0.23              |
| 4:5:219:VAL:O   | 4:9:335:ARG:C[1_554]   | 1.97                     | 0.23              |
| 4:3:300:SER:OG  | 4:7:107:GLU:OE1[1_554] | 1.97                     | 0.23              |
| 4:4:210:ARG:CA  | 4:8:69:TYR:CE2[1_554]  | 1.97                     | 0.23              |
| 4:3:173:HIS:ND1 | 4:8:267:ILE:N[1_554]   | 1.97                     | 0.23              |
| 4:5:289:ILE:CG2 | 4:W:39:ARG:CZ[1_554]   | 1.97                     | 0.23              |
| 4:5:214:GLU:N   | 4:9:16:LEU:CG[1_554]   | 1.97                     | 0.23              |
| 4:3:178:LEU:CD2 | 4:7:176:MET:O[1_554]   | 1.97                     | 0.23              |
| 4:5:75:ILE:CG1  | 4:V:194:THR:CA[1_554]  | 1.97                     | 0.23              |
| 4:4:193:LEU:CA  | 4:8:210:ARG:CG[1_554]  | 1.97                     | 0.23              |
| 4:3:335:ARG:NH2 | 4:7:106:THR:CB[1_554]  | 1.97                     | 0.23              |
| 4:4:15:GLY:O    | 4:8:77:THR:CG2[1_554]  | 1.97                     | 0.23              |
| 4:4:171:LEU:O   | 4:9:266:PHE:O[1_554]   | 1.97                     | 0.23              |
| 4:5:113:LYS:N   | 4:V:253:GLU:CB[1_554]  | 1.97                     | 0.23              |
| 4:3:286:ASP:CG  | 4:8:270:GLU:OE1[1_554] | 1.97                     | 0.23              |
| 4:5:141:SER:CB  | 4:9:116:ARG:CZ[1_554]  | 1.97                     | 0.23              |
| 4:5:370:VAL:CA  | 4:V:231:ALA:N[1_554]   | 1.97                     | 0.23              |
| 4:4:191:LYS:O   | 4:8:186:THR:CG2[1_554] | 1.97                     | 0.23              |
| 4:4:258:PRO:O   | 4:8:155:SER:CB[1_554]  | 1.97                     | 0.23              |
| 4:4:156:GLY:N   | 4:8:75:ILE:CD1[1_554]  | 1.97                     | 0.23              |
| 4:5:207:GLU:CD  | 4:9:67:LEU:CA[1_554]   | 1.97                     | 0.23              |
| 4:5:297:ASN:CB  | 4:9:165:ILE:CG2[1_554] | 1.97                     | 0.23              |
| 4:5:194:THR:O   | 4:9:209:VAL:CB[1_554]  | 1.97                     | 0.23              |
| 4:4:213:LYS:CB  | 4:8:15:GLY:C[1_554]    | 1.97                     | 0.23              |
| 4:4:348:SER:OG  | 4:8:366:GLY:CA[1_554]  | 1.97                     | 0.23              |
| 4:5:298:VAL:C   | 4:9:136:ILE:CB[1_554]  | 1.97                     | 0.23              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:294:TYR:CG  | 4:8:166:TYR:CD2[1_554] | 1.97                     | 0.23              |
| 4:3:207:GLU:CA  | 4:7:67:LEU:CD1[1_554]  | 1.97                     | 0.23              |
| 4:4:111:ASN:O   | 4:9:253:GLU:CG[1_554]  | 1.97                     | 0.23              |
| 4:4:196:ARG:C   | 4:8:208:ILE:O[1_554]   | 1.97                     | 0.23              |
| 4:5:263:GLN:O   | 4:9:274:ILE:CG1[1_554] | 1.97                     | 0.23              |
| 4:4:265:SER:CA  | 4:8:261:LEU:C[1_554]   | 1.97                     | 0.23              |
| 4:5:258:PRO:CB  | 4:9:301:GLY:C[1_554]   | 1.97                     | 0.23              |
| 4:5:30:VAL:CA   | 4:9:83:GLU:N[1_554]    | 1.97                     | 0.23              |
| 4:4:137:GLN:O   | 4:8:113:LYS:CB[1_554]  | 1.97                     | 0.23              |
| 4:4:143:TYR:N   | 4:8:372:ARG:C[1_554]   | 1.97                     | 0.23              |
| 4:5:26:ALA:CA   | 4:9:123:MET:N[1_554]   | 1.97                     | 0.23              |
| 4:2:367:PRO:CB  | 4:7:235:SER:C[1_554]   | 1.97                     | 0.23              |
| 4:4:18:LYS:CD   | 4:8:79:TRP:CZ3[1_554]  | 1.97                     | 0.23              |
| 4:2:110:LEU:O   | 4:7:192:ILE:C[1_554]   | 1.97                     | 0.23              |
| 4:5:210:ARG:C   | 4:9:15:GLY:O[1_554]    | 1.97                     | 0.23              |
| 4:4:180:LEU:CB  | 4:8:179:ASP:CA[1_554]  | 1.97                     | 0.23              |
| 4:2:171:LEU:C   | 4:7:266:PHE:O[1_554]   | 1.97                     | 0.23              |
| 4:3:337:TYR:CA  | 4:7:119:MET:SD[1_554]  | 1.97                     | 0.23              |
| 4:3:16:LEU:N    | 4:7:77:THR:CB[1_554]   | 1.97                     | 0.23              |
| 4:5:286:ASP:N   | 4:V:270:GLU:CG[1_554]  | 1.97                     | 0.23              |
| 4:5:340:TRP:CZ2 | 4:9:121:GLN:CB[1_554]  | 1.97                     | 0.23              |
| 4:5:166:TYR:CZ  | 4:W:39:ARG:CA[1_554]   | 1.97                     | 0.23              |
| 4:3:218:TYR:OH  | 4:7:27:PRO:CD[1_554]   | 1.97                     | 0.23              |
| 4:5:137:GLN:CG  | 4:9:112:PRO:CB[1_554]  | 1.97                     | 0.23              |
| 4:3:312:ARG:CD  | 4:7:299:MET:CA[1_554]  | 1.97                     | 0.23              |
| 4:3:270:GLU:C   | 4:7:272:ALA:C[1_554]   | 1.97                     | 0.23              |
| 4:4:261:LEU:CA  | 4:8:160:THR:CA[1_554]  | 1.97                     | 0.23              |
| 4:4:207:GLU:OE1 | 4:8:67:LEU:N[1_554]    | 1.97                     | 0.23              |
| 4:5:307:PRO:CG  | 4:9:337:TYR:CA[1_554]  | 1.97                     | 0.23              |
| 4:5:278:THR:OG1 | 4:9:164:PRO:CD[1_554]  | 1.97                     | 0.23              |
| 4:3:321:ALA:N   | 4:7:293:LEU:CD1[1_554] | 1.97                     | 0.23              |
| 4:3:177:ARG:CZ  | 4:8:194:THR:CB[1_554]  | 1.97                     | 0.23              |
| 4:5:214:GLU:OE1 | 4:9:33:SER:N[1_554]    | 1.97                     | 0.23              |
| 4:3:194:THR:N   | 4:7:209:VAL:CG1[1_554] | 1.97                     | 0.23              |
| 4:5:213:LYS:CA  | 4:9:16:LEU:CD2[1_554]  | 1.97                     | 0.23              |
| 4:3:24:ASP:CG   | 4:7:125:GLU:OE1[1_554] | 1.97                     | 0.23              |
| 4:5:273:GLY:CA  | 4:9:162:ASN:ND2[1_554] | 1.97                     | 0.23              |
| 4:3:317:ILE:N   | 4:7:151:ILE:N[1_554]   | 1.97                     | 0.23              |
| 4:5:109:PRO:C   | 4:V:195:GLU:CG[1_554]  | 1.97                     | 0.23              |
| 4:4:337:TYR:O   | 4:8:116:ARG:O[1_554]   | 1.97                     | 0.23              |
| 4:5:301:GLY:CA  | 4:9:107:GLU:CA[1_554]  | 1.97                     | 0.23              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:304:THR:N   | 4:7:137:GLN:CD[1_554]  | 1.97                     | 0.23              |
| 4:5:317:ILE:N   | 4:9:150:GLY:CA[1_554]  | 1.97                     | 0.23              |
| 4:5:346:LEU:CA  | 4:9:366:GLY:O[1_554]   | 1.97                     | 0.23              |
| 4:5:256:ARG:CA  | 4:9:303:THR:O[1_554]   | 1.97                     | 0.23              |
| 4:5:276:GLU:CB  | 4:9:281:SER:CB[1_554]  | 1.97                     | 0.23              |
| 4:3:367:PRO:CA  | 4:8:236:LEU:N[1_554]   | 1.97                     | 0.23              |
| 4:5:150:GLY:O   | 4:9:169:TYR:CZ[1_554]  | 1.97                     | 0.23              |
| 4:3:16:LEU:CB   | 4:7:78:ASN:CA[1_554]   | 1.97                     | 0.23              |
| 4:5:59:GLN:CA   | 4:9:68:LYS:CD[1_554]   | 1.97                     | 0.23              |
| 4:4:210:ARG:CZ  | 4:8:33:SER:C[1_554]    | 1.97                     | 0.23              |
| 4:2:372:ARG:CB  | 4:7:226:GLU:O[1_554]   | 1.97                     | 0.23              |
| 4:5:372:ARG:O   | 4:V:227:MET:CA[1_554]  | 1.97                     | 0.23              |
| 4:4:340:TRP:CE3 | 4:8:118:LYS:O[1_554]   | 1.97                     | 0.23              |
| 4:4:221:LEU:CB  | 4:8:332:PRO:CG[1_554]  | 1.97                     | 0.23              |
| 4:5:22:ALA:C    | 4:9:362:TYR:CZ[1_554]  | 1.97                     | 0.23              |
| 4:4:110:LEU:CB  | 4:9:192:ILE:CB[1_554]  | 1.98                     | 0.22              |
| 4:4:339:VAL:C   | 4:8:117:GLU:CA[1_554]  | 1.98                     | 0.22              |
| 4:5:259:GLU:CD  | 4:9:309:ILE:CB[1_554]  | 1.98                     | 0.22              |
| 4:5:186:THR:O   | 4:9:183:ARG:CA[1_554]  | 1.98                     | 0.22              |
| 4:5:334:GLU:CA  | 4:9:105:LEU:CB[1_554]  | 1.98                     | 0.22              |
| 4:3:151:ILE:CD1 | 4:7:171:LEU:CA[1_554]  | 1.98                     | 0.22              |
| 4:4:200:PHE:CB  | 4:8:206:ARG:NE[1_554]  | 1.98                     | 0.22              |
| 4:3:310:ALA:O   | 4:7:139:VAL:O[1_554]   | 1.98                     | 0.22              |
| 4:3:185:LEU:N   | 4:7:158:GLY:O[1_554]   | 1.98                     | 0.22              |
| 4:4:269:MET:CG  | 4:8:178:LEU:CD1[1_554] | 1.98                     | 0.22              |
| 4:3:166:TYR:CE1 | 4:9:40:HIS:ND1[1_554]  | 1.98                     | 0.22              |
| 4:3:284:LYS:O   | 4:8:268:GLY:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:257:CYS:O   | 4:7:156:GLY:C[1_554]   | 1.98                     | 0.22              |
| 4:5:311:ASP:OD1 | 4:9:144:ALA:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:335:ARG:NH1 | 4:7:106:THR:CB[1_554]  | 1.98                     | 0.22              |
| 4:4:311:ASP:O   | 4:8:142:LEU:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:335:ARG:CG  | 4:7:106:THR:N[1_554]   | 1.98                     | 0.22              |
| 4:2:79:TRP:CH2  | 4:7:249:THR:CB[1_554]  | 1.98                     | 0.22              |
| 4:3:368:SER:N   | 4:8:234:SER:OG[1_554]  | 1.98                     | 0.22              |
| 4:3:159:VAL:CA  | 4:7:177:ARG:CZ[1_554]  | 1.98                     | 0.22              |
| 4:1:292:ASP:CB  | 4:7:40:HIS:ND1[1_554]  | 1.98                     | 0.22              |
| 4:4:144:ALA:N   | 4:8:371:HIS:C[1_554]   | 1.98                     | 0.22              |
| 4:3:184:ASP:OD1 | 4:7:73:HIS:ND1[1_554]  | 1.98                     | 0.22              |
| 4:3:288:ASP:C   | 4:9:64:ILE:N[1_554]    | 1.98                     | 0.22              |
| 4:3:183:ARG:CD  | 4:7:72:GLU:OE1[1_554]  | 1.98                     | 0.22              |
| 4:4:201:VAL:CG2 | 4:8:203:THR:N[1_554]   | 1.98                     | 0.22              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:410:ASN:CG  | 4:4:226:GLU:OE2[1_556] | 1.98                     | 0.22              |
| 4:4:346:LEU:CA  | 4:8:368:SER:CB[1_554]  | 1.98                     | 0.22              |
| 4:5:192:ILE:CD1 | 4:9:306:TYR:OH[1_554]  | 1.98                     | 0.22              |
| 4:3:289:ILE:O   | 4:9:64:ILE:CG2[1_554]  | 1.98                     | 0.22              |
| 4:4:220:ALA:N   | 4:8:335:ARG:CB[1_554]  | 1.98                     | 0.22              |
| 4:5:266:PHE:CZ  | 4:9:261:LEU:CD1[1_554] | 1.98                     | 0.22              |
| 4:3:304:THR:CG2 | 4:7:107:GLU:O[1_554]   | 1.98                     | 0.22              |
| 4:4:118:LYS:CB  | 4:9:237:GLU:OE1[1_554] | 1.98                     | 0.22              |
| 4:4:218:TYR:O   | 4:8:302:GLY:N[1_554]   | 1.98                     | 0.22              |
| 4:3:275:HIS:CA  | 4:7:163:VAL:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:219:VAL:O   | 4:7:335:ARG:O[1_554]   | 1.98                     | 0.22              |
| 4:4:214:GLU:CB  | 4:8:16:LEU:C[1_554]    | 1.98                     | 0.22              |
| 4:5:109:PRO:CA  | 4:V:195:GLU:CG[1_554]  | 1.98                     | 0.22              |
| 4:2:286:ASP:CB  | 4:7:270:GLU:OE2[1_554] | 1.98                     | 0.22              |
| 4:4:160:THR:CG2 | 4:8:161:HIS:CD2[1_554] | 1.98                     | 0.22              |
| 4:5:255:PHE:O   | 4:9:305:MET:N[1_554]   | 1.98                     | 0.22              |
| 4:4:191:LYS:CG  | 4:8:185:LEU:CA[1_554]  | 1.98                     | 0.22              |
| 4:4:311:ASP:CB  | 4:8:144:ALA:CB[1_554]  | 1.98                     | 0.22              |
| 4:2:287:ILE:O   | 4:8:63:GLY:N[1_554]    | 1.98                     | 0.22              |
| 4:5:194:THR:OG1 | 4:9:190:MET:CB[1_554]  | 1.98                     | 0.22              |
| 4:5:309:ILE:CD1 | 4:9:154:ASP:OD1[1_554] | 1.98                     | 0.22              |
| 4:3:151:ILE:N   | 4:7:169:TYR:CE1[1_554] | 1.98                     | 0.22              |
| 4:3:192:ILE:O   | 4:7:213:LYS:CB[1_554]  | 1.98                     | 0.22              |
| 4:5:340:TRP:CD2 | 4:9:121:GLN:N[1_554]   | 1.98                     | 0.22              |
| 4:4:257:CYS:C   | 4:8:156:GLY:O[1_554]   | 1.98                     | 0.22              |
| 4:4:256:ARG:NH2 | 4:8:213:LYS:CG[1_554]  | 1.98                     | 0.22              |
| 4:4:16:LEU:CD1  | 4:8:78:ASN:C[1_554]    | 1.98                     | 0.22              |
| 4:4:75:ILE:CA   | 4:9:197:GLY:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:263:GLN:O   | 4:7:274:ILE:CD1[1_554] | 1.98                     | 0.22              |
| 4:4:140:LEU:CB  | 4:8:113:LYS:O[1_554]   | 1.98                     | 0.22              |
| 4:3:218:TYR:CZ  | 4:7:337:TYR:CZ[1_554]  | 1.98                     | 0.22              |
| 4:4:116:ARG:CB  | 4:9:252:ASN:CG[1_554]  | 1.98                     | 0.22              |
| 4:4:200:PHE:N   | 4:8:206:ARG:CD[1_554]  | 1.98                     | 0.22              |
| 4:4:345:ILE:CB  | 4:8:369:ILE:CG2[1_554] | 1.98                     | 0.22              |
| 4:2:117:GLU:OE1 | 4:7:254:ARG:NH1[1_554] | 1.98                     | 0.22              |
| 4:4:186:THR:CG2 | 4:8:183:ARG:NE[1_554]  | 1.98                     | 0.22              |
| 4:3:269:MET:CG  | 4:7:178:LEU:CD1[1_554] | 1.98                     | 0.22              |
| 4:5:237:GLU:OE2 | 4:9:215:LYS:CG[1_554]  | 1.98                     | 0.22              |
| 4:5:218:TYR:CE1 | 4:9:337:TYR:CE2[1_554] | 1.98                     | 0.22              |
| 4:3:300:SER:CA  | 4:7:107:GLU:OE1[1_554] | 1.98                     | 0.22              |
| 4:2:108:ALA:N   | 4:7:196:ARG:CA[1_554]  | 1.98                     | 0.22              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:26:ALA:O    | 4:8:121:GLN:O[1_554]   | 1.98                     | 0.22              |
| 1:D:542:PHE:CZ  | 4:5:328:LYS:CE[1_556]  | 1.98                     | 0.22              |
| 4:4:191:LYS:CA  | 4:8:186:THR:O[1_554]   | 1.98                     | 0.22              |
| 4:4:154:ASP:CA  | 4:8:109:PRO:C[1_554]   | 1.98                     | 0.22              |
| 4:3:283:MET:SD  | 4:7:286:ASP:N[1_554]   | 1.98                     | 0.22              |
| 4:4:328:LYS:O   | 4:8:168:GLY:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:110:LEU:CG  | 4:8:191:LYS:CG[1_554]  | 1.98                     | 0.22              |
| 4:3:312:ARG:NE  | 4:7:299:MET:O[1_554]   | 1.98                     | 0.22              |
| 4:3:326:LYS:O   | 4:7:167:GLU:C[1_554]   | 1.98                     | 0.22              |
| 4:4:173:HIS:NE2 | 4:9:265:SER:O[1_554]   | 1.98                     | 0.22              |
| 4:4:288:ASP:N   | 4:V:62:ARG:O[1_554]    | 1.98                     | 0.22              |
| 4:3:173:HIS:CB  | 4:8:267:ILE:N[1_554]   | 1.98                     | 0.22              |
| 4:4:26:ALA:C    | 4:8:122:ILE:CB[1_554]  | 1.98                     | 0.22              |
| 4:4:28:ARG:O    | 4:8:83:GLU:OE1[1_554]  | 1.98                     | 0.22              |
| 4:4:280:ASN:C   | 4:8:174:ALA:CB[1_554]  | 1.98                     | 0.22              |
| 4:4:186:THR:CA  | 4:8:183:ARG:CZ[1_554]  | 1.98                     | 0.22              |
| 4:4:199:SER:C   | 4:8:206:ARG:CA[1_554]  | 1.98                     | 0.22              |
| 4:5:301:GLY:N   | 4:9:107:GLU:CB[1_554]  | 1.98                     | 0.22              |
| 4:3:299:MET:CE  | 4:7:137:GLN:N[1_554]   | 1.98                     | 0.22              |
| 4:4:24:ASP:OD1  | 4:8:125:GLU:CB[1_554]  | 1.98                     | 0.22              |
| 4:3:281:SER:C   | 4:7:173:HIS:ND1[1_554] | 1.98                     | 0.22              |
| 4:5:31:PHE:N    | 4:9:80:ASP:N[1_554]    | 1.98                     | 0.22              |
| 4:5:273:GLY:O   | 4:9:162:ASN:ND2[1_554] | 1.98                     | 0.22              |
| 4:2:111:ASN:ND2 | 4:7:196:ARG:NE[1_554]  | 1.98                     | 0.22              |
| 4:4:193:LEU:C   | 4:8:210:ARG:CB[1_554]  | 1.98                     | 0.22              |
| 4:5:198:TYR:CE2 | 4:9:211:ASP:CB[1_554]  | 1.98                     | 0.22              |
| 4:5:256:ARG:NE  | 4:9:306:TYR:CE1[1_554] | 1.98                     | 0.22              |
| 4:4:317:ILE:C   | 4:8:150:GLY:C[1_554]   | 1.98                     | 0.22              |
| 4:5:336:LYS:N   | 4:9:106:THR:C[1_554]   | 1.98                     | 0.22              |
| 4:5:274:ILE:O   | 4:9:162:ASN:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:215:LYS:C   | 4:7:30:VAL:CG1[1_554]  | 1.98                     | 0.22              |
| 4:3:143:TYR:N   | 4:7:372:ARG:CA[1_554]  | 1.98                     | 0.22              |
| 4:1:326:LYS:CG  | 4:7:43:VAL:C[1_554]    | 1.98                     | 0.22              |
| 4:2:173:HIS:CG  | 4:7:264:PRO:O[1_554]   | 1.98                     | 0.22              |
| 4:2:292:ASP:OD1 | 4:8:40:HIS:O[1_554]    | 1.98                     | 0.22              |
| 4:4:213:LYS:C   | 4:8:15:GLY:C[1_554]    | 1.98                     | 0.22              |
| 4:3:18:LYS:CD   | 4:7:79:TRP:CE3[1_554]  | 1.98                     | 0.22              |
| 4:4:198:TYR:CA  | 4:8:208:ILE:N[1_554]   | 1.98                     | 0.22              |
| 4:5:157:ASP:O   | 4:9:72:GLU:O[1_554]    | 1.98                     | 0.22              |
| 4:4:117:GLU:CB  | 4:9:237:GLU:CA[1_554]  | 1.98                     | 0.22              |
| 4:3:267:ILE:CA  | 4:7:180:LEU:CD2[1_554] | 1.98                     | 0.22              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:287:ILE:O   | 4:V:63:GLY:C[1_554]    | 1.99                     | 0.21              |
| 4:4:286:ASP:OD1 | 4:9:270:GLU:OE1[1_554] | 1.99                     | 0.21              |
| 4:4:317:ILE:CD1 | 4:8:165:ILE:CG2[1_554] | 1.99                     | 0.21              |
| 4:3:154:ASP:C   | 4:7:110:LEU:N[1_554]   | 1.99                     | 0.21              |
| 4:4:213:LYS:O   | 4:8:16:LEU:CA[1_554]   | 1.99                     | 0.21              |
| 4:2:172:PRO:CA  | 4:7:188:TYR:CE1[1_554] | 1.99                     | 0.21              |
| 4:4:222:ASP:CA  | 4:8:331:ALA:N[1_554]   | 1.99                     | 0.21              |
| 4:3:328:LYS:O   | 4:7:168:GLY:C[1_554]   | 1.99                     | 0.21              |
| 4:4:284:LYS:O   | 4:9:269:MET:N[1_554]   | 1.99                     | 0.21              |
| 4:5:268:GLY:CA  | 4:9:264:PRO:C[1_554]   | 1.99                     | 0.21              |
| 4:5:145:SER:CB  | 4:9:372:ARG:NH2[1_554] | 1.99                     | 0.21              |
| 4:2:173:HIS:NE2 | 4:7:265:SER:N[1_554]   | 1.99                     | 0.21              |
| 4:5:108:ALA:CB  | 4:V:195:GLU:O[1_554]   | 1.99                     | 0.21              |
| 4:3:317:ILE:CG1 | 4:7:165:ILE:CA[1_554]  | 1.99                     | 0.21              |
| 4:4:314:GLN:CG  | 4:8:143:TYR:CA[1_554]  | 1.99                     | 0.21              |
| 4:2:371:HIS:ND1 | 4:7:252:ASN:N[1_554]   | 1.99                     | 0.21              |
| 4:3:116:ARG:CA  | 4:8:196:ARG:NH1[1_554] | 1.99                     | 0.21              |
| 4:3:211:ASP:C   | 4:7:32:PRO:N[1_554]    | 1.99                     | 0.21              |
| 4:5:307:PRO:CA  | 4:9:337:TYR:O[1_554]   | 1.99                     | 0.21              |
| 4:4:195:GLU:OE1 | 4:8:257:CYS:SG[1_554]  | 1.99                     | 0.21              |
| 4:3:113:LYS:O   | 4:8:251:GLY:O[1_554]   | 1.99                     | 0.21              |
| 4:5:112:PRO:CA  | 4:V:253:GLU:OE1[1_554] | 1.99                     | 0.21              |
| 4:5:110:LEU:C   | 4:V:192:ILE:C[1_554]   | 1.99                     | 0.21              |
| 4:5:280:ASN:CA  | 4:9:281:SER:O[1_554]   | 1.99                     | 0.21              |
| 4:2:72:GLU:C    | 4:7:199:SER:CB[1_554]  | 1.99                     | 0.21              |
| 4:3:156:GLY:O   | 4:7:73:HIS:O[1_554]    | 1.99                     | 0.21              |
| 4:2:109:PRO:CD  | 4:7:195:GLU:CB[1_554]  | 1.99                     | 0.21              |
| 4:3:191:LYS:CD  | 4:7:185:LEU:CA[1_554]  | 1.99                     | 0.21              |
| 4:4:215:LYS:N   | 4:8:31:PHE:O[1_554]    | 1.99                     | 0.21              |
| 4:4:277:THR:CA  | 4:8:281:SER:OG[1_554]  | 1.99                     | 0.21              |
| 4:3:62:ARG:NH2  | 4:7:67:LEU:O[1_554]    | 1.99                     | 0.21              |
| 4:3:309:ILE:O   | 4:7:141:SER:CB[1_554]  | 1.99                     | 0.21              |
| 4:4:316:GLU:OE1 | 4:8:151:ILE:O[1_554]   | 1.99                     | 0.21              |
| 4:4:138:ALA:N   | 4:8:113:LYS:N[1_554]   | 1.99                     | 0.21              |
| 4:3:366:GLY:C   | 4:8:234:SER:CA[1_554]  | 1.99                     | 0.21              |
| 4:5:180:LEU:CB  | 4:9:179:ASP:CA[1_554]  | 1.99                     | 0.21              |
| 4:4:208:ILE:CB  | 4:8:59:GLN:CB[1_554]   | 1.99                     | 0.21              |
| 4:5:264:PRO:CA  | 4:9:274:ILE:CD1[1_554] | 1.99                     | 0.21              |
| 4:4:196:ARG:CD  | 4:8:211:ASP:CB[1_554]  | 1.99                     | 0.21              |
| 4:5:266:PHE:CG  | 4:9:261:LEU:CD2[1_554] | 1.99                     | 0.21              |
| 4:3:30:VAL:CB   | 4:7:79:TRP:CA[1_554]   | 1.99                     | 0.21              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:293:LEU:O   | 4:7:169:TYR:CD1[1_554] | 1.99                     | 0.21              |
| 4:3:76:ILE:N    | 4:8:197:GLY:O[1_554]   | 1.99                     | 0.21              |
| 4:3:336:LYS:CE  | 4:7:86:TRP:CD1[1_554]  | 1.99                     | 0.21              |
| 4:4:190:MET:C   | 4:8:186:THR:CG2[1_554] | 1.99                     | 0.21              |
| 4:5:295:ALA:C   | 4:9:168:GLY:CA[1_554]  | 1.99                     | 0.21              |
| 4:5:215:LYS:CD  | 4:9:30:VAL:C[1_554]    | 1.99                     | 0.21              |
| 4:4:30:VAL:CG1  | 4:8:79:TRP:O[1_554]    | 1.99                     | 0.21              |
| 4:5:372:ARG:CA  | 4:V:227:MET:O[1_554]   | 1.99                     | 0.21              |
| 4:5:181:ALA:C   | 4:9:159:VAL:N[1_554]   | 1.99                     | 0.21              |
| 4:5:340:TRP:CZ3 | 4:9:121:GLN:N[1_554]   | 1.99                     | 0.21              |
| 4:5:288:ASP:C   | 4:W:63:GLY:O[1_554]    | 1.99                     | 0.21              |
| 4:3:316:GLU:CG  | 4:7:298:VAL:O[1_554]   | 1.99                     | 0.21              |
| 4:3:188:TYR:CE2 | 4:7:182:GLY:N[1_554]   | 1.99                     | 0.21              |
| 4:5:237:GLU:OE1 | 4:9:215:LYS:CD[1_554]  | 1.99                     | 0.21              |
| 4:5:256:ARG:CZ  | 4:9:217:CYS:CB[1_554]  | 1.99                     | 0.21              |
| 4:3:217:CYS:N   | 4:7:16:LEU:CG[1_554]   | 1.99                     | 0.21              |
| 4:5:140:LEU:N   | 4:9:371:HIS:NE2[1_554] | 1.99                     | 0.21              |
| 4:5:173:HIS:ND1 | 4:V:266:PHE:CA[1_554]  | 1.99                     | 0.21              |
| 4:2:117:GLU:OE1 | 4:7:236:LEU:O[1_554]   | 1.99                     | 0.21              |
| 4:5:300:SER:CA  | 4:9:107:GLU:O[1_554]   | 1.99                     | 0.21              |
| 4:4:310:ALA:CA  | 4:8:140:LEU:N[1_554]   | 1.99                     | 0.21              |
| 4:5:256:ARG:N   | 4:9:302:GLY:O[1_554]   | 1.99                     | 0.21              |
| 4:4:164:PRO:CB  | 4:8:172:PRO:CG[1_554]  | 1.99                     | 0.21              |
| 4:3:277:THR:C   | 4:7:174:ALA:O[1_554]   | 1.99                     | 0.21              |
| 4:4:193:LEU:CB  | 4:8:210:ARG:CD[1_554]  | 1.99                     | 0.21              |
| 4:5:276:GLU:O   | 4:9:281:SER:CA[1_554]  | 1.99                     | 0.21              |
| 4:3:191:LYS:CB  | 4:7:186:THR:N[1_554]   | 1.99                     | 0.21              |
| 4:3:371:HIS:ND1 | 4:8:252:ASN:CB[1_554]  | 1.99                     | 0.21              |
| 4:4:201:VAL:CG2 | 4:8:203:THR:CB[1_554]  | 1.99                     | 0.21              |
| 4:4:26:ALA:CA   | 4:8:122:ILE:O[1_554]   | 1.99                     | 0.21              |
| 4:4:319:ALA:N   | 4:8:296:ASN:CG[1_554]  | 1.99                     | 0.21              |
| 4:5:142:LEU:C   | 4:9:372:ARG:CG[1_554]  | 1.99                     | 0.21              |
| 4:3:298:VAL:CA  | 4:7:136:ILE:CD1[1_554] | 1.99                     | 0.21              |
| 4:4:277:THR:O   | 4:8:174:ALA:O[1_554]   | 1.99                     | 0.21              |
| 4:5:178:LEU:CD1 | 4:9:177:ARG:C[1_554]   | 1.99                     | 0.21              |
| 4:5:18:LYS:CG   | 4:9:79:TRP:CE3[1_554]  | 1.99                     | 0.21              |
| 4:5:28:ARG:NE   | 4:9:126:THR:N[1_554]   | 1.99                     | 0.21              |
| 4:3:279:TYR:CA  | 4:7:164:PRO:CB[1_554]  | 1.99                     | 0.21              |
| 4:3:173:HIS:NE2 | 4:8:266:PHE:N[1_554]   | 1.99                     | 0.21              |
| 4:3:215:LYS:CG  | 4:7:31:PHE:CD2[1_554]  | 1.99                     | 0.21              |
| 4:3:259:GLU:C   | 4:7:155:SER:OG[1_554]  | 1.99                     | 0.21              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:342:GLY:N   | 4:7:117:GLU:CA[1_554]  | 1.99                     | 0.21              |
| 4:5:322:PRO:N   | 4:9:291:LYS:NZ[1_554]  | 1.99                     | 0.21              |
| 4:4:196:ARG:NE  | 4:8:211:ASP:CB[1_554]  | 1.99                     | 0.21              |
| 4:4:185:LEU:CD1 | 4:8:158:GLY:C[1_554]   | 1.99                     | 0.21              |
| 4:3:266:PHE:C   | 4:7:180:LEU:CD1[1_554] | 1.99                     | 0.21              |
| 4:5:210:ARG:CD  | 4:9:69:TYR:CE2[1_554]  | 1.99                     | 0.21              |
| 4:3:293:LEU:CB  | 4:7:169:TYR:CZ[1_554]  | 1.99                     | 0.21              |
| 4:5:140:LEU:C   | 4:9:371:HIS:O[1_554]   | 1.99                     | 0.21              |
| 4:5:211:ASP:OD2 | 4:9:32:PRO:CD[1_554]   | 1.99                     | 0.21              |
| 4:4:211:ASP:CB  | 4:8:32:PRO:CG[1_554]   | 1.99                     | 0.21              |
| 4:5:199:SER:O   | 4:9:206:ARG:CB[1_554]  | 1.99                     | 0.21              |
| 4:4:160:THR:OG1 | 4:8:161:HIS:CE1[1_554] | 1.99                     | 0.21              |
| 4:5:29:ALA:CA   | 4:9:83:GLU:CD[1_554]   | 1.99                     | 0.21              |
| 4:5:332:PRO:CG  | 4:9:135:ALA:CB[1_554]  | 1.99                     | 0.21              |
| 4:4:205:GLU:C   | 4:8:62:ARG:NE[1_554]   | 1.99                     | 0.21              |
| 4:4:252:ASN:OD1 | 4:8:215:LYS:CA[1_554]  | 1.99                     | 0.21              |
| 4:5:157:ASP:C   | 4:9:73:HIS:CA[1_554]   | 1.99                     | 0.21              |
| 4:3:240:TYR:OH  | 4:7:55:GLY:C[1_554]    | 1.99                     | 0.21              |
| 4:4:221:LEU:O   | 4:8:332:PRO:CD[1_554]  | 1.99                     | 0.21              |
| 4:5:21:PHE:CB   | 4:9:125:GLU:CB[1_554]  | 1.99                     | 0.21              |
| 4:3:286:ASP:OD1 | 4:8:270:GLU:OE1[1_554] | 1.99                     | 0.21              |
| 4:5:180:LEU:CA  | 4:9:179:ASP:N[1_554]   | 1.99                     | 0.21              |
| 4:3:278:THR:CA  | 4:7:164:PRO:CD[1_554]  | 1.99                     | 0.21              |
| 4:5:223:PHE:CE2 | 4:9:304:THR:CG2[1_554] | 1.99                     | 0.21              |
| 4:5:340:TRP:N   | 4:9:116:ARG:CA[1_554]  | 1.99                     | 0.21              |
| 4:3:256:ARG:NH2 | 4:7:213:LYS:O[1_554]   | 1.99                     | 0.21              |
| 4:3:191:LYS:CE  | 4:7:185:LEU:CB[1_554]  | 1.99                     | 0.21              |
| 4:3:270:GLU:CB  | 4:7:271:SER:C[1_554]   | 1.99                     | 0.21              |
| 4:3:143:TYR:CA  | 4:7:371:HIS:C[1_554]   | 1.99                     | 0.21              |
| 4:5:166:TYR:CZ  | 4:W:39:ARG:CB[1_554]   | 1.99                     | 0.21              |
| 4:3:215:LYS:CD  | 4:7:31:PHE:CD2[1_554]  | 1.99                     | 0.21              |
| 4:4:172:PRO:CB  | 4:9:188:TYR:OH[1_554]  | 1.99                     | 0.21              |
| 4:5:372:ARG:C   | 4:V:227:MET:N[1_554]   | 1.99                     | 0.21              |
| 4:5:159:VAL:CB  | 4:9:177:ARG:NH1[1_554] | 1.99                     | 0.21              |
| 4:1:292:ASP:OD1 | 4:7:40:HIS:N[1_554]    | 1.99                     | 0.21              |
| 4:5:27:PRO:C    | 4:9:122:ILE:CB[1_554]  | 1.99                     | 0.21              |
| 4:3:197:GLY:N   | 4:7:209:VAL:CA[1_554]  | 1.99                     | 0.21              |
| 4:3:117:GLU:O   | 4:8:237:GLU:CB[1_554]  | 1.99                     | 0.21              |
| 4:5:210:ARG:NH2 | 4:9:33:SER:CA[1_554]   | 1.99                     | 0.21              |
| 4:3:116:ARG:C   | 4:8:237:GLU:CD[1_554]  | 2.00                     | 0.20              |
| 4:4:110:LEU:N   | 4:9:195:GLU:OE1[1_554] | 2.00                     | 0.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:186:THR:O   | 4:8:183:ARG:CB[1_554]  | 2.00                     | 0.20              |
| 4:3:312:ARG:N   | 4:7:141:SER:CB[1_554]  | 2.00                     | 0.20              |
| 4:4:214:GLU:N   | 4:8:15:GLY:O[1_554]    | 2.00                     | 0.20              |
| 4:3:319:ALA:O   | 4:7:292:ASP:C[1_554]   | 2.00                     | 0.20              |
| 4:5:319:ALA:N   | 4:9:296:ASN:CB[1_554]  | 2.00                     | 0.20              |
| 4:4:281:SER:CA  | 4:8:174:ALA:N[1_554]   | 2.00                     | 0.20              |
| 4:4:74:GLY:C    | 4:9:197:GLY:C[1_554]   | 2.00                     | 0.20              |
| 4:5:22:ALA:CB   | 4:9:362:TYR:OH[1_554]  | 2.00                     | 0.20              |
| 4:3:325:MET:CE  | 4:7:166:TYR:CZ[1_554]  | 2.00                     | 0.20              |
| 4:5:218:TYR:CD1 | 4:9:336:LYS:CB[1_554]  | 2.00                     | 0.20              |
| 4:5:166:TYR:CZ  | 4:W:39:ARG:O[1_554]    | 2.00                     | 0.20              |
| 4:5:114:ALA:C   | 4:V:251:GLY:N[1_554]   | 2.00                     | 0.20              |
| 4:5:113:LYS:CG  | 4:V:253:GLU:CA[1_554]  | 2.00                     | 0.20              |
| 4:3:157:ASP:OD1 | 4:7:72:GLU:CG[1_554]   | 2.00                     | 0.20              |
| 4:3:186:THR:N   | 4:7:183:ARG:NE[1_554]  | 2.00                     | 0.20              |
| 4:4:284:LYS:C   | 4:9:268:GLY:C[1_554]   | 2.00                     | 0.20              |
| 4:5:312:ARG:CD  | 4:9:298:VAL:C[1_554]   | 2.00                     | 0.20              |
| 4:5:316:GLU:C   | 4:9:151:ILE:N[1_554]   | 2.00                     | 0.20              |
| 4:3:342:GLY:C   | 4:7:117:GLU:CG[1_554]  | 2.00                     | 0.20              |
| 4:5:18:LYS:CE   | 4:9:79:TRP:CZ2[1_554]  | 2.00                     | 0.20              |
| 4:3:325:MET:CB  | 4:7:166:TYR:CE2[1_554] | 2.00                     | 0.20              |
| 4:3:327:ILE:CG1 | 4:7:149:THR:OG1[1_554] | 2.00                     | 0.20              |
| 4:5:19:ALA:C    | 4:9:121:GLN:OE1[1_554] | 2.00                     | 0.20              |
| 1:D:411:GLU:OE2 | 4:5:226:GLU:OE1[1_556] | 2.00                     | 0.20              |
| 4:3:191:LYS:CD  | 4:7:186:THR:N[1_554]   | 2.00                     | 0.20              |
| 4:4:371:HIS:NE2 | 4:9:255:PHE:CE2[1_554] | 2.00                     | 0.20              |
| 4:5:297:ASN:ND2 | 4:9:165:ILE:CD1[1_554] | 2.00                     | 0.20              |
| 4:3:112:PRO:O   | 4:8:253:GLU:CD[1_554]  | 2.00                     | 0.20              |
| 4:5:187:ASP:CA  | 4:9:183:ARG:CB[1_554]  | 2.00                     | 0.20              |
| 4:5:274:ILE:C   | 4:9:162:ASN:O[1_554]   | 2.00                     | 0.20              |
| 4:4:303:THR:CB  | 4:8:74:GLY:CA[1_554]   | 2.00                     | 0.20              |
| 4:5:283:MET:SD  | 4:9:286:ASP:C[1_554]   | 2.00                     | 0.20              |
| 4:3:159:VAL:CA  | 4:7:177:ARG:NH2[1_554] | 2.00                     | 0.20              |
| 4:3:222:ASP:O   | 4:7:332:PRO:C[1_554]   | 2.00                     | 0.20              |
| 4:4:75:ILE:CG1  | 4:9:194:THR:CA[1_554]  | 2.00                     | 0.20              |
| 4:5:311:ASP:O   | 4:9:298:VAL:CG1[1_554] | 2.00                     | 0.20              |
| 4:3:291:LYS:CD  | 4:9:64:ILE:CB[1_554]   | 2.00                     | 0.20              |
| 4:3:294:TYR:O   | 4:7:168:GLY:C[1_554]   | 2.00                     | 0.20              |
| 4:3:282:ILE:N   | 4:7:173:HIS:CE1[1_554] | 2.00                     | 0.20              |
| 4:5:106:THR:N   | 4:9:114:ALA:CB[1_554]  | 2.00                     | 0.20              |
| 4:5:184:ASP:OD2 | 4:9:179:ASP:O[1_554]   | 2.00                     | 0.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:166:TYR:OH  | 4:9:39:ARG:CA[1_554]   | 2.00                     | 0.20              |
| 4:4:315:LYS:N   | 4:8:142:LEU:CG[1_554]  | 2.00                     | 0.20              |
| 4:3:137:GLN:CB  | 4:7:112:PRO:CB[1_554]  | 2.00                     | 0.20              |
| 4:3:31:PHE:O    | 4:7:78:ASN:CG[1_554]   | 2.00                     | 0.20              |
| 4:3:257:CYS:SG  | 4:7:157:ASP:N[1_554]   | 2.00                     | 0.20              |
| 4:4:319:ALA:O   | 4:8:294:TYR:N[1_554]   | 2.00                     | 0.20              |
| 4:4:367:PRO:CD  | 4:9:235:SER:C[1_554]   | 2.00                     | 0.20              |
| 4:4:75:ILE:O    | 4:9:197:GLY:C[1_554]   | 2.00                     | 0.20              |
| 4:3:283:MET:CG  | 4:7:286:ASP:CB[1_554]  | 2.00                     | 0.20              |
| 4:5:208:ILE:CB  | 4:9:59:GLN:OE1[1_554]  | 2.00                     | 0.20              |
| 4:3:175:ILE:CG2 | 4:8:191:LYS:CD[1_554]  | 2.00                     | 0.20              |
| 4:4:372:ARG:CA  | 4:9:227:MET:O[1_554]   | 2.00                     | 0.20              |
| 4:4:183:ARG:CD  | 4:8:72:GLU:OE1[1_554]  | 2.00                     | 0.20              |
| 4:3:178:LEU:CD2 | 4:7:177:ARG:C[1_554]   | 2.00                     | 0.20              |
| 4:3:73:HIS:C    | 4:8:198:TYR:O[1_554]   | 2.00                     | 0.20              |
| 4:4:113:LYS:CB  | 4:9:252:ASN:O[1_554]   | 2.00                     | 0.20              |
| 4:3:372:ARG:C   | 4:8:227:MET:N[1_554]   | 2.00                     | 0.20              |
| 4:3:263:GLN:N   | 4:7:153:LEU:CD1[1_554] | 2.00                     | 0.20              |
| 4:3:215:LYS:CA  | 4:7:31:PHE:O[1_554]    | 2.00                     | 0.20              |
| 4:5:277:THR:O   | 4:9:174:ALA:CB[1_554]  | 2.00                     | 0.20              |
| 4:5:295:ALA:CB  | 4:9:167:GLU:C[1_554]   | 2.00                     | 0.20              |
| 4:2:166:TYR:CE1 | 4:8:40:HIS:NE2[1_554]  | 2.00                     | 0.20              |
| 4:5:198:TYR:CB  | 4:9:208:ILE:CA[1_554]  | 2.00                     | 0.20              |
| 4:3:320:LEU:C   | 4:7:293:LEU:CD1[1_554] | 2.00                     | 0.20              |
| 4:3:337:TYR:CB  | 4:7:119:MET:N[1_554]   | 2.00                     | 0.20              |
| 4:5:192:ILE:CD1 | 4:9:213:LYS:CE[1_554]  | 2.00                     | 0.20              |
| 4:3:308:GLY:CA  | 4:7:338:SER:CA[1_554]  | 2.00                     | 0.20              |
| 4:5:30:VAL:C    | 4:9:82:MET:N[1_554]    | 2.00                     | 0.20              |
| 4:3:25:ASP:O    | 4:7:120:THR:C[1_554]   | 2.00                     | 0.20              |
| 4:4:139:VAL:CA  | 4:8:371:HIS:NE2[1_554] | 2.00                     | 0.20              |
| 4:5:299:MET:CE  | 4:9:137:GLN:C[1_554]   | 2.00                     | 0.20              |
| 4:3:304:THR:CB  | 4:7:107:GLU:C[1_554]   | 2.00                     | 0.20              |
| 4:3:243:PRO:C   | 4:7:60:SER:CB[1_554]   | 2.00                     | 0.20              |
| 4:5:319:ALA:CA  | 4:9:292:ASP:O[1_554]   | 2.00                     | 0.20              |
| 4:4:250:ILE:CB  | 4:8:214:GLU:OE1[1_554] | 2.00                     | 0.20              |
| 4:5:213:LYS:CE  | 4:9:15:GLY:CA[1_554]   | 2.00                     | 0.20              |
| 4:5:13:GLY:CA   | 4:9:76:ILE:O[1_554]    | 2.00                     | 0.20              |
| 4:4:219:VAL:N   | 4:8:335:ARG:O[1_554]   | 2.00                     | 0.20              |
| 4:5:166:TYR:CA  | 4:W:40:HIS:NE2[1_554]  | 2.00                     | 0.20              |
| 4:2:112:PRO:O   | 4:7:250:ILE:CA[1_554]  | 2.00                     | 0.20              |
| 4:4:109:PRO:O   | 4:9:195:GLU:CD[1_554]  | 2.00                     | 0.20              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:24:ASP:OD2  | 4:8:125:GLU:CB[1_554]  | 2.00                     | 0.20              |
| 4:4:26:ALA:N    | 4:8:123:MET:C[1_554]   | 2.00                     | 0.20              |
| 4:3:181:ALA:CA  | 4:7:159:VAL:CG1[1_554] | 2.00                     | 0.20              |
| 4:4:257:CYS:SG  | 4:8:157:ASP:CA[1_554]  | 2.00                     | 0.20              |
| 4:4:331:ALA:C   | 4:8:135:ALA:CA[1_554]  | 2.00                     | 0.20              |
| 4:3:198:TYR:CD2 | 4:7:208:ILE:CA[1_554]  | 2.00                     | 0.20              |
| 4:3:366:GLY:O   | 4:8:234:SER:C[1_554]   | 2.00                     | 0.20              |
| 4:3:320:LEU:N   | 4:7:292:ASP:C[1_554]   | 2.00                     | 0.20              |
| 4:4:198:TYR:N   | 4:8:208:ILE:C[1_554]   | 2.00                     | 0.20              |
| 4:4:196:ARG:CA  | 4:8:209:VAL:O[1_554]   | 2.00                     | 0.20              |
| 4:4:308:GLY:C   | 4:8:141:SER:OG[1_554]  | 2.00                     | 0.20              |
| 4:4:213:LYS:CG  | 4:8:15:GLY:N[1_554]    | 2.00                     | 0.20              |
| 4:5:320:LEU:N   | 4:9:293:LEU:O[1_554]   | 2.00                     | 0.20              |
| 4:4:317:ILE:CG1 | 4:8:165:ILE:O[1_554]   | 2.00                     | 0.20              |
| 4:3:274:ILE:CA  | 4:7:162:ASN:CA[1_554]  | 2.00                     | 0.20              |
| 4:3:193:LEU:O   | 4:7:209:VAL:C[1_554]   | 2.00                     | 0.20              |
| 4:3:143:TYR:CD2 | 4:7:368:SER:CA[1_554]  | 2.00                     | 0.20              |
| 4:3:317:ILE:CA  | 4:7:150:GLY:N[1_554]   | 2.00                     | 0.20              |
| 4:5:156:GLY:CA  | 4:9:74:GLY:CA[1_554]   | 2.00                     | 0.20              |
| 4:3:257:CYS:O   | 4:7:156:GLY:CA[1_554]  | 2.00                     | 0.20              |
| 4:5:331:ALA:O   | 4:9:140:LEU:CG[1_554]  | 2.00                     | 0.20              |
| 4:4:110:LEU:O   | 4:9:192:ILE:CB[1_554]  | 2.00                     | 0.20              |
| 4:3:334:GLU:OE2 | 4:7:133:TYR:C[1_554]   | 2.00                     | 0.20              |
| 4:5:110:LEU:C   | 4:V:192:ILE:O[1_554]   | 2.00                     | 0.20              |
| 4:5:200:PHE:CZ  | 4:9:207:GLU:C[1_554]   | 2.00                     | 0.20              |
| 4:4:295:ALA:CB  | 4:8:167:GLU:O[1_554]   | 2.00                     | 0.20              |
| 4:3:267:ILE:CG2 | 4:7:180:LEU:C[1_554]   | 2.00                     | 0.20              |
| 4:3:139:VAL:C   | 4:7:371:HIS:CD2[1_554] | 2.01                     | 0.19              |
| 4:3:198:TYR:O   | 4:7:206:ARG:C[1_554]   | 2.01                     | 0.19              |
| 4:3:312:ARG:NH1 | 4:7:299:MET:CA[1_554]  | 2.01                     | 0.19              |
| 4:5:312:ARG:O   | 4:9:298:VAL:N[1_554]   | 2.01                     | 0.19              |
| 4:2:116:ARG:NE  | 4:7:252:ASN:CG[1_554]  | 2.01                     | 0.19              |
| 4:5:111:ASN:CG  | 4:V:196:ARG:CA[1_554]  | 2.01                     | 0.19              |
| 4:4:310:ALA:CB  | 4:8:141:SER:N[1_554]   | 2.01                     | 0.19              |
| 4:5:112:PRO:N   | 4:V:192:ILE:O[1_554]   | 2.01                     | 0.19              |
| 4:4:213:LYS:O   | 4:8:16:LEU:N[1_554]    | 2.01                     | 0.19              |
| 4:5:270:GLU:CG  | 4:9:271:SER:O[1_554]   | 2.01                     | 0.19              |
| 4:3:317:ILE:N   | 4:7:150:GLY:CA[1_554]  | 2.01                     | 0.19              |
| 4:4:313:MET:CB  | 4:8:138:ALA:C[1_554]   | 2.01                     | 0.19              |
| 4:4:320:LEU:CA  | 4:8:292:ASP:C[1_554]   | 2.01                     | 0.19              |
| 4:5:335:ARG:CG  | 4:9:106:THR:OG1[1_554] | 2.01                     | 0.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:143:TYR:CB  | 4:9:371:HIS:C[1_554]   | 2.01                     | 0.19              |
| 4:4:338:SER:N   | 4:8:119:MET:CG[1_554]  | 2.01                     | 0.19              |
| 4:3:328:LYS:C   | 4:7:168:GLY:O[1_554]   | 2.01                     | 0.19              |
| 4:5:261:LEU:C   | 4:9:160:THR:CG2[1_554] | 2.01                     | 0.19              |
| 4:5:371:HIS:CE1 | 4:V:252:ASN:CB[1_554]  | 2.01                     | 0.19              |
| 4:4:311:ASP:N   | 4:8:141:SER:N[1_554]   | 2.01                     | 0.19              |
| 4:5:335:ARG:CD  | 4:9:106:THR:CG2[1_554] | 2.01                     | 0.19              |
| 4:3:139:VAL:O   | 4:7:371:HIS:CE1[1_554] | 2.01                     | 0.19              |
| 4:3:297:ASN:CB  | 4:7:170:ALA:N[1_554]   | 2.01                     | 0.19              |
| 4:4:191:LYS:CB  | 4:8:186:THR:N[1_554]   | 2.01                     | 0.19              |
| 4:3:370:VAL:O   | 4:8:231:ALA:N[1_554]   | 2.01                     | 0.19              |
| 4:5:334:GLU:O   | 4:9:105:LEU:C[1_554]   | 2.01                     | 0.19              |
| 4:5:348:SER:C   | 4:9:366:GLY:N[1_554]   | 2.01                     | 0.19              |
| 4:2:112:PRO:O   | 4:7:250:ILE:CB[1_554]  | 2.01                     | 0.19              |
| 4:5:154:ASP:CA  | 4:9:110:LEU:N[1_554]   | 2.01                     | 0.19              |
| 4:3:116:ARG:CA  | 4:8:237:GLU:OE2[1_554] | 2.01                     | 0.19              |
| 4:3:115:ASN:N   | 4:8:249:THR:C[1_554]   | 2.01                     | 0.19              |
| 4:3:257:CYS:SG  | 4:7:157:ASP:CB[1_554]  | 2.01                     | 0.19              |
| 4:3:194:THR:OG1 | 4:7:209:VAL:CG1[1_554] | 2.01                     | 0.19              |
| 4:4:173:HIS:C   | 4:9:267:ILE:CB[1_554]  | 2.01                     | 0.19              |
| 4:4:372:ARG:CB  | 4:9:227:MET:O[1_554]   | 2.01                     | 0.19              |
| 4:5:174:ALA:CA  | 4:9:173:HIS:CB[1_554]  | 2.01                     | 0.19              |
| 4:4:372:ARG:N   | 4:9:227:MET:O[1_554]   | 2.01                     | 0.19              |
| 4:4:111:ASN:O   | 4:9:253:GLU:CB[1_554]  | 2.01                     | 0.19              |
| 4:3:59:GLN:CB   | 4:7:68:LYS:CD[1_554]   | 2.01                     | 0.19              |
| 4:2:116:ARG:NE  | 4:7:252:ASN:CB[1_554]  | 2.01                     | 0.19              |
| 4:4:183:ARG:CB  | 4:8:72:GLU:OE2[1_554]  | 2.01                     | 0.19              |
| 4:4:308:GLY:CA  | 4:8:338:SER:CB[1_554]  | 2.01                     | 0.19              |
| 4:3:114:ALA:CB  | 4:8:250:ILE:CB[1_554]  | 2.01                     | 0.19              |
| 4:4:367:PRO:CG  | 4:9:235:SER:CA[1_554]  | 2.01                     | 0.19              |
| 4:5:295:ALA:N   | 4:9:167:GLU:N[1_554]   | 2.01                     | 0.19              |
| 4:5:329:ILE:O   | 4:9:139:VAL:O[1_554]   | 2.01                     | 0.19              |
| 4:4:188:TYR:CD2 | 4:8:181:ALA:O[1_554]   | 2.01                     | 0.19              |
| 4:4:370:VAL:CB  | 4:9:230:ALA:C[1_554]   | 2.01                     | 0.19              |
| 4:2:370:VAL:CG2 | 4:7:230:ALA:C[1_554]   | 2.01                     | 0.19              |
| 4:2:117:GLU:CG  | 4:7:237:GLU:N[1_554]   | 2.01                     | 0.19              |
| 4:4:345:ILE:CG2 | 4:8:369:ILE:CA[1_554]  | 2.01                     | 0.19              |
| 4:3:140:LEU:O   | 4:7:371:HIS:CA[1_554]  | 2.01                     | 0.19              |
| 4:3:181:ALA:N   | 4:7:159:VAL:CG1[1_554] | 2.01                     | 0.19              |
| 4:4:191:LYS:NZ  | 4:8:257:CYS:SG[1_554]  | 2.01                     | 0.19              |
| 4:5:196:ARG:C   | 4:9:212:ILE:CG2[1_554] | 2.01                     | 0.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:114:ALA:C   | 4:9:250:ILE:N[1_554]   | 2.01                     | 0.19              |
| 4:5:11:ASP:OD2  | 4:9:115:ASN:C[1_554]   | 2.01                     | 0.19              |
| 4:4:283:MET:CA  | 4:8:286:ASP:N[1_554]   | 2.01                     | 0.19              |
| 4:4:182:GLY:N   | 4:8:74:GLY:N[1_554]    | 2.01                     | 0.19              |
| 4:4:115:ASN:CA  | 4:9:196:ARG:NE[1_554]  | 2.01                     | 0.19              |
| 4:4:326:LYS:CB  | 4:8:167:GLU:CD[1_554]  | 2.01                     | 0.19              |
| 4:5:337:TYR:O   | 4:9:119:MET:CG[1_554]  | 2.01                     | 0.19              |
| 4:5:255:PHE:CE2 | 4:9:305:MET:O[1_554]   | 2.01                     | 0.19              |
| 4:5:260:THR:OG1 | 4:9:303:THR:CG2[1_554] | 2.01                     | 0.19              |
| 4:5:294:TYR:CE2 | 4:9:166:TYR:CD1[1_554] | 2.01                     | 0.19              |
| 4:5:257:CYS:C   | 4:9:303:THR:CA[1_554]  | 2.01                     | 0.19              |
| 4:4:191:LYS:O   | 4:8:186:THR:O[1_554]   | 2.01                     | 0.19              |
| 4:4:242:LEU:CD1 | 4:8:207:GLU:OE1[1_554] | 2.01                     | 0.19              |
| 4:4:264:PRO:CD  | 4:8:274:ILE:CD1[1_554] | 2.01                     | 0.19              |
| 4:3:299:MET:CA  | 4:7:136:ILE:CA[1_554]  | 2.01                     | 0.19              |
| 4:4:316:GLU:CB  | 4:8:152:VAL:N[1_554]   | 2.01                     | 0.19              |
| 4:5:329:ILE:CG1 | 4:9:142:LEU:CG[1_554]  | 2.01                     | 0.19              |
| 4:5:297:ASN:N   | 4:9:169:TYR:N[1_554]   | 2.01                     | 0.19              |
| 4:4:340:TRP:CH2 | 4:8:121:GLN:C[1_554]   | 2.01                     | 0.19              |
| 4:5:340:TRP:CE3 | 4:9:121:GLN:N[1_554]   | 2.01                     | 0.19              |
| 4:4:110:LEU:CB  | 4:9:192:ILE:CG2[1_554] | 2.01                     | 0.19              |
| 4:3:265:SER:O   | 4:7:260:THR:C[1_554]   | 2.01                     | 0.19              |
| 4:4:183:ARG:CD  | 4:8:72:GLU:CD[1_554]   | 2.01                     | 0.19              |
| 4:4:283:MET:CE  | 4:8:289:ILE:CG2[1_554] | 2.01                     | 0.19              |
| 4:5:346:LEU:CD1 | 4:9:368:SER:OG[1_554]  | 2.01                     | 0.19              |
| 4:5:335:ARG:CZ  | 4:9:339:VAL:CG1[1_554] | 2.01                     | 0.19              |
| 4:4:309:ILE:CG2 | 4:8:339:VAL:CG1[1_554] | 2.01                     | 0.19              |
| 4:3:191:LYS:NZ  | 4:7:185:LEU:O[1_554]   | 2.01                     | 0.19              |
| 4:5:22:ALA:CA   | 4:9:362:TYR:CE2[1_554] | 2.01                     | 0.19              |
| 4:3:25:ASP:OD2  | 4:7:124:PHE:O[1_554]   | 2.01                     | 0.19              |
| 4:4:368:SER:CA  | 4:9:236:LEU:CB[1_554]  | 2.01                     | 0.19              |
| 4:4:274:ILE:CB  | 4:8:162:ASN:N[1_554]   | 2.01                     | 0.19              |
| 4:4:189:LEU:N   | 4:8:182:GLY:O[1_554]   | 2.01                     | 0.19              |
| 4:3:183:ARG:CD  | 4:7:72:GLU:OE2[1_554]  | 2.01                     | 0.19              |
| 4:3:113:LYS:CG  | 4:8:253:GLU:C[1_554]   | 2.01                     | 0.19              |
| 4:3:320:LEU:CB  | 4:7:293:LEU:CD1[1_554] | 2.01                     | 0.19              |
| 4:3:199:SER:CB  | 4:7:206:ARG:CB[1_554]  | 2.01                     | 0.19              |
| 4:4:185:LEU:N   | 4:8:158:GLY:O[1_554]   | 2.01                     | 0.19              |
| 4:4:242:LEU:CD2 | 4:8:207:GLU:OE1[1_554] | 2.01                     | 0.19              |
| 4:3:155:SER:C   | 4:7:75:ILE:CD1[1_554]  | 2.01                     | 0.19              |
| 4:5:370:VAL:C   | 4:V:231:ALA:CB[1_554]  | 2.01                     | 0.19              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:291:LYS:CB  | 4:9:64:ILE:CD1[1_554]  | 2.01                     | 0.19              |
| 4:2:109:PRO:N   | 4:7:195:GLU:CD[1_554]  | 2.01                     | 0.19              |
| 4:3:335:ARG:CZ  | 4:7:106:THR:CA[1_554]  | 2.01                     | 0.19              |
| 4:3:298:VAL:CG1 | 4:7:116:ARG:CZ[1_554]  | 2.01                     | 0.19              |
| 4:5:141:SER:N   | 4:9:116:ARG:NE[1_554]  | 2.01                     | 0.19              |
| 4:4:31:PHE:CA   | 4:8:78:ASN:ND2[1_554]  | 2.01                     | 0.19              |
| 4:5:262:PHE:CD2 | 4:9:153:LEU:C[1_554]   | 2.01                     | 0.19              |
| 4:2:369:ILE:O   | 4:7:229:THR:CA[1_554]  | 2.01                     | 0.19              |
| 4:5:173:HIS:O   | 4:V:267:ILE:CA[1_554]  | 2.01                     | 0.19              |
| 4:4:329:ILE:CB  | 4:8:139:VAL:O[1_554]   | 2.01                     | 0.19              |
| 4:4:336:LYS:N   | 4:8:119:MET:CE[1_554]  | 2.01                     | 0.19              |
| 4:4:272:ALA:CA  | 4:8:277:THR:CA[1_554]  | 2.01                     | 0.19              |
| 4:5:317:ILE:CB  | 4:9:150:GLY:CA[1_554]  | 2.01                     | 0.19              |
| 4:5:227:MET:CE  | 4:9:306:TYR:C[1_554]   | 2.01                     | 0.19              |
| 4:3:143:TYR:CE2 | 4:7:368:SER:OG[1_554]  | 2.01                     | 0.19              |
| 4:3:173:HIS:CE1 | 4:8:265:SER:CA[1_554]  | 2.01                     | 0.19              |
| 4:4:304:THR:C   | 4:8:137:GLN:NE2[1_554] | 2.01                     | 0.19              |
| 4:3:162:ASN:CG  | 4:7:175:ILE:CD1[1_554] | 2.01                     | 0.19              |
| 4:5:256:ARG:CG  | 4:9:306:TYR:CE1[1_554] | 2.01                     | 0.19              |
| 4:4:259:GLU:OE2 | 4:8:309:ILE:CG2[1_554] | 2.01                     | 0.19              |
| 4:2:117:GLU:CG  | 4:7:236:LEU:C[1_554]   | 2.01                     | 0.19              |
| 4:5:145:SER:C   | 4:9:372:ARG:NH2[1_554] | 2.01                     | 0.19              |
| 4:3:319:ALA:CB  | 4:7:296:ASN:ND2[1_554] | 2.01                     | 0.19              |
| 4:4:19:ALA:C    | 4:8:118:LYS:NZ[1_554]  | 2.01                     | 0.19              |
| 4:5:227:MET:N   | 4:9:307:PRO:CA[1_554]  | 2.02                     | 0.18              |
| 4:5:276:GLU:OE1 | 4:9:278:THR:C[1_554]   | 2.02                     | 0.18              |
| 4:4:255:PHE:CA  | 4:8:302:GLY:C[1_554]   | 2.02                     | 0.18              |
| 4:3:112:PRO:CB  | 4:8:250:ILE:CG1[1_554] | 2.02                     | 0.18              |
| 4:5:27:PRO:CG   | 4:9:86:TRP:CZ3[1_554]  | 2.02                     | 0.18              |
| 4:3:214:GLU:CA  | 4:7:17:VAL:N[1_554]    | 2.02                     | 0.18              |
| 4:2:113:LYS:C   | 4:7:250:ILE:C[1_554]   | 2.02                     | 0.18              |
| 4:3:188:TYR:CG  | 4:7:182:GLY:CA[1_554]  | 2.02                     | 0.18              |
| 4:3:79:TRP:NE1  | 4:8:247:VAL:O[1_554]   | 2.02                     | 0.18              |
| 4:5:154:ASP:C   | 4:9:109:PRO:CA[1_554]  | 2.02                     | 0.18              |
| 4:4:267:ILE:CG1 | 4:8:180:LEU:CD1[1_554] | 2.02                     | 0.18              |
| 4:4:211:ASP:CB  | 4:8:32:PRO:C[1_554]    | 2.02                     | 0.18              |
| 4:4:110:LEU:CG  | 4:9:191:LYS:CE[1_554]  | 2.02                     | 0.18              |
| 4:4:341:ILE:CA  | 4:8:120:THR:CG2[1_554] | 2.02                     | 0.18              |
| 4:5:183:ARG:CD  | 4:9:72:GLU:CD[1_554]   | 2.02                     | 0.18              |
| 4:4:180:LEU:C   | 4:8:179:ASP:OD1[1_554] | 2.02                     | 0.18              |
| 4:3:299:MET:O   | 4:7:107:GLU:CG[1_554]  | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:198:TYR:CD1 | 4:7:208:ILE:CB[1_554]  | 2.02                     | 0.18              |
| 4:5:331:ALA:CB  | 4:9:140:LEU:CD2[1_554] | 2.02                     | 0.18              |
| 4:5:151:ILE:N   | 4:9:169:TYR:CE1[1_554] | 2.02                     | 0.18              |
| 4:5:117:GLU:OE1 | 4:V:236:LEU:CG[1_554]  | 2.02                     | 0.18              |
| 4:3:204:ALA:CA  | 4:7:62:ARG:O[1_554]    | 2.02                     | 0.18              |
| 4:4:260:THR:CA  | 4:8:155:SER:CB[1_554]  | 2.02                     | 0.18              |
| 4:3:279:TYR:C   | 4:7:174:ALA:CB[1_554]  | 2.02                     | 0.18              |
| 4:4:314:GLN:O   | 4:8:142:LEU:CD1[1_554] | 2.02                     | 0.18              |
| 4:5:301:GLY:N   | 4:9:107:GLU:N[1_554]   | 2.02                     | 0.18              |
| 4:4:106:THR:CG2 | 4:8:114:ALA:CA[1_554]  | 2.02                     | 0.18              |
| 4:4:26:ALA:N    | 4:8:122:ILE:C[1_554]   | 2.02                     | 0.18              |
| 4:5:326:LYS:NZ  | 4:W:45:VAL:CG2[1_554]  | 2.02                     | 0.18              |
| 4:4:256:ARG:O   | 4:8:303:THR:C[1_554]   | 2.02                     | 0.18              |
| 4:3:255:PHE:C   | 4:7:303:THR:N[1_554]   | 2.02                     | 0.18              |
| 4:4:317:ILE:C   | 4:8:149:THR:C[1_554]   | 2.02                     | 0.18              |
| 4:4:226:GLU:OE1 | 4:8:333:PRO:C[1_554]   | 2.02                     | 0.18              |
| 4:5:200:PHE:CZ  | 4:9:207:GLU:CA[1_554]  | 2.02                     | 0.18              |
| 4:4:215:LYS:NZ  | 4:8:31:PHE:CD2[1_554]  | 2.02                     | 0.18              |
| 4:4:367:PRO:CA  | 4:9:234:SER:N[1_554]   | 2.02                     | 0.18              |
| 4:5:316:GLU:O   | 4:9:293:LEU:O[1_554]   | 2.02                     | 0.18              |
| 4:5:297:ASN:O   | 4:9:139:VAL:CG2[1_554] | 2.02                     | 0.18              |
| 4:5:304:THR:C   | 4:9:137:GLN:CG[1_554]  | 2.02                     | 0.18              |
| 4:4:282:ILE:CB  | 4:8:171:LEU:CG[1_554]  | 2.02                     | 0.18              |
| 4:4:306:TYR:O   | 4:8:339:VAL:CG2[1_554] | 2.02                     | 0.18              |
| 4:3:144:ALA:CA  | 4:7:370:VAL:O[1_554]   | 2.02                     | 0.18              |
| 4:3:349:LEU:CD2 | 4:7:365:ALA:O[1_554]   | 2.02                     | 0.18              |
| 1:A:411:GLU:CD  | 4:4:226:GLU:OE1[1_556] | 2.02                     | 0.18              |
| 4:5:338:SER:C   | 4:9:116:ARG:CG[1_554]  | 2.02                     | 0.18              |
| 4:5:227:MET:CB  | 4:9:307:PRO:O[1_554]   | 2.02                     | 0.18              |
| 4:4:332:PRO:CB  | 4:8:134:VAL:N[1_554]   | 2.02                     | 0.18              |
| 4:4:189:LEU:CB  | 4:8:157:ASP:OD1[1_554] | 2.02                     | 0.18              |
| 4:4:258:PRO:CA  | 4:8:156:GLY:CA[1_554]  | 2.02                     | 0.18              |
| 4:3:366:GLY:CA  | 4:8:235:SER:N[1_554]   | 2.02                     | 0.18              |
| 4:4:283:MET:SD  | 4:8:286:ASP:N[1_554]   | 2.02                     | 0.18              |
| 4:3:210:ARG:CG  | 4:7:69:TYR:CE2[1_554]  | 2.02                     | 0.18              |
| 4:4:255:PHE:CZ  | 4:8:305:MET:CE[1_554]  | 2.02                     | 0.18              |
| 4:4:154:ASP:N   | 4:8:109:PRO:CA[1_554]  | 2.02                     | 0.18              |
| 4:2:72:GLU:O    | 4:7:198:TYR:O[1_554]   | 2.02                     | 0.18              |
| 4:4:185:LEU:CD1 | 4:8:159:VAL:CA[1_554]  | 2.02                     | 0.18              |
| 4:3:277:THR:C   | 4:7:175:ILE:CA[1_554]  | 2.02                     | 0.18              |
| 4:4:144:ALA:CB  | 4:8:370:VAL:O[1_554]   | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:111:ASN:O   | 4:8:253:GLU:OE1[1_554] | 2.02                     | 0.18              |
| 4:3:272:ALA:CB  | 4:7:277:THR:O[1_554]   | 2.02                     | 0.18              |
| 4:3:76:ILE:O    | 4:8:198:TYR:CD1[1_554] | 2.02                     | 0.18              |
| 4:5:137:GLN:CG  | 4:9:113:LYS:N[1_554]   | 2.02                     | 0.18              |
| 4:3:270:GLU:CB  | 4:7:272:ALA:CB[1_554]  | 2.02                     | 0.18              |
| 4:3:227:MET:CE  | 4:7:305:MET:C[1_554]   | 2.02                     | 0.18              |
| 4:4:219:VAL:CG1 | 4:8:301:GLY:N[1_554]   | 2.02                     | 0.18              |
| 4:4:184:ASP:CA  | 4:8:73:HIS:CE1[1_554]  | 2.02                     | 0.18              |
| 4:3:188:TYR:CD2 | 4:7:181:ALA:O[1_554]   | 2.02                     | 0.18              |
| 4:5:76:ILE:N    | 4:V:197:GLY:C[1_554]   | 2.02                     | 0.18              |
| 4:4:312:ARG:CD  | 4:8:298:VAL:C[1_554]   | 2.02                     | 0.18              |
| 4:5:255:PHE:O   | 4:9:302:GLY:O[1_554]   | 2.02                     | 0.18              |
| 4:5:270:GLU:N   | 4:9:272:ALA:CA[1_554]  | 2.02                     | 0.18              |
| 4:3:166:TYR:CE1 | 4:9:40:HIS:NE2[1_554]  | 2.02                     | 0.18              |
| 4:5:151:ILE:CG1 | 4:9:172:PRO:N[1_554]   | 2.02                     | 0.18              |
| 4:5:273:GLY:O   | 4:9:162:ASN:OD1[1_554] | 2.02                     | 0.18              |
| 4:2:174:ALA:CB  | 4:7:268:GLY:N[1_554]   | 2.02                     | 0.18              |
| 4:3:281:SER:CB  | 4:7:173:HIS:C[1_554]   | 2.02                     | 0.18              |
| 4:1:288:ASP:C   | 4:7:39:ARG:CG[1_554]   | 2.02                     | 0.18              |
| 4:5:314:GLN:OE1 | 4:9:147:ARG:C[1_554]   | 2.02                     | 0.18              |
| 4:5:115:ASN:CB  | 4:V:196:ARG:CG[1_554]  | 2.02                     | 0.18              |
| 4:5:341:ILE:CB  | 4:9:132:MET:SD[1_554]  | 2.02                     | 0.18              |
| 4:4:303:THR:OG1 | 4:8:74:GLY:N[1_554]    | 2.02                     | 0.18              |
| 4:4:309:ILE:CG2 | 4:8:339:VAL:CG2[1_554] | 2.02                     | 0.18              |
| 4:4:304:THR:CB  | 4:8:137:GLN:NE2[1_554] | 2.02                     | 0.18              |
| 4:5:162:ASN:CG  | 4:9:175:ILE:CA[1_554]  | 2.02                     | 0.18              |
| 4:3:327:ILE:CG1 | 4:7:149:THR:CA[1_554]  | 2.02                     | 0.18              |
| 4:2:110:LEU:CA  | 4:7:192:ILE:CG2[1_554] | 2.02                     | 0.18              |
| 4:2:173:HIS:C   | 4:7:267:ILE:C[1_554]   | 2.02                     | 0.18              |
| 4:3:139:VAL:N   | 4:7:113:LYS:CD[1_554]  | 2.02                     | 0.18              |
| 4:5:60:SER:CB   | 4:9:37:ARG:CA[1_554]   | 2.02                     | 0.18              |
| 4:3:266:PHE:CD2 | 4:7:261:LEU:CD1[1_554] | 2.02                     | 0.18              |
| 4:5:292:ASP:OD1 | 4:W:64:ILE:CD1[1_554]  | 2.02                     | 0.18              |
| 4:5:11:ASP:OD1  | 4:9:115:ASN:N[1_554]   | 2.02                     | 0.18              |
| 4:2:115:ASN:N   | 4:7:250:ILE:CB[1_554]  | 2.02                     | 0.18              |
| 4:5:173:HIS:CD2 | 4:V:264:PRO:O[1_554]   | 2.02                     | 0.18              |
| 4:4:208:ILE:CD1 | 4:8:59:GLN:N[1_554]    | 2.02                     | 0.18              |
| 4:5:281:SER:CA  | 4:9:174:ALA:N[1_554]   | 2.02                     | 0.18              |
| 4:4:304:THR:CG2 | 4:8:107:GLU:O[1_554]   | 2.02                     | 0.18              |
| 4:3:153:LEU:C   | 4:7:109:PRO:CA[1_554]  | 2.02                     | 0.18              |
| 4:3:318:THR:C   | 4:7:149:THR:C[1_554]   | 2.02                     | 0.18              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:553:MLY:CH1 | 4:4:328:LYS:CE[1_556]  | 2.02                     | 0.18              |
| 4:3:337:TYR:CB  | 4:7:119:MET:CG[1_554]  | 2.02                     | 0.18              |
| 4:2:289:ILE:CG1 | 4:8:39:ARG:NH2[1_554]  | 2.02                     | 0.18              |
| 4:4:264:PRO:C   | 4:8:178:LEU:CD2[1_554] | 2.02                     | 0.18              |
| 4:5:210:ARG:CZ  | 4:9:33:SER:CA[1_554]   | 2.02                     | 0.18              |
| 4:5:194:THR:CG2 | 4:9:209:VAL:CG1[1_554] | 2.02                     | 0.18              |
| 4:5:142:LEU:N   | 4:9:116:ARG:NH1[1_554] | 2.02                     | 0.18              |
| 4:3:210:ARG:NE  | 4:7:33:SER:O[1_554]    | 2.02                     | 0.18              |
| 4:5:214:GLU:OE1 | 4:9:33:SER:OG[1_554]   | 2.02                     | 0.18              |
| 4:3:188:TYR:OH  | 4:7:306:TYR:OH[1_554]  | 2.02                     | 0.18              |
| 4:5:153:LEU:CG  | 4:9:163:VAL:CG2[1_554] | 2.02                     | 0.18              |
| 4:5:307:PRO:C   | 4:9:338:SER:CA[1_554]  | 2.02                     | 0.18              |
| 4:4:329:ILE:CD1 | 4:8:165:ILE:CG2[1_554] | 2.02                     | 0.18              |
| 4:3:159:VAL:CA  | 4:7:177:ARG:NH1[1_554] | 2.02                     | 0.18              |
| 4:3:341:ILE:CG1 | 4:7:120:THR:OG1[1_554] | 2.02                     | 0.18              |
| 4:4:115:ASN:ND2 | 4:9:198:TYR:OH[1_554]  | 2.02                     | 0.18              |
| 4:4:193:LEU:CA  | 4:8:210:ARG:N[1_554]   | 2.02                     | 0.18              |
| 4:3:334:GLU:CB  | 4:7:105:LEU:CD1[1_554] | 2.02                     | 0.18              |
| 4:3:314:GLN:CB  | 4:7:142:LEU:CA[1_554]  | 2.02                     | 0.18              |
| 4:1:288:ASP:O   | 4:7:39:ARG:CB[1_554]   | 2.02                     | 0.18              |
| 4:4:197:GLY:CA  | 4:8:212:ILE:CD1[1_554] | 2.02                     | 0.18              |
| 4:5:30:VAL:CG2  | 4:9:83:GLU:N[1_554]    | 2.02                     | 0.18              |
| 4:3:317:ILE:CG1 | 4:7:165:ILE:O[1_554]   | 2.03                     | 0.17              |
| 4:5:334:GLU:N   | 4:9:105:LEU:CA[1_554]  | 2.03                     | 0.17              |
| 4:4:265:SER:CB  | 4:8:261:LEU:C[1_554]   | 2.03                     | 0.17              |
| 4:3:173:HIS:ND1 | 4:8:266:PHE:CA[1_554]  | 2.03                     | 0.17              |
| 4:3:222:ASP:C   | 4:7:331:ALA:O[1_554]   | 2.03                     | 0.17              |
| 4:3:185:LEU:C   | 4:7:158:GLY:N[1_554]   | 2.03                     | 0.17              |
| 4:2:111:ASN:O   | 4:7:253:GLU:CD[1_554]  | 2.03                     | 0.17              |
| 4:2:75:ILE:CG2  | 4:7:198:TYR:CB[1_554]  | 2.03                     | 0.17              |
| 4:3:313:MET:N   | 4:7:152:VAL:CG2[1_554] | 2.03                     | 0.17              |
| 4:5:277:THR:O   | 4:9:175:ILE:N[1_554]   | 2.03                     | 0.17              |
| 4:4:332:PRO:CG  | 4:8:134:VAL:O[1_554]   | 2.03                     | 0.17              |
| 4:4:261:LEU:N   | 4:8:155:SER:CB[1_554]  | 2.03                     | 0.17              |
| 4:5:339:VAL:CB  | 4:9:116:ARG:CB[1_554]  | 2.03                     | 0.17              |
| 4:3:331:ALA:N   | 4:7:135:ALA:CA[1_554]  | 2.03                     | 0.17              |
| 4:3:175:ILE:CD1 | 4:8:191:LYS:CE[1_554]  | 2.03                     | 0.17              |
| 4:5:346:LEU:C   | 4:9:366:GLY:C[1_554]   | 2.03                     | 0.17              |
| 4:3:210:ARG:NE  | 4:7:69:TYR:CA[1_554]   | 2.03                     | 0.17              |
| 4:4:266:PHE:CD1 | 4:8:261:LEU:CB[1_554]  | 2.03                     | 0.17              |
| 4:4:289:ILE:N   | 4:V:39:ARG:NH1[1_554]  | 2.03                     | 0.17              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:166:TYR:CZ  | 4:8:39:ARG:O[1_554]    | 2.03                     | 0.17              |
| 4:4:290:ARG:NE  | 4:8:286:ASP:OD2[1_554] | 2.03                     | 0.17              |
| 4:4:196:ARG:NH1 | 4:8:211:ASP:O[1_554]   | 2.03                     | 0.17              |
| 4:3:343:GLY:CA  | 4:7:117:GLU:OE1[1_554] | 2.03                     | 0.17              |
| 4:4:372:ARG:O   | 4:9:227:MET:CG[1_554]  | 2.03                     | 0.17              |
| 4:5:270:GLU:CA  | 4:9:272:ALA:CB[1_554]  | 2.03                     | 0.17              |
| 4:4:164:PRO:N   | 4:8:172:PRO:CG[1_554]  | 2.03                     | 0.17              |
| 4:3:106:THR:CB  | 4:7:114:ALA:CB[1_554]  | 2.03                     | 0.17              |
| 4:4:279:TYR:CE2 | 4:8:285:CYS:CB[1_554]  | 2.03                     | 0.17              |
| 4:4:194:THR:N   | 4:8:210:ARG:N[1_554]   | 2.03                     | 0.17              |
| 4:4:277:THR:OG1 | 4:8:176:MET:CB[1_554]  | 2.03                     | 0.17              |
| 4:3:183:ARG:O   | 4:7:183:ARG:NH1[1_554] | 2.03                     | 0.17              |
| 4:5:259:GLU:N   | 4:9:304:THR:CG2[1_554] | 2.03                     | 0.17              |
| 4:3:339:VAL:CA  | 4:7:116:ARG:CA[1_554]  | 2.03                     | 0.17              |
| 4:4:16:LEU:C    | 4:8:77:THR:C[1_554]    | 2.03                     | 0.17              |
| 4:2:118:LYS:N   | 4:7:237:GLU:OE1[1_554] | 2.03                     | 0.17              |
| 4:5:258:PRO:O   | 4:9:155:SER:N[1_554]   | 2.03                     | 0.17              |
| 4:3:143:TYR:CG  | 4:7:368:SER:O[1_554]   | 2.03                     | 0.17              |
| 4:4:205:GLU:OE2 | 4:8:203:THR:CB[1_554]  | 2.03                     | 0.17              |
| 4:3:180:LEU:CD2 | 4:7:178:LEU:N[1_554]   | 2.03                     | 0.17              |
| 4:5:325:MET:CE  | 4:9:166:TYR:OH[1_554]  | 2.03                     | 0.17              |
| 4:5:21:PHE:N    | 4:9:121:GLN:NE2[1_554] | 2.03                     | 0.17              |
| 4:4:317:ILE:CA  | 4:8:151:ILE:N[1_554]   | 2.03                     | 0.17              |
| 4:4:142:LEU:O   | 4:8:372:ARG:CA[1_554]  | 2.03                     | 0.17              |
| 4:5:291:LYS:NZ  | 4:W:64:ILE:CB[1_554]   | 2.03                     | 0.17              |
| 4:5:223:PHE:CD2 | 4:9:304:THR:OG1[1_554] | 2.03                     | 0.17              |
| 4:3:110:LEU:CA  | 4:8:192:ILE:C[1_554]   | 2.03                     | 0.17              |
| 4:4:282:ILE:CA  | 4:8:173:HIS:NE2[1_554] | 2.03                     | 0.17              |
| 4:3:77:THR:O    | 4:8:246:GLN:CD[1_554]  | 2.03                     | 0.17              |
| 4:4:307:PRO:C   | 4:8:339:VAL:N[1_554]   | 2.03                     | 0.17              |
| 4:4:20:GLY:CA   | 4:8:121:GLN:NE2[1_554] | 2.03                     | 0.17              |
| 4:3:143:TYR:CA  | 4:7:372:ARG:CA[1_554]  | 2.03                     | 0.17              |
| 4:5:141:SER:CB  | 4:9:107:GLU:OE2[1_554] | 2.03                     | 0.17              |
| 4:5:256:ARG:CG  | 4:9:306:TYR:CG[1_554]  | 2.03                     | 0.17              |
| 4:5:340:TRP:CE3 | 4:9:120:THR:O[1_554]   | 2.03                     | 0.17              |
| 4:3:147:ARG:NE  | 4:7:372:ARG:CD[1_554]  | 2.03                     | 0.17              |
| 4:2:289:ILE:N   | 4:8:63:GLY:O[1_554]    | 2.03                     | 0.17              |
| 4:5:188:TYR:CD2 | 4:9:181:ALA:O[1_554]   | 2.03                     | 0.17              |
| 4:4:371:HIS:CB  | 4:9:236:LEU:CD1[1_554] | 2.03                     | 0.17              |
| 4:4:262:PHE:CE1 | 4:8:153:LEU:C[1_554]   | 2.03                     | 0.17              |
| 4:2:367:PRO:N   | 4:7:235:SER:CB[1_554]  | 2.03                     | 0.17              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:253:GLU:CD  | 4:9:213:LYS:C[1_554]   | 2.03                     | 0.17              |
| 4:3:198:TYR:O   | 4:7:206:ARG:CA[1_554]  | 2.03                     | 0.17              |
| 4:5:26:ALA:C    | 4:9:122:ILE:O[1_554]   | 2.03                     | 0.17              |
| 4:3:294:TYR:CB  | 4:7:166:TYR:C[1_554]   | 2.03                     | 0.17              |
| 4:2:110:LEU:N   | 4:7:192:ILE:CB[1_554]  | 2.03                     | 0.17              |
| 4:5:11:ASP:OD2  | 4:9:115:ASN:O[1_554]   | 2.03                     | 0.17              |
| 4:5:309:ILE:CA  | 4:9:141:SER:CB[1_554]  | 2.03                     | 0.17              |
| 4:4:266:PHE:O   | 4:8:185:LEU:CD1[1_554] | 2.03                     | 0.17              |
| 4:3:275:HIS:CG  | 4:7:152:VAL:O[1_554]   | 2.03                     | 0.17              |
| 4:5:162:ASN:O   | 4:9:172:PRO:O[1_554]   | 2.03                     | 0.17              |
| 4:3:367:PRO:N   | 4:8:236:LEU:N[1_554]   | 2.03                     | 0.17              |
| 4:3:155:SER:CA  | 4:7:108:ALA:CB[1_554]  | 2.03                     | 0.17              |
| 4:4:316:GLU:O   | 4:8:150:GLY:C[1_554]   | 2.03                     | 0.17              |
| 4:3:357:ILE:CB  | 4:8:232:SER:C[1_554]   | 2.03                     | 0.17              |
| 4:3:18:LYS:NZ   | 4:7:76:ILE:O[1_554]    | 2.03                     | 0.17              |
| 4:3:300:SER:C   | 4:7:107:GLU:CG[1_554]  | 2.03                     | 0.17              |
| 4:5:299:MET:CE  | 4:9:140:LEU:N[1_554]   | 2.03                     | 0.17              |
| 4:4:31:PHE:O    | 4:8:78:ASN:CB[1_554]   | 2.03                     | 0.17              |
| 4:5:219:VAL:CA  | 4:9:335:ARG:O[1_554]   | 2.03                     | 0.17              |
| 4:5:313:MET:N   | 4:9:298:VAL:CG1[1_554] | 2.03                     | 0.17              |
| 4:4:32:PRO:CA   | 4:8:78:ASN:CG[1_554]   | 2.03                     | 0.17              |
| 4:5:136:ILE:CA  | 4:9:113:LYS:CD[1_554]  | 2.03                     | 0.17              |
| 4:3:312:ARG:NH1 | 4:7:298:VAL:O[1_554]   | 2.03                     | 0.17              |
| 4:5:186:THR:CB  | 4:9:157:ASP:OD2[1_554] | 2.03                     | 0.17              |
| 4:5:265:SER:C   | 4:9:260:THR:O[1_554]   | 2.03                     | 0.17              |
| 4:5:157:ASP:C   | 4:9:73:HIS:CB[1_554]   | 2.03                     | 0.17              |
| 4:3:16:LEU:N    | 4:7:78:ASN:N[1_554]    | 2.03                     | 0.17              |
| 4:3:282:ILE:N   | 4:7:173:HIS:CD2[1_554] | 2.03                     | 0.17              |
| 4:5:262:PHE:CD1 | 4:9:153:LEU:O[1_554]   | 2.03                     | 0.17              |
| 4:3:319:ALA:CA  | 4:7:296:ASN:CG[1_554]  | 2.03                     | 0.17              |
| 4:3:255:PHE:O   | 4:7:302:GLY:O[1_554]   | 2.03                     | 0.17              |
| 4:3:357:ILE:CB  | 4:8:232:SER:N[1_554]   | 2.03                     | 0.17              |
| 4:4:338:SER:N   | 4:8:119:MET:SD[1_554]  | 2.03                     | 0.17              |
| 4:3:31:PHE:C    | 4:7:78:ASN:ND2[1_554]  | 2.03                     | 0.17              |
| 4:5:28:ARG:NE   | 4:9:126:THR:C[1_554]   | 2.03                     | 0.17              |
| 4:3:156:GLY:O   | 4:7:74:GLY:C[1_554]    | 2.03                     | 0.17              |
| 4:3:264:PRO:CB  | 4:7:178:LEU:CG[1_554]  | 2.03                     | 0.17              |
| 4:5:288:ASP:O   | 4:W:64:ILE:CA[1_554]   | 2.03                     | 0.17              |
| 4:4:291:LYS:CE  | 4:V:64:ILE:CD1[1_554]  | 2.03                     | 0.17              |
| 4:2:172:PRO:C   | 4:7:188:TYR:CE1[1_554] | 2.03                     | 0.17              |
| 4:3:110:LEU:O   | 4:8:192:ILE:CA[1_554]  | 2.03                     | 0.17              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:20:GLY:CA   | 4:9:121:GLN:CD[1_554]  | 2.03                     | 0.17              |
| 4:3:194:THR:C   | 4:7:209:VAL:C[1_554]   | 2.03                     | 0.17              |
| 4:3:294:TYR:CZ  | 4:7:166:TYR:CB[1_554]  | 2.03                     | 0.17              |
| 4:4:270:GLU:CA  | 4:8:272:ALA:CB[1_554]  | 2.03                     | 0.17              |
| 4:5:187:ASP:C   | 4:9:183:ARG:CA[1_554]  | 2.03                     | 0.17              |
| 4:3:312:ARG:CZ  | 4:7:299:MET:CG[1_554]  | 2.03                     | 0.17              |
| 4:4:210:ARG:NH2 | 4:8:34:ILE:N[1_554]    | 2.03                     | 0.17              |
| 4:3:265:SER:N   | 4:7:274:ILE:CD1[1_554] | 2.04                     | 0.16              |
| 4:3:75:ILE:CG1  | 4:8:193:LEU:C[1_554]   | 2.04                     | 0.16              |
| 4:2:117:GLU:CB  | 4:7:237:GLU:CB[1_554]  | 2.04                     | 0.16              |
| 4:5:276:GLU:OE1 | 4:9:279:TYR:O[1_554]   | 2.04                     | 0.16              |
| 4:4:223:PHE:CA  | 4:8:335:ARG:NH2[1_554] | 2.04                     | 0.16              |
| 4:3:140:LEU:N   | 4:7:113:LYS:CB[1_554]  | 2.04                     | 0.16              |
| 4:5:106:THR:CA  | 4:9:114:ALA:CA[1_554]  | 2.04                     | 0.16              |
| 4:5:18:LYS:C    | 4:9:122:ILE:CD1[1_554] | 2.04                     | 0.16              |
| 4:3:116:ARG:CD  | 4:8:252:ASN:CB[1_554]  | 2.04                     | 0.16              |
| 4:3:179:ASP:C   | 4:7:179:ASP:OD1[1_554] | 2.04                     | 0.16              |
| 4:3:321:ALA:C   | 4:7:292:ASP:CG[1_554]  | 2.04                     | 0.16              |
| 4:3:240:TYR:CE2 | 4:7:56:ASP:CG[1_554]   | 2.04                     | 0.16              |
| 4:4:115:ASN:N   | 4:9:251:GLY:N[1_554]   | 2.04                     | 0.16              |
| 4:5:372:ARG:C   | 4:V:227:MET:C[1_554]   | 2.04                     | 0.16              |
| 4:3:318:THR:N   | 4:7:149:THR:CA[1_554]  | 2.04                     | 0.16              |
| 4:5:263:GLN:CA  | 4:9:274:ILE:CD1[1_554] | 2.04                     | 0.16              |
| 4:5:269:MET:CB  | 4:9:271:SER:OG[1_554]  | 2.04                     | 0.16              |
| 4:4:308:GLY:N   | 4:8:340:TRP:N[1_554]   | 2.04                     | 0.16              |
| 4:4:279:TYR:N   | 4:8:164:PRO:CD[1_554]  | 2.04                     | 0.16              |
| 4:5:275:HIS:CA  | 4:9:151:ILE:CG1[1_554] | 2.04                     | 0.16              |
| 4:4:341:ILE:N   | 4:8:117:GLU:C[1_554]   | 2.04                     | 0.16              |
| 4:5:337:TYR:CZ  | 4:9:86:TRP:CH2[1_554]  | 2.04                     | 0.16              |
| 4:4:25:ASP:CG   | 4:8:124:PHE:CG[1_554]  | 2.04                     | 0.16              |
| 4:5:56:ASP:CG   | 4:9:37:ARG:NH1[1_554]  | 2.04                     | 0.16              |
| 4:5:320:LEU:O   | 4:9:290:ARG:CA[1_554]  | 2.04                     | 0.16              |
| 4:4:151:ILE:N   | 4:8:169:TYR:CD1[1_554] | 2.04                     | 0.16              |
| 4:5:166:TYR:OH  | 4:W:39:ARG:CB[1_554]   | 2.04                     | 0.16              |
| 4:5:219:VAL:C   | 4:9:335:ARG:C[1_554]   | 2.04                     | 0.16              |
| 4:3:279:TYR:N   | 4:7:164:PRO:CD[1_554]  | 2.04                     | 0.16              |
| 4:3:191:LYS:CG  | 4:7:185:LEU:CA[1_554]  | 2.04                     | 0.16              |
| 4:4:137:GLN:CB  | 4:8:112:PRO:CB[1_554]  | 2.04                     | 0.16              |
| 4:3:319:ALA:CA  | 4:7:292:ASP:O[1_554]   | 2.04                     | 0.16              |
| 4:4:41:GLN:NE2  | 4:7:224:GLU:OE2[1_554] | 2.04                     | 0.16              |
| 4:4:362:TYR:CG  | 4:9:233:SER:O[1_554]   | 2.04                     | 0.16              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:198:TYR:CE2 | 4:8:211:ASP:CB[1_554]  | 2.04                     | 0.16              |
| 4:4:115:ASN:CB  | 4:9:196:ARG:NH2[1_554] | 2.04                     | 0.16              |
| 4:5:186:THR:CA  | 4:9:157:ASP:OD2[1_554] | 2.04                     | 0.16              |
| 4:4:314:GLN:CD  | 4:8:147:ARG:C[1_554]   | 2.04                     | 0.16              |
| 4:5:31:PHE:C    | 4:9:78:ASN:CB[1_554]   | 2.04                     | 0.16              |
| 4:4:335:ARG:CG  | 4:8:106:THR:O[1_554]   | 2.04                     | 0.16              |
| 4:4:274:ILE:CA  | 4:8:161:HIS:C[1_554]   | 2.04                     | 0.16              |
| 4:4:141:SER:N   | 4:8:371:HIS:CE1[1_554] | 2.04                     | 0.16              |
| 4:5:17:VAL:CA   | 4:9:79:TRP:NE1[1_554]  | 2.04                     | 0.16              |
| 4:4:27:PRO:CB   | 4:8:122:ILE:CB[1_554]  | 2.04                     | 0.16              |
| 4:3:154:ASP:CG  | 4:7:112:PRO:N[1_554]   | 2.04                     | 0.16              |
| 4:5:299:MET:CG  | 4:9:137:GLN:C[1_554]   | 2.04                     | 0.16              |
| 4:3:18:LYS:N    | 4:7:79:TRP:CG[1_554]   | 2.04                     | 0.16              |
| 4:4:250:ILE:CG2 | 4:8:214:GLU:CD[1_554]  | 2.04                     | 0.16              |
| 4:4:136:ILE:C   | 4:8:113:LYS:CB[1_554]  | 2.04                     | 0.16              |
| 4:5:348:SER:O   | 4:9:365:ALA:N[1_554]   | 2.04                     | 0.16              |
| 4:5:316:GLU:CA  | 4:9:296:ASN:C[1_554]   | 2.04                     | 0.16              |
| 4:5:297:ASN:CA  | 4:9:168:GLY:O[1_554]   | 2.04                     | 0.16              |
| 4:5:191:LYS:CB  | 4:9:187:ASP:CA[1_554]  | 2.04                     | 0.16              |
| 4:3:222:ASP:O   | 4:7:331:ALA:O[1_554]   | 2.04                     | 0.16              |
| 4:5:219:VAL:O   | 4:9:335:ARG:O[1_554]   | 2.04                     | 0.16              |
| 4:4:362:TYR:CD1 | 4:9:233:SER:C[1_554]   | 2.04                     | 0.16              |
| 4:4:275:HIS:CD2 | 4:8:151:ILE:CG1[1_554] | 2.04                     | 0.16              |
| 4:4:144:ALA:N   | 4:8:372:ARG:N[1_554]   | 2.04                     | 0.16              |
| 4:3:218:TYR:CE2 | 4:7:337:TYR:CE1[1_554] | 2.04                     | 0.16              |
| 4:4:18:LYS:NZ   | 4:8:76:ILE:O[1_554]    | 2.04                     | 0.16              |
| 4:4:141:SER:CB  | 4:8:116:ARG:CD[1_554]  | 2.04                     | 0.16              |
| 4:5:289:ILE:CA  | 4:W:64:ILE:CA[1_554]   | 2.04                     | 0.16              |
| 4:5:112:PRO:CB  | 4:V:253:GLU:CG[1_554]  | 2.04                     | 0.16              |
| 4:4:325:MET:CG  | 4:8:166:TYR:CD2[1_554] | 2.04                     | 0.16              |
| 4:5:308:GLY:CA  | 4:9:338:SER:N[1_554]   | 2.04                     | 0.16              |
| 4:5:270:GLU:C   | 4:9:272:ALA:C[1_554]   | 2.04                     | 0.16              |
| 4:5:309:ILE:CA  | 4:9:300:SER:OG[1_554]  | 2.04                     | 0.16              |
| 4:3:327:ILE:CA  | 4:7:167:GLU:N[1_554]   | 2.04                     | 0.16              |
| 4:5:274:ILE:CA  | 4:9:162:ASN:CB[1_554]  | 2.04                     | 0.16              |
| 4:4:290:ARG:NE  | 4:8:286:ASP:CG[1_554]  | 2.04                     | 0.16              |
| 4:5:288:ASP:N   | 4:W:62:ARG:C[1_554]    | 2.04                     | 0.16              |
| 4:3:30:VAL:CB   | 4:7:80:ASP:N[1_554]    | 2.04                     | 0.16              |
| 4:4:26:ALA:O    | 4:8:122:ILE:C[1_554]   | 2.04                     | 0.16              |
| 4:3:191:LYS:C   | 4:7:186:THR:OG1[1_554] | 2.04                     | 0.16              |
| 4:4:300:SER:O   | 4:8:108:ALA:CA[1_554]  | 2.04                     | 0.16              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:33:SER:N    | 4:9:78:ASN:CB[1_554]   | 2.04                     | 0.16              |
| 4:3:222:ASP:OD1 | 4:7:331:ALA:C[1_554]   | 2.04                     | 0.16              |
| 4:2:169:TYR:CE1 | 4:7:266:PHE:CE1[1_554] | 2.04                     | 0.16              |
| 4:3:227:MET:SD  | 4:7:306:TYR:CA[1_554]  | 2.04                     | 0.16              |
| 4:4:261:LEU:O   | 4:8:161:HIS:C[1_554]   | 2.04                     | 0.16              |
| 4:5:157:ASP:N   | 4:9:74:GLY:C[1_554]    | 2.04                     | 0.16              |
| 4:4:372:ARG:CG  | 4:9:227:MET:CA[1_554]  | 2.04                     | 0.16              |
| 4:5:137:GLN:CD  | 4:9:112:PRO:CG[1_554]  | 2.04                     | 0.16              |
| 4:4:198:TYR:CG  | 4:8:207:GLU:O[1_554]   | 2.04                     | 0.16              |
| 4:5:299:MET:CB  | 4:9:136:ILE:CA[1_554]  | 2.04                     | 0.16              |
| 4:2:370:VAL:CA  | 4:7:230:ALA:C[1_554]   | 2.04                     | 0.16              |
| 4:5:16:LEU:N    | 4:9:78:ASN:N[1_554]    | 2.04                     | 0.16              |
| 4:4:327:ILE:CG1 | 4:8:148:THR:O[1_554]   | 2.04                     | 0.16              |
| 4:5:344:SER:N   | 4:9:367:PRO:CA[1_554]  | 2.04                     | 0.16              |
| 4:1:292:ASP:CB  | 4:7:40:HIS:CD2[1_554]  | 2.04                     | 0.16              |
| 4:5:345:ILE:C   | 4:9:369:ILE:CB[1_554]  | 2.04                     | 0.16              |
| 4:3:267:ILE:C   | 4:7:180:LEU:CG[1_554]  | 2.04                     | 0.16              |
| 4:5:182:GLY:O   | 4:9:158:GLY:CA[1_554]  | 2.04                     | 0.16              |
| 4:4:27:PRO:CA   | 4:8:122:ILE:CA[1_554]  | 2.04                     | 0.16              |
| 4:5:200:PHE:O   | 4:9:206:ARG:CD[1_554]  | 2.04                     | 0.16              |
| 4:5:253:GLU:OE2 | 4:9:214:GLU:N[1_554]   | 2.04                     | 0.16              |
| 4:4:136:ILE:O   | 4:8:113:LYS:CE[1_554]  | 2.04                     | 0.16              |
| 4:3:188:TYR:CB  | 4:7:183:ARG:N[1_554]   | 2.04                     | 0.16              |
| 4:4:140:LEU:CA  | 4:8:371:HIS:NE2[1_554] | 2.04                     | 0.16              |
| 4:5:28:ARG:N    | 4:9:126:THR:OG1[1_554] | 2.04                     | 0.16              |
| 4:4:327:ILE:C   | 4:8:168:GLY:N[1_554]   | 2.04                     | 0.16              |
| 4:3:276:GLU:CB  | 4:7:281:SER:OG[1_554]  | 2.04                     | 0.16              |
| 4:5:286:ASP:CB  | 4:V:270:GLU:OE2[1_554] | 2.04                     | 0.16              |
| 4:3:289:ILE:CG1 | 4:9:39:ARG:NH2[1_554]  | 2.04                     | 0.16              |
| 4:3:256:ARG:N   | 4:7:303:THR:N[1_554]   | 2.04                     | 0.16              |
| 4:5:326:LYS:CD  | 4:9:167:GLU:OE1[1_554] | 2.04                     | 0.16              |
| 4:3:315:LYS:CG  | 4:7:147:ARG:NE[1_554]  | 2.04                     | 0.16              |
| 4:4:312:ARG:NE  | 4:8:300:SER:N[1_554]   | 2.04                     | 0.16              |
| 4:4:154:ASP:OD1 | 4:8:111:ASN:N[1_554]   | 2.04                     | 0.16              |
| 4:2:108:ALA:C   | 4:7:195:GLU:C[1_554]   | 2.04                     | 0.16              |
| 4:3:288:ASP:C   | 4:9:39:ARG:NH1[1_554]  | 2.04                     | 0.16              |
| 4:3:276:GLU:CD  | 4:7:278:THR:CA[1_554]  | 2.05                     | 0.15              |
| 4:4:173:HIS:NE2 | 4:9:264:PRO:O[1_554]   | 2.05                     | 0.15              |
| 4:5:110:LEU:CG  | 4:V:191:LYS:CG[1_554]  | 2.05                     | 0.15              |
| 4:5:28:ARG:CA   | 4:9:126:THR:CG2[1_554] | 2.05                     | 0.15              |
| 4:4:200:PHE:C   | 4:8:206:ARG:CG[1_554]  | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:283:MET:CG  | 4:8:286:ASP:O[1_554]   | 2.05                     | 0.15              |
| 4:3:332:PRO:CD  | 4:7:135:ALA:CA[1_554]  | 2.05                     | 0.15              |
| 4:4:205:GLU:CB  | 4:8:62:ARG:CZ[1_554]   | 2.05                     | 0.15              |
| 4:4:337:TYR:OH  | 4:8:86:TRP:CH2[1_554]  | 2.05                     | 0.15              |
| 4:3:26:ALA:C    | 4:7:121:GLN:C[1_554]   | 2.05                     | 0.15              |
| 4:2:173:HIS:CG  | 4:7:267:ILE:CG1[1_554] | 2.05                     | 0.15              |
| 4:5:151:ILE:CD1 | 4:9:172:PRO:N[1_554]   | 2.05                     | 0.15              |
| 4:5:242:LEU:CG  | 4:9:207:GLU:CD[1_554]  | 2.05                     | 0.15              |
| 4:3:308:GLY:C   | 4:7:141:SER:OG[1_554]  | 2.05                     | 0.15              |
| 4:4:264:PRO:N   | 4:8:274:ILE:CG1[1_554] | 2.05                     | 0.15              |
| 4:2:118:LYS:CA  | 4:7:249:THR:OG1[1_554] | 2.05                     | 0.15              |
| 4:5:264:PRO:CD  | 4:9:274:ILE:CD1[1_554] | 2.05                     | 0.15              |
| 4:5:268:GLY:C   | 4:9:264:PRO:CG[1_554]  | 2.05                     | 0.15              |
| 4:3:18:LYS:C    | 4:7:118:LYS:NZ[1_554]  | 2.05                     | 0.15              |
| 4:5:198:TYR:CE1 | 4:9:208:ILE:CA[1_554]  | 2.05                     | 0.15              |
| 4:3:76:ILE:O    | 4:8:198:TYR:CZ[1_554]  | 2.05                     | 0.15              |
| 4:3:278:THR:CB  | 4:7:164:PRO:CD[1_554]  | 2.05                     | 0.15              |
| 4:3:117:GLU:CG  | 4:8:237:GLU:CA[1_554]  | 2.05                     | 0.15              |
| 4:2:372:ARG:CB  | 4:7:227:MET:N[1_554]   | 2.05                     | 0.15              |
| 4:3:333:PRO:CA  | 4:7:104:LEU:O[1_554]   | 2.05                     | 0.15              |
| 4:3:276:GLU:C   | 4:7:281:SER:CB[1_554]  | 2.05                     | 0.15              |
| 4:5:21:PHE:N    | 4:9:125:GLU:CB[1_554]  | 2.05                     | 0.15              |
| 4:5:256:ARG:NE  | 4:9:306:TYR:CD1[1_554] | 2.05                     | 0.15              |
| 4:5:297:ASN:CG  | 4:9:165:ILE:CB[1_554]  | 2.05                     | 0.15              |
| 4:4:311:ASP:N   | 4:8:140:LEU:C[1_554]   | 2.05                     | 0.15              |
| 4:5:195:GLU:OE1 | 4:9:257:CYS:CB[1_554]  | 2.05                     | 0.15              |
| 4:5:340:TRP:CB  | 4:9:119:MET:CB[1_554]  | 2.05                     | 0.15              |
| 4:5:335:ARG:CD  | 4:9:106:THR:CB[1_554]  | 2.05                     | 0.15              |
| 4:2:169:TYR:CE1 | 4:7:266:PHE:CZ[1_554]  | 2.05                     | 0.15              |
| 4:5:250:ILE:CG2 | 4:9:214:GLU:CG[1_554]  | 2.05                     | 0.15              |
| 4:4:349:LEU:CD2 | 4:8:365:ALA:C[1_554]   | 2.05                     | 0.15              |
| 4:4:262:PHE:CA  | 4:8:153:LEU:CD1[1_554] | 2.05                     | 0.15              |
| 4:3:310:ALA:C   | 4:7:140:LEU:CA[1_554]  | 2.05                     | 0.15              |
| 4:3:197:GLY:C   | 4:7:209:VAL:N[1_554]   | 2.05                     | 0.15              |
| 4:3:310:ALA:C   | 4:7:141:SER:CA[1_554]  | 2.05                     | 0.15              |
| 4:3:300:SER:CB  | 4:7:107:GLU:CG[1_554]  | 2.05                     | 0.15              |
| 4:5:227:MET:SD  | 4:9:306:TYR:O[1_554]   | 2.05                     | 0.15              |
| 4:3:294:TYR:O   | 4:7:166:TYR:O[1_554]   | 2.05                     | 0.15              |
| 4:5:296:ASN:CA  | 4:9:168:GLY:O[1_554]   | 2.05                     | 0.15              |
| 4:4:370:VAL:O   | 4:9:230:ALA:C[1_554]   | 2.05                     | 0.15              |
| 4:4:117:GLU:CB  | 4:9:237:GLU:CB[1_554]  | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:325:MET:CG  | 4:8:166:TYR:CE1[1_554] | 2.05                     | 0.15              |
| 4:5:255:PHE:CD1 | 4:9:306:TYR:N[1_554]   | 2.05                     | 0.15              |
| 4:2:73:HIS:CA   | 4:7:198:TYR:O[1_554]   | 2.05                     | 0.15              |
| 4:3:282:ILE:CD1 | 4:7:171:LEU:CD1[1_554] | 2.05                     | 0.15              |
| 4:2:75:ILE:C    | 4:7:197:GLY:O[1_554]   | 2.05                     | 0.15              |
| 4:5:60:SER:CA   | 4:9:37:ARG:CB[1_554]   | 2.05                     | 0.15              |
| 4:4:220:ALA:CB  | 4:8:335:ARG:N[1_554]   | 2.05                     | 0.15              |
| 4:3:172:PRO:CB  | 4:8:188:TYR:CZ[1_554]  | 2.05                     | 0.15              |
| 4:5:227:MET:CB  | 4:9:308:GLY:N[1_554]   | 2.05                     | 0.15              |
| 4:5:16:LEU:N    | 4:9:70:PRO:O[1_554]    | 2.05                     | 0.15              |
| 4:4:293:LEU:CG  | 4:8:169:TYR:OH[1_554]  | 2.05                     | 0.15              |
| 4:4:255:PHE:CA  | 4:8:302:GLY:O[1_554]   | 2.05                     | 0.15              |
| 4:5:262:PHE:CE1 | 4:9:152:VAL:C[1_554]   | 2.05                     | 0.15              |
| 4:4:197:GLY:C   | 4:8:208:ILE:CG2[1_554] | 2.05                     | 0.15              |
| 4:5:344:SER:CB  | 4:9:120:THR:CG2[1_554] | 2.05                     | 0.15              |
| 4:3:226:GLU:CG  | 4:7:333:PRO:O[1_554]   | 2.05                     | 0.15              |
| 4:5:215:LYS:CG  | 4:9:30:VAL:O[1_554]    | 2.05                     | 0.15              |
| 4:4:143:TYR:N   | 4:8:372:ARG:CB[1_554]  | 2.05                     | 0.15              |
| 4:5:327:ILE:CG1 | 4:9:149:THR:OG1[1_554] | 2.05                     | 0.15              |
| 4:4:331:ALA:CB  | 4:8:140:LEU:CD1[1_554] | 2.05                     | 0.15              |
| 4:5:276:GLU:CG  | 4:9:278:THR:CA[1_554]  | 2.05                     | 0.15              |
| 4:5:75:ILE:CG2  | 4:V:198:TYR:CD2[1_554] | 2.05                     | 0.15              |
| 4:2:369:ILE:C   | 4:7:229:THR:O[1_554]   | 2.05                     | 0.15              |
| 4:4:334:GLU:OE1 | 4:8:133:TYR:C[1_554]   | 2.05                     | 0.15              |
| 4:3:339:VAL:C   | 4:7:117:GLU:CA[1_554]  | 2.05                     | 0.15              |
| 4:3:181:ALA:O   | 4:7:158:GLY:C[1_554]   | 2.05                     | 0.15              |
| 4:3:372:ARG:CB  | 4:8:227:MET:CB[1_554]  | 2.05                     | 0.15              |
| 4:5:25:ASP:OD1  | 4:9:131:ALA:N[1_554]   | 2.05                     | 0.15              |
| 4:4:173:HIS:CD2 | 4:9:267:ILE:N[1_554]   | 2.05                     | 0.15              |
| 4:5:275:HIS:NE2 | 4:9:278:THR:CG2[1_554] | 2.05                     | 0.15              |
| 4:3:340:TRP:N   | 4:7:117:GLU:N[1_554]   | 2.05                     | 0.15              |
| 4:4:253:GLU:CG  | 4:8:214:GLU:CB[1_554]  | 2.05                     | 0.15              |
| 4:5:186:THR:CB  | 4:9:183:ARG:NH2[1_554] | 2.05                     | 0.15              |
| 4:4:226:GLU:OE1 | 4:8:333:PRO:O[1_554]   | 2.05                     | 0.15              |
| 4:5:196:ARG:CG  | 4:9:211:ASP:O[1_554]   | 2.05                     | 0.15              |
| 4:5:162:ASN:CB  | 4:9:172:PRO:O[1_554]   | 2.05                     | 0.15              |
| 4:4:368:SER:CA  | 4:9:234:SER:OG[1_554]  | 2.05                     | 0.15              |
| 4:3:182:GLY:N   | 4:7:73:HIS:N[1_554]    | 2.05                     | 0.15              |
| 4:3:333:PRO:N   | 4:7:104:LEU:C[1_554]   | 2.05                     | 0.15              |
| 4:3:277:THR:O   | 4:7:174:ALA:N[1_554]   | 2.05                     | 0.15              |
| 4:4:117:GLU:CD  | 4:9:236:LEU:O[1_554]   | 2.05                     | 0.15              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:161:HIS:C   | 4:9:110:LEU:CD1[1_554] | 2.05                     | 0.15              |
| 4:4:334:GLU:CD  | 4:8:133:TYR:O[1_554]   | 2.05                     | 0.15              |
| 4:3:280:ASN:C   | 4:7:174:ALA:CB[1_554]  | 2.05                     | 0.15              |
| 4:4:75:ILE:CB   | 4:9:198:TYR:CG[1_554]  | 2.05                     | 0.15              |
| 4:4:18:LYS:CD   | 4:8:79:TRP:CZ2[1_554]  | 2.05                     | 0.15              |
| 4:3:161:HIS:N   | 4:7:110:LEU:CB[1_554]  | 2.05                     | 0.15              |
| 4:3:349:LEU:CD2 | 4:7:365:ALA:CA[1_554]  | 2.05                     | 0.15              |
| 4:4:120:THR:CB  | 4:9:233:SER:OG[1_554]  | 2.05                     | 0.15              |
| 4:2:286:ASP:C   | 4:7:270:GLU:OE2[1_554] | 2.05                     | 0.15              |
| 4:4:328:LYS:C   | 4:8:168:GLY:CA[1_554]  | 2.05                     | 0.15              |
| 4:3:265:SER:CB  | 4:7:261:LEU:C[1_554]   | 2.05                     | 0.15              |
| 4:3:210:ARG:CG  | 4:7:69:TYR:CG[1_554]   | 2.05                     | 0.15              |
| 4:4:281:SER:CA  | 4:8:173:HIS:CG[1_554]  | 2.05                     | 0.15              |
| 4:4:191:LYS:C   | 4:8:186:THR:CG2[1_554] | 2.05                     | 0.15              |
| 4:2:289:ILE:CB  | 4:8:39:ARG:NH2[1_554]  | 2.05                     | 0.15              |
| 4:1:288:ASP:C   | 4:7:39:ARG:CD[1_554]   | 2.05                     | 0.15              |
| 4:5:15:GLY:N    | 4:9:77:THR:CA[1_554]   | 2.05                     | 0.15              |
| 4:3:137:GLN:CB  | 4:7:113:LYS:N[1_554]   | 2.05                     | 0.15              |
| 4:3:281:SER:CA  | 4:7:174:ALA:N[1_554]   | 2.05                     | 0.15              |
| 4:5:205:GLU:CB  | 4:9:62:ARG:NE[1_554]   | 2.05                     | 0.15              |
| 4:4:110:LEU:N   | 4:9:192:ILE:CA[1_554]  | 2.05                     | 0.15              |
| 4:5:270:GLU:N   | 4:9:272:ALA:C[1_554]   | 2.05                     | 0.15              |
| 4:4:309:ILE:C   | 4:8:141:SER:N[1_554]   | 2.05                     | 0.15              |
| 4:3:299:MET:CB  | 4:7:136:ILE:CG1[1_554] | 2.06                     | 0.14              |
| 4:5:186:THR:C   | 4:9:183:ARG:CD[1_554]  | 2.06                     | 0.14              |
| 4:5:198:TYR:CD1 | 4:9:208:ILE:C[1_554]   | 2.06                     | 0.14              |
| 4:3:75:ILE:C    | 4:8:198:TYR:CD1[1_554] | 2.06                     | 0.14              |
| 4:1:292:ASP:CA  | 4:7:40:HIS:CB[1_554]   | 2.06                     | 0.14              |
| 4:3:283:MET:CE  | 4:7:289:ILE:CG1[1_554] | 2.06                     | 0.14              |
| 4:5:252:ASN:CG  | 4:9:215:LYS:O[1_554]   | 2.06                     | 0.14              |
| 4:4:180:LEU:CA  | 4:8:179:ASP:CG[1_554]  | 2.06                     | 0.14              |
| 4:4:112:PRO:CD  | 4:9:193:LEU:CA[1_554]  | 2.06                     | 0.14              |
| 4:2:115:ASN:ND2 | 4:7:198:TYR:CZ[1_554]  | 2.06                     | 0.14              |
| 4:3:180:LEU:CB  | 4:7:178:LEU:O[1_554]   | 2.06                     | 0.14              |
| 4:4:18:LYS:CE   | 4:8:79:TRP:CD2[1_554]  | 2.06                     | 0.14              |
| 4:3:273:GLY:N   | 4:7:277:THR:CG2[1_554] | 2.06                     | 0.14              |
| 4:5:17:VAL:N    | 4:9:78:ASN:C[1_554]    | 2.06                     | 0.14              |
| 4:2:177:ARG:NH1 | 4:7:194:THR:OG1[1_554] | 2.06                     | 0.14              |
| 4:4:200:PHE:CB  | 4:8:206:ARG:CG[1_554]  | 2.06                     | 0.14              |
| 4:3:248:ILE:CD1 | 4:7:207:GLU:CD[1_554]  | 2.06                     | 0.14              |
| 4:5:204:ALA:O   | 4:9:62:ARG:NH1[1_554]  | 2.06                     | 0.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:243:PRO:CB  | 4:8:61:LYS:CA[1_554]   | 2.06                     | 0.14              |
| 4:3:185:LEU:CB  | 4:7:158:GLY:C[1_554]   | 2.06                     | 0.14              |
| 4:5:292:ASP:OD2 | 4:W:64:ILE:CB[1_554]   | 2.06                     | 0.14              |
| 4:2:110:LEU:N   | 4:7:192:ILE:N[1_554]   | 2.06                     | 0.14              |
| 4:3:315:LYS:CB  | 4:7:298:VAL:CG2[1_554] | 2.06                     | 0.14              |
| 4:5:185:LEU:N   | 4:9:158:GLY:C[1_554]   | 2.06                     | 0.14              |
| 4:4:289:ILE:C   | 4:V:64:ILE:CG2[1_554]  | 2.06                     | 0.14              |
| 4:4:113:LYS:CA  | 4:9:252:ASN:C[1_554]   | 2.06                     | 0.14              |
| 4:2:75:ILE:CG1  | 4:7:198:TYR:CB[1_554]  | 2.06                     | 0.14              |
| 4:4:185:LEU:O   | 4:8:157:ASP:CA[1_554]  | 2.06                     | 0.14              |
| 4:3:317:ILE:CG2 | 4:7:164:PRO:C[1_554]   | 2.06                     | 0.14              |
| 4:3:337:TYR:CE1 | 4:7:86:TRP:CH2[1_554]  | 2.06                     | 0.14              |
| 4:3:110:LEU:C   | 4:8:193:LEU:N[1_554]   | 2.06                     | 0.14              |
| 4:5:198:TYR:CA  | 4:9:209:VAL:N[1_554]   | 2.06                     | 0.14              |
| 4:4:137:GLN:C   | 4:8:113:LYS:CB[1_554]  | 2.06                     | 0.14              |
| 4:5:17:VAL:O    | 4:9:79:TRP:CG[1_554]   | 2.06                     | 0.14              |
| 4:4:115:ASN:CG  | 4:9:196:ARG:NE[1_554]  | 2.06                     | 0.14              |
| 4:4:199:SER:OG  | 4:8:206:ARG:N[1_554]   | 2.06                     | 0.14              |
| 4:4:210:ARG:NH2 | 4:8:33:SER:C[1_554]    | 2.06                     | 0.14              |
| 4:3:30:VAL:CA   | 4:7:79:TRP:CA[1_554]   | 2.06                     | 0.14              |
| 4:4:314:GLN:CA  | 4:8:142:LEU:CA[1_554]  | 2.06                     | 0.14              |
| 4:5:110:LEU:CA  | 4:V:192:ILE:CA[1_554]  | 2.06                     | 0.14              |
| 4:5:264:PRO:N   | 4:9:274:ILE:CG1[1_554] | 2.06                     | 0.14              |
| 4:2:371:HIS:ND1 | 4:7:251:GLY:O[1_554]   | 2.06                     | 0.14              |
| 4:4:200:PHE:CB  | 4:8:206:ARG:CD[1_554]  | 2.06                     | 0.14              |
| 4:5:341:ILE:CB  | 4:9:132:MET:CE[1_554]  | 2.06                     | 0.14              |
| 4:3:274:ILE:CD1 | 4:7:161:HIS:CA[1_554]  | 2.06                     | 0.14              |
| 4:4:191:LYS:C   | 4:8:186:THR:N[1_554]   | 2.06                     | 0.14              |
| 4:5:140:LEU:O   | 4:9:116:ARG:CD[1_554]  | 2.06                     | 0.14              |
| 4:5:336:LYS:C   | 4:9:119:MET:CE[1_554]  | 2.06                     | 0.14              |
| 4:3:16:LEU:CG   | 4:7:78:ASN:CA[1_554]   | 2.06                     | 0.14              |
| 4:5:215:LYS:CD  | 4:9:31:PHE:N[1_554]    | 2.06                     | 0.14              |
| 4:4:266:PHE:CE2 | 4:8:303:THR:O[1_554]   | 2.06                     | 0.14              |
| 4:3:183:ARG:CG  | 4:7:72:GLU:CD[1_554]   | 2.06                     | 0.14              |
| 4:3:335:ARG:NE  | 4:7:106:THR:CG2[1_554] | 2.06                     | 0.14              |
| 4:4:32:PRO:CD   | 4:8:78:ASN:CG[1_554]   | 2.06                     | 0.14              |
| 4:4:23:GLY:C    | 4:8:362:TYR:CE2[1_554] | 2.06                     | 0.14              |
| 4:4:75:ILE:CD1  | 4:9:196:ARG:N[1_554]   | 2.06                     | 0.14              |
| 4:5:192:ILE:CA  | 4:9:213:LYS:CD[1_554]  | 2.06                     | 0.14              |
| 4:4:276:GLU:CD  | 4:8:279:TYR:N[1_554]   | 2.06                     | 0.14              |
| 4:5:162:ASN:CB  | 4:9:175:ILE:CG1[1_554] | 2.06                     | 0.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:344:SER:O   | 4:8:367:PRO:N[1_554]   | 2.06                     | 0.14              |
| 4:5:288:ASP:C   | 4:W:63:GLY:N[1_554]    | 2.06                     | 0.14              |
| 4:3:166:TYR:CE1 | 4:9:39:ARG:O[1_554]    | 2.06                     | 0.14              |
| 4:4:209:VAL:CG1 | 4:8:69:TYR:OH[1_554]   | 2.06                     | 0.14              |
| 4:3:19:ALA:CA   | 4:7:118:LYS:NZ[1_554]  | 2.06                     | 0.14              |
| 4:4:345:ILE:C   | 4:8:367:PRO:N[1_554]   | 2.06                     | 0.14              |
| 4:4:200:PHE:CD2 | 4:8:206:ARG:NE[1_554]  | 2.06                     | 0.14              |
| 4:4:79:TRP:CH2  | 4:9:249:THR:CG2[1_554] | 2.06                     | 0.14              |
| 4:3:210:ARG:CZ  | 4:7:70:PRO:CD[1_554]   | 2.06                     | 0.14              |
| 4:5:180:LEU:CA  | 4:9:179:ASP:CA[1_554]  | 2.06                     | 0.14              |
| 4:3:256:ARG:CZ  | 4:7:306:TYR:CE1[1_554] | 2.06                     | 0.14              |
| 4:4:157:ASP:OD2 | 4:8:72:GLU:CA[1_554]   | 2.06                     | 0.14              |
| 4:5:322:PRO:O   | 4:9:291:LYS:NZ[1_554]  | 2.06                     | 0.14              |
| 4:3:265:SER:CA  | 4:7:261:LEU:C[1_554]   | 2.06                     | 0.14              |
| 4:5:254:ARG:NH2 | 4:9:336:LYS:CE[1_554]  | 2.06                     | 0.14              |
| 4:4:255:PHE:CD2 | 4:8:305:MET:CE[1_554]  | 2.06                     | 0.14              |
| 4:5:180:LEU:CD1 | 4:9:160:THR:CA[1_554]  | 2.06                     | 0.14              |
| 4:4:325:MET:CG  | 4:8:166:TYR:OH[1_554]  | 2.06                     | 0.14              |
| 4:3:184:ASP:CG  | 4:7:73:HIS:NE2[1_554]  | 2.06                     | 0.14              |
| 4:5:341:ILE:CG1 | 4:9:132:MET:SD[1_554]  | 2.06                     | 0.14              |
| 4:5:301:GLY:O   | 4:9:137:GLN:CD[1_554]  | 2.06                     | 0.14              |
| 4:4:18:LYS:N    | 4:8:79:TRP:CD2[1_554]  | 2.06                     | 0.14              |
| 4:3:218:TYR:CE2 | 4:7:337:TYR:CZ[1_554]  | 2.06                     | 0.14              |
| 4:3:277:THR:OG1 | 4:7:176:MET:CB[1_554]  | 2.06                     | 0.14              |
| 4:5:256:ARG:CB  | 4:9:306:TYR:CD1[1_554] | 2.06                     | 0.14              |
| 4:3:339:VAL:CA  | 4:7:115:ASN:C[1_554]   | 2.06                     | 0.14              |
| 4:3:154:ASP:OD1 | 4:7:111:ASN:N[1_554]   | 2.06                     | 0.14              |
| 4:4:332:PRO:CG  | 4:8:133:TYR:CD2[1_554] | 2.06                     | 0.14              |
| 4:5:199:SER:CB  | 4:9:206:ARG:CA[1_554]  | 2.06                     | 0.14              |
| 4:3:310:ALA:O   | 4:7:141:SER:N[1_554]   | 2.06                     | 0.14              |
| 4:4:188:TYR:OH  | 4:8:306:TYR:OH[1_554]  | 2.06                     | 0.14              |
| 4:5:316:GLU:CB  | 4:9:298:VAL:N[1_554]   | 2.06                     | 0.14              |
| 4:4:215:LYS:N   | 4:8:17:VAL:N[1_554]    | 2.06                     | 0.14              |
| 4:5:279:TYR:CE1 | 4:9:293:LEU:CD2[1_554] | 2.06                     | 0.14              |
| 4:3:211:ASP:O   | 4:7:31:PHE:O[1_554]    | 2.06                     | 0.14              |
| 4:3:306:TYR:N   | 4:7:11:ASP:CG[1_554]   | 2.06                     | 0.14              |
| 4:4:205:GLU:CD  | 4:8:203:THR:OG1[1_554] | 2.06                     | 0.14              |
| 4:3:367:PRO:C   | 4:8:236:LEU:N[1_554]   | 2.06                     | 0.14              |
| 4:5:213:LYS:CE  | 4:9:14:SER:C[1_554]    | 2.06                     | 0.14              |
| 4:5:187:ASP:O   | 4:9:184:ASP:N[1_554]   | 2.06                     | 0.14              |
| 4:5:339:VAL:C   | 4:9:116:ARG:CB[1_554]  | 2.06                     | 0.14              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:334:GLU:C   | 4:8:105:LEU:CD1[1_554] | 2.06                     | 0.14              |
| 4:4:157:ASP:N   | 4:8:75:ILE:CA[1_554]   | 2.06                     | 0.14              |
| 4:5:185:LEU:CB  | 4:9:157:ASP:O[1_554]   | 2.06                     | 0.14              |
| 4:4:243:PRO:O   | 4:8:60:SER:OG[1_554]   | 2.06                     | 0.14              |
| 4:1:324:THR:O   | 4:7:44:MET:CE[1_554]   | 2.06                     | 0.14              |
| 4:3:357:ILE:CG2 | 4:8:233:SER:N[1_554]   | 2.06                     | 0.14              |
| 4:4:183:ARG:NE  | 4:8:72:GLU:OE2[1_554]  | 2.06                     | 0.14              |
| 4:4:185:LEU:CG  | 4:8:158:GLY:N[1_554]   | 2.06                     | 0.14              |
| 4:3:266:PHE:CA  | 4:7:261:LEU:CA[1_554]  | 2.06                     | 0.14              |
| 4:4:113:LYS:CG  | 4:9:254:ARG:CA[1_554]  | 2.06                     | 0.14              |
| 4:4:187:ASP:CA  | 4:8:183:ARG:CB[1_554]  | 2.06                     | 0.14              |
| 4:4:284:LYS:CA  | 4:9:268:GLY:O[1_554]   | 2.06                     | 0.14              |
| 4:5:264:PRO:CD  | 4:9:274:ILE:CA[1_554]  | 2.06                     | 0.14              |
| 4:2:124:PHE:CE2 | 4:7:233:SER:O[1_554]   | 2.06                     | 0.14              |
| 4:3:186:THR:CA  | 4:7:183:ARG:CD[1_554]  | 2.06                     | 0.14              |
| 4:4:340:TRP:N   | 4:8:117:GLU:C[1_554]   | 2.06                     | 0.14              |
| 4:5:180:LEU:CG  | 4:9:178:LEU:CA[1_554]  | 2.06                     | 0.14              |
| 4:5:308:GLY:N   | 4:9:337:TYR:C[1_554]   | 2.06                     | 0.14              |
| 4:3:208:ILE:N   | 4:7:59:GLN:NE2[1_554]  | 2.06                     | 0.14              |
| 4:4:256:ARG:CA  | 4:8:303:THR:C[1_554]   | 2.06                     | 0.14              |
| 4:5:136:ILE:N   | 4:9:113:LYS:NZ[1_554]  | 2.06                     | 0.14              |
| 4:4:334:GLU:C   | 4:8:105:LEU:CG[1_554]  | 2.06                     | 0.14              |
| 4:3:289:ILE:CB  | 4:9:39:ARG:NH2[1_554]  | 2.06                     | 0.14              |
| 4:2:116:ARG:CG  | 4:7:252:ASN:ND2[1_554] | 2.06                     | 0.14              |
| 4:5:180:LEU:CG  | 4:9:178:LEU:N[1_554]   | 2.06                     | 0.14              |
| 4:2:370:VAL:CG2 | 4:7:233:SER:OG[1_554]  | 2.06                     | 0.14              |
| 4:5:208:ILE:CB  | 4:9:59:GLN:CB[1_554]   | 2.06                     | 0.14              |
| 4:5:276:GLU:OE1 | 4:9:278:THR:O[1_554]   | 2.06                     | 0.14              |
| 4:5:318:THR:O   | 4:9:292:ASP:CA[1_554]  | 2.06                     | 0.14              |
| 4:3:157:ASP:N   | 4:7:75:ILE:CB[1_554]   | 2.07                     | 0.13              |
| 4:4:275:HIS:O   | 4:8:164:PRO:CG[1_554]  | 2.07                     | 0.13              |
| 4:3:221:LEU:N   | 4:7:338:SER:OG[1_554]  | 2.07                     | 0.13              |
| 4:3:305:MET:O   | 4:7:11:ASP:CA[1_554]   | 2.07                     | 0.13              |
| 4:5:211:ASP:CB  | 4:9:32:PRO:N[1_554]    | 2.07                     | 0.13              |
| 4:2:290:ARG:N   | 4:8:63:GLY:O[1_554]    | 2.07                     | 0.13              |
| 4:5:223:PHE:O   | 4:9:309:ILE:CG2[1_554] | 2.07                     | 0.13              |
| 4:5:368:SER:C   | 4:V:230:ALA:CA[1_554]  | 2.07                     | 0.13              |
| 4:3:219:VAL:CG1 | 4:7:300:SER:CA[1_554]  | 2.07                     | 0.13              |
| 4:5:59:GLN:CG   | 4:9:68:LYS:CD[1_554]   | 2.07                     | 0.13              |
| 4:3:226:GLU:CG  | 4:7:305:MET:CE[1_554]  | 2.07                     | 0.13              |
| 4:5:337:TYR:CE2 | 4:9:86:TRP:CZ2[1_554]  | 2.07                     | 0.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:16:LEU:CA   | 4:7:78:ASN:CA[1_554]   | 2.07                     | 0.13              |
| 4:5:143:TYR:CG  | 4:9:372:ARG:CA[1_554]  | 2.07                     | 0.13              |
| 4:4:300:SER:O   | 4:8:107:GLU:C[1_554]   | 2.07                     | 0.13              |
| 4:4:161:HIS:N   | 4:8:110:LEU:CG[1_554]  | 2.07                     | 0.13              |
| 4:3:327:ILE:CG2 | 4:7:148:THR:CA[1_554]  | 2.07                     | 0.13              |
| 4:5:348:SER:O   | 4:9:364:GLU:CA[1_554]  | 2.07                     | 0.13              |
| 4:4:223:PHE:CD2 | 4:8:304:THR:CB[1_554]  | 2.07                     | 0.13              |
| 4:5:327:ILE:CB  | 4:9:148:THR:C[1_554]   | 2.07                     | 0.13              |
| 4:2:115:ASN:ND2 | 4:7:198:TYR:OH[1_554]  | 2.07                     | 0.13              |
| 4:5:162:ASN:CB  | 4:9:175:ILE:CD1[1_554] | 2.07                     | 0.13              |
| 4:3:240:TYR:OH  | 4:7:55:GLY:O[1_554]    | 2.07                     | 0.13              |
| 4:3:210:ARG:N   | 4:7:69:TYR:CZ[1_554]   | 2.07                     | 0.13              |
| 4:3:242:LEU:C   | 4:7:60:SER:N[1_554]    | 2.07                     | 0.13              |
| 4:4:255:PHE:C   | 4:8:303:THR:N[1_554]   | 2.07                     | 0.13              |
| 4:4:196:ARG:C   | 4:8:212:ILE:N[1_554]   | 2.07                     | 0.13              |
| 4:3:290:ARG:N   | 4:9:63:GLY:O[1_554]    | 2.07                     | 0.13              |
| 1:A:637:LYS:CD  | 4:4:311:ASP:OD1[1_556] | 2.07                     | 0.13              |
| 4:5:185:LEU:CD2 | 4:9:159:VAL:O[1_554]   | 2.07                     | 0.13              |
| 4:3:294:TYR:CE2 | 4:7:166:TYR:CG[1_554]  | 2.07                     | 0.13              |
| 4:5:62:ARG:NH1  | 4:9:66:THR:C[1_554]    | 2.07                     | 0.13              |
| 4:5:295:ALA:N   | 4:9:167:GLU:CB[1_554]  | 2.07                     | 0.13              |
| 4:5:367:PRO:CA  | 4:V:233:SER:N[1_554]   | 2.07                     | 0.13              |
| 4:4:116:ARG:CD  | 4:9:252:ASN:OD1[1_554] | 2.07                     | 0.13              |
| 4:4:341:ILE:CG2 | 4:8:120:THR:OG1[1_554] | 2.07                     | 0.13              |
| 4:4:184:ASP:CB  | 4:8:158:GLY:O[1_554]   | 2.07                     | 0.13              |
| 4:5:327:ILE:CB  | 4:9:149:THR:OG1[1_554] | 2.07                     | 0.13              |
| 4:3:191:LYS:CB  | 4:7:186:THR:CA[1_554]  | 2.07                     | 0.13              |
| 4:5:143:TYR:CA  | 4:9:372:ARG:N[1_554]   | 2.07                     | 0.13              |
| 4:5:32:PRO:CD   | 4:9:78:ASN:ND2[1_554]  | 2.07                     | 0.13              |
| 4:3:185:LEU:CD2 | 4:7:159:VAL:N[1_554]   | 2.07                     | 0.13              |
| 4:5:143:TYR:N   | 4:9:372:ARG:CG[1_554]  | 2.07                     | 0.13              |
| 4:5:154:ASP:OD2 | 4:9:111:ASN:O[1_554]   | 2.07                     | 0.13              |
| 4:5:293:LEU:O   | 4:9:169:TYR:CB[1_554]  | 2.07                     | 0.13              |
| 4:3:253:GLU:CG  | 4:7:214:GLU:OE2[1_554] | 2.07                     | 0.13              |
| 4:5:31:PHE:C    | 4:9:78:ASN:ND2[1_554]  | 2.07                     | 0.13              |
| 4:3:304:THR:O   | 4:7:137:GLN:CD[1_554]  | 2.07                     | 0.13              |
| 4:3:316:GLU:O   | 4:7:150:GLY:CA[1_554]  | 2.07                     | 0.13              |
| 4:4:319:ALA:O   | 4:8:293:LEU:O[1_554]   | 2.07                     | 0.13              |
| 4:5:215:LYS:CB  | 4:9:30:VAL:CG1[1_554]  | 2.07                     | 0.13              |
| 4:2:172:PRO:CD  | 4:7:266:PHE:CD1[1_554] | 2.07                     | 0.13              |
| 4:4:156:GLY:N   | 4:8:75:ILE:CG1[1_554]  | 2.07                     | 0.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:254:ARG:CZ  | 4:8:336:LYS:NZ[1_554]  | 2.07                     | 0.13              |
| 4:4:14:SER:C    | 4:8:77:THR:OG1[1_554]  | 2.07                     | 0.13              |
| 4:4:223:PHE:CG  | 4:8:335:ARG:NE[1_554]  | 2.07                     | 0.13              |
| 4:3:223:PHE:CE2 | 4:7:301:GLY:N[1_554]   | 2.07                     | 0.13              |
| 4:5:205:GLU:N   | 4:9:62:ARG:CZ[1_554]   | 2.07                     | 0.13              |
| 4:2:115:ASN:ND2 | 4:7:249:THR:O[1_554]   | 2.07                     | 0.13              |
| 4:4:153:LEU:CD2 | 4:8:109:PRO:CD[1_554]  | 2.07                     | 0.13              |
| 4:5:193:LEU:CG  | 4:9:210:ARG:C[1_554]   | 2.07                     | 0.13              |
| 4:3:213:LYS:N   | 4:7:15:GLY:O[1_554]    | 2.07                     | 0.13              |
| 4:3:259:GLU:N   | 4:7:155:SER:C[1_554]   | 2.07                     | 0.13              |
| 4:5:319:ALA:CB  | 4:9:295:ALA:O[1_554]   | 2.07                     | 0.13              |
| 4:5:293:LEU:O   | 4:9:169:TYR:CA[1_554]  | 2.07                     | 0.13              |
| 4:4:196:ARG:CB  | 4:8:211:ASP:CA[1_554]  | 2.07                     | 0.13              |
| 4:5:173:HIS:C   | 4:V:267:ILE:O[1_554]   | 2.07                     | 0.13              |
| 4:4:249:THR:CG2 | 4:8:211:ASP:OD2[1_554] | 2.07                     | 0.13              |
| 4:5:195:GLU:CB  | 4:9:189:LEU:CD1[1_554] | 2.07                     | 0.13              |
| 4:4:145:SER:CB  | 4:8:372:ARG:NH1[1_554] | 2.07                     | 0.13              |
| 4:3:240:TYR:CE2 | 4:7:32:PRO:CD[1_554]   | 2.07                     | 0.13              |
| 4:4:340:TRP:CB  | 4:8:118:LYS:O[1_554]   | 2.07                     | 0.13              |
| 4:5:317:ILE:CD1 | 4:9:165:ILE:C[1_554]   | 2.07                     | 0.13              |
| 4:3:76:ILE:C    | 4:8:198:TYR:CD1[1_554] | 2.07                     | 0.13              |
| 4:4:173:HIS:CE1 | 4:9:265:SER:O[1_554]   | 2.07                     | 0.13              |
| 4:3:19:ALA:CA   | 4:7:118:LYS:CE[1_554]  | 2.07                     | 0.13              |
| 4:3:371:HIS:ND1 | 4:8:252:ASN:N[1_554]   | 2.07                     | 0.13              |
| 4:3:113:LYS:CE  | 4:8:254:ARG:C[1_554]   | 2.07                     | 0.13              |
| 4:5:316:GLU:CG  | 4:9:297:ASN:C[1_554]   | 2.07                     | 0.13              |
| 4:4:369:ILE:C   | 4:9:230:ALA:N[1_554]   | 2.07                     | 0.13              |
| 4:3:275:HIS:CB  | 4:7:152:VAL:O[1_554]   | 2.07                     | 0.13              |
| 4:4:262:PHE:CE1 | 4:8:154:ASP:N[1_554]   | 2.07                     | 0.13              |
| 4:5:321:ALA:N   | 4:9:292:ASP:CA[1_554]  | 2.07                     | 0.13              |
| 4:4:62:ARG:NH1  | 4:8:67:LEU:O[1_554]    | 2.07                     | 0.13              |
| 4:3:114:ALA:N   | 4:8:250:ILE:CA[1_554]  | 2.07                     | 0.13              |
| 4:5:10:CYS:CA   | 4:9:118:LYS:CE[1_554]  | 2.07                     | 0.13              |
| 4:3:270:GLU:CA  | 4:7:272:ALA:CB[1_554]  | 2.07                     | 0.13              |
| 4:3:307:PRO:CD  | 4:7:11:ASP:OD2[1_554]  | 2.07                     | 0.13              |
| 4:4:333:PRO:N   | 4:8:104:LEU:CA[1_554]  | 2.07                     | 0.13              |
| 4:4:284:LYS:O   | 4:9:268:GLY:CA[1_554]  | 2.07                     | 0.13              |
| 4:4:261:LEU:N   | 4:8:155:SER:OG[1_554]  | 2.07                     | 0.13              |
| 4:4:227:MET:CE  | 4:8:306:TYR:O[1_554]   | 2.07                     | 0.13              |
| 4:3:198:TYR:CD2 | 4:7:207:GLU:C[1_554]   | 2.07                     | 0.13              |
| 4:3:213:LYS:CB  | 4:7:15:GLY:N[1_554]    | 2.07                     | 0.13              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:151:ILE:CG1 | 4:9:172:PRO:CD[1_554]  | 2.07                     | 0.13              |
| 4:4:262:PHE:CD2 | 4:8:154:ASP:N[1_554]   | 2.07                     | 0.13              |
| 4:5:281:SER:CA  | 4:9:173:HIS:CD2[1_554] | 2.07                     | 0.13              |
| 4:4:198:TYR:CG  | 4:8:208:ILE:C[1_554]   | 2.07                     | 0.13              |
| 4:3:172:PRO:O   | 4:8:188:TYR:CD1[1_554] | 2.07                     | 0.13              |
| 4:3:136:ILE:O   | 4:7:113:LYS:CG[1_554]  | 2.07                     | 0.13              |
| 4:3:113:LYS:C   | 4:8:250:ILE:C[1_554]   | 2.07                     | 0.13              |
| 4:4:113:LYS:CE  | 4:9:254:ARG:CG[1_554]  | 2.07                     | 0.13              |
| 4:3:272:ALA:N   | 4:7:277:THR:CG2[1_554] | 2.07                     | 0.13              |
| 4:5:253:GLU:N   | 4:9:214:GLU:CA[1_554]  | 2.07                     | 0.13              |
| 4:5:200:PHE:C   | 4:9:206:ARG:CD[1_554]  | 2.07                     | 0.13              |
| 4:4:309:ILE:N   | 4:8:339:VAL:CG2[1_554] | 2.07                     | 0.13              |
| 4:4:178:LEU:CD2 | 4:8:177:ARG:C[1_554]   | 2.07                     | 0.13              |
| 4:3:184:ASP:N   | 4:7:73:HIS:ND1[1_554]  | 2.07                     | 0.13              |
| 4:3:340:TRP:CG  | 4:7:118:LYS:CG[1_554]  | 2.07                     | 0.13              |
| 4:3:304:THR:CB  | 4:7:137:GLN:CD[1_554]  | 2.07                     | 0.13              |
| 4:3:184:ASP:O   | 4:7:184:ASP:OD1[1_554] | 2.07                     | 0.13              |
| 4:5:335:ARG:NH1 | 4:9:140:LEU:CD1[1_554] | 2.07                     | 0.13              |
| 4:4:282:ILE:CD1 | 4:8:171:LEU:CB[1_554]  | 2.07                     | 0.13              |
| 4:5:207:GLU:C   | 4:9:59:GLN:NE2[1_554]  | 2.07                     | 0.13              |
| 4:5:311:ASP:CG  | 4:9:144:ALA:C[1_554]   | 2.07                     | 0.13              |
| 4:5:28:ARG:CB   | 4:9:126:THR:OG1[1_554] | 2.07                     | 0.13              |
| 4:3:244:ASP:N   | 4:7:60:SER:O[1_554]    | 2.07                     | 0.13              |
| 4:5:337:TYR:CA  | 4:9:119:MET:SD[1_554]  | 2.07                     | 0.13              |
| 4:5:149:THR:OG1 | 4:W:40:HIS:CB[1_554]   | 2.07                     | 0.13              |
| 4:4:336:LYS:CD  | 4:8:86:TRP:CE2[1_554]  | 2.07                     | 0.13              |
| 4:5:140:LEU:N   | 4:9:371:HIS:CG[1_554]  | 2.07                     | 0.13              |
| 4:5:157:ASP:CA  | 4:9:73:HIS:N[1_554]    | 2.07                     | 0.13              |
| 4:3:154:ASP:OD2 | 4:7:112:PRO:CD[1_554]  | 2.07                     | 0.13              |
| 4:5:142:LEU:O   | 4:9:372:ARG:CG[1_554]  | 2.07                     | 0.13              |
| 4:5:319:ALA:C   | 4:9:292:ASP:O[1_554]   | 2.07                     | 0.13              |
| 4:5:340:TRP:O   | 4:9:120:THR:OG1[1_554] | 2.07                     | 0.13              |
| 4:5:368:SER:O   | 4:V:229:THR:O[1_554]   | 2.07                     | 0.13              |
| 4:2:291:LYS:N   | 4:8:64:ILE:CB[1_554]   | 2.07                     | 0.13              |
| 4:4:211:ASP:O   | 4:8:31:PHE:O[1_554]    | 2.08                     | 0.12              |
| 4:4:366:GLY:CA  | 4:9:234:SER:CB[1_554]  | 2.08                     | 0.12              |
| 4:5:338:SER:N   | 4:9:134:VAL:CG2[1_554] | 2.08                     | 0.12              |
| 4:5:156:GLY:C   | 4:9:73:HIS:C[1_554]    | 2.08                     | 0.12              |
| 4:5:73:HIS:CD2  | 4:V:199:SER:OG[1_554]  | 2.08                     | 0.12              |
| 4:2:284:LYS:C   | 4:7:268:GLY:CA[1_554]  | 2.08                     | 0.12              |
| 4:4:310:ALA:N   | 4:8:140:LEU:C[1_554]   | 2.08                     | 0.12              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:262:PHE:O   | 4:8:153:LEU:CG[1_554]  | 2.08                     | 0.12              |
| 4:5:117:GLU:N   | 4:V:252:ASN:OD1[1_554] | 2.08                     | 0.12              |
| 4:4:369:ILE:O   | 4:9:229:THR:N[1_554]   | 2.08                     | 0.12              |
| 4:5:344:SER:OG  | 4:9:362:TYR:CE1[1_554] | 2.08                     | 0.12              |
| 4:5:9:VAL:CB    | 4:9:121:GLN:CB[1_554]  | 2.08                     | 0.12              |
| 4:5:317:ILE:CB  | 4:9:151:ILE:N[1_554]   | 2.08                     | 0.12              |
| 4:4:310:ALA:CB  | 4:8:140:LEU:O[1_554]   | 2.08                     | 0.12              |
| 4:3:312:ARG:NE  | 4:7:299:MET:N[1_554]   | 2.08                     | 0.12              |
| 4:3:191:LYS:NZ  | 4:7:257:CYS:SG[1_554]  | 2.08                     | 0.12              |
| 4:4:334:GLU:CD  | 4:8:133:TYR:C[1_554]   | 2.08                     | 0.12              |
| 4:4:140:LEU:C   | 4:8:371:HIS:CE1[1_554] | 2.08                     | 0.12              |
| 4:2:367:PRO:C   | 4:7:235:SER:C[1_554]   | 2.08                     | 0.12              |
| 4:5:178:LEU:C   | 4:9:177:ARG:CB[1_554]  | 2.08                     | 0.12              |
| 4:4:195:GLU:CG  | 4:8:189:LEU:CD1[1_554] | 2.08                     | 0.12              |
| 4:3:112:PRO:CD  | 4:8:193:LEU:CG[1_554]  | 2.08                     | 0.12              |
| 4:5:312:ARG:NH1 | 4:9:299:MET:CG[1_554]  | 2.08                     | 0.12              |
| 4:4:113:LYS:C   | 4:9:251:GLY:CA[1_554]  | 2.08                     | 0.12              |
| 4:3:340:TRP:CD1 | 4:7:118:LYS:CB[1_554]  | 2.08                     | 0.12              |
| 4:3:243:PRO:CB  | 4:7:60:SER:O[1_554]    | 2.08                     | 0.12              |
| 4:5:294:TYR:C   | 4:9:167:GLU:CA[1_554]  | 2.08                     | 0.12              |
| 4:4:339:VAL:CG2 | 4:8:112:PRO:O[1_554]   | 2.08                     | 0.12              |
| 4:5:308:GLY:O   | 4:9:338:SER:CB[1_554]  | 2.08                     | 0.12              |
| 4:3:265:SER:OG  | 4:7:261:LEU:O[1_554]   | 2.08                     | 0.12              |
| 4:4:111:ASN:OD1 | 4:9:196:ARG:CA[1_554]  | 2.08                     | 0.12              |
| 4:3:340:TRP:NE1 | 4:7:118:LYS:CE[1_554]  | 2.08                     | 0.12              |
| 4:5:342:GLY:C   | 4:9:370:VAL:CG1[1_554] | 2.08                     | 0.12              |
| 4:5:314:GLN:N   | 4:9:142:LEU:CG[1_554]  | 2.08                     | 0.12              |
| 4:4:30:VAL:CA   | 4:8:79:TRP:CA[1_554]   | 2.08                     | 0.12              |
| 4:3:341:ILE:CA  | 4:7:120:THR:CB[1_554]  | 2.08                     | 0.12              |
| 4:3:115:ASN:CG  | 4:8:249:THR:C[1_554]   | 2.08                     | 0.12              |
| 4:3:317:ILE:CD1 | 4:7:165:ILE:O[1_554]   | 2.08                     | 0.12              |
| 4:1:289:ILE:CA  | 4:7:39:ARG:CZ[1_554]   | 2.08                     | 0.12              |
| 4:4:314:GLN:C   | 4:8:142:LEU:CD2[1_554] | 2.08                     | 0.12              |
| 4:4:223:PHE:CZ  | 4:8:301:GLY:N[1_554]   | 2.08                     | 0.12              |
| 4:3:204:ALA:CA  | 4:7:62:ARG:C[1_554]    | 2.08                     | 0.12              |
| 4:3:334:GLU:CA  | 4:7:105:LEU:CB[1_554]  | 2.08                     | 0.12              |
| 4:3:31:PHE:CA   | 4:7:78:ASN:ND2[1_554]  | 2.08                     | 0.12              |
| 4:4:185:LEU:C   | 4:8:158:GLY:N[1_554]   | 2.08                     | 0.12              |
| 4:5:274:ILE:CD1 | 4:9:161:HIS:CG[1_554]  | 2.08                     | 0.12              |
| 4:3:197:GLY:O   | 4:7:208:ILE:CG1[1_554] | 2.08                     | 0.12              |
| 4:5:312:ARG:O   | 4:9:298:VAL:CG2[1_554] | 2.08                     | 0.12              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:252:ASN:CA  | 4:9:214:GLU:O[1_554]   | 2.08                     | 0.12              |
| 4:3:339:VAL:CG2 | 4:7:116:ARG:N[1_554]   | 2.08                     | 0.12              |
| 4:3:218:TYR:CD2 | 4:7:337:TYR:CE1[1_554] | 2.08                     | 0.12              |
| 4:4:211:ASP:CG  | 4:8:32:PRO:CG[1_554]   | 2.08                     | 0.12              |
| 4:5:214:GLU:CB  | 4:9:16:LEU:CB[1_554]   | 2.08                     | 0.12              |
| 4:2:79:TRP:CZ3  | 4:7:249:THR:CG2[1_554] | 2.08                     | 0.12              |
| 4:1:289:ILE:O   | 4:7:40:HIS:CE1[1_554]  | 2.08                     | 0.12              |
| 4:3:215:LYS:NZ  | 4:7:31:PHE:CD2[1_554]  | 2.08                     | 0.12              |
| 4:1:326:LYS:CD  | 4:7:43:VAL:CG2[1_554]  | 2.08                     | 0.12              |
| 4:5:188:TYR:C   | 4:9:183:ARG:N[1_554]   | 2.08                     | 0.12              |
| 4:4:188:TYR:CZ  | 4:8:185:LEU:CG[1_554]  | 2.08                     | 0.12              |
| 4:2:287:ILE:C   | 4:8:63:GLY:C[1_554]    | 2.08                     | 0.12              |
| 4:5:31:PHE:CD1  | 4:9:79:TRP:C[1_554]    | 2.08                     | 0.12              |
| 4:5:190:MET:CB  | 4:9:187:ASP:OD1[1_554] | 2.08                     | 0.12              |
| 4:4:75:ILE:CD1  | 4:9:193:LEU:C[1_554]   | 2.08                     | 0.12              |
| 4:3:319:ALA:O   | 4:7:293:LEU:O[1_554]   | 2.08                     | 0.12              |
| 4:4:299:MET:SD  | 4:8:136:ILE:O[1_554]   | 2.08                     | 0.12              |
| 4:1:292:ASP:CG  | 4:7:40:HIS:N[1_554]    | 2.08                     | 0.12              |
| 4:5:162:ASN:OD1 | 4:9:175:ILE:CG1[1_554] | 2.08                     | 0.12              |
| 4:5:9:VAL:O     | 4:9:121:GLN:OE1[1_554] | 2.08                     | 0.12              |
| 4:4:288:ASP:O   | 4:V:63:GLY:C[1_554]    | 2.08                     | 0.12              |
| 4:4:142:LEU:C   | 4:8:372:ARG:N[1_554]   | 2.08                     | 0.12              |
| 4:1:291:LYS:CA  | 4:7:64:ILE:CB[1_554]   | 2.08                     | 0.12              |
| 4:5:173:HIS:CG  | 4:V:267:ILE:CA[1_554]  | 2.08                     | 0.12              |
| 4:3:151:ILE:CB  | 4:7:170:ALA:O[1_554]   | 2.08                     | 0.12              |
| 4:5:9:VAL:CG2   | 4:9:367:PRO:CG[1_554]  | 2.08                     | 0.12              |
| 4:5:24:ASP:CA   | 4:9:125:GLU:N[1_554]   | 2.08                     | 0.12              |
| 4:5:184:ASP:CB  | 4:9:158:GLY:O[1_554]   | 2.08                     | 0.12              |
| 4:4:207:GLU:CD  | 4:8:68:LYS:N[1_554]    | 2.08                     | 0.12              |
| 4:4:372:ARG:C   | 4:9:226:GLU:O[1_554]   | 2.08                     | 0.12              |
| 4:5:322:PRO:O   | 4:9:292:ASP:CG[1_554]  | 2.08                     | 0.12              |
| 4:4:161:HIS:O   | 4:8:110:LEU:CB[1_554]  | 2.08                     | 0.12              |
| 4:4:298:VAL:CA  | 4:8:136:ILE:CD1[1_554] | 2.08                     | 0.12              |
| 4:3:180:LEU:CD2 | 4:7:178:LEU:CB[1_554]  | 2.08                     | 0.12              |
| 4:3:299:MET:SD  | 4:7:136:ILE:O[1_554]   | 2.08                     | 0.12              |
| 4:4:276:GLU:OE1 | 4:8:279:TYR:C[1_554]   | 2.08                     | 0.12              |
| 4:5:280:ASN:ND2 | 4:9:282:ILE:C[1_554]   | 2.08                     | 0.12              |
| 4:3:193:LEU:N   | 4:7:186:THR:OG1[1_554] | 2.08                     | 0.12              |
| 4:3:142:LEU:C   | 4:7:372:ARG:C[1_554]   | 2.08                     | 0.12              |
| 4:3:222:ASP:OD2 | 4:7:331:ALA:O[1_554]   | 2.08                     | 0.12              |
| 4:5:18:LYS:NZ   | 4:9:76:ILE:CG2[1_554]  | 2.08                     | 0.12              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:113:LYS:CD  | 4:8:254:ARG:CB[1_554]  | 2.08                     | 0.12              |
| 4:2:75:ILE:CA   | 4:7:197:GLY:C[1_554]   | 2.08                     | 0.12              |
| 4:5:219:VAL:C   | 4:9:335:ARG:CA[1_554]  | 2.08                     | 0.12              |
| 4:3:337:TYR:CA  | 4:7:119:MET:CA[1_554]  | 2.08                     | 0.12              |
| 4:5:255:PHE:CD2 | 4:9:305:MET:CE[1_554]  | 2.08                     | 0.12              |
| 4:5:192:ILE:O   | 4:9:213:LYS:CA[1_554]  | 2.08                     | 0.12              |
| 4:3:283:MET:CB  | 4:7:285:CYS:O[1_554]   | 2.08                     | 0.12              |
| 4:4:218:TYR:CE2 | 4:8:337:TYR:CD1[1_554] | 2.08                     | 0.12              |
| 4:5:162:ASN:CA  | 4:9:110:LEU:CD2[1_554] | 2.08                     | 0.12              |
| 4:2:286:ASP:CB  | 4:7:270:GLU:OE1[1_554] | 2.08                     | 0.12              |
| 4:3:181:ALA:O   | 4:7:158:GLY:O[1_554]   | 2.08                     | 0.12              |
| 4:5:227:MET:CE  | 4:9:306:TYR:CA[1_554]  | 2.08                     | 0.12              |
| 4:4:160:THR:N   | 4:8:177:ARG:CD[1_554]  | 2.08                     | 0.12              |
| 4:4:191:LYS:CB  | 4:8:186:THR:CA[1_554]  | 2.08                     | 0.12              |
| 4:3:262:PHE:N   | 4:7:154:ASP:O[1_554]   | 2.08                     | 0.12              |
| 4:5:312:ARG:CB  | 4:9:299:MET:N[1_554]   | 2.08                     | 0.12              |
| 4:4:173:HIS:O   | 4:9:267:ILE:CB[1_554]  | 2.08                     | 0.12              |
| 4:5:326:LYS:O   | 4:9:167:GLU:OE2[1_554] | 2.08                     | 0.12              |
| 4:4:371:HIS:N   | 4:9:230:ALA:O[1_554]   | 2.08                     | 0.12              |
| 4:3:327:ILE:C   | 4:7:168:GLY:CA[1_554]  | 2.09                     | 0.11              |
| 4:4:339:VAL:C   | 4:8:116:ARG:N[1_554]   | 2.09                     | 0.11              |
| 4:3:282:ILE:CB  | 4:7:171:LEU:CG[1_554]  | 2.09                     | 0.11              |
| 4:4:26:ALA:CA   | 4:8:123:MET:CA[1_554]  | 2.09                     | 0.11              |
| 4:3:314:GLN:CG  | 4:7:143:TYR:CA[1_554]  | 2.09                     | 0.11              |
| 4:5:325:MET:SD  | 4:9:166:TYR:CE1[1_554] | 2.09                     | 0.11              |
| 4:5:116:ARG:CB  | 4:V:252:ASN:OD1[1_554] | 2.09                     | 0.11              |
| 4:5:289:ILE:CG2 | 4:W:39:ARG:NH2[1_554]  | 2.09                     | 0.11              |
| 4:4:187:ASP:CA  | 4:8:183:ARG:CD[1_554]  | 2.09                     | 0.11              |
| 4:5:250:ILE:CG2 | 4:9:214:GLU:OE2[1_554] | 2.09                     | 0.11              |
| 4:4:210:ARG:O   | 4:8:15:GLY:C[1_554]    | 2.09                     | 0.11              |
| 4:4:257:CYS:N   | 4:8:303:THR:CB[1_554]  | 2.09                     | 0.11              |
| 4:5:136:ILE:CA  | 4:9:113:LYS:CE[1_554]  | 2.09                     | 0.11              |
| 4:3:110:LEU:CD1 | 4:8:191:LYS:CD[1_554]  | 2.09                     | 0.11              |
| 4:4:218:TYR:C   | 4:8:336:LYS:CA[1_554]  | 2.09                     | 0.11              |
| 4:4:62:ARG:CZ   | 4:8:67:LEU:O[1_554]    | 2.09                     | 0.11              |
| 4:3:274:ILE:CA  | 4:7:162:ASN:O[1_554]   | 2.09                     | 0.11              |
| 4:4:321:ALA:O   | 4:8:292:ASP:CA[1_554]  | 2.09                     | 0.11              |
| 4:3:195:GLU:OE2 | 4:7:189:LEU:CB[1_554]  | 2.09                     | 0.11              |
| 4:3:315:LYS:NZ  | 4:7:147:ARG:NE[1_554]  | 2.09                     | 0.11              |
| 4:5:328:LYS:CB  | 4:9:148:THR:CG2[1_554] | 2.09                     | 0.11              |
| 4:5:309:ILE:CB  | 4:9:339:VAL:CG2[1_554] | 2.09                     | 0.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:317:ILE:C   | 4:7:150:GLY:C[1_554]   | 2.09                     | 0.11              |
| 4:4:309:ILE:O   | 4:8:141:SER:OG[1_554]  | 2.09                     | 0.11              |
| 4:5:227:MET:CA  | 4:9:307:PRO:N[1_554]   | 2.09                     | 0.11              |
| 4:4:195:GLU:OE2 | 4:8:189:LEU:CB[1_554]  | 2.09                     | 0.11              |
| 1:D:637:LYS:CG  | 4:5:311:ASP:CG[1_556]  | 2.09                     | 0.11              |
| 4:3:162:ASN:CG  | 4:7:175:ILE:CG1[1_554] | 2.09                     | 0.11              |
| 4:4:308:GLY:CA  | 4:8:338:SER:N[1_554]   | 2.09                     | 0.11              |
| 4:3:221:LEU:C   | 4:7:332:PRO:N[1_554]   | 2.09                     | 0.11              |
| 4:5:318:THR:CG2 | 4:9:149:THR:O[1_554]   | 2.09                     | 0.11              |
| 4:4:154:ASP:OD2 | 4:8:111:ASN:N[1_554]   | 2.09                     | 0.11              |
| 4:5:196:ARG:N   | 4:9:209:VAL:O[1_554]   | 2.09                     | 0.11              |
| 4:5:314:GLN:CD  | 4:9:147:ARG:CG[1_554]  | 2.09                     | 0.11              |
| 4:3:144:ALA:N   | 4:7:372:ARG:N[1_554]   | 2.09                     | 0.11              |
| 4:4:336:LYS:CD  | 4:8:86:TRP:CZ2[1_554]  | 2.09                     | 0.11              |
| 4:2:173:HIS:C   | 4:7:267:ILE:CG2[1_554] | 2.09                     | 0.11              |
| 4:5:189:LEU:C   | 4:9:186:THR:CB[1_554]  | 2.09                     | 0.11              |
| 4:2:109:PRO:CB  | 4:7:195:GLU:CB[1_554]  | 2.09                     | 0.11              |
| 4:3:270:GLU:N   | 4:7:271:SER:C[1_554]   | 2.09                     | 0.11              |
| 4:2:371:HIS:NE2 | 4:7:252:ASN:O[1_554]   | 2.09                     | 0.11              |
| 4:3:277:THR:CA  | 4:7:175:ILE:N[1_554]   | 2.09                     | 0.11              |
| 4:5:108:ALA:O   | 4:V:195:GLU:CG[1_554]  | 2.09                     | 0.11              |
| 4:3:194:THR:O   | 4:7:209:VAL:CG1[1_554] | 2.09                     | 0.11              |
| 4:3:370:VAL:N   | 4:8:229:THR:C[1_554]   | 2.09                     | 0.11              |
| 4:4:344:SER:CB  | 4:8:367:PRO:CG[1_554]  | 2.09                     | 0.11              |
| 4:5:135:ALA:C   | 4:9:113:LYS:CE[1_554]  | 2.09                     | 0.11              |
| 4:5:315:LYS:NZ  | 4:9:295:ALA:O[1_554]   | 2.09                     | 0.11              |
| 4:3:23:GLY:C    | 4:7:125:GLU:CD[1_554]  | 2.09                     | 0.11              |
| 4:4:336:LYS:CD  | 4:8:12:ASN:OD1[1_554]  | 2.09                     | 0.11              |
| 4:4:368:SER:O   | 4:9:230:ALA:N[1_554]   | 2.09                     | 0.11              |
| 4:4:197:GLY:C   | 4:8:208:ILE:C[1_554]   | 2.09                     | 0.11              |
| 4:1:326:LYS:NZ  | 4:7:43:VAL:CG2[1_554]  | 2.09                     | 0.11              |
| 4:5:227:MET:O   | 4:9:307:PRO:CG[1_554]  | 2.09                     | 0.11              |
| 4:3:325:MET:CE  | 4:7:166:TYR:CE2[1_554] | 2.09                     | 0.11              |
| 4:4:215:LYS:O   | 4:8:30:VAL:CA[1_554]   | 2.09                     | 0.11              |
| 4:4:279:TYR:CD2 | 4:8:285:CYS:CB[1_554]  | 2.09                     | 0.11              |
| 4:3:154:ASP:C   | 4:7:111:ASN:N[1_554]   | 2.09                     | 0.11              |
| 4:3:143:TYR:C   | 4:7:371:HIS:C[1_554]   | 2.09                     | 0.11              |
| 4:3:223:PHE:CZ  | 4:7:301:GLY:C[1_554]   | 2.09                     | 0.11              |
| 4:4:348:SER:OG  | 4:8:366:GLY:N[1_554]   | 2.09                     | 0.11              |
| 4:4:187:ASP:C   | 4:8:183:ARG:O[1_554]   | 2.09                     | 0.11              |
| 4:3:220:ALA:C   | 4:7:335:ARG:CA[1_554]  | 2.09                     | 0.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:156:GLY:O   | 4:9:74:GLY:C[1_554]    | 2.09                     | 0.11              |
| 4:4:140:LEU:CG  | 4:8:117:GLU:OE2[1_554] | 2.09                     | 0.11              |
| 4:5:31:PHE:C    | 4:9:78:ASN:C[1_554]    | 2.09                     | 0.11              |
| 4:5:17:VAL:C    | 4:9:79:TRP:CA[1_554]   | 2.09                     | 0.11              |
| 4:5:316:GLU:N   | 4:9:298:VAL:N[1_554]   | 2.09                     | 0.11              |
| 4:4:30:VAL:CG1  | 4:8:79:TRP:CA[1_554]   | 2.09                     | 0.11              |
| 4:5:110:LEU:CA  | 4:V:192:ILE:CG2[1_554] | 2.09                     | 0.11              |
| 4:4:278:THR:OG1 | 4:8:163:VAL:CB[1_554]  | 2.09                     | 0.11              |
| 4:3:140:LEU:CD2 | 4:7:117:GLU:OE1[1_554] | 2.09                     | 0.11              |
| 4:5:173:HIS:CA  | 4:V:266:PHE:C[1_554]   | 2.09                     | 0.11              |
| 4:5:31:PHE:CD1  | 4:9:80:ASP:CB[1_554]   | 2.09                     | 0.11              |
| 4:5:269:MET:CG  | 4:9:178:LEU:CD1[1_554] | 2.09                     | 0.11              |
| 4:2:173:HIS:CA  | 4:7:267:ILE:N[1_554]   | 2.09                     | 0.11              |
| 4:3:316:GLU:OE2 | 4:7:153:LEU:N[1_554]   | 2.09                     | 0.11              |
| 4:5:261:LEU:N   | 4:9:160:THR:OG1[1_554] | 2.09                     | 0.11              |
| 4:5:214:GLU:O   | 4:9:18:LYS:CD[1_554]   | 2.09                     | 0.11              |
| 4:3:338:SER:CA  | 4:7:116:ARG:C[1_554]   | 2.09                     | 0.11              |
| 4:4:345:ILE:N   | 4:8:367:PRO:CD[1_554]  | 2.09                     | 0.11              |
| 4:4:110:LEU:N   | 4:9:195:GLU:CD[1_554]  | 2.09                     | 0.11              |
| 4:5:219:VAL:CG1 | 4:9:300:SER:CB[1_554]  | 2.09                     | 0.11              |
| 4:4:276:GLU:CA  | 4:8:281:SER:OG[1_554]  | 2.09                     | 0.11              |
| 4:2:75:ILE:CG1  | 4:7:193:LEU:C[1_554]   | 2.09                     | 0.11              |
| 4:4:304:THR:C   | 4:8:137:GLN:OE1[1_554] | 2.09                     | 0.11              |
| 4:3:215:LYS:NZ  | 4:7:55:GLY:CA[1_554]   | 2.09                     | 0.11              |
| 4:4:223:PHE:CG  | 4:8:335:ARG:CD[1_554]  | 2.09                     | 0.11              |
| 4:3:320:LEU:N   | 4:7:292:ASP:O[1_554]   | 2.09                     | 0.11              |
| 4:5:299:MET:CG  | 4:9:137:GLN:N[1_554]   | 2.09                     | 0.11              |
| 4:2:367:PRO:CB  | 4:7:236:LEU:N[1_554]   | 2.09                     | 0.11              |
| 4:4:367:PRO:CG  | 4:9:234:SER:C[1_554]   | 2.09                     | 0.11              |
| 4:5:274:ILE:CG1 | 4:9:162:ASN:N[1_554]   | 2.09                     | 0.11              |
| 4:5:367:PRO:CB  | 4:V:233:SER:CA[1_554]  | 2.09                     | 0.11              |
| 4:5:344:SER:OG  | 4:9:362:TYR:CZ[1_554]  | 2.09                     | 0.11              |
| 4:3:18:LYS:N    | 4:7:79:TRP:NE1[1_554]  | 2.09                     | 0.11              |
| 4:5:257:CYS:O   | 4:9:303:THR:CG2[1_554] | 2.09                     | 0.11              |
| 4:2:113:LYS:CD  | 4:7:254:ARG:CB[1_554]  | 2.09                     | 0.11              |
| 4:4:226:GLU:OE1 | 4:8:333:PRO:CB[1_554]  | 2.09                     | 0.11              |
| 4:3:208:ILE:CG1 | 4:7:59:GLN:CA[1_554]   | 2.09                     | 0.11              |
| 4:5:336:LYS:NZ  | 4:9:10:CYS:SG[1_554]   | 2.09                     | 0.11              |
| 4:5:310:ALA:N   | 4:9:141:SER:C[1_554]   | 2.09                     | 0.11              |
| 4:3:186:THR:N   | 4:7:183:ARG:CZ[1_554]  | 2.09                     | 0.11              |
| 4:4:294:TYR:CD1 | 4:8:166:TYR:CG[1_554]  | 2.09                     | 0.11              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:172:PRO:CB  | 4:9:266:PHE:CB[1_554]  | 2.09                     | 0.11              |
| 4:2:285:CYS:N   | 4:7:268:GLY:O[1_554]   | 2.09                     | 0.11              |
| 4:4:281:SER:CB  | 4:8:173:HIS:C[1_554]   | 2.09                     | 0.11              |
| 4:4:120:THR:OG1 | 4:9:233:SER:OG[1_554]  | 2.09                     | 0.11              |
| 4:3:140:LEU:CA  | 4:7:371:HIS:ND1[1_554] | 2.09                     | 0.11              |
| 4:3:160:THR:N   | 4:7:177:ARG:CZ[1_554]  | 2.09                     | 0.11              |
| 4:4:184:ASP:OD1 | 4:8:73:HIS:CG[1_554]   | 2.09                     | 0.11              |
| 4:5:366:GLY:CA  | 4:V:234:SER:CA[1_554]  | 2.09                     | 0.11              |
| 4:3:334:GLU:CG  | 4:7:132:MET:SD[1_554]  | 2.09                     | 0.11              |
| 4:3:191:LYS:C   | 4:7:186:THR:N[1_554]   | 2.09                     | 0.11              |
| 4:5:173:HIS:CB  | 4:V:267:ILE:C[1_554]   | 2.09                     | 0.11              |
| 4:5:280:ASN:CG  | 4:9:280:ASN:O[1_554]   | 2.09                     | 0.11              |
| 4:3:277:THR:OG1 | 4:7:176:MET:CA[1_554]  | 2.09                     | 0.11              |
| 4:3:335:ARG:NH1 | 4:7:106:THR:CA[1_554]  | 2.09                     | 0.11              |
| 4:3:312:ARG:O   | 4:7:152:VAL:CG2[1_554] | 2.09                     | 0.11              |
| 4:4:264:PRO:CB  | 4:8:178:LEU:CG[1_554]  | 2.09                     | 0.11              |
| 4:5:258:PRO:N   | 4:9:303:THR:CB[1_554]  | 2.09                     | 0.11              |
| 4:4:267:ILE:CG2 | 4:8:180:LEU:CD1[1_554] | 2.09                     | 0.11              |
| 4:2:113:LYS:CG  | 4:7:255:PHE:N[1_554]   | 2.09                     | 0.11              |
| 4:2:173:HIS:CE1 | 4:7:266:PHE:CA[1_554]  | 2.09                     | 0.11              |
| 4:5:182:GLY:C   | 4:9:158:GLY:CA[1_554]  | 2.09                     | 0.11              |
| 4:3:140:LEU:CB  | 4:7:113:LYS:O[1_554]   | 2.09                     | 0.11              |
| 4:3:219:VAL:CG1 | 4:7:300:SER:C[1_554]   | 2.09                     | 0.11              |
| 4:3:343:GLY:N   | 4:7:117:GLU:CD[1_554]  | 2.09                     | 0.11              |
| 4:5:173:HIS:CA  | 4:V:267:ILE:C[1_554]   | 2.09                     | 0.11              |
| 4:5:185:LEU:CA  | 4:9:158:GLY:N[1_554]   | 2.09                     | 0.11              |
| 4:3:214:GLU:O   | 4:7:17:VAL:C[1_554]    | 2.09                     | 0.11              |
| 4:5:273:GLY:N   | 4:9:162:ASN:OD1[1_554] | 2.09                     | 0.11              |
| 4:3:276:GLU:CA  | 4:7:151:ILE:CD1[1_554] | 2.09                     | 0.11              |
| 4:4:249:THR:CG2 | 4:8:215:LYS:NZ[1_554]  | 2.09                     | 0.11              |
| 4:3:56:ASP:OD2  | 4:7:81:ASP:OD1[1_554]  | 2.10                     | 0.10              |
| 4:5:321:ALA:O   | 4:9:292:ASP:CG[1_554]  | 2.10                     | 0.10              |
| 4:4:25:ASP:CA   | 4:8:124:PHE:C[1_554]   | 2.10                     | 0.10              |
| 4:4:327:ILE:CA  | 4:8:167:GLU:N[1_554]   | 2.10                     | 0.10              |
| 4:3:186:THR:CG2 | 4:7:183:ARG:NE[1_554]  | 2.10                     | 0.10              |
| 4:4:370:VAL:N   | 4:9:229:THR:C[1_554]   | 2.10                     | 0.10              |
| 4:3:211:ASP:O   | 4:7:32:PRO:CB[1_554]   | 2.10                     | 0.10              |
| 4:4:315:LYS:O   | 4:8:296:ASN:O[1_554]   | 2.10                     | 0.10              |
| 4:5:111:ASN:N   | 4:V:192:ILE:O[1_554]   | 2.10                     | 0.10              |
| 4:4:22:ALA:C    | 4:8:125:GLU:OE2[1_554] | 2.10                     | 0.10              |
| 4:3:260:THR:N   | 4:7:155:SER:CA[1_554]  | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:187:ASP:N   | 4:7:183:ARG:NE[1_554]  | 2.10                     | 0.10              |
| 4:3:317:ILE:CG2 | 4:7:150:GLY:O[1_554]   | 2.10                     | 0.10              |
| 4:5:26:ALA:N    | 4:9:124:PHE:N[1_554]   | 2.10                     | 0.10              |
| 4:4:319:ALA:CA  | 4:8:296:ASN:CG[1_554]  | 2.10                     | 0.10              |
| 4:5:214:GLU:N   | 4:9:16:LEU:CD2[1_554]  | 2.10                     | 0.10              |
| 4:2:173:HIS:N   | 4:7:267:ILE:N[1_554]   | 2.10                     | 0.10              |
| 4:4:275:HIS:O   | 4:8:164:PRO:CA[1_554]  | 2.10                     | 0.10              |
| 4:3:166:TYR:CE1 | 4:9:40:HIS:CG[1_554]   | 2.10                     | 0.10              |
| 4:4:316:GLU:C   | 4:8:296:ASN:O[1_554]   | 2.10                     | 0.10              |
| 4:5:41:GLN:CG   | 4:8:224:GLU:CD[1_554]  | 2.10                     | 0.10              |
| 4:3:339:VAL:CG1 | 4:7:114:ALA:N[1_554]   | 2.10                     | 0.10              |
| 4:3:315:LYS:CD  | 4:7:147:ARG:CZ[1_554]  | 2.10                     | 0.10              |
| 4:3:367:PRO:CA  | 4:8:235:SER:N[1_554]   | 2.10                     | 0.10              |
| 4:3:160:THR:CB  | 4:7:177:ARG:CD[1_554]  | 2.10                     | 0.10              |
| 4:3:109:PRO:CG  | 4:8:195:GLU:CD[1_554]  | 2.10                     | 0.10              |
| 4:5:154:ASP:CB  | 4:9:108:ALA:O[1_554]   | 2.10                     | 0.10              |
| 4:3:372:ARG:CB  | 4:8:227:MET:O[1_554]   | 2.10                     | 0.10              |
| 4:3:266:PHE:CD2 | 4:7:303:THR:CG2[1_554] | 2.10                     | 0.10              |
| 4:4:262:PHE:CZ  | 4:8:152:VAL:CG1[1_554] | 2.10                     | 0.10              |
| 4:3:26:ALA:CA   | 4:7:121:GLN:O[1_554]   | 2.10                     | 0.10              |
| 4:3:112:PRO:C   | 4:8:253:GLU:OE2[1_554] | 2.10                     | 0.10              |
| 4:4:278:THR:CB  | 4:8:164:PRO:O[1_554]   | 2.10                     | 0.10              |
| 4:3:308:GLY:N   | 4:7:338:SER:C[1_554]   | 2.10                     | 0.10              |
| 4:3:332:PRO:CB  | 4:7:133:TYR:O[1_554]   | 2.10                     | 0.10              |
| 4:5:300:SER:O   | 4:9:108:ALA:O[1_554]   | 2.10                     | 0.10              |
| 4:3:198:TYR:CB  | 4:7:208:ILE:CA[1_554]  | 2.10                     | 0.10              |
| 4:3:340:TRP:CD2 | 4:7:121:GLN:CB[1_554]  | 2.10                     | 0.10              |
| 4:4:113:LYS:NZ  | 4:9:254:ARG:CG[1_554]  | 2.10                     | 0.10              |
| 4:3:223:PHE:CG  | 4:7:335:ARG:CD[1_554]  | 2.10                     | 0.10              |
| 4:3:332:PRO:CB  | 4:7:134:VAL:C[1_554]   | 2.10                     | 0.10              |
| 4:5:369:ILE:O   | 4:V:228:ALA:C[1_554]   | 2.10                     | 0.10              |
| 4:5:75:ILE:N    | 4:V:197:GLY:C[1_554]   | 2.10                     | 0.10              |
| 4:3:186:THR:O   | 4:7:183:ARG:CD[1_554]  | 2.10                     | 0.10              |
| 4:4:370:VAL:O   | 4:9:230:ALA:CB[1_554]  | 2.10                     | 0.10              |
| 4:5:193:LEU:CD1 | 4:9:210:ARG:CB[1_554]  | 2.10                     | 0.10              |
| 4:5:334:GLU:CG  | 4:9:104:LEU:CA[1_554]  | 2.10                     | 0.10              |
| 4:4:276:GLU:CA  | 4:8:281:SER:CB[1_554]  | 2.10                     | 0.10              |
| 4:3:23:GLY:O    | 4:7:362:TYR:CE2[1_554] | 2.10                     | 0.10              |
| 4:5:294:TYR:O   | 4:9:166:TYR:O[1_554]   | 2.10                     | 0.10              |
| 4:5:72:GLU:O    | 4:V:198:TYR:C[1_554]   | 2.10                     | 0.10              |
| 4:4:223:PHE:CD1 | 4:8:335:ARG:CD[1_554]  | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:161:HIS:N   | 4:8:110:LEU:CB[1_554]  | 2.10                     | 0.10              |
| 4:3:243:PRO:C   | 4:7:60:SER:C[1_554]    | 2.10                     | 0.10              |
| 4:5:204:ALA:N   | 4:9:62:ARG:CB[1_554]   | 2.10                     | 0.10              |
| 4:2:169:TYR:CE2 | 4:7:266:PHE:CE1[1_554] | 2.10                     | 0.10              |
| 4:3:326:LYS:O   | 4:7:167:GLU:CG[1_554]  | 2.10                     | 0.10              |
| 4:5:334:GLU:N   | 4:9:104:LEU:CA[1_554]  | 2.10                     | 0.10              |
| 4:3:312:ARG:CZ  | 4:7:299:MET:C[1_554]   | 2.10                     | 0.10              |
| 4:5:349:LEU:C   | 4:9:365:ALA:CA[1_554]  | 2.10                     | 0.10              |
| 4:5:198:TYR:OH  | 4:9:211:ASP:CB[1_554]  | 2.10                     | 0.10              |
| 4:5:204:ALA:CB  | 4:9:62:ARG:N[1_554]    | 2.10                     | 0.10              |
| 4:3:317:ILE:C   | 4:7:150:GLY:O[1_554]   | 2.10                     | 0.10              |
| 4:5:217:CYS:O   | 4:9:336:LYS:O[1_554]   | 2.10                     | 0.10              |
| 4:3:313:MET:N   | 4:7:138:ALA:O[1_554]   | 2.10                     | 0.10              |
| 4:3:211:ASP:CB  | 4:7:32:PRO:CB[1_554]   | 2.10                     | 0.10              |
| 4:5:254:ARG:O   | 4:9:302:GLY:CA[1_554]  | 2.10                     | 0.10              |
| 4:4:223:PHE:N   | 4:8:331:ALA:CA[1_554]  | 2.10                     | 0.10              |
| 4:5:221:LEU:N   | 4:9:332:PRO:N[1_554]   | 2.10                     | 0.10              |
| 4:4:316:GLU:CG  | 4:8:298:VAL:N[1_554]   | 2.10                     | 0.10              |
| 4:5:347:ALA:O   | 4:9:366:GLY:CA[1_554]  | 2.10                     | 0.10              |
| 4:3:25:ASP:CG   | 4:7:124:PHE:CG[1_554]  | 2.10                     | 0.10              |
| 4:5:316:GLU:C   | 4:9:296:ASN:C[1_554]   | 2.10                     | 0.10              |
| 4:5:110:LEU:CB  | 4:V:192:ILE:CG2[1_554] | 2.10                     | 0.10              |
| 4:3:314:GLN:N   | 4:7:142:LEU:CG[1_554]  | 2.10                     | 0.10              |
| 4:3:326:LYS:C   | 4:7:167:GLU:CD[1_554]  | 2.10                     | 0.10              |
| 4:3:336:LYS:CD  | 4:7:86:TRP:NE1[1_554]  | 2.10                     | 0.10              |
| 4:4:207:GLU:CG  | 4:8:67:LEU:CA[1_554]   | 2.10                     | 0.10              |
| 4:4:341:ILE:N   | 4:8:120:THR:CB[1_554]  | 2.10                     | 0.10              |
| 4:3:267:ILE:CG2 | 4:7:181:ALA:N[1_554]   | 2.10                     | 0.10              |
| 4:4:28:ARG:C    | 4:8:83:GLU:OE1[1_554]  | 2.10                     | 0.10              |
| 4:3:272:ALA:C   | 4:7:162:ASN:OD1[1_554] | 2.10                     | 0.10              |
| 4:1:291:LYS:CB  | 4:7:64:ILE:CG1[1_554]  | 2.10                     | 0.10              |
| 4:3:76:ILE:N    | 4:8:198:TYR:CD1[1_554] | 2.10                     | 0.10              |
| 4:4:345:ILE:N   | 4:8:366:GLY:O[1_554]   | 2.10                     | 0.10              |
| 4:5:24:ASP:CB   | 4:9:125:GLU:CA[1_554]  | 2.10                     | 0.10              |
| 4:5:188:TYR:CD2 | 4:9:182:GLY:CA[1_554]  | 2.10                     | 0.10              |
| 4:4:157:ASP:CB  | 4:8:72:GLU:CA[1_554]   | 2.10                     | 0.10              |
| 4:3:339:VAL:N   | 4:7:117:GLU:N[1_554]   | 2.10                     | 0.10              |
| 4:3:300:SER:OG  | 4:7:107:GLU:OE2[1_554] | 2.10                     | 0.10              |
| 4:2:77:THR:CA   | 4:7:246:GLN:CD[1_554]  | 2.10                     | 0.10              |
| 4:3:144:ALA:C   | 4:7:371:HIS:N[1_554]   | 2.10                     | 0.10              |
| 4:3:218:TYR:CG  | 4:7:336:LYS:O[1_554]   | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:317:ILE:CB  | 4:7:165:ILE:O[1_554]   | 2.10                     | 0.10              |
| 4:5:106:THR:OG1 | 4:9:114:ALA:CA[1_554]  | 2.10                     | 0.10              |
| 4:4:300:SER:O   | 4:8:108:ALA:C[1_554]   | 2.10                     | 0.10              |
| 4:4:275:HIS:C   | 4:8:151:ILE:CG1[1_554] | 2.10                     | 0.10              |
| 4:3:309:ILE:C   | 4:7:141:SER:OG[1_554]  | 2.10                     | 0.10              |
| 4:5:193:LEU:O   | 4:9:209:VAL:N[1_554]   | 2.10                     | 0.10              |
| 4:5:115:ASN:CG  | 4:V:196:ARG:CG[1_554]  | 2.10                     | 0.10              |
| 4:3:171:LEU:O   | 4:8:266:PHE:C[1_554]   | 2.10                     | 0.10              |
| 4:3:187:ASP:C   | 4:7:184:ASP:N[1_554]   | 2.10                     | 0.10              |
| 4:4:60:SER:O    | 4:8:66:THR:OG1[1_554]  | 2.10                     | 0.10              |
| 4:3:161:HIS:O   | 4:7:110:LEU:CA[1_554]  | 2.10                     | 0.10              |
| 4:5:328:LYS:N   | 4:9:148:THR:CA[1_554]  | 2.10                     | 0.10              |
| 4:5:218:TYR:CA  | 4:9:336:LYS:C[1_554]   | 2.10                     | 0.10              |
| 4:4:196:ARG:CD  | 4:8:212:ILE:N[1_554]   | 2.10                     | 0.10              |
| 4:4:335:ARG:CD  | 4:8:135:ALA:O[1_554]   | 2.10                     | 0.10              |
| 4:3:215:LYS:CE  | 4:7:31:PHE:CB[1_554]   | 2.10                     | 0.10              |
| 4:4:26:ALA:C    | 4:8:122:ILE:O[1_554]   | 2.10                     | 0.10              |
| 4:4:267:ILE:CG1 | 4:8:180:LEU:CA[1_554]  | 2.10                     | 0.10              |
| 4:5:200:PHE:CG  | 4:9:206:ARG:NE[1_554]  | 2.10                     | 0.10              |
| 4:2:357:ILE:N   | 4:7:232:SER:CA[1_554]  | 2.10                     | 0.10              |
| 4:4:370:VAL:N   | 4:9:230:ALA:O[1_554]   | 2.10                     | 0.10              |
| 4:4:30:VAL:C    | 4:8:80:ASP:C[1_554]    | 2.10                     | 0.10              |
| 4:4:259:GLU:O   | 4:8:155:SER:CB[1_554]  | 2.10                     | 0.10              |
| 4:4:293:LEU:O   | 4:8:169:TYR:CD2[1_554] | 2.10                     | 0.10              |
| 4:3:24:ASP:CA   | 4:7:125:GLU:OE2[1_554] | 2.10                     | 0.10              |
| 4:3:316:GLU:CA  | 4:7:151:ILE:O[1_554]   | 2.10                     | 0.10              |
| 4:2:115:ASN:OD1 | 4:7:249:THR:O[1_554]   | 2.10                     | 0.10              |
| 4:4:198:TYR:C   | 4:8:205:GLU:C[1_554]   | 2.10                     | 0.10              |
| 4:4:339:VAL:CB  | 4:8:115:ASN:N[1_554]   | 2.10                     | 0.10              |
| 4:3:211:ASP:OD1 | 4:7:32:PRO:CG[1_554]   | 2.10                     | 0.10              |
| 4:3:316:GLU:C   | 4:7:150:GLY:CA[1_554]  | 2.10                     | 0.10              |
| 4:3:270:GLU:CG  | 4:7:272:ALA:CA[1_554]  | 2.10                     | 0.10              |
| 4:5:295:ALA:CA  | 4:9:167:GLU:CB[1_554]  | 2.10                     | 0.10              |
| 4:5:290:ARG:CZ  | 4:9:286:ASP:CG[1_554]  | 2.10                     | 0.10              |
| 4:4:109:PRO:N   | 4:9:195:GLU:CB[1_554]  | 2.10                     | 0.10              |
| 4:4:332:PRO:CB  | 4:8:133:TYR:C[1_554]   | 2.10                     | 0.10              |
| 4:4:267:ILE:CD1 | 4:8:180:LEU:C[1_554]   | 2.10                     | 0.10              |
| 4:3:214:GLU:C   | 4:7:16:LEU:O[1_554]    | 2.10                     | 0.10              |
| 4:4:287:ILE:N   | 4:9:270:GLU:OE1[1_554] | 2.10                     | 0.10              |
| 4:4:25:ASP:CG   | 4:8:124:PHE:CB[1_554]  | 2.10                     | 0.10              |
| 4:4:275:HIS:CB  | 4:8:152:VAL:O[1_554]   | 2.10                     | 0.10              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:167:GLU:N   | 4:W:40:HIS:CD2[1_554]  | 2.10                     | 0.10              |
| 4:3:371:HIS:CD2 | 4:8:255:PHE:CE2[1_554] | 2.10                     | 0.10              |
| 4:4:147:ARG:CG  | 4:8:372:ARG:CG[1_554]  | 2.10                     | 0.10              |
| 4:5:195:GLU:CD  | 4:9:189:LEU:CB[1_554]  | 2.10                     | 0.10              |
| 4:5:143:TYR:CD2 | 4:9:368:SER:O[1_554]   | 2.10                     | 0.10              |
| 4:5:113:LYS:CE  | 4:V:255:PHE:N[1_554]   | 2.10                     | 0.10              |
| 4:2:114:ALA:O   | 4:7:250:ILE:O[1_554]   | 2.10                     | 0.10              |
| 4:3:26:ALA:C    | 4:7:122:ILE:CB[1_554]  | 2.10                     | 0.10              |
| 4:2:111:ASN:CB  | 4:7:196:ARG:CB[1_554]  | 2.10                     | 0.10              |
| 4:4:288:ASP:CA  | 4:V:63:GLY:C[1_554]    | 2.10                     | 0.10              |
| 4:2:114:ALA:CA  | 4:7:250:ILE:C[1_554]   | 2.10                     | 0.10              |
| 4:5:60:SER:OG   | 4:9:37:ARG:CB[1_554]   | 2.10                     | 0.10              |
| 4:5:299:MET:N   | 4:9:136:ILE:CA[1_554]  | 2.10                     | 0.10              |
| 4:3:367:PRO:CD  | 4:8:235:SER:O[1_554]   | 2.11                     | 0.09              |
| 4:5:205:GLU:O   | 4:9:59:GLN:OE1[1_554]  | 2.11                     | 0.09              |
| 4:4:221:LEU:C   | 4:8:332:PRO:CA[1_554]  | 2.11                     | 0.09              |
| 4:4:283:MET:SD  | 4:8:289:ILE:CG1[1_554] | 2.11                     | 0.09              |
| 4:5:320:LEU:CB  | 4:9:294:TYR:N[1_554]   | 2.11                     | 0.09              |
| 4:5:340:TRP:CH2 | 4:9:120:THR:C[1_554]   | 2.11                     | 0.09              |
| 4:5:266:PHE:CB  | 4:9:261:LEU:CA[1_554]  | 2.11                     | 0.09              |
| 4:5:75:ILE:CD1  | 4:V:195:GLU:N[1_554]   | 2.11                     | 0.09              |
| 4:4:313:MET:O   | 4:8:142:LEU:CD1[1_554] | 2.11                     | 0.09              |
| 4:3:215:LYS:CB  | 4:7:31:PHE:CB[1_554]   | 2.11                     | 0.09              |
| 4:5:343:GLY:CA  | 4:9:367:PRO:C[1_554]   | 2.11                     | 0.09              |
| 4:4:243:PRO:CA  | 4:8:61:LYS:N[1_554]    | 2.11                     | 0.09              |
| 4:4:266:PHE:C   | 4:8:180:LEU:CD1[1_554] | 2.11                     | 0.09              |
| 4:3:316:GLU:CB  | 4:7:152:VAL:CA[1_554]  | 2.11                     | 0.09              |
| 4:5:75:ILE:CD1  | 4:V:197:GLY:N[1_554]   | 2.11                     | 0.09              |
| 4:5:344:SER:N   | 4:9:367:PRO:CB[1_554]  | 2.11                     | 0.09              |
| 4:3:25:ASP:O    | 4:7:124:PHE:N[1_554]   | 2.11                     | 0.09              |
| 4:5:260:THR:CB  | 4:9:155:SER:OG[1_554]  | 2.11                     | 0.09              |
| 4:4:117:GLU:N   | 4:9:237:GLU:CD[1_554]  | 2.11                     | 0.09              |
| 4:3:222:ASP:CA  | 4:7:331:ALA:O[1_554]   | 2.11                     | 0.09              |
| 4:4:346:LEU:N   | 4:8:366:GLY:O[1_554]   | 2.11                     | 0.09              |
| 4:3:332:PRO:C   | 4:7:133:TYR:O[1_554]   | 2.11                     | 0.09              |
| 4:3:173:HIS:NE2 | 4:8:265:SER:N[1_554]   | 2.11                     | 0.09              |
| 4:5:304:THR:O   | 4:9:339:VAL:CG1[1_554] | 2.11                     | 0.09              |
| 4:4:211:ASP:O   | 4:8:32:PRO:CD[1_554]   | 2.11                     | 0.09              |
| 4:4:215:LYS:CB  | 4:8:31:PHE:C[1_554]    | 2.11                     | 0.09              |
| 4:3:213:LYS:CA  | 4:7:15:GLY:CA[1_554]   | 2.11                     | 0.09              |
| 4:3:166:TYR:CB  | 4:9:40:HIS:NE2[1_554]  | 2.11                     | 0.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:312:ARG:O   | 4:9:298:VAL:C[1_554]   | 2.11                     | 0.09              |
| 4:3:114:ALA:N   | 4:8:250:ILE:CB[1_554]  | 2.11                     | 0.09              |
| 4:4:310:ALA:O   | 4:8:142:LEU:CA[1_554]  | 2.11                     | 0.09              |
| 4:3:219:VAL:CA  | 4:7:335:ARG:O[1_554]   | 2.11                     | 0.09              |
| 4:3:115:ASN:CA  | 4:8:250:ILE:N[1_554]   | 2.11                     | 0.09              |
| 4:3:261:LEU:CB  | 4:7:154:ASP:C[1_554]   | 2.11                     | 0.09              |
| 4:3:111:ASN:CB  | 4:8:196:ARG:CB[1_554]  | 2.11                     | 0.09              |
| 4:5:25:ASP:CG   | 4:9:129:VAL:C[1_554]   | 2.11                     | 0.09              |
| 4:5:243:PRO:C   | 4:9:60:SER:CB[1_554]   | 2.11                     | 0.09              |
| 4:4:341:ILE:N   | 4:8:116:ARG:O[1_554]   | 2.11                     | 0.09              |
| 4:4:269:MET:SD  | 4:8:178:LEU:CD1[1_554] | 2.11                     | 0.09              |
| 4:5:18:LYS:O    | 4:9:118:LYS:CD[1_554]  | 2.11                     | 0.09              |
| 4:5:198:TYR:CE1 | 4:9:208:ILE:CD1[1_554] | 2.11                     | 0.09              |
| 4:5:207:GLU:OE1 | 4:9:67:LEU:CB[1_554]   | 2.11                     | 0.09              |
| 4:4:173:HIS:CB  | 4:9:267:ILE:CG2[1_554] | 2.11                     | 0.09              |
| 4:5:201:VAL:CG2 | 4:9:202:THR:C[1_554]   | 2.11                     | 0.09              |
| 4:3:175:ILE:CG1 | 4:8:191:LYS:NZ[1_554]  | 2.11                     | 0.09              |
| 4:2:109:PRO:CA  | 4:7:195:GLU:CB[1_554]  | 2.11                     | 0.09              |
| 4:4:113:LYS:CE  | 4:9:254:ARG:CA[1_554]  | 2.11                     | 0.09              |
| 4:5:28:ARG:O    | 4:9:83:GLU:CG[1_554]   | 2.11                     | 0.09              |
| 4:4:305:MET:CA  | 4:8:11:ASP:CG[1_554]   | 2.11                     | 0.09              |
| 4:3:281:SER:CA  | 4:7:173:HIS:CA[1_554]  | 2.11                     | 0.09              |
| 4:2:72:GLU:C    | 4:7:199:SER:N[1_554]   | 2.11                     | 0.09              |
| 4:2:114:ALA:N   | 4:7:250:ILE:C[1_554]   | 2.11                     | 0.09              |
| 4:4:188:TYR:CG  | 4:8:182:GLY:CA[1_554]  | 2.11                     | 0.09              |
| 4:3:339:VAL:CG1 | 4:7:114:ALA:O[1_554]   | 2.11                     | 0.09              |
| 4:2:113:LYS:CA  | 4:7:254:ARG:N[1_554]   | 2.11                     | 0.09              |
| 4:4:113:LYS:CB  | 4:9:254:ARG:CB[1_554]  | 2.11                     | 0.09              |
| 4:5:242:LEU:CD1 | 4:9:207:GLU:CD[1_554]  | 2.11                     | 0.09              |
| 4:3:274:ILE:CB  | 4:7:161:HIS:C[1_554]   | 2.11                     | 0.09              |
| 4:5:153:LEU:O   | 4:9:136:ILE:CG2[1_554] | 2.11                     | 0.09              |
| 4:3:187:ASP:C   | 4:7:183:ARG:CA[1_554]  | 2.11                     | 0.09              |
| 4:3:223:PHE:N   | 4:7:335:ARG:CD[1_554]  | 2.11                     | 0.09              |
| 4:3:157:ASP:O   | 4:7:73:HIS:CB[1_554]   | 2.11                     | 0.09              |
| 4:4:312:ARG:NH1 | 4:8:299:MET:CA[1_554]  | 2.11                     | 0.09              |
| 4:5:199:SER:O   | 4:9:207:GLU:N[1_554]   | 2.11                     | 0.09              |
| 4:4:195:GLU:CD  | 4:8:257:CYS:SG[1_554]  | 2.11                     | 0.09              |
| 4:4:142:LEU:CB  | 4:8:372:ARG:O[1_554]   | 2.11                     | 0.09              |
| 4:4:270:GLU:CB  | 4:8:272:ALA:CB[1_554]  | 2.11                     | 0.09              |
| 4:4:194:THR:OG1 | 4:8:209:VAL:CG1[1_554] | 2.11                     | 0.09              |
| 4:5:257:CYS:C   | 4:9:303:THR:N[1_554]   | 2.11                     | 0.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:256:ARG:C   | 4:8:303:THR:C[1_554]   | 2.11                     | 0.09              |
| 4:5:261:LEU:CA  | 4:9:154:ASP:O[1_554]   | 2.11                     | 0.09              |
| 4:3:221:LEU:O   | 4:7:332:PRO:C[1_554]   | 2.11                     | 0.09              |
| 4:3:199:SER:OG  | 4:7:206:ARG:N[1_554]   | 2.11                     | 0.09              |
| 4:3:339:VAL:N   | 4:7:115:ASN:C[1_554]   | 2.11                     | 0.09              |
| 4:4:372:ARG:O   | 4:9:227:MET:SD[1_554]  | 2.11                     | 0.09              |
| 4:5:298:VAL:O   | 4:9:136:ILE:CB[1_554]  | 2.11                     | 0.09              |
| 4:5:292:ASP:CG  | 4:W:64:ILE:CD1[1_554]  | 2.11                     | 0.09              |
| 4:2:172:PRO:N   | 4:7:266:PHE:CB[1_554]  | 2.11                     | 0.09              |
| 4:4:287:ILE:C   | 4:V:63:GLY:N[1_554]    | 2.11                     | 0.09              |
| 4:1:292:ASP:OD2 | 4:7:40:HIS:CD2[1_554]  | 2.11                     | 0.09              |
| 4:3:173:HIS:CE1 | 4:8:265:SER:N[1_554]   | 2.11                     | 0.09              |
| 4:4:227:MET:SD  | 4:8:307:PRO:N[1_554]   | 2.11                     | 0.09              |
| 4:4:256:ARG:CD  | 4:8:306:TYR:CD1[1_554] | 2.11                     | 0.09              |
| 4:5:316:GLU:CA  | 4:9:151:ILE:O[1_554]   | 2.11                     | 0.09              |
| 4:2:113:LYS:C   | 4:7:250:ILE:O[1_554]   | 2.11                     | 0.09              |
| 4:5:205:GLU:CB  | 4:9:62:ARG:CZ[1_554]   | 2.11                     | 0.09              |
| 4:5:215:LYS:NZ  | 4:9:31:PHE:CA[1_554]   | 2.11                     | 0.09              |
| 4:3:204:ALA:CA  | 4:7:62:ARG:CA[1_554]   | 2.11                     | 0.09              |
| 4:4:184:ASP:N   | 4:8:73:HIS:ND1[1_554]  | 2.11                     | 0.09              |
| 4:4:173:HIS:CD2 | 4:9:268:GLY:N[1_554]   | 2.11                     | 0.09              |
| 4:5:151:ILE:CG1 | 4:9:171:LEU:C[1_554]   | 2.11                     | 0.09              |
| 4:4:198:TYR:CB  | 4:8:207:GLU:O[1_554]   | 2.11                     | 0.09              |
| 4:5:15:GLY:C    | 4:9:70:PRO:O[1_554]    | 2.11                     | 0.09              |
| 4:3:211:ASP:CG  | 4:7:55:GLY:CA[1_554]   | 2.11                     | 0.09              |
| 4:3:255:PHE:CZ  | 4:7:305:MET:CG[1_554]  | 2.11                     | 0.09              |
| 4:3:195:GLU:N   | 4:7:209:VAL:C[1_554]   | 2.11                     | 0.09              |
| 4:4:172:PRO:CD  | 4:9:266:PHE:CA[1_554]  | 2.11                     | 0.09              |
| 4:4:277:THR:O   | 4:8:174:ALA:CB[1_554]  | 2.11                     | 0.09              |
| 4:4:117:GLU:C   | 4:9:237:GLU:OE1[1_554] | 2.11                     | 0.09              |
| 4:4:188:TYR:CD1 | 4:8:185:LEU:N[1_554]   | 2.11                     | 0.09              |
| 4:4:140:LEU:N   | 4:8:371:HIS:CG[1_554]  | 2.11                     | 0.09              |
| 4:5:186:THR:CA  | 4:9:183:ARG:CB[1_554]  | 2.11                     | 0.09              |
| 4:4:113:LYS:N   | 4:9:253:GLU:CD[1_554]  | 2.11                     | 0.09              |
| 4:5:294:TYR:O   | 4:9:167:GLU:CA[1_554]  | 2.11                     | 0.09              |
| 4:3:115:ASN:CB  | 4:8:196:ARG:CZ[1_554]  | 2.11                     | 0.09              |
| 4:5:153:LEU:CD2 | 4:9:109:PRO:CG[1_554]  | 2.11                     | 0.09              |
| 4:3:157:ASP:CB  | 4:7:72:GLU:O[1_554]    | 2.11                     | 0.09              |
| 4:3:211:ASP:OD1 | 4:7:55:GLY:CA[1_554]   | 2.11                     | 0.09              |
| 4:4:195:GLU:CD  | 4:8:189:LEU:CB[1_554]  | 2.11                     | 0.09              |
| 4:3:264:PRO:CD  | 4:7:274:ILE:CD1[1_554] | 2.11                     | 0.09              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:75:ILE:CB   | 4:7:198:TYR:CA[1_554]  | 2.11                     | 0.09              |
| 4:5:188:TYR:C   | 4:9:183:ARG:C[1_554]   | 2.11                     | 0.09              |
| 4:5:200:PHE:N   | 4:9:206:ARG:CD[1_554]  | 2.11                     | 0.09              |
| 4:5:113:LYS:C   | 4:V:253:GLU:OE2[1_554] | 2.11                     | 0.09              |
| 4:5:317:ILE:CD1 | 4:9:150:GLY:O[1_554]   | 2.11                     | 0.09              |
| 4:3:279:TYR:CE1 | 4:7:289:ILE:CG1[1_554] | 2.11                     | 0.09              |
| 4:5:335:ARG:CA  | 4:9:106:THR:C[1_554]   | 2.11                     | 0.09              |
| 4:4:111:ASN:OD1 | 4:9:196:ARG:CD[1_554]  | 2.11                     | 0.09              |
| 4:4:115:ASN:N   | 4:9:250:ILE:N[1_554]   | 2.11                     | 0.09              |
| 4:5:188:TYR:CA  | 4:9:184:ASP:CA[1_554]  | 2.11                     | 0.09              |
| 4:4:218:TYR:CG  | 4:8:336:LYS:C[1_554]   | 2.11                     | 0.09              |
| 4:3:113:LYS:N   | 4:8:253:GLU:CG[1_554]  | 2.11                     | 0.09              |
| 4:5:290:ARG:NE  | 4:9:286:ASP:OD1[1_554] | 2.11                     | 0.09              |
| 4:4:316:GLU:N   | 4:8:142:LEU:CD1[1_554] | 2.11                     | 0.09              |
| 4:4:274:ILE:CA  | 4:8:162:ASN:O[1_554]   | 2.11                     | 0.09              |
| 4:5:265:SER:CA  | 4:9:261:LEU:C[1_554]   | 2.11                     | 0.09              |
| 4:3:172:PRO:O   | 4:8:188:TYR:CE1[1_554] | 2.11                     | 0.09              |
| 4:4:140:LEU:CG  | 4:8:117:GLU:CD[1_554]  | 2.11                     | 0.09              |
| 4:5:16:LEU:N    | 4:9:77:THR:C[1_554]    | 2.12                     | 0.08              |
| 4:4:187:ASP:C   | 4:8:183:ARG:CG[1_554]  | 2.12                     | 0.08              |
| 4:5:338:SER:O   | 4:9:116:ARG:CG[1_554]  | 2.12                     | 0.08              |
| 4:3:171:LEU:C   | 4:8:266:PHE:O[1_554]   | 2.12                     | 0.08              |
| 4:3:276:GLU:CG  | 4:7:151:ILE:CD1[1_554] | 2.12                     | 0.08              |
| 4:5:293:LEU:O   | 4:9:169:TYR:N[1_554]   | 2.12                     | 0.08              |
| 4:5:110:LEU:CD2 | 4:V:191:LYS:CD[1_554]  | 2.12                     | 0.08              |
| 4:3:120:THR:CG2 | 4:8:233:SER:OG[1_554]  | 2.12                     | 0.08              |
| 4:3:299:MET:N   | 4:7:136:ILE:CB[1_554]  | 2.12                     | 0.08              |
| 4:5:253:GLU:OE1 | 4:9:214:GLU:C[1_554]   | 2.12                     | 0.08              |
| 4:4:325:MET:C   | 4:8:167:GLU:CD[1_554]  | 2.12                     | 0.08              |
| 4:3:223:PHE:CD1 | 4:7:335:ARG:CG[1_554]  | 2.12                     | 0.08              |
| 4:5:191:LYS:CG  | 4:9:184:ASP:O[1_554]   | 2.12                     | 0.08              |
| 4:5:256:ARG:NH2 | 4:9:217:CYS:CB[1_554]  | 2.12                     | 0.08              |
| 4:3:194:THR:N   | 4:7:210:ARG:N[1_554]   | 2.12                     | 0.08              |
| 4:5:17:VAL:C    | 4:9:79:TRP:CD1[1_554]  | 2.12                     | 0.08              |
| 4:3:267:ILE:CG1 | 4:7:180:LEU:O[1_554]   | 2.12                     | 0.08              |
| 4:5:330:ILE:O   | 4:9:139:VAL:CB[1_554]  | 2.12                     | 0.08              |
| 4:3:313:MET:CG  | 4:7:138:ALA:C[1_554]   | 2.12                     | 0.08              |
| 4:4:198:TYR:O   | 4:8:206:ARG:O[1_554]   | 2.12                     | 0.08              |
| 4:2:112:PRO:CD  | 4:7:193:LEU:CB[1_554]  | 2.12                     | 0.08              |
| 4:4:293:LEU:CA  | 4:8:169:TYR:CE2[1_554] | 2.12                     | 0.08              |
| 4:5:191:LYS:CE  | 4:9:185:LEU:O[1_554]   | 2.12                     | 0.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:32:PRO:CD   | 4:7:78:ASN:CG[1_554]   | 2.12                     | 0.08              |
| 4:2:371:HIS:CE1 | 4:7:252:ASN:CA[1_554]  | 2.12                     | 0.08              |
| 4:4:242:LEU:C   | 4:8:60:SER:CA[1_554]   | 2.12                     | 0.08              |
| 4:4:219:VAL:CB  | 4:8:301:GLY:N[1_554]   | 2.12                     | 0.08              |
| 4:4:259:GLU:CG  | 4:8:304:THR:CG2[1_554] | 2.12                     | 0.08              |
| 4:5:337:TYR:CE2 | 4:9:86:TRP:NE1[1_554]  | 2.12                     | 0.08              |
| 4:4:23:GLY:N    | 4:8:125:GLU:OE2[1_554] | 2.12                     | 0.08              |
| 4:3:26:ALA:O    | 4:7:122:ILE:CA[1_554]  | 2.12                     | 0.08              |
| 4:4:344:SER:C   | 4:8:366:GLY:C[1_554]   | 2.12                     | 0.08              |
| 4:5:274:ILE:CB  | 4:9:162:ASN:CA[1_554]  | 2.12                     | 0.08              |
| 4:5:222:ASP:N   | 4:9:331:ALA:O[1_554]   | 2.12                     | 0.08              |
| 4:2:115:ASN:OD1 | 4:7:249:THR:C[1_554]   | 2.12                     | 0.08              |
| 4:2:74:GLY:O    | 4:7:198:TYR:N[1_554]   | 2.12                     | 0.08              |
| 4:3:335:ARG:O   | 4:7:119:MET:SD[1_554]  | 2.12                     | 0.08              |
| 4:4:23:GLY:O    | 4:8:362:TYR:CD2[1_554] | 2.12                     | 0.08              |
| 4:4:285:CYS:C   | 4:9:270:GLU:OE2[1_554] | 2.12                     | 0.08              |
| 4:4:341:ILE:O   | 4:8:367:PRO:CA[1_554]  | 2.12                     | 0.08              |
| 4:5:185:LEU:O   | 4:9:183:ARG:N[1_554]   | 2.12                     | 0.08              |
| 4:5:160:THR:CB  | 4:9:161:HIS:CD2[1_554] | 2.12                     | 0.08              |
| 1:D:542:PHE:CE2 | 4:5:328:LYS:CE[1_556]  | 2.12                     | 0.08              |
| 4:5:166:TYR:CD2 | 4:W:40:HIS:CG[1_554]   | 2.12                     | 0.08              |
| 4:4:340:TRP:CD2 | 4:8:118:LYS:C[1_554]   | 2.12                     | 0.08              |
| 4:3:345:ILE:CG1 | 4:7:366:GLY:C[1_554]   | 2.12                     | 0.08              |
| 4:4:272:ALA:N   | 4:8:277:THR:CG2[1_554] | 2.12                     | 0.08              |
| 4:3:270:GLU:CB  | 4:7:272:ALA:C[1_554]   | 2.12                     | 0.08              |
| 4:4:223:PHE:CE2 | 4:8:300:SER:C[1_554]   | 2.12                     | 0.08              |
| 4:2:173:HIS:C   | 4:7:267:ILE:N[1_554]   | 2.12                     | 0.08              |
| 4:4:196:ARG:CB  | 4:8:210:ARG:C[1_554]   | 2.12                     | 0.08              |
| 4:3:291:LYS:NZ  | 4:9:64:ILE:C[1_554]    | 2.12                     | 0.08              |
| 4:3:315:LYS:N   | 4:7:142:LEU:CB[1_554]  | 2.12                     | 0.08              |
| 4:3:196:ARG:O   | 4:7:212:ILE:N[1_554]   | 2.12                     | 0.08              |
| 4:4:368:SER:N   | 4:9:236:LEU:CB[1_554]  | 2.12                     | 0.08              |
| 4:5:135:ALA:CB  | 4:9:117:GLU:OE2[1_554] | 2.12                     | 0.08              |
| 4:5:334:GLU:OE2 | 4:9:104:LEU:CA[1_554]  | 2.12                     | 0.08              |
| 4:5:112:PRO:CG  | 4:V:193:LEU:CA[1_554]  | 2.12                     | 0.08              |
| 4:5:161:HIS:O   | 4:9:110:LEU:CG[1_554]  | 2.12                     | 0.08              |
| 4:2:289:ILE:N   | 4:8:39:ARG:NH2[1_554]  | 2.12                     | 0.08              |
| 4:5:183:ARG:NE  | 4:9:72:GLU:CG[1_554]   | 2.12                     | 0.08              |
| 4:3:335:ARG:NH1 | 4:7:106:THR:N[1_554]   | 2.12                     | 0.08              |
| 4:4:173:HIS:CE1 | 4:9:265:SER:N[1_554]   | 2.12                     | 0.08              |
| 4:5:370:VAL:CG1 | 4:V:231:ALA:CA[1_554]  | 2.12                     | 0.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:309:ILE:C   | 4:9:141:SER:CA[1_554]  | 2.12                     | 0.08              |
| 4:4:243:PRO:CD  | 4:8:60:SER:C[1_554]    | 2.12                     | 0.08              |
| 4:4:309:ILE:C   | 4:8:141:SER:CA[1_554]  | 2.12                     | 0.08              |
| 4:5:140:LEU:CA  | 4:9:371:HIS:O[1_554]   | 2.12                     | 0.08              |
| 4:3:336:LYS:O   | 4:7:76:ILE:CD1[1_554]  | 2.12                     | 0.08              |
| 4:4:115:ASN:CB  | 4:9:249:THR:O[1_554]   | 2.12                     | 0.08              |
| 4:3:267:ILE:CD1 | 4:7:180:LEU:C[1_554]   | 2.12                     | 0.08              |
| 4:5:294:TYR:CG  | 4:9:166:TYR:CA[1_554]  | 2.12                     | 0.08              |
| 4:2:326:LYS:CE  | 4:8:44:MET:O[1_554]    | 2.12                     | 0.08              |
| 4:5:191:LYS:O   | 4:9:186:THR:C[1_554]   | 2.12                     | 0.08              |
| 4:2:291:LYS:CE  | 4:8:64:ILE:C[1_554]    | 2.12                     | 0.08              |
| 4:4:337:TYR:N   | 4:8:119:MET:CG[1_554]  | 2.12                     | 0.08              |
| 4:5:21:PHE:N    | 4:9:125:GLU:OE1[1_554] | 2.12                     | 0.08              |
| 4:5:366:GLY:C   | 4:V:234:SER:CA[1_554]  | 2.12                     | 0.08              |
| 4:5:343:GLY:O   | 4:9:367:PRO:CG[1_554]  | 2.12                     | 0.08              |
| 4:3:75:ILE:CG2  | 4:8:198:TYR:CE2[1_554] | 2.12                     | 0.08              |
| 4:3:334:GLU:OE2 | 4:7:133:TYR:O[1_554]   | 2.12                     | 0.08              |
| 4:1:289:ILE:CA  | 4:7:39:ARG:NE[1_554]   | 2.12                     | 0.08              |
| 4:3:221:LEU:C   | 4:7:332:PRO:CG[1_554]  | 2.12                     | 0.08              |
| 4:4:279:TYR:CA  | 4:8:285:CYS:SG[1_554]  | 2.12                     | 0.08              |
| 4:4:198:TYR:CA  | 4:8:209:VAL:N[1_554]   | 2.12                     | 0.08              |
| 4:4:370:VAL:CB  | 4:9:231:ALA:N[1_554]   | 2.12                     | 0.08              |
| 4:3:157:ASP:C   | 4:7:72:GLU:C[1_554]    | 2.12                     | 0.08              |
| 4:3:304:THR:OG1 | 4:7:107:GLU:N[1_554]   | 2.12                     | 0.08              |
| 4:5:349:LEU:CA  | 4:9:364:GLU:O[1_554]   | 2.12                     | 0.08              |
| 4:4:16:LEU:CD1  | 4:8:78:ASN:CA[1_554]   | 2.12                     | 0.08              |
| 4:4:317:ILE:CB  | 4:8:150:GLY:C[1_554]   | 2.12                     | 0.08              |
| 4:4:262:PHE:CD2 | 4:8:154:ASP:CA[1_554]  | 2.12                     | 0.08              |
| 4:5:190:MET:SD  | 4:9:206:ARG:CZ[1_554]  | 2.12                     | 0.08              |
| 4:5:193:LEU:C   | 4:9:210:ARG:CA[1_554]  | 2.12                     | 0.08              |
| 4:3:115:ASN:N   | 4:8:251:GLY:N[1_554]   | 2.12                     | 0.08              |
| 4:5:75:ILE:CD1  | 4:V:194:THR:O[1_554]   | 2.12                     | 0.08              |
| 4:5:369:ILE:C   | 4:V:231:ALA:N[1_554]   | 2.12                     | 0.08              |
| 4:4:262:PHE:CD1 | 4:8:152:VAL:C[1_554]   | 2.12                     | 0.08              |
| 4:5:164:PRO:CA  | 4:9:169:TYR:OH[1_554]  | 2.12                     | 0.08              |
| 4:4:319:ALA:CB  | 4:8:296:ASN:ND2[1_554] | 2.12                     | 0.08              |
| 4:5:204:ALA:N   | 4:9:62:ARG:CG[1_554]   | 2.12                     | 0.08              |
| 4:5:369:ILE:CA  | 4:V:232:SER:N[1_554]   | 2.12                     | 0.08              |
| 4:5:349:LEU:CA  | 4:9:365:ALA:C[1_554]   | 2.12                     | 0.08              |
| 4:4:143:TYR:C   | 4:8:370:VAL:C[1_554]   | 2.12                     | 0.08              |
| 4:5:56:ASP:CA   | 4:9:37:ARG:CZ[1_554]   | 2.12                     | 0.08              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:330:ILE:O   | 4:7:136:ILE:N[1_554]   | 2.12                     | 0.08              |
| 4:4:191:LYS:CG  | 4:8:185:LEU:O[1_554]   | 2.12                     | 0.08              |
| 4:5:106:THR:CG2 | 4:9:114:ALA:CB[1_554]  | 2.13                     | 0.07              |
| 4:4:323:SER:N   | 4:8:292:ASP:OD1[1_554] | 2.13                     | 0.07              |
| 4:5:62:ARG:NH2  | 4:9:67:LEU:CB[1_554]   | 2.13                     | 0.07              |
| 4:3:114:ALA:N   | 4:8:251:GLY:N[1_554]   | 2.13                     | 0.07              |
| 4:4:28:ARG:CA   | 4:8:126:THR:CG2[1_554] | 2.13                     | 0.07              |
| 4:3:75:ILE:CB   | 4:8:198:TYR:CD2[1_554] | 2.13                     | 0.07              |
| 4:3:370:VAL:C   | 4:8:231:ALA:N[1_554]   | 2.13                     | 0.07              |
| 4:3:166:TYR:CD1 | 4:9:40:HIS:CG[1_554]   | 2.13                     | 0.07              |
| 4:5:280:ASN:N   | 4:9:285:CYS:SG[1_554]  | 2.13                     | 0.07              |
| 4:5:14:SER:O    | 4:9:77:THR:CB[1_554]   | 2.13                     | 0.07              |
| 4:3:174:ALA:CB  | 4:8:268:GLY:N[1_554]   | 2.13                     | 0.07              |
| 4:5:198:TYR:CD2 | 4:9:209:VAL:N[1_554]   | 2.13                     | 0.07              |
| 4:3:214:GLU:CB  | 4:7:33:SER:OG[1_554]   | 2.13                     | 0.07              |
| 4:3:281:SER:CB  | 4:7:172:PRO:C[1_554]   | 2.13                     | 0.07              |
| 4:3:371:HIS:ND1 | 4:8:252:ASN:C[1_554]   | 2.13                     | 0.07              |
| 4:3:277:THR:OG1 | 4:7:175:ILE:C[1_554]   | 2.13                     | 0.07              |
| 4:3:222:ASP:C   | 4:7:331:ALA:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:188:TYR:CD2 | 4:9:181:ALA:C[1_554]   | 2.13                     | 0.07              |
| 4:4:249:THR:C   | 4:8:211:ASP:OD2[1_554] | 2.13                     | 0.07              |
| 4:3:332:PRO:CA  | 4:7:135:ALA:N[1_554]   | 2.13                     | 0.07              |
| 4:2:288:ASP:N   | 4:8:39:ARG:NH1[1_554]  | 2.13                     | 0.07              |
| 4:5:219:VAL:C   | 4:9:335:ARG:O[1_554]   | 2.13                     | 0.07              |
| 4:4:77:THR:C    | 4:9:246:GLN:NE2[1_554] | 2.13                     | 0.07              |
| 4:4:183:ARG:NH2 | 4:8:72:GLU:OE1[1_554]  | 2.13                     | 0.07              |
| 4:5:315:LYS:O   | 4:9:296:ASN:CB[1_554]  | 2.13                     | 0.07              |
| 4:4:177:ARG:NH1 | 4:9:194:THR:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:279:TYR:CA  | 4:9:164:PRO:CB[1_554]  | 2.13                     | 0.07              |
| 4:3:144:ALA:CA  | 4:7:371:HIS:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:31:PHE:CA   | 4:9:80:ASP:C[1_554]    | 2.13                     | 0.07              |
| 4:2:367:PRO:CG  | 4:7:235:SER:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:276:GLU:CD  | 4:9:278:THR:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:281:SER:O   | 4:9:173:HIS:CE1[1_554] | 2.13                     | 0.07              |
| 4:3:211:ASP:CB  | 4:7:32:PRO:C[1_554]    | 2.13                     | 0.07              |
| 4:4:192:ILE:CB  | 4:8:213:LYS:NZ[1_554]  | 2.13                     | 0.07              |
| 4:4:75:ILE:C    | 4:9:198:TYR:N[1_554]   | 2.13                     | 0.07              |
| 4:3:210:ARG:NH1 | 4:7:33:SER:O[1_554]    | 2.13                     | 0.07              |
| 4:5:281:SER:O   | 4:9:173:HIS:CG[1_554]  | 2.13                     | 0.07              |
| 4:5:186:THR:N   | 4:9:157:ASP:C[1_554]   | 2.13                     | 0.07              |
| 4:5:331:ALA:CB  | 4:9:140:LEU:N[1_554]   | 2.13                     | 0.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:342:GLY:CA  | 4:7:117:GLU:CG[1_554]  | 2.13                     | 0.07              |
| 4:3:136:ILE:O   | 4:7:113:LYS:NZ[1_554]  | 2.13                     | 0.07              |
| 4:5:199:SER:CA  | 4:9:206:ARG:CB[1_554]  | 2.13                     | 0.07              |
| 4:5:199:SER:O   | 4:9:206:ARG:CA[1_554]  | 2.13                     | 0.07              |
| 4:3:320:LEU:CG  | 4:7:293:LEU:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:311:ASP:O   | 4:9:298:VAL:CG2[1_554] | 2.13                     | 0.07              |
| 4:2:370:VAL:CA  | 4:7:229:THR:O[1_554]   | 2.13                     | 0.07              |
| 4:3:110:LEU:CG  | 4:8:191:LYS:CD[1_554]  | 2.13                     | 0.07              |
| 4:3:184:ASP:OD1 | 4:7:73:HIS:CG[1_554]   | 2.13                     | 0.07              |
| 4:3:195:GLU:N   | 4:7:209:VAL:CB[1_554]  | 2.13                     | 0.07              |
| 4:5:198:TYR:OH  | 4:9:211:ASP:CG[1_554]  | 2.13                     | 0.07              |
| 4:3:349:LEU:CD2 | 4:7:365:ALA:C[1_554]   | 2.13                     | 0.07              |
| 4:3:249:THR:O   | 4:7:211:ASP:OD2[1_554] | 2.13                     | 0.07              |
| 4:2:371:HIS:N   | 4:7:236:LEU:CG[1_554]  | 2.13                     | 0.07              |
| 4:1:287:ILE:C   | 4:7:63:GLY:O[1_554]    | 2.13                     | 0.07              |
| 4:4:276:GLU:OE2 | 4:8:278:THR:CB[1_554]  | 2.13                     | 0.07              |
| 4:4:31:PHE:CA   | 4:8:80:ASP:N[1_554]    | 2.13                     | 0.07              |
| 4:4:262:PHE:CB  | 4:8:153:LEU:CD2[1_554] | 2.13                     | 0.07              |
| 4:5:346:LEU:N   | 4:9:369:ILE:CG2[1_554] | 2.13                     | 0.07              |
| 4:3:76:ILE:N    | 4:8:198:TYR:CE1[1_554] | 2.13                     | 0.07              |
| 4:4:191:LYS:CD  | 4:8:185:LEU:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:140:LEU:CA  | 4:9:371:HIS:CE1[1_554] | 2.13                     | 0.07              |
| 4:5:275:HIS:CB  | 4:9:151:ILE:CG1[1_554] | 2.13                     | 0.07              |
| 4:4:258:PRO:O   | 4:8:155:SER:O[1_554]   | 2.13                     | 0.07              |
| 4:4:297:ASN:CB  | 4:8:170:ALA:N[1_554]   | 2.13                     | 0.07              |
| 4:5:312:ARG:CA  | 4:9:298:VAL:CB[1_554]  | 2.13                     | 0.07              |
| 4:3:370:VAL:C   | 4:8:230:ALA:N[1_554]   | 2.13                     | 0.07              |
| 4:3:340:TRP:N   | 4:7:115:ASN:O[1_554]   | 2.13                     | 0.07              |
| 4:3:195:GLU:CB  | 4:7:189:LEU:CG[1_554]  | 2.13                     | 0.07              |
| 4:3:157:ASP:CG  | 4:7:72:GLU:CG[1_554]   | 2.13                     | 0.07              |
| 4:5:218:TYR:OH  | 4:9:337:TYR:CZ[1_554]  | 2.13                     | 0.07              |
| 4:4:322:PRO:CD  | 4:8:289:ILE:CA[1_554]  | 2.13                     | 0.07              |
| 4:4:24:ASP:CA   | 4:8:125:GLU:CA[1_554]  | 2.13                     | 0.07              |
| 4:3:195:GLU:N   | 4:7:209:VAL:CG1[1_554] | 2.13                     | 0.07              |
| 4:2:110:LEU:CD1 | 4:7:191:LYS:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:340:TRP:CB  | 4:9:119:MET:CG[1_554]  | 2.13                     | 0.07              |
| 4:5:288:ASP:CA  | 4:W:63:GLY:C[1_554]    | 2.13                     | 0.07              |
| 4:3:195:GLU:CA  | 4:7:189:LEU:CD2[1_554] | 2.13                     | 0.07              |
| 4:5:191:LYS:CG  | 4:9:185:LEU:CA[1_554]  | 2.13                     | 0.07              |
| 4:4:115:ASN:CB  | 4:9:196:ARG:CD[1_554]  | 2.13                     | 0.07              |
| 4:3:171:LEU:CB  | 4:8:265:SER:O[1_554]   | 2.13                     | 0.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:288:ASP:CB  | 4:W:62:ARG:C[1_554]    | 2.13                     | 0.07              |
| 4:4:197:GLY:N   | 4:8:208:ILE:O[1_554]   | 2.13                     | 0.07              |
| 4:5:154:ASP:C   | 4:9:110:LEU:N[1_554]   | 2.13                     | 0.07              |
| 4:2:171:LEU:C   | 4:7:266:PHE:CA[1_554]  | 2.13                     | 0.07              |
| 4:3:281:SER:N   | 4:7:173:HIS:C[1_554]   | 2.13                     | 0.07              |
| 4:3:154:ASP:OD2 | 4:7:112:PRO:CA[1_554]  | 2.13                     | 0.07              |
| 4:4:291:LYS:NZ  | 4:V:64:ILE:CD1[1_554]  | 2.13                     | 0.07              |
| 4:5:223:PHE:C   | 4:9:309:ILE:CG2[1_554] | 2.13                     | 0.07              |
| 4:3:300:SER:OG  | 4:7:111:ASN:CB[1_554]  | 2.13                     | 0.07              |
| 4:5:257:CYS:SG  | 4:9:156:GLY:O[1_554]   | 2.13                     | 0.07              |
| 4:5:188:TYR:CD1 | 4:9:185:LEU:CA[1_554]  | 2.13                     | 0.07              |
| 4:4:164:PRO:N   | 4:8:172:PRO:CB[1_554]  | 2.13                     | 0.07              |
| 4:4:15:GLY:O    | 4:8:77:THR:C[1_554]    | 2.13                     | 0.07              |
| 4:4:218:TYR:OH  | 4:8:337:TYR:CD2[1_554] | 2.13                     | 0.07              |
| 4:2:79:TRP:CG   | 4:7:247:VAL:O[1_554]   | 2.13                     | 0.07              |
| 4:4:294:TYR:C   | 4:8:169:TYR:N[1_554]   | 2.13                     | 0.07              |
| 4:3:217:CYS:SG  | 4:7:16:LEU:CD2[1_554]  | 2.13                     | 0.07              |
| 4:4:312:ARG:CG  | 4:8:300:SER:N[1_554]   | 2.13                     | 0.07              |
| 4:3:75:ILE:CB   | 4:8:198:TYR:N[1_554]   | 2.13                     | 0.07              |
| 4:4:172:PRO:CG  | 4:9:266:PHE:CA[1_554]  | 2.13                     | 0.07              |
| 4:4:41:GLN:CD   | 4:7:224:GLU:OE1[1_554] | 2.13                     | 0.07              |
| 4:5:56:ASP:OD2  | 4:9:81:ASP:CG[1_554]   | 2.13                     | 0.07              |
| 4:3:270:GLU:CA  | 4:7:273:GLY:N[1_554]   | 2.13                     | 0.07              |
| 4:5:140:LEU:O   | 4:9:371:HIS:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:210:ARG:NE  | 4:9:33:SER:C[1_554]    | 2.13                     | 0.07              |
| 4:3:173:HIS:CE1 | 4:8:266:PHE:CA[1_554]  | 2.13                     | 0.07              |
| 4:4:288:ASP:N   | 4:V:63:GLY:CA[1_554]   | 2.13                     | 0.07              |
| 4:3:186:THR:O   | 4:7:183:ARG:CB[1_554]  | 2.13                     | 0.07              |
| 4:4:25:ASP:CG   | 4:8:124:PHE:CA[1_554]  | 2.13                     | 0.07              |
| 4:3:285:CYS:N   | 4:8:268:GLY:O[1_554]   | 2.13                     | 0.07              |
| 4:4:188:TYR:CE2 | 4:8:182:GLY:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:221:LEU:O   | 4:9:332:PRO:CA[1_554]  | 2.13                     | 0.07              |
| 4:4:288:ASP:OD1 | 4:V:65:LEU:O[1_554]    | 2.13                     | 0.07              |
| 4:4:195:GLU:O   | 4:8:212:ILE:CB[1_554]  | 2.13                     | 0.07              |
| 4:4:280:ASN:N   | 4:8:285:CYS:SG[1_554]  | 2.13                     | 0.07              |
| 4:5:164:PRO:CG  | 4:9:172:PRO:CD[1_554]  | 2.13                     | 0.07              |
| 4:4:191:LYS:CB  | 4:8:187:ASP:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:210:ARG:CG  | 4:9:69:TYR:CD2[1_554]  | 2.13                     | 0.07              |
| 4:3:318:THR:CG2 | 4:7:148:THR:N[1_554]   | 2.13                     | 0.07              |
| 4:4:113:LYS:N   | 4:9:253:GLU:OE2[1_554] | 2.13                     | 0.07              |
| 4:5:17:VAL:CA   | 4:9:79:TRP:CB[1_554]   | 2.13                     | 0.07              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:337:TYR:CB  | 4:9:119:MET:CE[1_554]  | 2.13                     | 0.07              |
| 4:3:214:GLU:CA  | 4:7:16:LEU:N[1_554]    | 2.13                     | 0.07              |
| 4:5:162:ASN:C   | 4:9:172:PRO:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:22:ALA:O    | 4:9:125:GLU:OE2[1_554] | 2.13                     | 0.07              |
| 4:5:208:ILE:N   | 4:9:59:GLN:OE1[1_554]  | 2.13                     | 0.07              |
| 4:4:276:GLU:N   | 4:8:151:ILE:CD1[1_554] | 2.13                     | 0.07              |
| 4:5:188:TYR:CD1 | 4:9:185:LEU:N[1_554]   | 2.13                     | 0.07              |
| 4:4:299:MET:N   | 4:8:136:ILE:N[1_554]   | 2.13                     | 0.07              |
| 4:5:348:SER:N   | 4:9:366:GLY:C[1_554]   | 2.13                     | 0.07              |
| 4:4:186:THR:N   | 4:8:183:ARG:NE[1_554]  | 2.13                     | 0.07              |
| 4:2:109:PRO:C   | 4:7:192:ILE:CA[1_554]  | 2.13                     | 0.07              |
| 4:5:174:ALA:C   | 4:9:173:HIS:CA[1_554]  | 2.13                     | 0.07              |
| 4:2:288:ASP:C   | 4:8:63:GLY:O[1_554]    | 2.13                     | 0.07              |
| 4:1:324:THR:C   | 4:7:44:MET:CE[1_554]   | 2.13                     | 0.07              |
| 4:5:186:THR:C   | 4:9:183:ARG:CA[1_554]  | 2.13                     | 0.07              |
| 4:3:222:ASP:O   | 4:7:331:ALA:C[1_554]   | 2.14                     | 0.06              |
| 4:5:181:ALA:CB  | 4:9:159:VAL:CG1[1_554] | 2.14                     | 0.06              |
| 4:2:171:LEU:CB  | 4:7:265:SER:O[1_554]   | 2.14                     | 0.06              |
| 4:4:265:SER:N   | 4:8:261:LEU:O[1_554]   | 2.14                     | 0.06              |
| 4:3:297:ASN:OD1 | 4:7:169:TYR:C[1_554]   | 2.14                     | 0.06              |
| 4:3:337:TYR:O   | 4:7:119:MET:N[1_554]   | 2.14                     | 0.06              |
| 4:4:213:LYS:CD  | 4:8:15:GLY:CA[1_554]   | 2.14                     | 0.06              |
| 1:A:542:PHE:CZ  | 4:4:328:LYS:NZ[1_556]  | 2.14                     | 0.06              |
| 4:3:262:PHE:CG  | 4:7:154:ASP:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:144:ALA:CB  | 4:8:371:HIS:N[1_554]   | 2.14                     | 0.06              |
| 4:5:279:TYR:OH  | 4:9:290:ARG:CA[1_554]  | 2.14                     | 0.06              |
| 4:5:321:ALA:C   | 4:9:292:ASP:CG[1_554]  | 2.14                     | 0.06              |
| 4:5:151:ILE:O   | 4:9:170:ALA:CB[1_554]  | 2.14                     | 0.06              |
| 4:4:116:ARG:CA  | 4:9:252:ASN:OD1[1_554] | 2.14                     | 0.06              |
| 4:5:186:THR:OG1 | 4:9:183:ARG:NE[1_554]  | 2.14                     | 0.06              |
| 4:4:156:GLY:CA  | 4:8:75:ILE:CB[1_554]   | 2.14                     | 0.06              |
| 4:4:336:LYS:CG  | 4:8:12:ASN:ND2[1_554]  | 2.14                     | 0.06              |
| 4:4:136:ILE:CG1 | 4:8:113:LYS:NZ[1_554]  | 2.14                     | 0.06              |
| 4:4:214:GLU:CB  | 4:8:17:VAL:N[1_554]    | 2.14                     | 0.06              |
| 4:4:30:VAL:CG1  | 4:8:79:TRP:C[1_554]    | 2.14                     | 0.06              |
| 4:3:336:LYS:CA  | 4:7:119:MET:CE[1_554]  | 2.14                     | 0.06              |
| 4:3:312:ARG:CD  | 4:7:300:SER:N[1_554]   | 2.14                     | 0.06              |
| 4:3:339:VAL:CB  | 4:7:114:ALA:C[1_554]   | 2.14                     | 0.06              |
| 4:4:75:ILE:CA   | 4:9:198:TYR:CA[1_554]  | 2.14                     | 0.06              |
| 4:5:207:GLU:CB  | 4:9:67:LEU:CG[1_554]   | 2.14                     | 0.06              |
| 4:3:316:GLU:O   | 4:7:296:ASN:O[1_554]   | 2.14                     | 0.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:110:LEU:CB  | 4:7:192:ILE:CG1[1_554] | 2.14                     | 0.06              |
| 4:5:141:SER:CA  | 4:9:116:ARG:NH1[1_554] | 2.14                     | 0.06              |
| 4:4:188:TYR:CB  | 4:8:183:ARG:N[1_554]   | 2.14                     | 0.06              |
| 4:4:172:PRO:CG  | 4:9:266:PHE:CD1[1_554] | 2.14                     | 0.06              |
| 4:4:211:ASP:CG  | 4:8:32:PRO:C[1_554]    | 2.14                     | 0.06              |
| 4:3:153:LEU:O   | 4:7:109:PRO:O[1_554]   | 2.14                     | 0.06              |
| 4:5:141:SER:C   | 4:9:116:ARG:NH2[1_554] | 2.14                     | 0.06              |
| 4:4:223:PHE:CA  | 4:8:335:ARG:CD[1_554]  | 2.14                     | 0.06              |
| 4:3:312:ARG:NH2 | 4:7:299:MET:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:180:LEU:CD2 | 4:8:178:LEU:N[1_554]   | 2.14                     | 0.06              |
| 4:5:317:ILE:O   | 4:9:293:LEU:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:281:SER:CB  | 4:8:173:HIS:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:161:HIS:CB  | 4:8:110:LEU:CG[1_554]  | 2.14                     | 0.06              |
| 4:5:113:LYS:CA  | 4:V:252:ASN:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:250:ILE:CD1 | 4:8:210:ARG:CZ[1_554]  | 2.14                     | 0.06              |
| 4:4:191:LYS:O   | 4:8:186:THR:C[1_554]   | 2.14                     | 0.06              |
| 4:4:319:ALA:N   | 4:8:296:ASN:ND2[1_554] | 2.14                     | 0.06              |
| 4:4:334:GLU:N   | 4:8:105:LEU:CG[1_554]  | 2.14                     | 0.06              |
| 4:4:314:GLN:CG  | 4:8:142:LEU:C[1_554]   | 2.14                     | 0.06              |
| 4:5:151:ILE:C   | 4:9:170:ALA:O[1_554]   | 2.14                     | 0.06              |
| 4:4:330:ILE:N   | 4:8:139:VAL:CG1[1_554] | 2.14                     | 0.06              |
| 4:4:366:GLY:CA  | 4:9:235:SER:N[1_554]   | 2.14                     | 0.06              |
| 4:4:370:VAL:N   | 4:9:231:ALA:N[1_554]   | 2.14                     | 0.06              |
| 4:3:156:GLY:O   | 4:7:74:GLY:CA[1_554]   | 2.14                     | 0.06              |
| 4:4:280:ASN:OD1 | 4:8:281:SER:N[1_554]   | 2.14                     | 0.06              |
| 4:4:333:PRO:CA  | 4:8:105:LEU:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:218:TYR:OH  | 4:8:27:PRO:CG[1_554]   | 2.14                     | 0.06              |
| 4:3:186:THR:CA  | 4:7:157:ASP:OD2[1_554] | 2.14                     | 0.06              |
| 4:4:279:TYR:CD2 | 4:8:285:CYS:SG[1_554]  | 2.14                     | 0.06              |
| 4:4:369:ILE:O   | 4:9:228:ALA:C[1_554]   | 2.14                     | 0.06              |
| 4:2:110:LEU:CD1 | 4:7:188:TYR:O[1_554]   | 2.14                     | 0.06              |
| 4:3:224:GLU:N   | 4:7:335:ARG:NH2[1_554] | 2.14                     | 0.06              |
| 4:2:175:ILE:CG1 | 4:7:191:LYS:CE[1_554]  | 2.14                     | 0.06              |
| 4:4:320:LEU:C   | 4:8:293:LEU:CA[1_554]  | 2.14                     | 0.06              |
| 4:3:243:PRO:CG  | 4:7:60:SER:N[1_554]    | 2.14                     | 0.06              |
| 4:2:291:LYS:CG  | 4:8:64:ILE:CB[1_554]   | 2.14                     | 0.06              |
| 4:3:333:PRO:CA  | 4:7:104:LEU:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:18:LYS:NZ   | 4:8:79:TRP:CZ2[1_554]  | 2.14                     | 0.06              |
| 4:4:255:PHE:CD1 | 4:8:305:MET:N[1_554]   | 2.14                     | 0.06              |
| 4:4:173:HIS:N   | 4:9:267:ILE:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:340:TRP:CB  | 4:8:118:LYS:CB[1_554]  | 2.14                     | 0.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:322:PRO:O   | 4:9:292:ASP:OD1[1_554] | 2.14                     | 0.06              |
| 4:3:326:LYS:O   | 4:7:167:GLU:N[1_554]   | 2.14                     | 0.06              |
| 4:5:327:ILE:CA  | 4:9:148:THR:O[1_554]   | 2.14                     | 0.06              |
| 4:3:198:TYR:C   | 4:7:205:GLU:C[1_554]   | 2.14                     | 0.06              |
| 4:4:188:TYR:CD1 | 4:8:185:LEU:CD1[1_554] | 2.14                     | 0.06              |
| 4:5:174:ALA:O   | 4:9:173:HIS:CG[1_554]  | 2.14                     | 0.06              |
| 4:4:56:ASP:CB   | 4:8:37:ARG:CZ[1_554]   | 2.14                     | 0.06              |
| 4:5:27:PRO:O    | 4:9:127:PHE:CE2[1_554] | 2.14                     | 0.06              |
| 4:4:221:LEU:C   | 4:8:332:PRO:CG[1_554]  | 2.14                     | 0.06              |
| 4:4:180:LEU:CG  | 4:8:178:LEU:N[1_554]   | 2.14                     | 0.06              |
| 4:5:274:ILE:CG2 | 4:9:152:VAL:O[1_554]   | 2.14                     | 0.06              |
| 4:4:218:TYR:C   | 4:8:336:LYS:C[1_554]   | 2.14                     | 0.06              |
| 4:5:196:ARG:NE  | 4:9:211:ASP:OD1[1_554] | 2.14                     | 0.06              |
| 4:5:334:GLU:O   | 4:9:105:LEU:CG[1_554]  | 2.14                     | 0.06              |
| 4:5:30:VAL:CG1  | 4:9:82:MET:C[1_554]    | 2.14                     | 0.06              |
| 4:4:305:MET:CB  | 4:8:11:ASP:C[1_554]    | 2.14                     | 0.06              |
| 4:4:305:MET:N   | 4:8:11:ASP:OD1[1_554]  | 2.14                     | 0.06              |
| 4:4:322:PRO:CB  | 4:8:291:LYS:NZ[1_554]  | 2.14                     | 0.06              |
| 4:5:136:ILE:N   | 4:9:113:LYS:CB[1_554]  | 2.14                     | 0.06              |
| 4:3:287:ILE:C   | 4:9:63:GLY:C[1_554]    | 2.14                     | 0.06              |
| 4:3:140:LEU:CA  | 4:7:371:HIS:NE2[1_554] | 2.14                     | 0.06              |
| 4:4:154:ASP:CB  | 4:8:110:LEU:CA[1_554]  | 2.14                     | 0.06              |
| 4:3:223:PHE:CE2 | 4:7:304:THR:OG1[1_554] | 2.14                     | 0.06              |
| 4:5:334:GLU:CD  | 4:9:133:TYR:C[1_554]   | 2.14                     | 0.06              |
| 4:4:143:TYR:C   | 4:8:371:HIS:N[1_554]   | 2.14                     | 0.06              |
| 4:5:342:GLY:CA  | 4:9:371:HIS:N[1_554]   | 2.14                     | 0.06              |
| 4:5:333:PRO:CG  | 4:9:104:LEU:CG[1_554]  | 2.14                     | 0.06              |
| 4:3:320:LEU:CG  | 4:7:293:LEU:CG[1_554]  | 2.14                     | 0.06              |
| 4:3:75:ILE:N    | 4:8:197:GLY:CA[1_554]  | 2.14                     | 0.06              |
| 4:2:77:THR:CB   | 4:7:246:GLN:CD[1_554]  | 2.14                     | 0.06              |
| 4:2:117:GLU:N   | 4:7:237:GLU:CD[1_554]  | 2.14                     | 0.06              |
| 4:2:169:TYR:CZ  | 4:7:266:PHE:CD1[1_554] | 2.14                     | 0.06              |
| 4:3:278:THR:O   | 4:7:171:LEU:CA[1_554]  | 2.14                     | 0.06              |
| 4:5:325:MET:SD  | 4:9:166:TYR:CE2[1_554] | 2.14                     | 0.06              |
| 4:3:74:GLY:C    | 4:8:197:GLY:N[1_554]   | 2.14                     | 0.06              |
| 4:2:109:PRO:CB  | 4:7:195:GLU:OE1[1_554] | 2.14                     | 0.06              |
| 4:5:343:GLY:C   | 4:9:367:PRO:O[1_554]   | 2.14                     | 0.06              |
| 4:4:193:LEU:CD1 | 4:8:210:ARG:CB[1_554]  | 2.14                     | 0.06              |
| 4:3:338:SER:N   | 4:7:119:MET:SD[1_554]  | 2.14                     | 0.06              |
| 4:5:268:GLY:O   | 4:9:269:MET:CB[1_554]  | 2.14                     | 0.06              |
| 4:5:173:HIS:ND1 | 4:V:266:PHE:C[1_554]   | 2.14                     | 0.06              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:342:GLY:O   | 4:9:367:PRO:C[1_554]   | 2.14                     | 0.06              |
| 4:5:271:SER:O   | 4:9:277:THR:CB[1_554]  | 2.14                     | 0.06              |
| 4:3:111:ASN:OD1 | 4:8:196:ARG:CD[1_554]  | 2.14                     | 0.06              |
| 4:4:372:ARG:N   | 4:9:226:GLU:O[1_554]   | 2.14                     | 0.06              |
| 4:5:316:GLU:CB  | 4:9:151:ILE:C[1_554]   | 2.14                     | 0.06              |
| 4:5:283:MET:N   | 4:9:286:ASP:N[1_554]   | 2.14                     | 0.06              |
| 4:3:173:HIS:N   | 4:8:267:ILE:CG2[1_554] | 2.14                     | 0.06              |
| 4:4:340:TRP:CE2 | 4:8:121:GLN:OE1[1_554] | 2.14                     | 0.06              |
| 4:5:75:ILE:CB   | 4:V:198:TYR:CA[1_554]  | 2.14                     | 0.06              |
| 4:4:199:SER:CB  | 4:8:205:GLU:C[1_554]   | 2.14                     | 0.06              |
| 4:4:25:ASP:O    | 4:8:123:MET:CB[1_554]  | 2.14                     | 0.06              |
| 4:3:274:ILE:C   | 4:7:163:VAL:CA[1_554]  | 2.14                     | 0.06              |
| 4:3:156:GLY:C   | 4:7:75:ILE:CB[1_554]   | 2.14                     | 0.06              |
| 4:4:327:ILE:CG1 | 4:8:148:THR:C[1_554]   | 2.14                     | 0.06              |
| 4:4:336:LYS:CB  | 4:8:12:ASN:ND2[1_554]  | 2.14                     | 0.06              |
| 4:3:207:GLU:C   | 4:7:67:LEU:CD1[1_554]  | 2.15                     | 0.05              |
| 4:4:174:ALA:C   | 4:8:173:HIS:CB[1_554]  | 2.15                     | 0.05              |
| 4:3:338:SER:OG  | 4:7:116:ARG:CG[1_554]  | 2.15                     | 0.05              |
| 4:3:195:GLU:CA  | 4:7:209:VAL:CG2[1_554] | 2.15                     | 0.05              |
| 4:5:75:ILE:C    | 4:V:198:TYR:N[1_554]   | 2.15                     | 0.05              |
| 1:D:553:MLY:CH1 | 4:5:328:LYS:CE[1_556]  | 2.15                     | 0.05              |
| 4:3:319:ALA:N   | 4:7:296:ASN:CB[1_554]  | 2.15                     | 0.05              |
| 4:5:178:LEU:CD2 | 4:9:177:ARG:C[1_554]   | 2.15                     | 0.05              |
| 4:3:188:TYR:CD1 | 4:7:185:LEU:N[1_554]   | 2.15                     | 0.05              |
| 4:5:341:ILE:C   | 4:9:120:THR:CG2[1_554] | 2.15                     | 0.05              |
| 4:4:335:ARG:C   | 4:8:119:MET:CE[1_554]  | 2.15                     | 0.05              |
| 4:4:308:GLY:N   | 4:8:339:VAL:C[1_554]   | 2.15                     | 0.05              |
| 4:3:367:PRO:CB  | 4:8:236:LEU:N[1_554]   | 2.15                     | 0.05              |
| 4:3:335:ARG:N   | 4:7:105:LEU:CB[1_554]  | 2.15                     | 0.05              |
| 4:3:213:LYS:C   | 4:7:16:LEU:CB[1_554]   | 2.15                     | 0.05              |
| 4:5:219:VAL:CG2 | 4:9:300:SER:O[1_554]   | 2.15                     | 0.05              |
| 4:3:340:TRP:CE2 | 4:7:121:GLN:OE1[1_554] | 2.15                     | 0.05              |
| 4:4:286:ASP:OD2 | 4:V:39:ARG:CZ[1_554]   | 2.15                     | 0.05              |
| 4:3:215:LYS:CA  | 4:7:17:VAL:O[1_554]    | 2.15                     | 0.05              |
| 4:3:219:VAL:O   | 4:7:338:SER:CB[1_554]  | 2.15                     | 0.05              |
| 4:4:204:ALA:CA  | 4:8:62:ARG:CG[1_554]   | 2.15                     | 0.05              |
| 4:3:308:GLY:O   | 4:7:339:VAL:N[1_554]   | 2.15                     | 0.05              |
| 4:3:250:ILE:CG2 | 4:7:214:GLU:OE2[1_554] | 2.15                     | 0.05              |
| 4:4:332:PRO:CB  | 4:8:133:TYR:CD2[1_554] | 2.15                     | 0.05              |
| 4:4:318:THR:CA  | 4:8:150:GLY:N[1_554]   | 2.15                     | 0.05              |
| 4:3:262:PHE:CZ  | 4:7:152:VAL:CG1[1_554] | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:294:TYR:CB  | 4:8:166:TYR:CB[1_554]  | 2.15                     | 0.05              |
| 4:2:110:LEU:O   | 4:7:189:LEU:O[1_554]   | 2.15                     | 0.05              |
| 4:4:340:TRP:CG  | 4:8:118:LYS:CB[1_554]  | 2.15                     | 0.05              |
| 4:4:306:TYR:N   | 4:8:11:ASP:CG[1_554]   | 2.15                     | 0.05              |
| 4:5:334:GLU:OE1 | 4:9:134:VAL:N[1_554]   | 2.15                     | 0.05              |
| 4:4:333:PRO:N   | 4:8:104:LEU:CD2[1_554] | 2.15                     | 0.05              |
| 4:4:312:ARG:C   | 4:8:298:VAL:CG1[1_554] | 2.15                     | 0.05              |
| 4:3:185:LEU:O   | 4:7:157:ASP:CA[1_554]  | 2.15                     | 0.05              |
| 4:4:222:ASP:O   | 4:8:331:ALA:C[1_554]   | 2.15                     | 0.05              |
| 4:2:110:LEU:CG  | 4:7:191:LYS:CG[1_554]  | 2.15                     | 0.05              |
| 4:1:289:ILE:CA  | 4:7:39:ARG:NH2[1_554]  | 2.15                     | 0.05              |
| 4:4:257:CYS:O   | 4:8:156:GLY:N[1_554]   | 2.15                     | 0.05              |
| 4:4:15:GLY:CA   | 4:8:77:THR:CA[1_554]   | 2.15                     | 0.05              |
| 4:5:140:LEU:CA  | 4:9:371:HIS:CA[1_554]  | 2.15                     | 0.05              |
| 4:4:344:SER:N   | 4:8:367:PRO:CA[1_554]  | 2.15                     | 0.05              |
| 4:3:327:ILE:CG1 | 4:7:148:THR:C[1_554]   | 2.15                     | 0.05              |
| 4:3:309:ILE:C   | 4:7:141:SER:N[1_554]   | 2.15                     | 0.05              |
| 4:4:283:MET:CG  | 4:8:286:ASP:CB[1_554]  | 2.15                     | 0.05              |
| 4:3:337:TYR:O   | 4:7:119:MET:CG[1_554]  | 2.15                     | 0.05              |
| 4:5:205:GLU:N   | 4:9:62:ARG:CG[1_554]   | 2.15                     | 0.05              |
| 4:5:224:GLU:N   | 4:9:310:ALA:CB[1_554]  | 2.15                     | 0.05              |
| 4:2:292:ASP:N   | 4:8:64:ILE:CG2[1_554]  | 2.15                     | 0.05              |
| 4:3:217:CYS:O   | 4:7:18:LYS:CE[1_554]   | 2.15                     | 0.05              |
| 4:5:188:TYR:CD2 | 4:9:182:GLY:N[1_554]   | 2.15                     | 0.05              |
| 4:3:17:VAL:C    | 4:7:79:TRP:CG[1_554]   | 2.15                     | 0.05              |
| 4:4:142:LEU:C   | 4:8:371:HIS:C[1_554]   | 2.15                     | 0.05              |
| 4:2:109:PRO:CA  | 4:7:195:GLU:OE2[1_554] | 2.15                     | 0.05              |
| 4:4:143:TYR:CE2 | 4:8:368:SER:CA[1_554]  | 2.15                     | 0.05              |
| 4:5:210:ARG:CZ  | 4:9:34:ILE:N[1_554]    | 2.15                     | 0.05              |
| 4:5:143:TYR:CE2 | 4:9:368:SER:O[1_554]   | 2.15                     | 0.05              |
| 4:2:172:PRO:CA  | 4:7:188:TYR:CZ[1_554]  | 2.15                     | 0.05              |
| 4:5:188:TYR:OH  | 4:9:185:LEU:CG[1_554]  | 2.15                     | 0.05              |
| 4:5:296:ASN:N   | 4:9:168:GLY:N[1_554]   | 2.15                     | 0.05              |
| 4:4:263:GLN:CD  | 4:8:153:LEU:CD2[1_554] | 2.15                     | 0.05              |
| 4:5:175:ILE:CD1 | 4:V:191:LYS:NZ[1_554]  | 2.15                     | 0.05              |
| 4:4:144:ALA:O   | 4:8:370:VAL:CA[1_554]  | 2.15                     | 0.05              |
| 4:4:320:LEU:CD2 | 4:8:293:LEU:CB[1_554]  | 2.15                     | 0.05              |
| 4:4:172:PRO:CD  | 4:9:266:PHE:CG[1_554]  | 2.15                     | 0.05              |
| 4:4:193:LEU:N   | 4:8:210:ARG:CA[1_554]  | 2.15                     | 0.05              |
| 4:5:304:THR:N   | 4:9:137:GLN:NE2[1_554] | 2.15                     | 0.05              |
| 4:3:25:ASP:C    | 4:7:121:GLN:O[1_554]   | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:30:VAL:O    | 4:9:82:MET:N[1_554]    | 2.15                     | 0.05              |
| 4:5:220:ALA:CB  | 4:9:335:ARG:CZ[1_554]  | 2.15                     | 0.05              |
| 4:3:338:SER:OG  | 4:7:134:VAL:CG1[1_554] | 2.15                     | 0.05              |
| 4:5:218:TYR:CD1 | 4:9:336:LYS:CD[1_554]  | 2.15                     | 0.05              |
| 4:4:75:ILE:CG1  | 4:9:193:LEU:C[1_554]   | 2.15                     | 0.05              |
| 4:3:267:ILE:CB  | 4:7:180:LEU:CA[1_554]  | 2.15                     | 0.05              |
| 4:5:286:ASP:OD2 | 4:W:39:ARG:CZ[1_554]   | 2.15                     | 0.05              |
| 4:3:315:LYS:CB  | 4:7:145:SER:OG[1_554]  | 2.15                     | 0.05              |
| 4:5:294:TYR:CD2 | 4:9:166:TYR:CB[1_554]  | 2.15                     | 0.05              |
| 4:3:345:ILE:CB  | 4:7:368:SER:N[1_554]   | 2.15                     | 0.05              |
| 4:4:299:MET:CB  | 4:8:137:GLN:N[1_554]   | 2.15                     | 0.05              |
| 4:5:269:MET:C   | 4:9:272:ALA:C[1_554]   | 2.15                     | 0.05              |
| 4:5:254:ARG:NE  | 4:9:336:LYS:CD[1_554]  | 2.15                     | 0.05              |
| 4:4:196:ARG:NE  | 4:8:211:ASP:OD2[1_554] | 2.15                     | 0.05              |
| 4:4:222:ASP:O   | 4:8:335:ARG:NH1[1_554] | 2.15                     | 0.05              |
| 4:5:182:GLY:O   | 4:9:158:GLY:N[1_554]   | 2.15                     | 0.05              |
| 4:4:339:VAL:O   | 4:8:116:ARG:C[1_554]   | 2.15                     | 0.05              |
| 4:4:173:HIS:CG  | 4:9:267:ILE:CA[1_554]  | 2.15                     | 0.05              |
| 4:4:299:MET:C   | 4:8:136:ILE:CG1[1_554] | 2.15                     | 0.05              |
| 4:3:218:TYR:CG  | 4:7:337:TYR:CG[1_554]  | 2.15                     | 0.05              |
| 4:3:329:ILE:CD1 | 4:7:165:ILE:CG2[1_554] | 2.15                     | 0.05              |
| 4:3:256:ARG:O   | 4:7:303:THR:N[1_554]   | 2.15                     | 0.05              |
| 4:4:27:PRO:N    | 4:8:122:ILE:CG2[1_554] | 2.15                     | 0.05              |
| 4:4:314:GLN:CG  | 4:8:147:ARG:O[1_554]   | 2.15                     | 0.05              |
| 4:3:186:THR:CG2 | 4:7:183:ARG:CZ[1_554]  | 2.15                     | 0.05              |
| 4:4:18:LYS:O    | 4:8:118:LYS:CD[1_554]  | 2.15                     | 0.05              |
| 4:5:275:HIS:N   | 4:9:162:ASN:C[1_554]   | 2.15                     | 0.05              |
| 4:5:215:LYS:CE  | 4:9:30:VAL:O[1_554]    | 2.15                     | 0.05              |
| 4:4:311:ASP:OD1 | 4:8:144:ALA:C[1_554]   | 2.15                     | 0.05              |
| 4:3:198:TYR:C   | 4:7:207:GLU:N[1_554]   | 2.15                     | 0.05              |
| 4:4:292:ASP:N   | 4:V:64:ILE:CG2[1_554]  | 2.15                     | 0.05              |
| 4:3:309:ILE:CG1 | 4:7:137:GLN:CB[1_554]  | 2.15                     | 0.05              |
| 4:3:316:GLU:OE2 | 4:7:298:VAL:O[1_554]   | 2.15                     | 0.05              |
| 4:5:340:TRP:O   | 4:9:117:GLU:O[1_554]   | 2.15                     | 0.05              |
| 4:2:368:SER:O   | 4:7:236:LEU:CB[1_554]  | 2.15                     | 0.05              |
| 4:5:328:LYS:N   | 4:9:148:THR:CB[1_554]  | 2.15                     | 0.05              |
| 4:5:329:ILE:CG2 | 4:9:139:VAL:O[1_554]   | 2.15                     | 0.05              |
| 4:5:261:LEU:CB  | 4:9:155:SER:N[1_554]   | 2.15                     | 0.05              |
| 4:5:214:GLU:CB  | 4:9:16:LEU:O[1_554]    | 2.15                     | 0.05              |
| 4:4:41:GLN:CD   | 4:7:224:GLU:CD[1_554]  | 2.15                     | 0.05              |
| 4:5:212:ILE:O   | 4:9:16:LEU:CG[1_554]   | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:299:MET:CA  | 4:8:136:ILE:N[1_554]   | 2.15                     | 0.05              |
| 4:3:306:TYR:O   | 4:7:11:ASP:OD2[1_554]  | 2.15                     | 0.05              |
| 4:3:213:LYS:CD  | 4:7:15:GLY:CA[1_554]   | 2.15                     | 0.05              |
| 4:5:41:GLN:CB   | 4:8:224:GLU:OE2[1_554] | 2.15                     | 0.05              |
| 4:5:310:ALA:C   | 4:9:142:LEU:CA[1_554]  | 2.15                     | 0.05              |
| 4:5:334:GLU:C   | 4:9:106:THR:N[1_554]   | 2.15                     | 0.05              |
| 4:4:18:LYS:CG   | 4:8:79:TRP:CH2[1_554]  | 2.15                     | 0.05              |
| 4:2:74:GLY:C    | 4:7:197:GLY:O[1_554]   | 2.15                     | 0.05              |
| 4:5:294:TYR:C   | 4:9:166:TYR:CA[1_554]  | 2.15                     | 0.05              |
| 4:3:25:ASP:CA   | 4:7:124:PHE:C[1_554]   | 2.15                     | 0.05              |
| 4:4:160:THR:N   | 4:8:177:ARG:CZ[1_554]  | 2.15                     | 0.05              |
| 4:2:371:HIS:ND1 | 4:7:251:GLY:C[1_554]   | 2.15                     | 0.05              |
| 4:3:281:SER:OG  | 4:7:172:PRO:O[1_554]   | 2.15                     | 0.05              |
| 4:4:153:LEU:CD1 | 4:8:109:PRO:CB[1_554]  | 2.15                     | 0.05              |
| 4:4:335:ARG:CB  | 4:8:107:GLU:N[1_554]   | 2.15                     | 0.05              |
| 4:4:326:LYS:NZ  | 4:V:45:VAL:CA[1_554]   | 2.15                     | 0.05              |
| 4:5:280:ASN:C   | 4:9:174:ALA:CB[1_554]  | 2.15                     | 0.05              |
| 4:4:276:GLU:O   | 4:8:281:SER:CB[1_554]  | 2.15                     | 0.05              |
| 4:3:337:TYR:CZ  | 4:7:86:TRP:CE3[1_554]  | 2.15                     | 0.05              |
| 4:3:182:GLY:CA  | 4:7:73:HIS:CA[1_554]   | 2.15                     | 0.05              |
| 4:3:309:ILE:CD1 | 4:7:137:GLN:CB[1_554]  | 2.15                     | 0.05              |
| 4:4:144:ALA:CB  | 4:8:370:VAL:CB[1_554]  | 2.15                     | 0.05              |
| 4:4:183:ARG:CG  | 4:8:72:GLU:CD[1_554]   | 2.15                     | 0.05              |
| 4:3:357:ILE:CD1 | 4:8:232:SER:CA[1_554]  | 2.15                     | 0.05              |
| 4:4:226:GLU:CD  | 4:8:333:PRO:C[1_554]   | 2.15                     | 0.05              |
| 4:4:141:SER:CB  | 4:8:116:ARG:NE[1_554]  | 2.15                     | 0.05              |
| 4:3:278:THR:CB  | 4:7:164:PRO:N[1_554]   | 2.15                     | 0.05              |
| 4:4:334:GLU:OE1 | 4:8:133:TYR:N[1_554]   | 2.15                     | 0.05              |
| 4:3:172:PRO:O   | 4:8:266:PHE:O[1_554]   | 2.15                     | 0.05              |
| 4:4:279:TYR:CG  | 4:8:285:CYS:SG[1_554]  | 2.15                     | 0.05              |
| 4:5:16:LEU:N    | 4:9:76:ILE:C[1_554]    | 2.15                     | 0.05              |
| 4:5:349:LEU:C   | 4:9:364:GLU:C[1_554]   | 2.15                     | 0.05              |
| 4:3:299:MET:SD  | 4:7:136:ILE:CB[1_554]  | 2.15                     | 0.05              |
| 4:3:335:ARG:CB  | 4:7:106:THR:C[1_554]   | 2.15                     | 0.05              |
| 4:5:21:PHE:C    | 4:9:125:GLU:OE2[1_554] | 2.15                     | 0.05              |
| 4:1:288:ASP:OD1 | 4:7:66:THR:CA[1_554]   | 2.15                     | 0.05              |
| 4:3:312:ARG:CD  | 4:7:299:MET:N[1_554]   | 2.15                     | 0.05              |
| 4:4:346:LEU:CD2 | 4:8:368:SER:OG[1_554]  | 2.15                     | 0.05              |
| 4:3:172:PRO:CD  | 4:8:266:PHE:CA[1_554]  | 2.15                     | 0.05              |
| 4:5:173:HIS:CA  | 4:V:267:ILE:CG2[1_554] | 2.15                     | 0.05              |
| 4:4:326:LYS:CE  | 4:V:44:MET:C[1_554]    | 2.15                     | 0.05              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:218:TYR:CD2 | 4:7:337:TYR:CB[1_554]  | 2.15                     | 0.05              |
| 4:5:178:LEU:C   | 4:9:177:ARG:CG[1_554]  | 2.15                     | 0.05              |
| 4:4:294:TYR:O   | 4:8:168:GLY:CA[1_554]  | 2.15                     | 0.05              |
| 4:5:204:ALA:O   | 4:9:62:ARG:NE[1_554]   | 2.15                     | 0.05              |
| 4:3:166:TYR:CE1 | 4:9:40:HIS:CD2[1_554]  | 2.16                     | 0.04              |
| 4:4:181:ALA:CB  | 4:8:73:HIS:C[1_554]    | 2.16                     | 0.04              |
| 4:5:266:PHE:N   | 4:9:261:LEU:CB[1_554]  | 2.16                     | 0.04              |
| 4:5:289:ILE:CB  | 4:W:63:GLY:O[1_554]    | 2.16                     | 0.04              |
| 4:5:139:VAL:C   | 4:9:371:HIS:NE2[1_554] | 2.16                     | 0.04              |
| 4:5:319:ALA:C   | 4:9:294:TYR:CA[1_554]  | 2.16                     | 0.04              |
| 1:D:411:GLU:OE1 | 4:5:226:GLU:OE2[1_556] | 2.16                     | 0.04              |
| 4:5:21:PHE:CA   | 4:9:125:GLU:CB[1_554]  | 2.16                     | 0.04              |
| 4:3:329:ILE:CB  | 4:7:139:VAL:CA[1_554]  | 2.16                     | 0.04              |
| 4:2:73:HIS:CB   | 4:7:199:SER:OG[1_554]  | 2.16                     | 0.04              |
| 4:4:311:ASP:O   | 4:8:141:SER:O[1_554]   | 2.16                     | 0.04              |
| 4:1:287:ILE:O   | 4:7:39:ARG:NH1[1_554]  | 2.16                     | 0.04              |
| 4:5:113:LYS:C   | 4:V:252:ASN:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:218:TYR:CE2 | 4:8:337:TYR:CZ[1_554]  | 2.16                     | 0.04              |
| 4:4:255:PHE:O   | 4:8:304:THR:N[1_554]   | 2.16                     | 0.04              |
| 4:3:173:HIS:C   | 4:8:267:ILE:N[1_554]   | 2.16                     | 0.04              |
| 4:3:113:LYS:N   | 4:8:250:ILE:CG2[1_554] | 2.16                     | 0.04              |
| 4:4:204:ALA:CA  | 4:8:62:ARG:C[1_554]    | 2.16                     | 0.04              |
| 4:2:370:VAL:C   | 4:7:230:ALA:CB[1_554]  | 2.16                     | 0.04              |
| 4:5:276:GLU:OE2 | 4:9:279:TYR:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:218:TYR:CE1 | 4:8:337:TYR:CG[1_554]  | 2.16                     | 0.04              |
| 4:3:223:PHE:C   | 4:7:335:ARG:NH1[1_554] | 2.16                     | 0.04              |
| 4:4:114:ALA:N   | 4:9:250:ILE:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:212:ILE:O   | 4:8:16:LEU:CD2[1_554]  | 2.16                     | 0.04              |
| 4:5:223:PHE:CB  | 4:9:309:ILE:CG2[1_554] | 2.16                     | 0.04              |
| 4:5:16:LEU:CA   | 4:9:77:THR:N[1_554]    | 2.16                     | 0.04              |
| 4:5:192:ILE:N   | 4:9:185:LEU:O[1_554]   | 2.16                     | 0.04              |
| 4:3:177:ARG:NH1 | 4:8:194:THR:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:371:HIS:N   | 4:9:230:ALA:N[1_554]   | 2.16                     | 0.04              |
| 4:5:288:ASP:OD1 | 4:W:62:ARG:O[1_554]    | 2.16                     | 0.04              |
| 4:3:277:THR:CA  | 4:7:175:ILE:CA[1_554]  | 2.16                     | 0.04              |
| 4:3:116:ARG:O   | 4:8:237:GLU:CD[1_554]  | 2.16                     | 0.04              |
| 4:3:181:ALA:CA  | 4:7:73:HIS:CB[1_554]   | 2.16                     | 0.04              |
| 4:3:221:LEU:O   | 4:7:332:PRO:N[1_554]   | 2.16                     | 0.04              |
| 4:4:371:HIS:CE1 | 4:9:252:ASN:CB[1_554]  | 2.16                     | 0.04              |
| 4:4:337:TYR:CB  | 4:8:119:MET:C[1_554]   | 2.16                     | 0.04              |
| 4:4:313:MET:CE  | 4:8:163:VAL:CG1[1_554] | 2.16                     | 0.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:155:SER:O   | 4:7:108:ALA:CB[1_554]  | 2.16                     | 0.04              |
| 4:3:371:HIS:NE2 | 4:8:255:PHE:CD2[1_554] | 2.16                     | 0.04              |
| 4:3:26:ALA:N    | 4:7:122:ILE:N[1_554]   | 2.16                     | 0.04              |
| 4:3:218:TYR:CB  | 4:7:336:LYS:CA[1_554]  | 2.16                     | 0.04              |
| 4:5:334:GLU:CA  | 4:9:104:LEU:O[1_554]   | 2.16                     | 0.04              |
| 4:4:41:GLN:CB   | 4:7:224:GLU:OE1[1_554] | 2.16                     | 0.04              |
| 4:3:256:ARG:NH1 | 4:7:306:TYR:CZ[1_554]  | 2.16                     | 0.04              |
| 4:5:224:GLU:OE2 | 4:9:311:ASP:OD1[1_554] | 2.16                     | 0.04              |
| 4:5:367:PRO:CB  | 4:V:233:SER:CB[1_554]  | 2.16                     | 0.04              |
| 4:3:340:TRP:CE3 | 4:7:118:LYS:O[1_554]   | 2.16                     | 0.04              |
| 4:5:26:ALA:CB   | 4:9:123:MET:CA[1_554]  | 2.16                     | 0.04              |
| 4:5:341:ILE:CA  | 4:9:120:THR:CG2[1_554] | 2.16                     | 0.04              |
| 4:4:333:PRO:C   | 4:8:104:LEU:O[1_554]   | 2.16                     | 0.04              |
| 4:5:213:LYS:C   | 4:9:16:LEU:CG[1_554]   | 2.16                     | 0.04              |
| 4:3:180:LEU:CG  | 4:7:178:LEU:N[1_554]   | 2.16                     | 0.04              |
| 4:4:198:TYR:CE1 | 4:8:208:ILE:CB[1_554]  | 2.16                     | 0.04              |
| 4:3:26:ALA:O    | 4:7:121:GLN:O[1_554]   | 2.16                     | 0.04              |
| 4:5:345:ILE:CD1 | 4:9:357:ILE:CG1[1_554] | 2.16                     | 0.04              |
| 4:5:30:VAL:CB   | 4:9:82:MET:CB[1_554]   | 2.16                     | 0.04              |
| 4:4:181:ALA:O   | 4:8:159:VAL:N[1_554]   | 2.16                     | 0.04              |
| 4:4:164:PRO:CA  | 4:8:172:PRO:CG[1_554]  | 2.16                     | 0.04              |
| 4:4:294:TYR:OH  | 4:8:289:ILE:CG1[1_554] | 2.16                     | 0.04              |
| 4:3:220:ALA:O   | 4:7:300:SER:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:27:PRO:CD   | 4:8:122:ILE:CA[1_554]  | 2.16                     | 0.04              |
| 4:5:275:HIS:CE1 | 4:9:278:THR:OG1[1_554] | 2.16                     | 0.04              |
| 4:5:227:MET:C   | 4:9:307:PRO:CG[1_554]  | 2.16                     | 0.04              |
| 4:3:322:PRO:CA  | 4:7:291:LYS:NZ[1_554]  | 2.16                     | 0.04              |
| 4:3:112:PRO:C   | 4:8:253:GLU:CD[1_554]  | 2.16                     | 0.04              |
| 4:4:344:SER:O   | 4:8:366:GLY:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:339:VAL:CA  | 4:8:115:ASN:C[1_554]   | 2.16                     | 0.04              |
| 4:3:335:ARG:CD  | 4:7:106:THR:CB[1_554]  | 2.16                     | 0.04              |
| 4:4:310:ALA:CA  | 4:8:141:SER:CA[1_554]  | 2.16                     | 0.04              |
| 4:5:181:ALA:C   | 4:9:158:GLY:C[1_554]   | 2.16                     | 0.04              |
| 4:3:193:LEU:O   | 4:7:210:ARG:CB[1_554]  | 2.16                     | 0.04              |
| 4:5:30:VAL:CB   | 4:9:82:MET:CA[1_554]   | 2.16                     | 0.04              |
| 4:3:277:THR:O   | 4:7:174:ALA:O[1_554]   | 2.16                     | 0.04              |
| 4:4:161:HIS:O   | 4:8:110:LEU:CD2[1_554] | 2.16                     | 0.04              |
| 4:5:307:PRO:CG  | 4:9:337:TYR:CB[1_554]  | 2.16                     | 0.04              |
| 4:3:145:SER:CA  | 4:7:370:VAL:O[1_554]   | 2.16                     | 0.04              |
| 4:4:179:ASP:C   | 4:8:179:ASP:CG[1_554]  | 2.16                     | 0.04              |
| 4:3:334:GLU:CD  | 4:7:132:MET:SD[1_554]  | 2.16                     | 0.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:138:ALA:C   | 4:7:113:LYS:CG[1_554]  | 2.16                     | 0.04              |
| 4:4:339:VAL:C   | 4:8:116:ARG:CA[1_554]  | 2.16                     | 0.04              |
| 4:5:204:ALA:CB  | 4:9:62:ARG:C[1_554]    | 2.16                     | 0.04              |
| 4:5:299:MET:CA  | 4:9:136:ILE:O[1_554]   | 2.16                     | 0.04              |
| 4:3:367:PRO:CD  | 4:8:236:LEU:N[1_554]   | 2.16                     | 0.04              |
| 4:4:337:TYR:CD2 | 4:8:86:TRP:CH2[1_554]  | 2.16                     | 0.04              |
| 4:3:370:VAL:CG2 | 4:8:231:ALA:CA[1_554]  | 2.16                     | 0.04              |
| 4:3:281:SER:CB  | 4:7:171:LEU:O[1_554]   | 2.16                     | 0.04              |
| 4:5:16:LEU:O    | 4:9:76:ILE:C[1_554]    | 2.16                     | 0.04              |
| 4:5:110:LEU:O   | 4:V:193:LEU:N[1_554]   | 2.16                     | 0.04              |
| 4:4:315:LYS:CE  | 4:8:147:ARG:NH2[1_554] | 2.16                     | 0.04              |
| 4:3:341:ILE:CD1 | 4:7:120:THR:OG1[1_554] | 2.16                     | 0.04              |
| 4:5:218:TYR:CG  | 4:9:336:LYS:CD[1_554]  | 2.16                     | 0.04              |
| 4:5:188:TYR:CZ  | 4:9:185:LEU:CB[1_554]  | 2.16                     | 0.04              |
| 4:4:188:TYR:N   | 4:8:183:ARG:N[1_554]   | 2.16                     | 0.04              |
| 4:3:18:LYS:NZ   | 4:7:79:TRP:NE1[1_554]  | 2.16                     | 0.04              |
| 4:3:157:ASP:OD1 | 4:7:71:ILE:C[1_554]    | 2.16                     | 0.04              |
| 4:5:345:ILE:CD1 | 4:9:357:ILE:CB[1_554]  | 2.16                     | 0.04              |
| 4:4:196:ARG:CD  | 4:8:211:ASP:CG[1_554]  | 2.16                     | 0.04              |
| 4:2:75:ILE:N    | 4:7:197:GLY:O[1_554]   | 2.16                     | 0.04              |
| 4:3:173:HIS:NE2 | 4:8:264:PRO:C[1_554]   | 2.16                     | 0.04              |
| 4:4:193:LEU:N   | 4:8:186:THR:OG1[1_554] | 2.16                     | 0.04              |
| 4:1:292:ASP:OD1 | 4:7:41:GLN:N[1_554]    | 2.16                     | 0.04              |
| 4:4:30:VAL:O    | 4:8:80:ASP:CB[1_554]   | 2.16                     | 0.04              |
| 4:3:144:ALA:CA  | 4:7:370:VAL:N[1_554]   | 2.16                     | 0.04              |
| 4:4:283:MET:CB  | 4:8:286:ASP:CA[1_554]  | 2.16                     | 0.04              |
| 4:3:221:LEU:O   | 4:7:332:PRO:CD[1_554]  | 2.16                     | 0.04              |
| 4:4:344:SER:C   | 4:8:367:PRO:CA[1_554]  | 2.16                     | 0.04              |
| 4:5:166:TYR:CD2 | 4:W:40:HIS:ND1[1_554]  | 2.16                     | 0.04              |
| 4:3:335:ARG:CD  | 4:7:135:ALA:O[1_554]   | 2.16                     | 0.04              |
| 4:5:179:ASP:C   | 4:9:179:ASP:CG[1_554]  | 2.16                     | 0.04              |
| 4:5:312:ARG:C   | 4:9:298:VAL:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:16:LEU:CA   | 4:8:77:THR:CA[1_554]   | 2.16                     | 0.04              |
| 4:4:111:ASN:O   | 4:9:253:GLU:CD[1_554]  | 2.16                     | 0.04              |
| 4:2:111:ASN:CB  | 4:7:196:ARG:CG[1_554]  | 2.16                     | 0.04              |
| 4:4:116:ARG:O   | 4:9:237:GLU:OE2[1_554] | 2.16                     | 0.04              |
| 4:3:188:TYR:CD1 | 4:7:185:LEU:CB[1_554]  | 2.16                     | 0.04              |
| 4:3:345:ILE:CA  | 4:7:367:PRO:CD[1_554]  | 2.16                     | 0.04              |
| 4:4:173:HIS:ND1 | 4:9:266:PHE:C[1_554]   | 2.16                     | 0.04              |
| 4:5:255:PHE:CB  | 4:9:305:MET:CA[1_554]  | 2.16                     | 0.04              |
| 4:4:27:PRO:CD   | 4:8:122:ILE:CG1[1_554] | 2.16                     | 0.04              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:191:LYS:CG  | 4:8:184:ASP:O[1_554]   | 2.16                     | 0.04              |
| 4:3:325:MET:CE  | 4:7:166:TYR:OH[1_554]  | 2.16                     | 0.04              |
| 4:4:305:MET:CE  | 4:8:11:ASP:N[1_554]    | 2.16                     | 0.04              |
| 4:5:327:ILE:O   | 4:9:148:THR:CG2[1_554] | 2.16                     | 0.04              |
| 4:3:320:LEU:CA  | 4:7:292:ASP:C[1_554]   | 2.16                     | 0.04              |
| 4:2:371:HIS:ND1 | 4:7:252:ASN:C[1_554]   | 2.16                     | 0.04              |
| 4:2:370:VAL:CB  | 4:7:233:SER:CA[1_554]  | 2.16                     | 0.04              |
| 4:5:161:HIS:N   | 4:9:110:LEU:CG[1_554]  | 2.16                     | 0.04              |
| 4:3:182:GLY:CA  | 4:7:73:HIS:N[1_554]    | 2.16                     | 0.04              |
| 4:4:143:TYR:CA  | 4:8:372:ARG:C[1_554]   | 2.16                     | 0.04              |
| 4:3:192:ILE:CD1 | 4:7:213:LYS:CE[1_554]  | 2.16                     | 0.04              |
| 4:3:196:ARG:O   | 4:7:212:ILE:CG1[1_554] | 2.16                     | 0.04              |
| 4:4:273:GLY:CA  | 4:8:162:ASN:ND2[1_554] | 2.16                     | 0.04              |
| 4:2:368:SER:O   | 4:7:236:LEU:CD1[1_554] | 2.16                     | 0.04              |
| 4:3:346:LEU:CB  | 4:7:368:SER:OG[1_554]  | 2.16                     | 0.04              |
| 4:2:166:TYR:CE1 | 4:8:39:ARG:O[1_554]    | 2.16                     | 0.04              |
| 4:4:254:ARG:NH2 | 4:8:337:TYR:CZ[1_554]  | 2.16                     | 0.04              |
| 4:4:325:MET:CB  | 4:8:166:TYR:CE1[1_554] | 2.16                     | 0.04              |
| 4:4:164:PRO:CD  | 4:8:172:PRO:CG[1_554]  | 2.16                     | 0.04              |
| 4:2:76:ILE:N    | 4:7:198:TYR:CZ[1_554]  | 2.17                     | 0.03              |
| 4:4:108:ALA:CA  | 4:9:195:GLU:C[1_554]   | 2.17                     | 0.03              |
| 4:3:25:ASP:N    | 4:7:125:GLU:CA[1_554]  | 2.17                     | 0.03              |
| 4:5:328:LYS:CD  | 4:W:45:VAL:CG2[1_554]  | 2.17                     | 0.03              |
| 4:3:191:LYS:O   | 4:7:186:THR:O[1_554]   | 2.17                     | 0.03              |
| 4:3:326:LYS:NZ  | 4:9:45:VAL:N[1_554]    | 2.17                     | 0.03              |
| 4:4:340:TRP:CE2 | 4:8:121:GLN:CG[1_554]  | 2.17                     | 0.03              |
| 4:4:262:PHE:CB  | 4:8:153:LEU:O[1_554]   | 2.17                     | 0.03              |
| 4:4:335:ARG:N   | 4:8:105:LEU:C[1_554]   | 2.17                     | 0.03              |
| 4:4:25:ASP:C    | 4:8:124:PHE:CA[1_554]  | 2.17                     | 0.03              |
| 4:5:262:PHE:CA  | 4:9:153:LEU:CD2[1_554] | 2.17                     | 0.03              |
| 4:3:211:ASP:OD1 | 4:7:32:PRO:O[1_554]    | 2.17                     | 0.03              |
| 4:3:243:PRO:CG  | 4:7:62:ARG:N[1_554]    | 2.17                     | 0.03              |
| 4:5:188:TYR:CG  | 4:9:181:ALA:C[1_554]   | 2.17                     | 0.03              |
| 4:4:173:HIS:CA  | 4:9:266:PHE:C[1_554]   | 2.17                     | 0.03              |
| 4:4:208:ILE:CA  | 4:8:59:GLN:CD[1_554]   | 2.17                     | 0.03              |
| 4:3:254:ARG:NH2 | 4:7:337:TYR:CZ[1_554]  | 2.17                     | 0.03              |
| 4:3:149:THR:CG2 | 4:9:40:HIS:CG[1_554]   | 2.17                     | 0.03              |
| 4:4:198:TYR:CD2 | 4:8:208:ILE:C[1_554]   | 2.17                     | 0.03              |
| 4:4:326:LYS:NZ  | 4:V:45:VAL:CG2[1_554]  | 2.17                     | 0.03              |
| 4:3:264:PRO:O   | 4:7:178:LEU:CD2[1_554] | 2.17                     | 0.03              |
| 4:5:338:SER:N   | 4:9:134:VAL:CG1[1_554] | 2.17                     | 0.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:369:ILE:CG2 | 4:9:232:SER:C[1_554]   | 2.17                     | 0.03              |
| 4:4:320:LEU:O   | 4:8:293:LEU:N[1_554]   | 2.17                     | 0.03              |
| 4:5:31:PHE:N    | 4:9:79:TRP:O[1_554]    | 2.17                     | 0.03              |
| 4:5:343:GLY:O   | 4:9:367:PRO:CD[1_554]  | 2.17                     | 0.03              |
| 4:5:318:THR:N   | 4:9:296:ASN:CB[1_554]  | 2.17                     | 0.03              |
| 4:3:215:LYS:O   | 4:7:30:VAL:CB[1_554]   | 2.17                     | 0.03              |
| 4:3:357:ILE:CD1 | 4:8:232:SER:OG[1_554]  | 2.17                     | 0.03              |
| 4:3:264:PRO:CB  | 4:7:178:LEU:CB[1_554]  | 2.17                     | 0.03              |
| 4:5:31:PHE:CD2  | 4:9:80:ASP:CB[1_554]   | 2.17                     | 0.03              |
| 4:5:300:SER:CA  | 4:9:107:GLU:C[1_554]   | 2.17                     | 0.03              |
| 4:4:333:PRO:N   | 4:8:104:LEU:CB[1_554]  | 2.17                     | 0.03              |
| 4:5:266:PHE:CE1 | 4:9:261:LEU:CD1[1_554] | 2.17                     | 0.03              |
| 1:A:637:LYS:CB  | 4:4:311:ASP:CG[1_556]  | 2.17                     | 0.03              |
| 4:5:294:TYR:CD2 | 4:9:166:TYR:CE1[1_554] | 2.17                     | 0.03              |
| 4:5:117:GLU:CD  | 4:V:236:LEU:CD1[1_554] | 2.17                     | 0.03              |
| 4:3:115:ASN:ND2 | 4:8:249:THR:O[1_554]   | 2.17                     | 0.03              |
| 4:3:215:LYS:C   | 4:7:17:VAL:O[1_554]    | 2.17                     | 0.03              |
| 4:5:31:PHE:CA   | 4:9:81:ASP:CA[1_554]   | 2.17                     | 0.03              |
| 4:5:336:LYS:CE  | 4:9:12:ASN:OD1[1_554]  | 2.17                     | 0.03              |
| 4:4:110:LEU:CA  | 4:9:192:ILE:N[1_554]   | 2.17                     | 0.03              |
| 4:5:370:VAL:CB  | 4:V:231:ALA:C[1_554]   | 2.17                     | 0.03              |
| 4:5:154:ASP:N   | 4:9:110:LEU:N[1_554]   | 2.17                     | 0.03              |
| 4:4:191:LYS:O   | 4:8:186:THR:CB[1_554]  | 2.17                     | 0.03              |
| 4:4:366:GLY:CA  | 4:9:234:SER:CA[1_554]  | 2.17                     | 0.03              |
| 4:5:28:ARG:NH2  | 4:9:125:GLU:C[1_554]   | 2.17                     | 0.03              |
| 4:4:266:PHE:N   | 4:8:261:LEU:CD2[1_554] | 2.17                     | 0.03              |
| 4:4:266:PHE:CE2 | 4:8:261:LEU:CD1[1_554] | 2.17                     | 0.03              |
| 4:3:145:SER:OG  | 4:7:372:ARG:NH2[1_554] | 2.17                     | 0.03              |
| 4:3:255:PHE:N   | 4:7:302:GLY:CA[1_554]  | 2.17                     | 0.03              |
| 4:4:60:SER:C    | 4:8:66:THR:OG1[1_554]  | 2.17                     | 0.03              |
| 4:3:172:PRO:C   | 4:8:266:PHE:C[1_554]   | 2.17                     | 0.03              |
| 4:3:256:ARG:N   | 4:7:302:GLY:CA[1_554]  | 2.17                     | 0.03              |
| 4:4:260:THR:C   | 4:8:155:SER:CB[1_554]  | 2.17                     | 0.03              |
| 4:5:331:ALA:N   | 4:9:140:LEU:CD2[1_554] | 2.17                     | 0.03              |
| 4:5:255:PHE:C   | 4:9:305:MET:N[1_554]   | 2.17                     | 0.03              |
| 4:4:187:ASP:O   | 4:8:184:ASP:N[1_554]   | 2.17                     | 0.03              |
| 4:5:369:ILE:C   | 4:V:232:SER:N[1_554]   | 2.17                     | 0.03              |
| 4:5:334:GLU:OE1 | 4:9:133:TYR:N[1_554]   | 2.17                     | 0.03              |
| 4:4:332:PRO:C   | 4:8:104:LEU:CG[1_554]  | 2.17                     | 0.03              |
| 4:5:156:GLY:C   | 4:9:73:HIS:O[1_554]    | 2.17                     | 0.03              |
| 4:4:243:PRO:CA  | 4:8:60:SER:N[1_554]    | 2.17                     | 0.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:300:SER:CB  | 4:9:107:GLU:CB[1_554]  | 2.17                     | 0.03              |
| 4:3:243:PRO:O   | 4:7:60:SER:OG[1_554]   | 2.17                     | 0.03              |
| 4:4:111:ASN:CG  | 4:9:196:ARG:CA[1_554]  | 2.17                     | 0.03              |
| 4:3:371:HIS:NE2 | 4:8:255:PHE:CE2[1_554] | 2.17                     | 0.03              |
| 4:3:312:ARG:CG  | 4:7:299:MET:O[1_554]   | 2.17                     | 0.03              |
| 4:3:291:LYS:CB  | 4:9:64:ILE:CG1[1_554]  | 2.17                     | 0.03              |
| 4:3:153:LEU:CB  | 4:7:109:PRO:CA[1_554]  | 2.17                     | 0.03              |
| 4:3:340:TRP:CE2 | 4:7:118:LYS:CD[1_554]  | 2.17                     | 0.03              |
| 4:4:195:GLU:C   | 4:8:189:LEU:CD2[1_554] | 2.17                     | 0.03              |
| 4:5:76:ILE:CA   | 4:V:197:GLY:O[1_554]   | 2.17                     | 0.03              |
| 4:3:275:HIS:ND1 | 4:7:152:VAL:C[1_554]   | 2.17                     | 0.03              |
| 4:5:75:ILE:N    | 4:V:198:TYR:N[1_554]   | 2.17                     | 0.03              |
| 4:4:222:ASP:CA  | 4:8:331:ALA:CB[1_554]  | 2.17                     | 0.03              |
| 4:3:267:ILE:CG1 | 4:7:180:LEU:CD1[1_554] | 2.17                     | 0.03              |
| 4:3:214:GLU:CB  | 4:7:33:SER:CB[1_554]   | 2.17                     | 0.03              |
| 4:4:263:GLN:CA  | 4:8:274:ILE:CD1[1_554] | 2.17                     | 0.03              |
| 4:5:271:SER:N   | 4:9:272:ALA:N[1_554]   | 2.17                     | 0.03              |
| 4:3:275:HIS:O   | 4:7:163:VAL:C[1_554]   | 2.17                     | 0.03              |
| 4:3:191:LYS:CB  | 4:7:187:ASP:CA[1_554]  | 2.17                     | 0.03              |
| 4:4:213:LYS:CE  | 4:8:15:GLY:CA[1_554]   | 2.17                     | 0.03              |
| 4:5:309:ILE:CA  | 4:9:300:SER:CB[1_554]  | 2.17                     | 0.03              |
| 4:3:370:VAL:CA  | 4:8:229:THR:O[1_554]   | 2.17                     | 0.03              |
| 4:4:199:SER:N   | 4:8:206:ARG:O[1_554]   | 2.17                     | 0.03              |
| 4:3:179:ASP:O   | 4:7:179:ASP:OD2[1_554] | 2.17                     | 0.03              |
| 4:3:318:THR:OG1 | 4:7:147:ARG:CG[1_554]  | 2.17                     | 0.03              |
| 4:4:114:ALA:N   | 4:9:250:ILE:CG2[1_554] | 2.17                     | 0.03              |
| 4:5:211:ASP:N   | 4:9:32:PRO:CB[1_554]   | 2.17                     | 0.03              |
| 4:3:327:ILE:N   | 4:7:167:GLU:C[1_554]   | 2.17                     | 0.03              |
| 4:4:153:LEU:CA  | 4:8:109:PRO:C[1_554]   | 2.17                     | 0.03              |
| 4:3:271:SER:O   | 4:7:277:THR:CG2[1_554] | 2.17                     | 0.03              |
| 4:5:192:ILE:N   | 4:9:185:LEU:C[1_554]   | 2.17                     | 0.03              |
| 4:4:307:PRO:N   | 4:8:11:ASP:OD2[1_554]  | 2.17                     | 0.03              |
| 4:5:340:TRP:CZ2 | 4:9:121:GLN:O[1_554]   | 2.17                     | 0.03              |
| 4:4:308:GLY:C   | 4:8:338:SER:CA[1_554]  | 2.17                     | 0.03              |
| 4:3:113:LYS:NZ  | 4:8:254:ARG:C[1_554]   | 2.17                     | 0.03              |
| 4:3:153:LEU:CD1 | 4:7:109:PRO:CG[1_554]  | 2.17                     | 0.03              |
| 4:4:114:ALA:N   | 4:9:250:ILE:O[1_554]   | 2.17                     | 0.03              |
| 4:4:157:ASP:OD1 | 4:8:71:ILE:O[1_554]    | 2.17                     | 0.03              |
| 4:4:194:THR:C   | 4:8:209:VAL:C[1_554]   | 2.17                     | 0.03              |
| 4:5:23:GLY:C    | 4:9:124:PHE:CB[1_554]  | 2.17                     | 0.03              |
| 4:5:162:ASN:O   | 4:9:172:PRO:C[1_554]   | 2.17                     | 0.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:145:SER:OG  | 4:9:372:ARG:CZ[1_554]  | 2.17                     | 0.03              |
| 4:4:190:MET:O   | 4:8:186:THR:CB[1_554]  | 2.17                     | 0.03              |
| 4:5:335:ARG:NH2 | 4:9:339:VAL:CB[1_554]  | 2.17                     | 0.03              |
| 4:4:26:ALA:O    | 4:8:122:ILE:N[1_554]   | 2.17                     | 0.03              |
| 4:3:337:TYR:C   | 4:7:119:MET:CB[1_554]  | 2.17                     | 0.03              |
| 4:3:172:PRO:CD  | 4:8:266:PHE:CD1[1_554] | 2.17                     | 0.03              |
| 4:4:259:GLU:C   | 4:8:155:SER:OG[1_554]  | 2.17                     | 0.03              |
| 4:3:114:ALA:O   | 4:8:250:ILE:C[1_554]   | 2.17                     | 0.03              |
| 4:5:260:THR:O   | 4:9:160:THR:OG1[1_554] | 2.17                     | 0.03              |
| 4:5:137:GLN:CB  | 4:9:112:PRO:N[1_554]   | 2.17                     | 0.03              |
| 4:5:346:LEU:CA  | 4:9:368:SER:C[1_554]   | 2.17                     | 0.03              |
| 4:5:261:LEU:CD1 | 4:9:154:ASP:O[1_554]   | 2.17                     | 0.03              |
| 4:3:294:TYR:CG  | 4:7:166:TYR:CA[1_554]  | 2.17                     | 0.03              |
| 4:4:276:GLU:CG  | 4:8:278:THR:C[1_554]   | 2.17                     | 0.03              |
| 4:3:240:TYR:CZ  | 4:7:56:ASP:OD2[1_554]  | 2.17                     | 0.03              |
| 4:4:157:ASP:N   | 4:8:75:ILE:CB[1_554]   | 2.17                     | 0.03              |
| 4:5:231:ALA:CB  | 4:9:218:TYR:OH[1_554]  | 2.17                     | 0.03              |
| 4:4:313:MET:CG  | 4:8:138:ALA:CA[1_554]  | 2.17                     | 0.03              |
| 4:5:366:GLY:O   | 4:V:232:SER:C[1_554]   | 2.17                     | 0.03              |
| 4:4:198:TYR:C   | 4:8:206:ARG:CA[1_554]  | 2.17                     | 0.03              |
| 4:5:176:MET:CG  | 4:9:173:HIS:O[1_554]   | 2.17                     | 0.03              |
| 4:5:110:LEU:C   | 4:V:192:ILE:CB[1_554]  | 2.17                     | 0.03              |
| 4:4:367:PRO:CA  | 4:9:234:SER:CA[1_554]  | 2.17                     | 0.03              |
| 4:4:305:MET:CA  | 4:8:106:THR:OG1[1_554] | 2.17                     | 0.03              |
| 4:5:326:LYS:O   | 4:9:167:GLU:N[1_554]   | 2.17                     | 0.03              |
| 4:3:75:ILE:CA   | 4:8:198:TYR:CB[1_554]  | 2.17                     | 0.03              |
| 4:5:249:THR:OG1 | 4:9:215:LYS:CE[1_554]  | 2.17                     | 0.03              |
| 4:3:196:ARG:NE  | 4:7:211:ASP:CA[1_554]  | 2.17                     | 0.03              |
| 4:3:218:TYR:CA  | 4:7:336:LYS:C[1_554]   | 2.17                     | 0.03              |
| 4:2:74:GLY:CA   | 4:7:198:TYR:N[1_554]   | 2.17                     | 0.03              |
| 4:4:210:ARG:C   | 4:8:15:GLY:O[1_554]    | 2.17                     | 0.03              |
| 4:2:72:GLU:OE1  | 4:7:201:VAL:CG2[1_554] | 2.17                     | 0.03              |
| 4:4:115:ASN:N   | 4:9:250:ILE:C[1_554]   | 2.17                     | 0.03              |
| 4:4:223:PHE:CD1 | 4:8:335:ARG:NE[1_554]  | 2.17                     | 0.03              |
| 4:4:210:ARG:CD  | 4:8:69:TYR:CB[1_554]   | 2.17                     | 0.03              |
| 4:4:343:GLY:O   | 4:8:367:PRO:CG[1_554]  | 2.17                     | 0.03              |
| 4:3:255:PHE:C   | 4:7:302:GLY:N[1_554]   | 2.17                     | 0.03              |
| 4:5:262:PHE:CG  | 4:9:153:LEU:CD2[1_554] | 2.17                     | 0.03              |
| 4:3:262:PHE:CD1 | 4:7:152:VAL:C[1_554]   | 2.17                     | 0.03              |
| 4:5:349:LEU:O   | 4:9:364:GLU:O[1_554]   | 2.17                     | 0.03              |
| 4:3:312:ARG:NE  | 4:7:299:MET:CB[1_554]  | 2.17                     | 0.03              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:154:ASP:N   | 4:9:109:PRO:N[1_554]   | 2.18                     | 0.02              |
| 4:4:312:ARG:CD  | 4:8:299:MET:O[1_554]   | 2.18                     | 0.02              |
| 4:3:191:LYS:CG  | 4:7:184:ASP:O[1_554]   | 2.18                     | 0.02              |
| 4:3:207:GLU:CG  | 4:7:68:LYS:N[1_554]    | 2.18                     | 0.02              |
| 4:5:255:PHE:C   | 4:9:302:GLY:C[1_554]   | 2.18                     | 0.02              |
| 4:3:310:ALA:CA  | 4:7:140:LEU:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:294:TYR:CB  | 4:8:166:TYR:CD2[1_554] | 2.18                     | 0.02              |
| 4:3:199:SER:N   | 4:7:205:GLU:C[1_554]   | 2.18                     | 0.02              |
| 4:4:311:ASP:C   | 4:8:142:LEU:N[1_554]   | 2.18                     | 0.02              |
| 4:5:194:THR:N   | 4:9:209:VAL:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:313:MET:N   | 4:9:152:VAL:CG2[1_554] | 2.18                     | 0.02              |
| 4:4:340:TRP:CZ3 | 4:8:122:ILE:N[1_554]   | 2.18                     | 0.02              |
| 4:4:154:ASP:CG  | 4:8:111:ASN:O[1_554]   | 2.18                     | 0.02              |
| 4:5:106:THR:OG1 | 4:9:115:ASN:N[1_554]   | 2.18                     | 0.02              |
| 4:5:339:VAL:C   | 4:9:117:GLU:N[1_554]   | 2.18                     | 0.02              |
| 4:4:314:GLN:CB  | 4:8:142:LEU:CG[1_554]  | 2.18                     | 0.02              |
| 4:2:172:PRO:CB  | 4:7:266:PHE:CD2[1_554] | 2.18                     | 0.02              |
| 4:4:113:LYS:NZ  | 4:9:254:ARG:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:178:LEU:O   | 4:9:177:ARG:NE[1_554]  | 2.18                     | 0.02              |
| 4:3:118:LYS:CB  | 4:8:249:THR:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:306:TYR:OH  | 4:9:157:ASP:N[1_554]   | 2.18                     | 0.02              |
| 4:4:270:GLU:N   | 4:8:272:ALA:CA[1_554]  | 2.18                     | 0.02              |
| 4:5:370:VAL:CB  | 4:V:231:ALA:O[1_554]   | 2.18                     | 0.02              |
| 4:3:75:ILE:N    | 4:8:197:GLY:O[1_554]   | 2.18                     | 0.02              |
| 4:3:115:ASN:CB  | 4:8:196:ARG:NH2[1_554] | 2.18                     | 0.02              |
| 4:4:11:ASP:O    | 4:8:79:TRP:NE1[1_554]  | 2.18                     | 0.02              |
| 4:3:191:LYS:O   | 4:7:186:THR:C[1_554]   | 2.18                     | 0.02              |
| 4:3:275:HIS:CA  | 4:7:162:ASN:C[1_554]   | 2.18                     | 0.02              |
| 4:4:140:LEU:C   | 4:8:371:HIS:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:256:ARG:CD  | 4:9:306:TYR:CG[1_554]  | 2.18                     | 0.02              |
| 4:2:177:ARG:CZ  | 4:7:194:THR:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:76:ILE:N    | 4:V:197:GLY:CA[1_554]  | 2.18                     | 0.02              |
| 4:5:191:LYS:O   | 4:9:186:THR:CA[1_554]  | 2.18                     | 0.02              |
| 4:3:260:THR:C   | 4:7:160:THR:CB[1_554]  | 2.18                     | 0.02              |
| 4:3:366:GLY:CA  | 4:8:235:SER:OG[1_554]  | 2.18                     | 0.02              |
| 4:4:269:MET:O   | 4:8:273:GLY:CA[1_554]  | 2.18                     | 0.02              |
| 4:2:118:LYS:N   | 4:7:237:GLU:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:315:LYS:CD  | 4:8:147:ARG:NH1[1_554] | 2.18                     | 0.02              |
| 4:5:219:VAL:N   | 4:9:336:LYS:N[1_554]   | 2.18                     | 0.02              |
| 4:5:293:LEU:C   | 4:9:166:TYR:O[1_554]   | 2.18                     | 0.02              |
| 4:5:315:LYS:CE  | 4:9:330:ILE:CD1[1_554] | 2.18                     | 0.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:327:ILE:CG2 | 4:9:149:THR:O[1_554]   | 2.18                     | 0.02              |
| 4:5:256:ARG:O   | 4:9:303:THR:CB[1_554]  | 2.18                     | 0.02              |
| 4:2:113:LYS:CA  | 4:7:254:ARG:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:158:GLY:N   | 4:8:72:GLU:O[1_554]    | 2.18                     | 0.02              |
| 4:5:183:ARG:NH1 | 4:9:72:GLU:OE1[1_554]  | 2.18                     | 0.02              |
| 4:3:154:ASP:OD1 | 4:7:111:ASN:OD1[1_554] | 2.18                     | 0.02              |
| 4:3:336:LYS:C   | 4:7:119:MET:CE[1_554]  | 2.18                     | 0.02              |
| 4:5:199:SER:O   | 4:9:206:ARG:N[1_554]   | 2.18                     | 0.02              |
| 4:2:370:VAL:C   | 4:7:230:ALA:C[1_554]   | 2.18                     | 0.02              |
| 4:4:213:LYS:CA  | 4:8:15:GLY:C[1_554]    | 2.18                     | 0.02              |
| 4:4:299:MET:CE  | 4:8:137:GLN:C[1_554]   | 2.18                     | 0.02              |
| 4:5:327:ILE:CG1 | 4:9:149:THR:N[1_554]   | 2.18                     | 0.02              |
| 4:4:257:CYS:CA  | 4:8:303:THR:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:321:ALA:CA  | 4:8:292:ASP:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:275:HIS:ND1 | 4:8:152:VAL:O[1_554]   | 2.18                     | 0.02              |
| 4:4:147:ARG:CG  | 4:8:372:ARG:CD[1_554]  | 2.18                     | 0.02              |
| 4:5:151:ILE:CD1 | 4:9:171:LEU:O[1_554]   | 2.18                     | 0.02              |
| 4:3:222:ASP:CB  | 4:7:332:PRO:CD[1_554]  | 2.18                     | 0.02              |
| 4:4:166:TYR:OH  | 4:V:39:ARG:CB[1_554]   | 2.18                     | 0.02              |
| 4:3:340:TRP:CZ3 | 4:7:121:GLN:C[1_554]   | 2.18                     | 0.02              |
| 4:2:79:TRP:CZ2  | 4:7:249:THR:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:199:SER:C   | 4:9:207:GLU:N[1_554]   | 2.18                     | 0.02              |
| 4:3:316:GLU:CD  | 4:7:298:VAL:O[1_554]   | 2.18                     | 0.02              |
| 4:2:114:ALA:CA  | 4:7:238:LYS:O[1_554]   | 2.18                     | 0.02              |
| 4:5:367:PRO:CG  | 4:V:233:SER:C[1_554]   | 2.18                     | 0.02              |
| 4:3:255:PHE:CA  | 4:7:302:GLY:N[1_554]   | 2.18                     | 0.02              |
| 4:3:341:ILE:CG2 | 4:7:120:THR:OG1[1_554] | 2.18                     | 0.02              |
| 4:5:262:PHE:CE1 | 4:9:154:ASP:N[1_554]   | 2.18                     | 0.02              |
| 4:3:157:ASP:N   | 4:7:75:ILE:N[1_554]    | 2.18                     | 0.02              |
| 4:3:25:ASP:CA   | 4:7:124:PHE:N[1_554]   | 2.18                     | 0.02              |
| 4:3:144:ALA:N   | 4:7:371:HIS:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:112:PRO:CG  | 4:9:193:LEU:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:313:MET:CE  | 4:8:163:VAL:O[1_554]   | 2.18                     | 0.02              |
| 4:5:191:LYS:CG  | 4:9:186:THR:N[1_554]   | 2.18                     | 0.02              |
| 4:4:173:HIS:ND1 | 4:9:265:SER:C[1_554]   | 2.18                     | 0.02              |
| 4:3:211:ASP:CG  | 4:7:32:PRO:C[1_554]    | 2.18                     | 0.02              |
| 4:3:18:LYS:CD   | 4:7:79:TRP:CD1[1_554]  | 2.18                     | 0.02              |
| 4:3:172:PRO:N   | 4:8:266:PHE:O[1_554]   | 2.18                     | 0.02              |
| 4:5:18:LYS:CA   | 4:9:79:TRP:CZ3[1_554]  | 2.18                     | 0.02              |
| 4:5:155:SER:OG  | 4:9:161:HIS:ND1[1_554] | 2.18                     | 0.02              |
| 4:5:166:TYR:CE1 | 4:W:40:HIS:CG[1_554]   | 2.18                     | 0.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:2:366:GLY:C   | 4:7:235:SER:OG[1_554]  | 2.18                     | 0.02              |
| 4:5:75:ILE:CG1  | 4:V:193:LEU:O[1_554]   | 2.18                     | 0.02              |
| 4:4:243:PRO:N   | 4:8:60:SER:C[1_554]    | 2.18                     | 0.02              |
| 4:3:321:ALA:O   | 4:7:292:ASP:OD1[1_554] | 2.18                     | 0.02              |
| 4:4:282:ILE:CG1 | 4:8:171:LEU:CD1[1_554] | 2.18                     | 0.02              |
| 4:5:370:VAL:CB  | 4:V:231:ALA:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:281:SER:OG  | 4:8:172:PRO:O[1_554]   | 2.18                     | 0.02              |
| 4:5:213:LYS:CD  | 4:9:157:ASP:OD2[1_554] | 2.18                     | 0.02              |
| 4:5:198:TYR:OH  | 4:9:240:TYR:OH[1_554]  | 2.18                     | 0.02              |
| 4:3:172:PRO:N   | 4:8:266:PHE:CA[1_554]  | 2.18                     | 0.02              |
| 4:4:198:TYR:CE1 | 4:8:208:ILE:CG1[1_554] | 2.18                     | 0.02              |
| 4:5:258:PRO:CG  | 4:9:155:SER:O[1_554]   | 2.18                     | 0.02              |
| 4:3:30:VAL:C    | 4:7:80:ASP:CB[1_554]   | 2.18                     | 0.02              |
| 4:4:166:TYR:CE1 | 4:V:39:ARG:O[1_554]    | 2.18                     | 0.02              |
| 4:5:188:TYR:N   | 4:9:183:ARG:N[1_554]   | 2.18                     | 0.02              |
| 4:5:244:ASP:OD2 | 4:7:291:LYS:CE[1_554]  | 2.18                     | 0.02              |
| 4:4:336:LYS:NZ  | 4:8:86:TRP:CD2[1_554]  | 2.18                     | 0.02              |
| 4:3:25:ASP:CB   | 4:7:125:GLU:N[1_554]   | 2.18                     | 0.02              |
| 4:4:269:MET:N   | 4:8:264:PRO:CG[1_554]  | 2.18                     | 0.02              |
| 4:3:282:ILE:CA  | 4:7:173:HIS:CE1[1_554] | 2.18                     | 0.02              |
| 4:5:178:LEU:CA  | 4:9:177:ARG:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:255:PHE:CE1 | 4:8:305:MET:O[1_554]   | 2.18                     | 0.02              |
| 4:5:334:GLU:CB  | 4:9:104:LEU:C[1_554]   | 2.18                     | 0.02              |
| 4:4:335:ARG:CD  | 4:8:106:THR:C[1_554]   | 2.18                     | 0.02              |
| 4:4:153:LEU:CD1 | 4:8:163:VAL:CG2[1_554] | 2.18                     | 0.02              |
| 4:5:32:PRO:O    | 4:9:78:ASN:ND2[1_554]  | 2.18                     | 0.02              |
| 4:4:299:MET:SD  | 4:8:136:ILE:C[1_554]   | 2.18                     | 0.02              |
| 4:5:326:LYS:C   | 4:9:149:THR:OG1[1_554] | 2.18                     | 0.02              |
| 4:5:153:LEU:C   | 4:9:109:PRO:C[1_554]   | 2.18                     | 0.02              |
| 4:4:177:ARG:CZ  | 4:9:194:THR:OG1[1_554] | 2.18                     | 0.02              |
| 4:5:280:ASN:OD1 | 4:9:281:SER:O[1_554]   | 2.18                     | 0.02              |
| 4:5:305:MET:C   | 4:9:11:ASP:CG[1_554]   | 2.18                     | 0.02              |
| 4:3:258:PRO:C   | 4:7:155:SER:N[1_554]   | 2.18                     | 0.02              |
| 4:3:215:LYS:C   | 4:7:31:PHE:N[1_554]    | 2.18                     | 0.02              |
| 4:5:164:PRO:CA  | 4:9:172:PRO:CD[1_554]  | 2.18                     | 0.02              |
| 4:4:164:PRO:CD  | 4:8:172:PRO:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:266:PHE:N   | 4:9:261:LEU:N[1_554]   | 2.18                     | 0.02              |
| 4:4:193:LEU:CB  | 4:8:210:ARG:CA[1_554]  | 2.18                     | 0.02              |
| 4:5:151:ILE:CG2 | 4:9:171:LEU:N[1_554]   | 2.18                     | 0.02              |
| 4:3:265:SER:O   | 4:7:261:LEU:O[1_554]   | 2.18                     | 0.02              |
| 4:3:210:ARG:N   | 4:7:69:TYR:CE2[1_554]  | 2.18                     | 0.02              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:186:THR:CA  | 4:7:183:ARG:NH2[1_554] | 2.18                     | 0.02              |
| 1:A:637:LYS:NZ  | 4:4:311:ASP:CA[1_556]  | 2.18                     | 0.02              |
| 4:2:174:ALA:N   | 4:7:266:PHE:O[1_554]   | 2.18                     | 0.02              |
| 4:4:111:ASN:C   | 4:9:253:GLU:OE1[1_554] | 2.18                     | 0.02              |
| 4:4:322:PRO:CG  | 4:8:288:ASP:O[1_554]   | 2.18                     | 0.02              |
| 4:4:114:ALA:CB  | 4:9:250:ILE:N[1_554]   | 2.18                     | 0.02              |
| 4:4:289:ILE:CG2 | 4:V:39:ARG:NH1[1_554]  | 2.18                     | 0.02              |
| 4:3:185:LEU:CG  | 4:7:158:GLY:C[1_554]   | 2.18                     | 0.02              |
| 4:4:316:GLU:C   | 4:8:150:GLY:CA[1_554]  | 2.18                     | 0.02              |
| 4:4:56:ASP:OD1  | 4:8:80:ASP:CG[1_554]   | 2.18                     | 0.02              |
| 4:3:317:ILE:CG1 | 4:7:165:ILE:C[1_554]   | 2.18                     | 0.02              |
| 4:5:29:ALA:N    | 4:9:83:GLU:CD[1_554]   | 2.18                     | 0.02              |
| 4:3:141:SER:CA  | 4:7:116:ARG:CD[1_554]  | 2.18                     | 0.02              |
| 4:5:262:PHE:C   | 4:9:153:LEU:CG[1_554]  | 2.18                     | 0.02              |
| 4:4:144:ALA:CA  | 4:8:370:VAL:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:320:LEU:N   | 4:8:293:LEU:C[1_554]   | 2.18                     | 0.02              |
| 4:3:154:ASP:CA  | 4:7:110:LEU:CA[1_554]  | 2.18                     | 0.02              |
| 4:3:368:SER:C   | 4:8:234:SER:OG[1_554]  | 2.18                     | 0.02              |
| 4:5:219:VAL:CB  | 4:9:300:SER:CB[1_554]  | 2.18                     | 0.02              |
| 4:3:117:GLU:CA  | 4:8:237:GLU:OE2[1_554] | 2.18                     | 0.02              |
| 4:5:319:ALA:O   | 4:9:294:TYR:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:207:GLU:OE1 | 4:8:67:LEU:CB[1_554]   | 2.18                     | 0.02              |
| 4:5:30:VAL:C    | 4:9:79:TRP:C[1_554]    | 2.18                     | 0.02              |
| 4:5:19:ALA:N    | 4:9:122:ILE:CG1[1_554] | 2.18                     | 0.02              |
| 4:5:218:TYR:O   | 4:9:302:GLY:CA[1_554]  | 2.18                     | 0.02              |
| 4:5:293:LEU:O   | 4:9:169:TYR:C[1_554]   | 2.18                     | 0.02              |
| 4:5:214:GLU:CA  | 4:9:16:LEU:CG[1_554]   | 2.18                     | 0.02              |
| 4:3:262:PHE:CE2 | 4:7:154:ASP:CB[1_554]  | 2.18                     | 0.02              |
| 4:5:299:MET:CA  | 4:9:136:ILE:N[1_554]   | 2.18                     | 0.02              |
| 4:4:26:ALA:CA   | 4:8:122:ILE:N[1_554]   | 2.18                     | 0.02              |
| 4:4:150:GLY:O   | 4:8:169:TYR:CE1[1_554] | 2.18                     | 0.02              |
| 4:2:362:TYR:CD1 | 4:7:235:SER:N[1_554]   | 2.18                     | 0.02              |
| 4:4:154:ASP:N   | 4:8:110:LEU:CA[1_554]  | 2.18                     | 0.02              |
| 4:4:307:PRO:CG  | 4:8:340:TRP:CB[1_554]  | 2.18                     | 0.02              |
| 4:4:282:ILE:CB  | 4:8:171:LEU:CD1[1_554] | 2.18                     | 0.02              |
| 4:3:295:ALA:CA  | 4:7:167:GLU:O[1_554]   | 2.19                     | 0.01              |
| 4:5:240:TYR:CZ  | 4:9:56:ASP:OD2[1_554]  | 2.19                     | 0.01              |
| 4:3:161:HIS:N   | 4:7:110:LEU:CG[1_554]  | 2.19                     | 0.01              |
| 4:3:267:ILE:N   | 4:7:180:LEU:CG[1_554]  | 2.19                     | 0.01              |
| 4:4:186:THR:CA  | 4:8:183:ARG:CD[1_554]  | 2.19                     | 0.01              |
| 4:3:257:CYS:N   | 4:7:303:THR:CA[1_554]  | 2.19                     | 0.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:109:PRO:C   | 4:9:195:GLU:CG[1_554]  | 2.19                     | 0.01              |
| 4:3:276:GLU:CA  | 4:7:281:SER:CB[1_554]  | 2.19                     | 0.01              |
| 4:3:188:TYR:O   | 4:7:183:ARG:N[1_554]   | 2.19                     | 0.01              |
| 4:5:9:VAL:N     | 4:9:121:GLN:CG[1_554]  | 2.19                     | 0.01              |
| 4:5:17:VAL:C    | 4:9:79:TRP:CE3[1_554]  | 2.19                     | 0.01              |
| 4:5:219:VAL:C   | 4:9:335:ARG:CG[1_554]  | 2.19                     | 0.01              |
| 4:3:276:GLU:OE2 | 4:7:278:THR:CB[1_554]  | 2.19                     | 0.01              |
| 4:3:117:GLU:N   | 4:8:251:GLY:CA[1_554]  | 2.19                     | 0.01              |
| 4:4:208:ILE:CD1 | 4:8:59:GLN:CG[1_554]   | 2.19                     | 0.01              |
| 4:5:298:VAL:C   | 4:9:136:ILE:CD1[1_554] | 2.19                     | 0.01              |
| 4:5:110:LEU:CG  | 4:V:191:LYS:NZ[1_554]  | 2.19                     | 0.01              |
| 4:4:117:GLU:CD  | 4:9:237:GLU:N[1_554]   | 2.19                     | 0.01              |
| 4:4:293:LEU:O   | 4:8:169:TYR:C[1_554]   | 2.19                     | 0.01              |
| 4:5:75:ILE:CA   | 4:V:197:GLY:O[1_554]   | 2.19                     | 0.01              |
| 4:4:137:GLN:C   | 4:8:112:PRO:C[1_554]   | 2.19                     | 0.01              |
| 4:3:345:ILE:CB  | 4:7:367:PRO:CA[1_554]  | 2.19                     | 0.01              |
| 4:3:200:PHE:CB  | 4:7:206:ARG:NE[1_554]  | 2.19                     | 0.01              |
| 4:5:334:GLU:CG  | 4:9:133:TYR:O[1_554]   | 2.19                     | 0.01              |
| 4:5:369:ILE:C   | 4:V:231:ALA:CB[1_554]  | 2.19                     | 0.01              |
| 4:5:249:THR:O   | 4:9:211:ASP:CA[1_554]  | 2.19                     | 0.01              |
| 4:3:76:ILE:CA   | 4:8:198:TYR:CE1[1_554] | 2.19                     | 0.01              |
| 4:3:18:LYS:CB   | 4:7:118:LYS:CG[1_554]  | 2.19                     | 0.01              |
| 4:5:154:ASP:CA  | 4:9:109:PRO:O[1_554]   | 2.19                     | 0.01              |
| 4:5:204:ALA:C   | 4:9:62:ARG:CB[1_554]   | 2.19                     | 0.01              |
| 4:3:184:ASP:N   | 4:7:73:HIS:NE2[1_554]  | 2.19                     | 0.01              |
| 4:5:283:MET:SD  | 4:9:286:ASP:N[1_554]   | 2.19                     | 0.01              |
| 4:5:218:TYR:CG  | 4:9:336:LYS:CA[1_554]  | 2.19                     | 0.01              |
| 4:4:214:GLU:O   | 4:8:16:LEU:CB[1_554]   | 2.19                     | 0.01              |
| 4:4:300:SER:CB  | 4:8:107:GLU:CB[1_554]  | 2.19                     | 0.01              |
| 4:4:196:ARG:NE  | 4:8:211:ASP:CA[1_554]  | 2.19                     | 0.01              |
| 4:5:348:SER:C   | 4:9:362:TYR:O[1_554]   | 2.19                     | 0.01              |
| 4:5:290:ARG:CD  | 4:9:286:ASP:CG[1_554]  | 2.19                     | 0.01              |
| 4:5:340:TRP:CE2 | 4:9:121:GLN:CA[1_554]  | 2.19                     | 0.01              |
| 4:5:315:LYS:CB  | 4:9:298:VAL:CG2[1_554] | 2.19                     | 0.01              |
| 4:4:340:TRP:N   | 4:8:116:ARG:O[1_554]   | 2.19                     | 0.01              |
| 4:4:211:ASP:N   | 4:8:32:PRO:CB[1_554]   | 2.19                     | 0.01              |
| 4:4:321:ALA:N   | 4:8:293:LEU:CD1[1_554] | 2.19                     | 0.01              |
| 4:5:192:ILE:CD1 | 4:9:213:LYS:CD[1_554]  | 2.19                     | 0.01              |
| 4:4:304:THR:OG1 | 4:8:137:GLN:NE2[1_554] | 2.19                     | 0.01              |
| 4:3:304:THR:CG2 | 4:7:107:GLU:C[1_554]   | 2.19                     | 0.01              |
| 4:5:41:GLN:CD   | 4:8:224:GLU:OE2[1_554] | 2.19                     | 0.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:5:312:ARG:CG  | 4:9:299:MET:CB[1_554]  | 2.19                     | 0.01              |
| 4:4:218:TYR:CG  | 4:8:337:TYR:CE1[1_554] | 2.19                     | 0.01              |
| 4:3:294:TYR:CG  | 4:7:166:TYR:CD2[1_554] | 2.19                     | 0.01              |
| 4:4:214:GLU:O   | 4:8:16:LEU:O[1_554]    | 2.19                     | 0.01              |
| 4:4:314:GLN:CA  | 4:8:142:LEU:CD1[1_554] | 2.19                     | 0.01              |
| 4:2:74:GLY:C    | 4:7:197:GLY:N[1_554]   | 2.19                     | 0.01              |
| 4:5:157:ASP:O   | 4:9:73:HIS:CG[1_554]   | 2.19                     | 0.01              |
| 4:3:205:GLU:OE2 | 4:7:203:THR:CB[1_554]  | 2.19                     | 0.01              |
| 4:5:196:ARG:NH2 | 4:9:215:LYS:CB[1_554]  | 2.19                     | 0.01              |
| 4:3:110:LEU:O   | 4:8:192:ILE:O[1_554]   | 2.19                     | 0.01              |
| 4:4:329:ILE:CB  | 4:8:139:VAL:CA[1_554]  | 2.19                     | 0.01              |
| 4:5:154:ASP:CB  | 4:9:109:PRO:O[1_554]   | 2.19                     | 0.01              |
| 4:3:193:LEU:N   | 4:7:210:ARG:CA[1_554]  | 2.19                     | 0.01              |
| 4:5:19:ALA:O    | 4:9:122:ILE:CB[1_554]  | 2.19                     | 0.01              |
| 4:3:258:PRO:N   | 4:7:156:GLY:N[1_554]   | 2.19                     | 0.01              |
| 4:5:294:TYR:CD1 | 4:9:166:TYR:CA[1_554]  | 2.19                     | 0.01              |
| 4:3:345:ILE:CB  | 4:7:367:PRO:C[1_554]   | 2.19                     | 0.01              |
| 4:5:188:TYR:N   | 4:9:184:ASP:CA[1_554]  | 2.19                     | 0.01              |
| 4:3:110:LEU:CD1 | 4:8:191:LYS:CA[1_554]  | 2.19                     | 0.01              |
| 4:5:297:ASN:C   | 4:9:139:VAL:CG2[1_554] | 2.19                     | 0.01              |
| 4:5:24:ASP:N    | 4:9:124:PHE:C[1_554]   | 2.19                     | 0.01              |
| 4:4:179:ASP:O   | 4:8:179:ASP:OD2[1_554] | 2.19                     | 0.01              |
| 4:3:213:LYS:N   | 4:7:15:GLY:C[1_554]    | 2.19                     | 0.01              |
| 4:5:368:SER:N   | 4:V:229:THR:O[1_554]   | 2.19                     | 0.01              |
| 4:5:198:TYR:CD1 | 4:9:208:ILE:N[1_554]   | 2.19                     | 0.01              |
| 4:3:27:PRO:CG   | 4:7:122:ILE:CB[1_554]  | 2.19                     | 0.01              |
| 4:4:56:ASP:CG   | 4:8:80:ASP:OD1[1_554]  | 2.19                     | 0.01              |
| 4:3:218:TYR:CZ  | 4:7:337:TYR:CD2[1_554] | 2.19                     | 0.01              |
| 4:5:255:PHE:CA  | 4:9:302:GLY:C[1_554]   | 2.19                     | 0.01              |
| 4:4:30:VAL:N    | 4:8:79:TRP:C[1_554]    | 2.19                     | 0.01              |
| 4:4:327:ILE:CD1 | 4:8:149:THR:CG2[1_554] | 2.19                     | 0.01              |
| 4:5:185:LEU:CG  | 4:9:181:ALA:CB[1_554]  | 2.19                     | 0.01              |
| 4:4:197:GLY:N   | 4:8:209:VAL:CA[1_554]  | 2.19                     | 0.01              |
| 4:2:115:ASN:CB  | 4:7:250:ILE:N[1_554]   | 2.19                     | 0.01              |
| 4:3:357:ILE:CB  | 4:8:231:ALA:C[1_554]   | 2.19                     | 0.01              |
| 4:4:113:LYS:CD  | 4:9:252:ASN:O[1_554]   | 2.19                     | 0.01              |
| 4:1:292:ASP:OD1 | 4:7:40:HIS:O[1_554]    | 2.19                     | 0.01              |
| 4:3:157:ASP:CB  | 4:7:72:GLU:CB[1_554]   | 2.19                     | 0.01              |
| 4:5:281:SER:CB  | 4:9:173:HIS:C[1_554]   | 2.19                     | 0.01              |
| 4:3:260:THR:CG2 | 4:7:160:THR:OG1[1_554] | 2.19                     | 0.01              |
| 4:2:132:MET:O   | 4:7:231:ALA:O[1_554]   | 2.19                     | 0.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:4:23:GLY:CA   | 4:8:125:GLU:OE2[1_554] | 2.19                     | 0.01              |
| 4:3:197:GLY:N   | 4:7:208:ILE:C[1_554]   | 2.19                     | 0.01              |
| 4:4:204:ALA:CB  | 4:8:62:ARG:N[1_554]    | 2.19                     | 0.01              |
| 4:4:345:ILE:CA  | 4:8:366:GLY:CA[1_554]  | 2.19                     | 0.01              |
| 4:2:286:ASP:OD1 | 4:7:270:GLU:OE1[1_554] | 2.19                     | 0.01              |
| 4:4:308:GLY:N   | 4:8:338:SER:O[1_554]   | 2.19                     | 0.01              |
| 4:4:372:ARG:CA  | 4:9:226:GLU:C[1_554]   | 2.19                     | 0.01              |
| 4:4:195:GLU:CA  | 4:8:209:VAL:CG2[1_554] | 2.19                     | 0.01              |
| 4:4:317:ILE:CB  | 4:8:165:ILE:N[1_554]   | 2.19                     | 0.01              |
| 4:3:182:GLY:C   | 4:7:73:HIS:N[1_554]    | 2.19                     | 0.01              |
| 4:3:257:CYS:O   | 4:7:155:SER:C[1_554]   | 2.19                     | 0.01              |
| 4:3:312:ARG:CG  | 4:7:299:MET:C[1_554]   | 2.19                     | 0.01              |
| 4:4:317:ILE:CG1 | 4:8:165:ILE:CB[1_554]  | 2.19                     | 0.01              |
| 4:5:178:LEU:CD1 | 4:9:177:ARG:N[1_554]   | 2.19                     | 0.01              |
| 4:5:315:LYS:CA  | 4:9:298:VAL:CG2[1_554] | 2.19                     | 0.01              |
| 4:5:270:GLU:CA  | 4:9:272:ALA:O[1_554]   | 2.19                     | 0.01              |
| 4:3:217:CYS:N   | 4:7:16:LEU:CD2[1_554]  | 2.19                     | 0.01              |
| 4:3:72:GLU:O    | 4:8:198:TYR:CA[1_554]  | 2.19                     | 0.01              |
| 4:4:113:LYS:CG  | 4:9:255:PHE:N[1_554]   | 2.19                     | 0.01              |
| 4:3:279:TYR:OH  | 4:7:286:ASP:O[1_554]   | 2.19                     | 0.01              |
| 4:5:297:ASN:CB  | 4:9:165:ILE:CG1[1_554] | 2.19                     | 0.01              |
| 4:5:17:VAL:CG1  | 4:9:79:TRP:CG[1_554]   | 2.19                     | 0.01              |
| 4:5:191:LYS:C   | 4:9:186:THR:N[1_554]   | 2.19                     | 0.01              |
| 4:5:32:PRO:CA   | 4:9:78:ASN:ND2[1_554]  | 2.19                     | 0.01              |
| 4:5:286:ASP:OD1 | 4:V:270:GLU:OE1[1_554] | 2.19                     | 0.01              |
| 4:5:297:ASN:CA  | 4:9:170:ALA:N[1_554]   | 2.19                     | 0.01              |
| 4:5:196:ARG:N   | 4:9:189:LEU:CD2[1_554] | 2.19                     | 0.01              |
| 4:3:255:PHE:CD1 | 4:7:305:MET:SD[1_554]  | 2.19                     | 0.01              |
| 4:4:321:ALA:N   | 4:8:292:ASP:CB[1_554]  | 2.19                     | 0.01              |
| 4:3:141:SER:C   | 4:7:116:ARG:CD[1_554]  | 2.19                     | 0.01              |
| 4:3:197:GLY:O   | 4:7:208:ILE:CA[1_554]  | 2.19                     | 0.01              |
| 4:4:283:MET:SD  | 4:8:286:ASP:O[1_554]   | 2.19                     | 0.01              |
| 4:3:259:GLU:OE2 | 4:7:304:THR:C[1_554]   | 2.19                     | 0.01              |
| 4:3:279:TYR:CG  | 4:7:293:LEU:CD2[1_554] | 2.19                     | 0.01              |
| 4:3:294:TYR:N   | 4:7:169:TYR:CD2[1_554] | 2.19                     | 0.01              |
| 4:5:196:ARG:CG  | 4:9:212:ILE:O[1_554]   | 2.19                     | 0.01              |
| 4:5:190:MET:CA  | 4:9:186:THR:CB[1_554]  | 2.19                     | 0.01              |
| 4:2:118:LYS:CB  | 4:7:249:THR:CB[1_554]  | 2.19                     | 0.01              |
| 4:3:207:GLU:OE2 | 4:7:67:LEU:N[1_554]    | 2.19                     | 0.01              |
| 4:5:219:VAL:CG1 | 4:9:301:GLY:N[1_554]   | 2.19                     | 0.01              |
| 4:4:267:ILE:CG2 | 4:8:180:LEU:C[1_554]   | 2.19                     | 0.01              |

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| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 4:3:110:LEU:CB  | 4:8:192:ILE:CG2[1_554] | 2.19                     | 0.01              |
| 4:4:207:GLU:CD  | 4:8:67:LEU:N[1_554]    | 2.19                     | 0.01              |
| 4:3:269:MET:SD  | 4:7:178:LEU:CD1[1_554] | 2.19                     | 0.01              |
| 4:3:24:ASP:CA   | 4:7:125:GLU:OE1[1_554] | 2.19                     | 0.01              |
| 4:4:337:TYR:CE2 | 4:8:86:TRP:CZ2[1_554]  | 2.19                     | 0.01              |
| 4:3:276:GLU:OE1 | 4:7:281:SER:N[1_554]   | 2.19                     | 0.01              |
| 4:4:318:THR:CG2 | 4:8:149:THR:N[1_554]   | 2.19                     | 0.01              |
| 4:5:265:SER:C   | 4:9:262:PHE:N[1_554]   | 2.19                     | 0.01              |
| 4:4:27:PRO:N    | 4:8:122:ILE:C[1_554]   | 2.19                     | 0.01              |
| 4:4:366:GLY:C   | 4:9:234:SER:N[1_554]   | 2.19                     | 0.01              |
| 4:4:283:MET:CE  | 4:8:289:ILE:CB[1_554]  | 2.19                     | 0.01              |
| 4:3:262:PHE:CE1 | 4:7:154:ASP:N[1_554]   | 2.19                     | 0.01              |
| 4:3:316:GLU:O   | 4:7:151:ILE:CA[1_554]  | 2.19                     | 0.01              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|-----------|----------|-------------|----|
| 1   | A     | 789/840 (94%) | 651 (82%) | 112 (14%) | 26 (3%)  | 5           | 40 |
| 1   | D     | 789/840 (94%) | 651 (82%) | 112 (14%) | 26 (3%)  | 5           | 40 |
| 1   | G     | 791/840 (94%) | 652 (82%) | 112 (14%) | 27 (3%)  | 5           | 40 |
| 1   | J     | 791/840 (94%) | 652 (82%) | 112 (14%) | 27 (3%)  | 5           | 40 |
| 1   | M     | 786/840 (94%) | 649 (83%) | 111 (14%) | 26 (3%)  | 5           | 40 |
| 1   | P     | 789/840 (94%) | 649 (82%) | 114 (14%) | 26 (3%)  | 5           | 40 |
| 2   | B     | 143/145 (99%) | 126 (88%) | 9 (6%)    | 8 (6%)   | 2           | 28 |
| 2   | E     | 143/145 (99%) | 126 (88%) | 9 (6%)    | 8 (6%)   | 2           | 28 |
| 2   | H     | 143/145 (99%) | 126 (88%) | 9 (6%)    | 8 (6%)   | 2           | 28 |
| 2   | K     | 143/145 (99%) | 126 (88%) | 9 (6%)    | 8 (6%)   | 2           | 28 |
| 2   | N     | 143/145 (99%) | 126 (88%) | 9 (6%)    | 8 (6%)   | 2           | 28 |

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| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 2   | Q     | 143/145 (99%)     | 126 (88%)   | 9 (6%)     | 8 (6%)   | 2           | 28  |
| 3   | C     | 143/147 (97%)     | 133 (93%)   | 10 (7%)    | 0        | 100         | 100 |
| 3   | F     | 143/147 (97%)     | 133 (93%)   | 10 (7%)    | 0        | 100         | 100 |
| 3   | I     | 143/147 (97%)     | 133 (93%)   | 10 (7%)    | 0        | 100         | 100 |
| 3   | L     | 143/147 (97%)     | 133 (93%)   | 10 (7%)    | 0        | 100         | 100 |
| 3   | O     | 143/147 (97%)     | 133 (93%)   | 10 (7%)    | 0        | 100         | 100 |
| 3   | R     | 143/147 (97%)     | 133 (93%)   | 10 (7%)    | 0        | 100         | 100 |
| 4   | 0     | 370/375 (99%)     | 333 (90%)   | 31 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 1     | 370/375 (99%)     | 335 (90%)   | 29 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 2     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 3     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 4     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 5     | 370/375 (99%)     | 335 (90%)   | 29 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 7     | 370/375 (99%)     | 335 (90%)   | 29 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 8     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | 9     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | V     | 370/375 (99%)     | 335 (90%)   | 29 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | W     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | X     | 370/375 (99%)     | 335 (90%)   | 29 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | Y     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| 4   | Z     | 370/375 (99%)     | 334 (90%)   | 30 (8%)    | 6 (2%)   | 12          | 56  |
| All | All   | 11631/12042 (97%) | 10138 (87%) | 1203 (10%) | 290 (2%) | 11          | 46  |

All (290) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 73  | LYS  |
| 1   | A     | 202 | SER  |
| 1   | A     | 572 | LYS  |
| 1   | A     | 712 | PRO  |
| 1   | A     | 729 | ALA  |
| 1   | A     | 757 | GLN  |
| 1   | A     | 762 | HIS  |
| 2   | B     | 131 | GLU  |
| 2   | B     | 141 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 73  | LYS  |
| 1   | D     | 202 | SER  |
| 1   | D     | 572 | LYS  |
| 1   | D     | 712 | PRO  |
| 1   | D     | 729 | ALA  |
| 1   | D     | 757 | GLN  |
| 1   | D     | 762 | HIS  |
| 2   | E     | 131 | GLU  |
| 2   | E     | 141 | PRO  |
| 1   | G     | 73  | LYS  |
| 1   | G     | 202 | SER  |
| 1   | G     | 572 | LYS  |
| 1   | G     | 712 | PRO  |
| 1   | G     | 729 | ALA  |
| 1   | G     | 757 | GLN  |
| 1   | G     | 762 | HIS  |
| 2   | H     | 131 | GLU  |
| 2   | H     | 141 | PRO  |
| 1   | J     | 73  | LYS  |
| 1   | J     | 202 | SER  |
| 1   | J     | 572 | LYS  |
| 1   | J     | 712 | PRO  |
| 1   | J     | 729 | ALA  |
| 1   | J     | 757 | GLN  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 785 | GLU  |
| 2   | K     | 131 | GLU  |
| 2   | K     | 141 | PRO  |
| 1   | M     | 73  | LYS  |
| 1   | M     | 202 | SER  |
| 1   | M     | 572 | LYS  |
| 1   | M     | 712 | PRO  |
| 1   | M     | 729 | ALA  |
| 1   | M     | 757 | GLN  |
| 1   | M     | 762 | HIS  |
| 2   | N     | 131 | GLU  |
| 2   | N     | 141 | PRO  |
| 1   | P     | 73  | LYS  |
| 1   | P     | 202 | SER  |
| 1   | P     | 572 | LYS  |
| 1   | P     | 712 | PRO  |
| 1   | P     | 729 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 757 | GLN  |
| 1   | P     | 762 | HIS  |
| 2   | Q     | 131 | GLU  |
| 2   | Q     | 141 | PRO  |
| 4   | 0     | 246 | GLN  |
| 4   | 1     | 246 | GLN  |
| 4   | 2     | 246 | GLN  |
| 4   | 3     | 246 | GLN  |
| 4   | 4     | 246 | GLN  |
| 4   | 5     | 246 | GLN  |
| 4   | 7     | 246 | GLN  |
| 4   | 8     | 246 | GLN  |
| 4   | 9     | 246 | GLN  |
| 4   | V     | 246 | GLN  |
| 4   | W     | 246 | GLN  |
| 4   | X     | 246 | GLN  |
| 4   | Y     | 246 | GLN  |
| 4   | Z     | 246 | GLN  |
| 1   | A     | 11  | GLY  |
| 1   | A     | 21  | GLU  |
| 1   | A     | 219 | GLU  |
| 1   | A     | 517 | MET  |
| 1   | A     | 532 | ILE  |
| 1   | A     | 637 | LYS  |
| 2   | B     | 130 | PRO  |
| 2   | B     | 147 | ASN  |
| 2   | B     | 151 | LYS  |
| 2   | B     | 161 | GLU  |
| 1   | D     | 11  | GLY  |
| 1   | D     | 21  | GLU  |
| 1   | D     | 219 | GLU  |
| 1   | D     | 517 | MET  |
| 1   | D     | 637 | LYS  |
| 2   | E     | 130 | PRO  |
| 2   | E     | 147 | ASN  |
| 2   | E     | 151 | LYS  |
| 2   | E     | 161 | GLU  |
| 1   | G     | 11  | GLY  |
| 1   | G     | 21  | GLU  |
| 1   | G     | 219 | GLU  |
| 1   | G     | 517 | MET  |
| 1   | G     | 532 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 637 | LYS  |
| 1   | G     | 785 | GLU  |
| 2   | H     | 130 | PRO  |
| 2   | H     | 147 | ASN  |
| 2   | H     | 151 | LYS  |
| 1   | J     | 11  | GLY  |
| 1   | J     | 21  | GLU  |
| 1   | J     | 219 | GLU  |
| 1   | J     | 517 | MET  |
| 1   | J     | 637 | LYS  |
| 2   | K     | 130 | PRO  |
| 2   | K     | 147 | ASN  |
| 2   | K     | 151 | LYS  |
| 1   | M     | 11  | GLY  |
| 1   | M     | 21  | GLU  |
| 1   | M     | 219 | GLU  |
| 1   | M     | 517 | MET  |
| 1   | M     | 637 | LYS  |
| 2   | N     | 130 | PRO  |
| 2   | N     | 147 | ASN  |
| 2   | N     | 151 | LYS  |
| 2   | N     | 161 | GLU  |
| 1   | P     | 11  | GLY  |
| 1   | P     | 21  | GLU  |
| 1   | P     | 219 | GLU  |
| 1   | P     | 517 | MET  |
| 1   | P     | 637 | LYS  |
| 2   | Q     | 130 | PRO  |
| 2   | Q     | 147 | ASN  |
| 2   | Q     | 151 | LYS  |
| 2   | Q     | 161 | GLU  |
| 4   | 0     | 274 | ILE  |
| 4   | 1     | 274 | ILE  |
| 4   | 2     | 274 | ILE  |
| 4   | 3     | 274 | ILE  |
| 4   | 4     | 274 | ILE  |
| 4   | 5     | 274 | ILE  |
| 4   | 7     | 274 | ILE  |
| 4   | 8     | 274 | ILE  |
| 4   | 9     | 274 | ILE  |
| 4   | V     | 274 | ILE  |
| 4   | W     | 274 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | X     | 274 | ILE  |
| 4   | Y     | 274 | ILE  |
| 4   | Z     | 274 | ILE  |
| 1   | A     | 58  | GLY  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 644 | SER  |
| 1   | D     | 58  | GLY  |
| 1   | D     | 294 | ASN  |
| 1   | D     | 532 | ILE  |
| 1   | D     | 644 | SER  |
| 1   | G     | 58  | GLY  |
| 1   | G     | 294 | ASN  |
| 1   | G     | 644 | SER  |
| 2   | H     | 161 | GLU  |
| 1   | J     | 58  | GLY  |
| 1   | J     | 294 | ASN  |
| 1   | J     | 532 | ILE  |
| 1   | J     | 644 | SER  |
| 2   | K     | 161 | GLU  |
| 1   | M     | 58  | GLY  |
| 1   | M     | 294 | ASN  |
| 1   | M     | 532 | ILE  |
| 1   | M     | 644 | SER  |
| 1   | P     | 58  | GLY  |
| 1   | P     | 294 | ASN  |
| 1   | P     | 532 | ILE  |
| 1   | P     | 644 | SER  |
| 4   | 0     | 233 | SER  |
| 4   | 1     | 233 | SER  |
| 4   | 2     | 233 | SER  |
| 4   | 3     | 233 | SER  |
| 4   | 4     | 233 | SER  |
| 4   | 5     | 233 | SER  |
| 4   | 7     | 233 | SER  |
| 4   | 8     | 233 | SER  |
| 4   | 9     | 233 | SER  |
| 4   | V     | 233 | SER  |
| 4   | W     | 233 | SER  |
| 4   | X     | 233 | SER  |
| 4   | Y     | 233 | SER  |
| 4   | Z     | 233 | SER  |
| 1   | A     | 435 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 817 | GLN  |
| 1   | D     | 269 | LEU  |
| 1   | D     | 435 | GLU  |
| 1   | D     | 817 | GLN  |
| 1   | G     | 269 | LEU  |
| 1   | G     | 435 | GLU  |
| 1   | G     | 817 | GLN  |
| 1   | J     | 269 | LEU  |
| 1   | J     | 435 | GLU  |
| 1   | J     | 817 | GLN  |
| 1   | M     | 435 | GLU  |
| 1   | M     | 817 | GLN  |
| 1   | P     | 435 | GLU  |
| 1   | P     | 817 | GLN  |
| 4   | 0     | 2   | GLU  |
| 4   | 0     | 253 | GLU  |
| 4   | 1     | 2   | GLU  |
| 4   | 2     | 2   | GLU  |
| 4   | 3     | 2   | GLU  |
| 4   | 4     | 2   | GLU  |
| 4   | 5     | 2   | GLU  |
| 4   | 7     | 2   | GLU  |
| 4   | 7     | 253 | GLU  |
| 4   | 8     | 2   | GLU  |
| 4   | 8     | 253 | GLU  |
| 4   | 9     | 2   | GLU  |
| 4   | V     | 2   | GLU  |
| 4   | W     | 2   | GLU  |
| 4   | W     | 253 | GLU  |
| 4   | X     | 2   | GLU  |
| 4   | Y     | 2   | GLU  |
| 4   | Y     | 253 | GLU  |
| 4   | Z     | 2   | GLU  |
| 1   | A     | 8   | ALA  |
| 1   | A     | 269 | LEU  |
| 1   | A     | 578 | HIS  |
| 2   | B     | 140 | PHE  |
| 1   | D     | 8   | ALA  |
| 1   | D     | 556 | ASP  |
| 1   | D     | 578 | HIS  |
| 2   | E     | 140 | PHE  |
| 1   | G     | 8   | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 79  | SER  |
| 1   | G     | 578 | HIS  |
| 2   | H     | 140 | PHE  |
| 1   | J     | 8   | ALA  |
| 1   | J     | 578 | HIS  |
| 2   | K     | 140 | PHE  |
| 1   | M     | 8   | ALA  |
| 1   | M     | 269 | LEU  |
| 1   | M     | 556 | ASP  |
| 1   | M     | 578 | HIS  |
| 1   | P     | 8   | ALA  |
| 1   | P     | 269 | LEU  |
| 1   | P     | 578 | HIS  |
| 2   | Q     | 140 | PHE  |
| 4   | 1     | 253 | GLU  |
| 4   | 2     | 253 | GLU  |
| 4   | 3     | 253 | GLU  |
| 4   | 4     | 253 | GLU  |
| 4   | 5     | 253 | GLU  |
| 4   | 9     | 253 | GLU  |
| 4   | V     | 253 | GLU  |
| 4   | X     | 253 | GLU  |
| 4   | Z     | 253 | GLU  |
| 1   | A     | 79  | SER  |
| 1   | A     | 199 | ILE  |
| 1   | A     | 556 | ASP  |
| 2   | B     | 142 | PRO  |
| 1   | D     | 79  | SER  |
| 1   | D     | 199 | ILE  |
| 2   | E     | 142 | PRO  |
| 1   | G     | 199 | ILE  |
| 1   | G     | 556 | ASP  |
| 2   | H     | 142 | PRO  |
| 1   | J     | 79  | SER  |
| 1   | J     | 199 | ILE  |
| 1   | J     | 556 | ASP  |
| 2   | K     | 142 | PRO  |
| 1   | M     | 79  | SER  |
| 1   | M     | 199 | ILE  |
| 2   | N     | 140 | PHE  |
| 2   | N     | 142 | PRO  |
| 1   | P     | 79  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 199 | ILE  |
| 1   | P     | 556 | ASP  |
| 2   | Q     | 142 | PRO  |
| 1   | A     | 840 | PRO  |
| 1   | D     | 840 | PRO  |
| 1   | G     | 840 | PRO  |
| 1   | J     | 287 | ILE  |
| 1   | J     | 840 | PRO  |
| 1   | M     | 840 | PRO  |
| 1   | P     | 287 | ILE  |
| 1   | P     | 840 | PRO  |
| 4   | 0     | 242 | LEU  |
| 4   | 1     | 242 | LEU  |
| 4   | 2     | 242 | LEU  |
| 4   | 3     | 242 | LEU  |
| 4   | 4     | 242 | LEU  |
| 4   | 5     | 242 | LEU  |
| 4   | 7     | 242 | LEU  |
| 4   | 8     | 242 | LEU  |
| 4   | 9     | 242 | LEU  |
| 4   | V     | 242 | LEU  |
| 4   | W     | 242 | LEU  |
| 4   | X     | 242 | LEU  |
| 4   | Y     | 242 | LEU  |
| 4   | Z     | 242 | LEU  |
| 1   | A     | 287 | ILE  |
| 1   | D     | 287 | ILE  |
| 1   | G     | 287 | ILE  |
| 1   | M     | 287 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric | Outliers  | Percentiles       |
|-----|-------|----------------|-----------|-----------|-------------------|
| 1   | A     | 672/672 (100%) | 510 (76%) | 162 (24%) | <b>1</b> <b>6</b> |
| 1   | D     | 672/672 (100%) | 514 (76%) | 158 (24%) | <b>1</b> <b>7</b> |

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| Mol | Chain | Analysed         | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|------------------|------------|------------|-------------|----|
| 1   | G     | 672/672 (100%)   | 513 (76%)  | 159 (24%)  | 1           | 7  |
| 1   | J     | 672/672 (100%)   | 515 (77%)  | 157 (23%)  | 1           | 7  |
| 1   | M     | 672/672 (100%)   | 514 (76%)  | 158 (24%)  | 1           | 7  |
| 1   | P     | 672/672 (100%)   | 514 (76%)  | 158 (24%)  | 1           | 7  |
| 2   | B     | 120/120 (100%)   | 119 (99%)  | 1 (1%)     | 86          | 94 |
| 2   | E     | 120/120 (100%)   | 119 (99%)  | 1 (1%)     | 86          | 94 |
| 2   | H     | 120/120 (100%)   | 119 (99%)  | 1 (1%)     | 86          | 94 |
| 2   | K     | 120/120 (100%)   | 119 (99%)  | 1 (1%)     | 86          | 94 |
| 2   | N     | 120/120 (100%)   | 119 (99%)  | 1 (1%)     | 86          | 94 |
| 2   | Q     | 120/120 (100%)   | 119 (99%)  | 1 (1%)     | 86          | 94 |
| 3   | C     | 117/117 (100%)   | 112 (96%)  | 5 (4%)     | 35          | 70 |
| 3   | F     | 117/117 (100%)   | 112 (96%)  | 5 (4%)     | 35          | 70 |
| 3   | I     | 117/117 (100%)   | 112 (96%)  | 5 (4%)     | 35          | 70 |
| 3   | L     | 117/117 (100%)   | 112 (96%)  | 5 (4%)     | 35          | 70 |
| 3   | O     | 117/117 (100%)   | 112 (96%)  | 5 (4%)     | 35          | 70 |
| 3   | R     | 117/117 (100%)   | 112 (96%)  | 5 (4%)     | 35          | 70 |
| 4   | 0     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 4           | 24 |
| 4   | 1     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 4           | 23 |
| 4   | 2     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 4           | 23 |
| 4   | 3     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 4           | 24 |
| 4   | 4     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 4           | 24 |
| 4   | 5     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 4           | 23 |
| 4   | 7     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 4           | 24 |
| 4   | 8     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 4           | 23 |
| 4   | 9     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 4           | 24 |
| 4   | V     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 4           | 23 |
| 4   | W     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 4           | 24 |
| 4   | X     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 4           | 23 |
| 4   | Y     | 315/318 (99%)    | 268 (85%)  | 47 (15%)   | 4           | 23 |
| 4   | Z     | 315/318 (99%)    | 269 (85%)  | 46 (15%)   | 4           | 24 |
| All | All   | 9864/9906 (100%) | 8225 (83%) | 1639 (17%) | 6           | 19 |

All (1639) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASP  |
| 1   | A     | 7   | MET  |
| 1   | A     | 12  | GLU  |
| 1   | A     | 15  | PRO  |
| 1   | A     | 17  | LEU  |
| 1   | A     | 20  | SER  |
| 1   | A     | 22  | LYS  |
| 1   | A     | 36  | SER  |
| 1   | A     | 37  | SER  |
| 1   | A     | 40  | VAL  |
| 1   | A     | 46  | SER  |
| 1   | A     | 61  | THR  |
| 1   | A     | 69  | THR  |
| 1   | A     | 70  | LEU  |
| 1   | A     | 72  | VAL  |
| 1   | A     | 73  | LYS  |
| 1   | A     | 75  | ASP  |
| 1   | A     | 76  | GLN  |
| 1   | A     | 97  | LEU  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 109 | ARG  |
| 1   | A     | 114 | MET  |
| 1   | A     | 117 | THR  |
| 1   | A     | 121 | LEU  |
| 1   | A     | 126 | VAL  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 135 | TYR  |
| 1   | A     | 136 | ASN  |
| 1   | A     | 146 | LYS  |
| 1   | A     | 149 | GLN  |
| 1   | A     | 155 | ILE  |
| 1   | A     | 157 | SER  |
| 1   | A     | 158 | ILE  |
| 1   | A     | 159 | SER  |
| 1   | A     | 165 | PHE  |
| 1   | A     | 167 | LEU  |
| 1   | A     | 169 | ASP  |
| 1   | A     | 173 | GLN  |
| 1   | A     | 178 | THR  |
| 1   | A     | 185 | LYS  |
| 1   | A     | 186 | THR  |
| 1   | A     | 187 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 189 | THR  |
| 1   | A     | 191 | ARG  |
| 1   | A     | 193 | ILE  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 198 | THR  |
| 1   | A     | 199 | ILE  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 219 | GLU  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 223 | ILE  |
| 1   | A     | 227 | PRO  |
| 1   | A     | 229 | LEU  |
| 1   | A     | 244 | SER  |
| 1   | A     | 245 | ARG  |
| 1   | A     | 251 | ARG  |
| 1   | A     | 264 | ASP  |
| 1   | A     | 273 | SER  |
| 1   | A     | 274 | ARG  |
| 1   | A     | 278 | GLN  |
| 1   | A     | 282 | GLU  |
| 1   | A     | 287 | ILE  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 298 | GLU  |
| 1   | A     | 300 | ILE  |
| 1   | A     | 325 | ILE  |
| 1   | A     | 331 | LEU  |
| 1   | A     | 336 | SER  |
| 1   | A     | 351 | ILE  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 364 | LEU  |
| 1   | A     | 365 | LYS  |
| 1   | A     | 372 | GLU  |
| 1   | A     | 376 | GLU  |
| 1   | A     | 381 | GLU  |
| 1   | A     | 389 | LEU  |
| 1   | A     | 392 | LEU  |
| 1   | A     | 394 | SER  |
| 1   | A     | 399 | LYS  |
| 1   | A     | 405 | ARG  |
| 1   | A     | 410 | ASN  |
| 1   | A     | 439 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 447 | GLN  |
| 1   | A     | 448 | GLN  |
| 1   | A     | 449 | LEU  |
| 1   | A     | 452 | LYS  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 455 | ARG  |
| 1   | A     | 457 | TYR  |
| 1   | A     | 462 | LEU  |
| 1   | A     | 471 | ASP  |
| 1   | A     | 474 | SER  |
| 1   | A     | 480 | ILE  |
| 1   | A     | 487 | LEU  |
| 1   | A     | 495 | MET  |
| 1   | A     | 499 | GLU  |
| 1   | A     | 506 | GLU  |
| 1   | A     | 513 | ILE  |
| 1   | A     | 518 | ASP  |
| 1   | A     | 524 | GLU  |
| 1   | A     | 532 | ILE  |
| 1   | A     | 534 | SER  |
| 1   | A     | 537 | GLU  |
| 1   | A     | 543 | PRO  |
| 1   | A     | 549 | SER  |
| 1   | A     | 561 | LYS  |
| 1   | A     | 562 | SER  |
| 1   | A     | 563 | ASN  |
| 1   | A     | 569 | LYS  |
| 1   | A     | 580 | SER  |
| 1   | A     | 593 | SER  |
| 1   | A     | 597 | GLU  |
| 1   | A     | 604 | ASN  |
| 1   | A     | 608 | ILE  |
| 1   | A     | 610 | LEU  |
| 1   | A     | 615 | SER  |
| 1   | A     | 621 | LEU  |
| 1   | A     | 625 | THR  |
| 1   | A     | 664 | LEU  |
| 1   | A     | 666 | SER  |
| 1   | A     | 673 | ARG  |
| 1   | A     | 675 | ILE  |
| 1   | A     | 676 | ILE  |
| 1   | A     | 686 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 689 | GLU  |
| 1   | A     | 690 | LEU  |
| 1   | A     | 693 | HIS  |
| 1   | A     | 698 | ASN  |
| 1   | A     | 701 | LEU  |
| 1   | A     | 702 | GLU  |
| 1   | A     | 704 | ILE  |
| 1   | A     | 708 | ARG  |
| 1   | A     | 713 | SER  |
| 1   | A     | 714 | ARG  |
| 1   | A     | 716 | LEU  |
| 1   | A     | 719 | ASP  |
| 1   | A     | 722 | GLN  |
| 1   | A     | 723 | ARG  |
| 1   | A     | 727 | LEU  |
| 1   | A     | 728 | ASN  |
| 1   | A     | 745 | GLU  |
| 1   | A     | 752 | ASP  |
| 1   | A     | 753 | VAL  |
| 1   | A     | 754 | ASP  |
| 1   | A     | 762 | HIS  |
| 1   | A     | 774 | LEU  |
| 1   | A     | 785 | GLU  |
| 1   | A     | 787 | ILE  |
| 1   | A     | 793 | ARG  |
| 1   | A     | 799 | MET  |
| 1   | A     | 802 | GLU  |
| 1   | A     | 804 | ARG  |
| 1   | A     | 810 | ARG  |
| 1   | A     | 816 | ILE  |
| 1   | A     | 822 | SER  |
| 1   | A     | 832 | MET  |
| 1   | A     | 834 | LEU  |
| 1   | A     | 838 | ILE  |
| 1   | A     | 842 | LEU  |
| 1   | A     | 843 | LYS  |
| 2   | B     | 142 | PRO  |
| 3   | C     | 48  | LYS  |
| 3   | C     | 68  | PHE  |
| 3   | C     | 83  | THR  |
| 3   | C     | 95  | ASP  |
| 3   | C     | 96  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 4   | ASP  |
| 1   | D     | 7   | MET  |
| 1   | D     | 12  | GLU  |
| 1   | D     | 15  | PRO  |
| 1   | D     | 17  | LEU  |
| 1   | D     | 20  | SER  |
| 1   | D     | 22  | LYS  |
| 1   | D     | 36  | SER  |
| 1   | D     | 37  | SER  |
| 1   | D     | 46  | SER  |
| 1   | D     | 61  | THR  |
| 1   | D     | 69  | THR  |
| 1   | D     | 70  | LEU  |
| 1   | D     | 72  | VAL  |
| 1   | D     | 73  | LYS  |
| 1   | D     | 75  | ASP  |
| 1   | D     | 76  | GLN  |
| 1   | D     | 97  | LEU  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 109 | ARG  |
| 1   | D     | 114 | MET  |
| 1   | D     | 117 | THR  |
| 1   | D     | 121 | LEU  |
| 1   | D     | 126 | VAL  |
| 1   | D     | 127 | ASN  |
| 1   | D     | 135 | TYR  |
| 1   | D     | 136 | ASN  |
| 1   | D     | 146 | LYS  |
| 1   | D     | 149 | GLN  |
| 1   | D     | 155 | ILE  |
| 1   | D     | 157 | SER  |
| 1   | D     | 158 | ILE  |
| 1   | D     | 159 | SER  |
| 1   | D     | 165 | PHE  |
| 1   | D     | 167 | LEU  |
| 1   | D     | 169 | ASP  |
| 1   | D     | 173 | GLN  |
| 1   | D     | 178 | THR  |
| 1   | D     | 185 | LYS  |
| 1   | D     | 186 | THR  |
| 1   | D     | 187 | VAL  |
| 1   | D     | 189 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 191 | ARG  |
| 1   | D     | 193 | ILE  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 198 | THR  |
| 1   | D     | 199 | ILE  |
| 1   | D     | 218 | LEU  |
| 1   | D     | 219 | GLU  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 223 | ILE  |
| 1   | D     | 229 | LEU  |
| 1   | D     | 244 | SER  |
| 1   | D     | 245 | ARG  |
| 1   | D     | 251 | ARG  |
| 1   | D     | 264 | ASP  |
| 1   | D     | 273 | SER  |
| 1   | D     | 274 | ARG  |
| 1   | D     | 278 | GLN  |
| 1   | D     | 282 | GLU  |
| 1   | D     | 287 | ILE  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 294 | ASN  |
| 1   | D     | 298 | GLU  |
| 1   | D     | 300 | ILE  |
| 1   | D     | 325 | ILE  |
| 1   | D     | 331 | LEU  |
| 1   | D     | 336 | SER  |
| 1   | D     | 351 | ILE  |
| 1   | D     | 354 | LEU  |
| 1   | D     | 364 | LEU  |
| 1   | D     | 365 | LYS  |
| 1   | D     | 372 | GLU  |
| 1   | D     | 376 | GLU  |
| 1   | D     | 381 | GLU  |
| 1   | D     | 389 | LEU  |
| 1   | D     | 392 | LEU  |
| 1   | D     | 394 | SER  |
| 1   | D     | 399 | LYS  |
| 1   | D     | 405 | ARG  |
| 1   | D     | 410 | ASN  |
| 1   | D     | 439 | LEU  |
| 1   | D     | 447 | GLN  |
| 1   | D     | 448 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 449 | LEU  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 455 | ARG  |
| 1   | D     | 457 | TYR  |
| 1   | D     | 462 | LEU  |
| 1   | D     | 471 | ASP  |
| 1   | D     | 474 | SER  |
| 1   | D     | 480 | ILE  |
| 1   | D     | 487 | LEU  |
| 1   | D     | 495 | MET  |
| 1   | D     | 499 | GLU  |
| 1   | D     | 506 | GLU  |
| 1   | D     | 513 | ILE  |
| 1   | D     | 518 | ASP  |
| 1   | D     | 524 | GLU  |
| 1   | D     | 532 | ILE  |
| 1   | D     | 534 | SER  |
| 1   | D     | 537 | GLU  |
| 1   | D     | 549 | SER  |
| 1   | D     | 561 | LYS  |
| 1   | D     | 562 | SER  |
| 1   | D     | 563 | ASN  |
| 1   | D     | 569 | LYS  |
| 1   | D     | 580 | SER  |
| 1   | D     | 593 | SER  |
| 1   | D     | 597 | GLU  |
| 1   | D     | 604 | ASN  |
| 1   | D     | 608 | ILE  |
| 1   | D     | 610 | LEU  |
| 1   | D     | 615 | SER  |
| 1   | D     | 621 | LEU  |
| 1   | D     | 625 | THR  |
| 1   | D     | 664 | LEU  |
| 1   | D     | 666 | SER  |
| 1   | D     | 673 | ARG  |
| 1   | D     | 675 | ILE  |
| 1   | D     | 676 | ILE  |
| 1   | D     | 686 | MET  |
| 1   | D     | 689 | GLU  |
| 1   | D     | 690 | LEU  |
| 1   | D     | 693 | HIS  |
| 1   | D     | 698 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 701 | LEU  |
| 1   | D     | 702 | GLU  |
| 1   | D     | 704 | ILE  |
| 1   | D     | 708 | ARG  |
| 1   | D     | 713 | SER  |
| 1   | D     | 714 | ARG  |
| 1   | D     | 716 | LEU  |
| 1   | D     | 719 | ASP  |
| 1   | D     | 722 | GLN  |
| 1   | D     | 723 | ARG  |
| 1   | D     | 727 | LEU  |
| 1   | D     | 728 | ASN  |
| 1   | D     | 745 | GLU  |
| 1   | D     | 752 | ASP  |
| 1   | D     | 753 | VAL  |
| 1   | D     | 754 | ASP  |
| 1   | D     | 762 | HIS  |
| 1   | D     | 774 | LEU  |
| 1   | D     | 785 | GLU  |
| 1   | D     | 787 | ILE  |
| 1   | D     | 793 | ARG  |
| 1   | D     | 799 | MET  |
| 1   | D     | 802 | GLU  |
| 1   | D     | 804 | ARG  |
| 1   | D     | 810 | ARG  |
| 1   | D     | 816 | ILE  |
| 1   | D     | 822 | SER  |
| 1   | D     | 832 | MET  |
| 1   | D     | 834 | LEU  |
| 1   | D     | 838 | ILE  |
| 1   | D     | 842 | LEU  |
| 1   | D     | 843 | LYS  |
| 2   | E     | 142 | PRO  |
| 3   | F     | 48  | LYS  |
| 3   | F     | 68  | PHE  |
| 3   | F     | 83  | THR  |
| 3   | F     | 95  | ASP  |
| 3   | F     | 96  | LYS  |
| 1   | G     | 4   | ASP  |
| 1   | G     | 7   | MET  |
| 1   | G     | 12  | GLU  |
| 1   | G     | 15  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 17  | LEU  |
| 1   | G     | 20  | SER  |
| 1   | G     | 22  | LYS  |
| 1   | G     | 36  | SER  |
| 1   | G     | 37  | SER  |
| 1   | G     | 46  | SER  |
| 1   | G     | 61  | THR  |
| 1   | G     | 69  | THR  |
| 1   | G     | 70  | LEU  |
| 1   | G     | 72  | VAL  |
| 1   | G     | 73  | LYS  |
| 1   | G     | 75  | ASP  |
| 1   | G     | 76  | GLN  |
| 1   | G     | 97  | LEU  |
| 1   | G     | 106 | LEU  |
| 1   | G     | 109 | ARG  |
| 1   | G     | 114 | MET  |
| 1   | G     | 117 | THR  |
| 1   | G     | 121 | LEU  |
| 1   | G     | 126 | VAL  |
| 1   | G     | 127 | ASN  |
| 1   | G     | 135 | TYR  |
| 1   | G     | 136 | ASN  |
| 1   | G     | 146 | LYS  |
| 1   | G     | 149 | GLN  |
| 1   | G     | 155 | ILE  |
| 1   | G     | 157 | SER  |
| 1   | G     | 158 | ILE  |
| 1   | G     | 159 | SER  |
| 1   | G     | 165 | PHE  |
| 1   | G     | 167 | LEU  |
| 1   | G     | 169 | ASP  |
| 1   | G     | 173 | GLN  |
| 1   | G     | 178 | THR  |
| 1   | G     | 185 | LYS  |
| 1   | G     | 186 | THR  |
| 1   | G     | 187 | VAL  |
| 1   | G     | 189 | THR  |
| 1   | G     | 191 | ARG  |
| 1   | G     | 193 | ILE  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 198 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 199 | ILE  |
| 1   | G     | 218 | LEU  |
| 1   | G     | 219 | GLU  |
| 1   | G     | 221 | GLN  |
| 1   | G     | 223 | ILE  |
| 1   | G     | 229 | LEU  |
| 1   | G     | 244 | SER  |
| 1   | G     | 245 | ARG  |
| 1   | G     | 251 | ARG  |
| 1   | G     | 264 | ASP  |
| 1   | G     | 273 | SER  |
| 1   | G     | 274 | ARG  |
| 1   | G     | 278 | GLN  |
| 1   | G     | 282 | GLU  |
| 1   | G     | 287 | ILE  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 294 | ASN  |
| 1   | G     | 298 | GLU  |
| 1   | G     | 300 | ILE  |
| 1   | G     | 325 | ILE  |
| 1   | G     | 331 | LEU  |
| 1   | G     | 336 | SER  |
| 1   | G     | 351 | ILE  |
| 1   | G     | 354 | LEU  |
| 1   | G     | 364 | LEU  |
| 1   | G     | 365 | LYS  |
| 1   | G     | 372 | GLU  |
| 1   | G     | 376 | GLU  |
| 1   | G     | 381 | GLU  |
| 1   | G     | 389 | LEU  |
| 1   | G     | 392 | LEU  |
| 1   | G     | 394 | SER  |
| 1   | G     | 399 | LYS  |
| 1   | G     | 405 | ARG  |
| 1   | G     | 410 | ASN  |
| 1   | G     | 439 | LEU  |
| 1   | G     | 447 | GLN  |
| 1   | G     | 448 | GLN  |
| 1   | G     | 449 | LEU  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 455 | ARG  |
| 1   | G     | 457 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 462 | LEU  |
| 1   | G     | 471 | ASP  |
| 1   | G     | 474 | SER  |
| 1   | G     | 480 | ILE  |
| 1   | G     | 487 | LEU  |
| 1   | G     | 495 | MET  |
| 1   | G     | 499 | GLU  |
| 1   | G     | 506 | GLU  |
| 1   | G     | 513 | ILE  |
| 1   | G     | 518 | ASP  |
| 1   | G     | 524 | GLU  |
| 1   | G     | 532 | ILE  |
| 1   | G     | 534 | SER  |
| 1   | G     | 537 | GLU  |
| 1   | G     | 543 | PRO  |
| 1   | G     | 549 | SER  |
| 1   | G     | 561 | LYS  |
| 1   | G     | 562 | SER  |
| 1   | G     | 563 | ASN  |
| 1   | G     | 569 | LYS  |
| 1   | G     | 580 | SER  |
| 1   | G     | 593 | SER  |
| 1   | G     | 597 | GLU  |
| 1   | G     | 604 | ASN  |
| 1   | G     | 608 | ILE  |
| 1   | G     | 610 | LEU  |
| 1   | G     | 615 | SER  |
| 1   | G     | 621 | LEU  |
| 1   | G     | 625 | THR  |
| 1   | G     | 664 | LEU  |
| 1   | G     | 666 | SER  |
| 1   | G     | 673 | ARG  |
| 1   | G     | 675 | ILE  |
| 1   | G     | 676 | ILE  |
| 1   | G     | 686 | MET  |
| 1   | G     | 689 | GLU  |
| 1   | G     | 690 | LEU  |
| 1   | G     | 693 | HIS  |
| 1   | G     | 698 | ASN  |
| 1   | G     | 701 | LEU  |
| 1   | G     | 702 | GLU  |
| 1   | G     | 704 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 708 | ARG  |
| 1   | G     | 713 | SER  |
| 1   | G     | 714 | ARG  |
| 1   | G     | 716 | LEU  |
| 1   | G     | 719 | ASP  |
| 1   | G     | 722 | GLN  |
| 1   | G     | 723 | ARG  |
| 1   | G     | 727 | LEU  |
| 1   | G     | 728 | ASN  |
| 1   | G     | 745 | GLU  |
| 1   | G     | 752 | ASP  |
| 1   | G     | 753 | VAL  |
| 1   | G     | 754 | ASP  |
| 1   | G     | 762 | HIS  |
| 1   | G     | 774 | LEU  |
| 1   | G     | 785 | GLU  |
| 1   | G     | 787 | ILE  |
| 1   | G     | 793 | ARG  |
| 1   | G     | 799 | MET  |
| 1   | G     | 802 | GLU  |
| 1   | G     | 804 | ARG  |
| 1   | G     | 810 | ARG  |
| 1   | G     | 816 | ILE  |
| 1   | G     | 822 | SER  |
| 1   | G     | 832 | MET  |
| 1   | G     | 834 | LEU  |
| 1   | G     | 838 | ILE  |
| 1   | G     | 842 | LEU  |
| 1   | G     | 843 | LYS  |
| 2   | H     | 142 | PRO  |
| 3   | I     | 48  | LYS  |
| 3   | I     | 68  | PHE  |
| 3   | I     | 83  | THR  |
| 3   | I     | 95  | ASP  |
| 3   | I     | 96  | LYS  |
| 1   | J     | 4   | ASP  |
| 1   | J     | 7   | MET  |
| 1   | J     | 12  | GLU  |
| 1   | J     | 15  | PRO  |
| 1   | J     | 17  | LEU  |
| 1   | J     | 20  | SER  |
| 1   | J     | 22  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 36  | SER  |
| 1   | J     | 37  | SER  |
| 1   | J     | 46  | SER  |
| 1   | J     | 61  | THR  |
| 1   | J     | 69  | THR  |
| 1   | J     | 70  | LEU  |
| 1   | J     | 72  | VAL  |
| 1   | J     | 73  | LYS  |
| 1   | J     | 75  | ASP  |
| 1   | J     | 76  | GLN  |
| 1   | J     | 97  | LEU  |
| 1   | J     | 106 | LEU  |
| 1   | J     | 109 | ARG  |
| 1   | J     | 114 | MET  |
| 1   | J     | 117 | THR  |
| 1   | J     | 121 | LEU  |
| 1   | J     | 126 | VAL  |
| 1   | J     | 127 | ASN  |
| 1   | J     | 135 | TYR  |
| 1   | J     | 136 | ASN  |
| 1   | J     | 146 | LYS  |
| 1   | J     | 149 | GLN  |
| 1   | J     | 155 | ILE  |
| 1   | J     | 157 | SER  |
| 1   | J     | 158 | ILE  |
| 1   | J     | 159 | SER  |
| 1   | J     | 165 | PHE  |
| 1   | J     | 167 | LEU  |
| 1   | J     | 169 | ASP  |
| 1   | J     | 173 | GLN  |
| 1   | J     | 178 | THR  |
| 1   | J     | 185 | LYS  |
| 1   | J     | 186 | THR  |
| 1   | J     | 187 | VAL  |
| 1   | J     | 191 | ARG  |
| 1   | J     | 193 | ILE  |
| 1   | J     | 194 | GLN  |
| 1   | J     | 198 | THR  |
| 1   | J     | 199 | ILE  |
| 1   | J     | 218 | LEU  |
| 1   | J     | 219 | GLU  |
| 1   | J     | 221 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 223 | ILE  |
| 1   | J     | 229 | LEU  |
| 1   | J     | 244 | SER  |
| 1   | J     | 245 | ARG  |
| 1   | J     | 251 | ARG  |
| 1   | J     | 264 | ASP  |
| 1   | J     | 273 | SER  |
| 1   | J     | 274 | ARG  |
| 1   | J     | 278 | GLN  |
| 1   | J     | 282 | GLU  |
| 1   | J     | 287 | ILE  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 294 | ASN  |
| 1   | J     | 298 | GLU  |
| 1   | J     | 300 | ILE  |
| 1   | J     | 325 | ILE  |
| 1   | J     | 331 | LEU  |
| 1   | J     | 336 | SER  |
| 1   | J     | 351 | ILE  |
| 1   | J     | 354 | LEU  |
| 1   | J     | 364 | LEU  |
| 1   | J     | 365 | LYS  |
| 1   | J     | 372 | GLU  |
| 1   | J     | 376 | GLU  |
| 1   | J     | 381 | GLU  |
| 1   | J     | 389 | LEU  |
| 1   | J     | 392 | LEU  |
| 1   | J     | 394 | SER  |
| 1   | J     | 399 | LYS  |
| 1   | J     | 405 | ARG  |
| 1   | J     | 410 | ASN  |
| 1   | J     | 439 | LEU  |
| 1   | J     | 447 | GLN  |
| 1   | J     | 448 | GLN  |
| 1   | J     | 449 | LEU  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 455 | ARG  |
| 1   | J     | 457 | TYR  |
| 1   | J     | 462 | LEU  |
| 1   | J     | 471 | ASP  |
| 1   | J     | 474 | SER  |
| 1   | J     | 480 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 487 | LEU  |
| 1   | J     | 495 | MET  |
| 1   | J     | 499 | GLU  |
| 1   | J     | 506 | GLU  |
| 1   | J     | 513 | ILE  |
| 1   | J     | 518 | ASP  |
| 1   | J     | 524 | GLU  |
| 1   | J     | 532 | ILE  |
| 1   | J     | 534 | SER  |
| 1   | J     | 537 | GLU  |
| 1   | J     | 543 | PRO  |
| 1   | J     | 549 | SER  |
| 1   | J     | 561 | LYS  |
| 1   | J     | 562 | SER  |
| 1   | J     | 563 | ASN  |
| 1   | J     | 569 | LYS  |
| 1   | J     | 580 | SER  |
| 1   | J     | 593 | SER  |
| 1   | J     | 597 | GLU  |
| 1   | J     | 604 | ASN  |
| 1   | J     | 608 | ILE  |
| 1   | J     | 610 | LEU  |
| 1   | J     | 615 | SER  |
| 1   | J     | 621 | LEU  |
| 1   | J     | 625 | THR  |
| 1   | J     | 664 | LEU  |
| 1   | J     | 666 | SER  |
| 1   | J     | 673 | ARG  |
| 1   | J     | 675 | ILE  |
| 1   | J     | 676 | ILE  |
| 1   | J     | 686 | MET  |
| 1   | J     | 689 | GLU  |
| 1   | J     | 690 | LEU  |
| 1   | J     | 693 | HIS  |
| 1   | J     | 698 | ASN  |
| 1   | J     | 701 | LEU  |
| 1   | J     | 702 | GLU  |
| 1   | J     | 708 | ARG  |
| 1   | J     | 713 | SER  |
| 1   | J     | 714 | ARG  |
| 1   | J     | 716 | LEU  |
| 1   | J     | 719 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 722 | GLN  |
| 1   | J     | 723 | ARG  |
| 1   | J     | 727 | LEU  |
| 1   | J     | 728 | ASN  |
| 1   | J     | 745 | GLU  |
| 1   | J     | 752 | ASP  |
| 1   | J     | 753 | VAL  |
| 1   | J     | 754 | ASP  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 774 | LEU  |
| 1   | J     | 785 | GLU  |
| 1   | J     | 787 | ILE  |
| 1   | J     | 793 | ARG  |
| 1   | J     | 799 | MET  |
| 1   | J     | 802 | GLU  |
| 1   | J     | 804 | ARG  |
| 1   | J     | 810 | ARG  |
| 1   | J     | 816 | ILE  |
| 1   | J     | 822 | SER  |
| 1   | J     | 832 | MET  |
| 1   | J     | 834 | LEU  |
| 1   | J     | 838 | ILE  |
| 1   | J     | 842 | LEU  |
| 1   | J     | 843 | LYS  |
| 2   | K     | 142 | PRO  |
| 3   | L     | 48  | LYS  |
| 3   | L     | 68  | PHE  |
| 3   | L     | 83  | THR  |
| 3   | L     | 95  | ASP  |
| 3   | L     | 96  | LYS  |
| 1   | M     | 4   | ASP  |
| 1   | M     | 7   | MET  |
| 1   | M     | 12  | GLU  |
| 1   | M     | 15  | PRO  |
| 1   | M     | 17  | LEU  |
| 1   | M     | 20  | SER  |
| 1   | M     | 22  | LYS  |
| 1   | M     | 36  | SER  |
| 1   | M     | 37  | SER  |
| 1   | M     | 46  | SER  |
| 1   | M     | 61  | THR  |
| 1   | M     | 69  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 70  | LEU  |
| 1   | M     | 72  | VAL  |
| 1   | M     | 73  | LYS  |
| 1   | M     | 75  | ASP  |
| 1   | M     | 76  | GLN  |
| 1   | M     | 97  | LEU  |
| 1   | M     | 106 | LEU  |
| 1   | M     | 109 | ARG  |
| 1   | M     | 114 | MET  |
| 1   | M     | 117 | THR  |
| 1   | M     | 121 | LEU  |
| 1   | M     | 126 | VAL  |
| 1   | M     | 127 | ASN  |
| 1   | M     | 135 | TYR  |
| 1   | M     | 136 | ASN  |
| 1   | M     | 146 | LYS  |
| 1   | M     | 149 | GLN  |
| 1   | M     | 155 | ILE  |
| 1   | M     | 157 | SER  |
| 1   | M     | 158 | ILE  |
| 1   | M     | 159 | SER  |
| 1   | M     | 165 | PHE  |
| 1   | M     | 167 | LEU  |
| 1   | M     | 169 | ASP  |
| 1   | M     | 173 | GLN  |
| 1   | M     | 178 | THR  |
| 1   | M     | 185 | LYS  |
| 1   | M     | 186 | THR  |
| 1   | M     | 187 | VAL  |
| 1   | M     | 189 | THR  |
| 1   | M     | 191 | ARG  |
| 1   | M     | 193 | ILE  |
| 1   | M     | 194 | GLN  |
| 1   | M     | 198 | THR  |
| 1   | M     | 199 | ILE  |
| 1   | M     | 218 | LEU  |
| 1   | M     | 219 | GLU  |
| 1   | M     | 221 | GLN  |
| 1   | M     | 223 | ILE  |
| 1   | M     | 229 | LEU  |
| 1   | M     | 244 | SER  |
| 1   | M     | 245 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 251 | ARG  |
| 1   | M     | 264 | ASP  |
| 1   | M     | 273 | SER  |
| 1   | M     | 274 | ARG  |
| 1   | M     | 278 | GLN  |
| 1   | M     | 282 | GLU  |
| 1   | M     | 287 | ILE  |
| 1   | M     | 290 | GLN  |
| 1   | M     | 294 | ASN  |
| 1   | M     | 298 | GLU  |
| 1   | M     | 300 | ILE  |
| 1   | M     | 325 | ILE  |
| 1   | M     | 331 | LEU  |
| 1   | M     | 336 | SER  |
| 1   | M     | 351 | ILE  |
| 1   | M     | 354 | LEU  |
| 1   | M     | 364 | LEU  |
| 1   | M     | 365 | LYS  |
| 1   | M     | 372 | GLU  |
| 1   | M     | 376 | GLU  |
| 1   | M     | 381 | GLU  |
| 1   | M     | 389 | LEU  |
| 1   | M     | 392 | LEU  |
| 1   | M     | 394 | SER  |
| 1   | M     | 399 | LYS  |
| 1   | M     | 405 | ARG  |
| 1   | M     | 410 | ASN  |
| 1   | M     | 439 | LEU  |
| 1   | M     | 447 | GLN  |
| 1   | M     | 448 | GLN  |
| 1   | M     | 449 | LEU  |
| 1   | M     | 453 | GLN  |
| 1   | M     | 455 | ARG  |
| 1   | M     | 457 | TYR  |
| 1   | M     | 462 | LEU  |
| 1   | M     | 471 | ASP  |
| 1   | M     | 474 | SER  |
| 1   | M     | 480 | ILE  |
| 1   | M     | 487 | LEU  |
| 1   | M     | 495 | MET  |
| 1   | M     | 499 | GLU  |
| 1   | M     | 506 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 513 | ILE  |
| 1   | M     | 518 | ASP  |
| 1   | M     | 524 | GLU  |
| 1   | M     | 532 | ILE  |
| 1   | M     | 534 | SER  |
| 1   | M     | 537 | GLU  |
| 1   | M     | 543 | PRO  |
| 1   | M     | 549 | SER  |
| 1   | M     | 561 | LYS  |
| 1   | M     | 562 | SER  |
| 1   | M     | 563 | ASN  |
| 1   | M     | 569 | LYS  |
| 1   | M     | 580 | SER  |
| 1   | M     | 593 | SER  |
| 1   | M     | 597 | GLU  |
| 1   | M     | 604 | ASN  |
| 1   | M     | 608 | ILE  |
| 1   | M     | 610 | LEU  |
| 1   | M     | 615 | SER  |
| 1   | M     | 621 | LEU  |
| 1   | M     | 625 | THR  |
| 1   | M     | 664 | LEU  |
| 1   | M     | 666 | SER  |
| 1   | M     | 673 | ARG  |
| 1   | M     | 675 | ILE  |
| 1   | M     | 676 | ILE  |
| 1   | M     | 686 | MET  |
| 1   | M     | 689 | GLU  |
| 1   | M     | 690 | LEU  |
| 1   | M     | 693 | HIS  |
| 1   | M     | 698 | ASN  |
| 1   | M     | 701 | LEU  |
| 1   | M     | 702 | GLU  |
| 1   | M     | 708 | ARG  |
| 1   | M     | 713 | SER  |
| 1   | M     | 714 | ARG  |
| 1   | M     | 716 | LEU  |
| 1   | M     | 719 | ASP  |
| 1   | M     | 722 | GLN  |
| 1   | M     | 723 | ARG  |
| 1   | M     | 727 | LEU  |
| 1   | M     | 728 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 745 | GLU  |
| 1   | M     | 752 | ASP  |
| 1   | M     | 753 | VAL  |
| 1   | M     | 754 | ASP  |
| 1   | M     | 762 | HIS  |
| 1   | M     | 774 | LEU  |
| 1   | M     | 785 | GLU  |
| 1   | M     | 787 | ILE  |
| 1   | M     | 793 | ARG  |
| 1   | M     | 799 | MET  |
| 1   | M     | 802 | GLU  |
| 1   | M     | 804 | ARG  |
| 1   | M     | 810 | ARG  |
| 1   | M     | 816 | ILE  |
| 1   | M     | 822 | SER  |
| 1   | M     | 832 | MET  |
| 1   | M     | 834 | LEU  |
| 1   | M     | 838 | ILE  |
| 1   | M     | 842 | LEU  |
| 1   | M     | 843 | LYS  |
| 2   | N     | 142 | PRO  |
| 3   | O     | 48  | LYS  |
| 3   | O     | 68  | PHE  |
| 3   | O     | 83  | THR  |
| 3   | O     | 95  | ASP  |
| 3   | O     | 96  | LYS  |
| 1   | P     | 4   | ASP  |
| 1   | P     | 7   | MET  |
| 1   | P     | 12  | GLU  |
| 1   | P     | 15  | PRO  |
| 1   | P     | 17  | LEU  |
| 1   | P     | 20  | SER  |
| 1   | P     | 22  | LYS  |
| 1   | P     | 36  | SER  |
| 1   | P     | 37  | SER  |
| 1   | P     | 46  | SER  |
| 1   | P     | 61  | THR  |
| 1   | P     | 69  | THR  |
| 1   | P     | 70  | LEU  |
| 1   | P     | 72  | VAL  |
| 1   | P     | 73  | LYS  |
| 1   | P     | 75  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 76  | GLN  |
| 1   | P     | 97  | LEU  |
| 1   | P     | 106 | LEU  |
| 1   | P     | 109 | ARG  |
| 1   | P     | 114 | MET  |
| 1   | P     | 117 | THR  |
| 1   | P     | 121 | LEU  |
| 1   | P     | 126 | VAL  |
| 1   | P     | 127 | ASN  |
| 1   | P     | 135 | TYR  |
| 1   | P     | 136 | ASN  |
| 1   | P     | 146 | LYS  |
| 1   | P     | 149 | GLN  |
| 1   | P     | 155 | ILE  |
| 1   | P     | 157 | SER  |
| 1   | P     | 158 | ILE  |
| 1   | P     | 159 | SER  |
| 1   | P     | 165 | PHE  |
| 1   | P     | 167 | LEU  |
| 1   | P     | 169 | ASP  |
| 1   | P     | 173 | GLN  |
| 1   | P     | 178 | THR  |
| 1   | P     | 185 | LYS  |
| 1   | P     | 186 | THR  |
| 1   | P     | 187 | VAL  |
| 1   | P     | 189 | THR  |
| 1   | P     | 191 | ARG  |
| 1   | P     | 193 | ILE  |
| 1   | P     | 194 | GLN  |
| 1   | P     | 198 | THR  |
| 1   | P     | 199 | ILE  |
| 1   | P     | 218 | LEU  |
| 1   | P     | 219 | GLU  |
| 1   | P     | 221 | GLN  |
| 1   | P     | 223 | ILE  |
| 1   | P     | 229 | LEU  |
| 1   | P     | 244 | SER  |
| 1   | P     | 245 | ARG  |
| 1   | P     | 251 | ARG  |
| 1   | P     | 264 | ASP  |
| 1   | P     | 273 | SER  |
| 1   | P     | 274 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 278 | GLN  |
| 1   | P     | 282 | GLU  |
| 1   | P     | 287 | ILE  |
| 1   | P     | 290 | GLN  |
| 1   | P     | 294 | ASN  |
| 1   | P     | 298 | GLU  |
| 1   | P     | 300 | ILE  |
| 1   | P     | 325 | ILE  |
| 1   | P     | 331 | LEU  |
| 1   | P     | 336 | SER  |
| 1   | P     | 351 | ILE  |
| 1   | P     | 354 | LEU  |
| 1   | P     | 364 | LEU  |
| 1   | P     | 365 | LYS  |
| 1   | P     | 372 | GLU  |
| 1   | P     | 376 | GLU  |
| 1   | P     | 381 | GLU  |
| 1   | P     | 389 | LEU  |
| 1   | P     | 392 | LEU  |
| 1   | P     | 394 | SER  |
| 1   | P     | 399 | LYS  |
| 1   | P     | 405 | ARG  |
| 1   | P     | 410 | ASN  |
| 1   | P     | 439 | LEU  |
| 1   | P     | 447 | GLN  |
| 1   | P     | 448 | GLN  |
| 1   | P     | 449 | LEU  |
| 1   | P     | 453 | GLN  |
| 1   | P     | 455 | ARG  |
| 1   | P     | 457 | TYR  |
| 1   | P     | 462 | LEU  |
| 1   | P     | 471 | ASP  |
| 1   | P     | 474 | SER  |
| 1   | P     | 480 | ILE  |
| 1   | P     | 487 | LEU  |
| 1   | P     | 495 | MET  |
| 1   | P     | 499 | GLU  |
| 1   | P     | 506 | GLU  |
| 1   | P     | 513 | ILE  |
| 1   | P     | 518 | ASP  |
| 1   | P     | 524 | GLU  |
| 1   | P     | 532 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 534 | SER  |
| 1   | P     | 537 | GLU  |
| 1   | P     | 543 | PRO  |
| 1   | P     | 549 | SER  |
| 1   | P     | 561 | LYS  |
| 1   | P     | 562 | SER  |
| 1   | P     | 563 | ASN  |
| 1   | P     | 569 | LYS  |
| 1   | P     | 580 | SER  |
| 1   | P     | 593 | SER  |
| 1   | P     | 597 | GLU  |
| 1   | P     | 604 | ASN  |
| 1   | P     | 608 | ILE  |
| 1   | P     | 610 | LEU  |
| 1   | P     | 615 | SER  |
| 1   | P     | 621 | LEU  |
| 1   | P     | 625 | THR  |
| 1   | P     | 664 | LEU  |
| 1   | P     | 666 | SER  |
| 1   | P     | 673 | ARG  |
| 1   | P     | 675 | ILE  |
| 1   | P     | 676 | ILE  |
| 1   | P     | 686 | MET  |
| 1   | P     | 689 | GLU  |
| 1   | P     | 690 | LEU  |
| 1   | P     | 693 | HIS  |
| 1   | P     | 698 | ASN  |
| 1   | P     | 701 | LEU  |
| 1   | P     | 702 | GLU  |
| 1   | P     | 708 | ARG  |
| 1   | P     | 713 | SER  |
| 1   | P     | 714 | ARG  |
| 1   | P     | 716 | LEU  |
| 1   | P     | 719 | ASP  |
| 1   | P     | 722 | GLN  |
| 1   | P     | 723 | ARG  |
| 1   | P     | 727 | LEU  |
| 1   | P     | 728 | ASN  |
| 1   | P     | 745 | GLU  |
| 1   | P     | 752 | ASP  |
| 1   | P     | 753 | VAL  |
| 1   | P     | 754 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 762 | HIS  |
| 1   | P     | 774 | LEU  |
| 1   | P     | 785 | GLU  |
| 1   | P     | 787 | ILE  |
| 1   | P     | 793 | ARG  |
| 1   | P     | 799 | MET  |
| 1   | P     | 802 | GLU  |
| 1   | P     | 804 | ARG  |
| 1   | P     | 810 | ARG  |
| 1   | P     | 816 | ILE  |
| 1   | P     | 822 | SER  |
| 1   | P     | 832 | MET  |
| 1   | P     | 834 | LEU  |
| 1   | P     | 838 | ILE  |
| 1   | P     | 842 | LEU  |
| 1   | P     | 843 | LYS  |
| 2   | Q     | 142 | PRO  |
| 3   | R     | 48  | LYS  |
| 3   | R     | 68  | PHE  |
| 3   | R     | 83  | THR  |
| 3   | R     | 95  | ASP  |
| 3   | R     | 96  | LYS  |
| 4   | 0     | 33  | SER  |
| 4   | 0     | 34  | ILE  |
| 4   | 0     | 37  | ARG  |
| 4   | 0     | 66  | THR  |
| 4   | 0     | 72  | GLU  |
| 4   | 0     | 80  | ASP  |
| 4   | 0     | 100 | GLU  |
| 4   | 0     | 109 | PRO  |
| 4   | 0     | 116 | ARG  |
| 4   | 0     | 145 | SER  |
| 4   | 0     | 153 | LEU  |
| 4   | 0     | 159 | VAL  |
| 4   | 0     | 180 | LEU  |
| 4   | 0     | 191 | LYS  |
| 4   | 0     | 196 | ARG  |
| 4   | 0     | 199 | SER  |
| 4   | 0     | 201 | VAL  |
| 4   | 0     | 206 | ARG  |
| 4   | 0     | 221 | LEU  |
| 4   | 0     | 223 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 0     | 229 | THR  |
| 4   | 0     | 239 | SER  |
| 4   | 0     | 242 | LEU  |
| 4   | 0     | 246 | GLN  |
| 4   | 0     | 263 | GLN  |
| 4   | 0     | 281 | SER  |
| 4   | 0     | 283 | MET  |
| 4   | 0     | 287 | ILE  |
| 4   | 0     | 291 | LYS  |
| 4   | 0     | 293 | LEU  |
| 4   | 0     | 297 | ASN  |
| 4   | 0     | 299 | MET  |
| 4   | 0     | 312 | ARG  |
| 4   | 0     | 315 | LYS  |
| 4   | 0     | 318 | THR  |
| 4   | 0     | 320 | LEU  |
| 4   | 0     | 327 | ILE  |
| 4   | 0     | 334 | GLU  |
| 4   | 0     | 349 | LEU  |
| 4   | 0     | 350 | SER  |
| 4   | 0     | 351 | THR  |
| 4   | 0     | 354 | GLN  |
| 4   | 0     | 359 | LYS  |
| 4   | 0     | 360 | GLN  |
| 4   | 0     | 361 | GLU  |
| 4   | 0     | 368 | SER  |
| 4   | 1     | 16  | LEU  |
| 4   | 1     | 33  | SER  |
| 4   | 1     | 34  | ILE  |
| 4   | 1     | 37  | ARG  |
| 4   | 1     | 66  | THR  |
| 4   | 1     | 72  | GLU  |
| 4   | 1     | 80  | ASP  |
| 4   | 1     | 100 | GLU  |
| 4   | 1     | 109 | PRO  |
| 4   | 1     | 116 | ARG  |
| 4   | 1     | 145 | SER  |
| 4   | 1     | 153 | LEU  |
| 4   | 1     | 159 | VAL  |
| 4   | 1     | 180 | LEU  |
| 4   | 1     | 191 | LYS  |
| 4   | 1     | 196 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 1     | 199 | SER  |
| 4   | 1     | 201 | VAL  |
| 4   | 1     | 206 | ARG  |
| 4   | 1     | 221 | LEU  |
| 4   | 1     | 223 | PHE  |
| 4   | 1     | 229 | THR  |
| 4   | 1     | 239 | SER  |
| 4   | 1     | 242 | LEU  |
| 4   | 1     | 246 | GLN  |
| 4   | 1     | 263 | GLN  |
| 4   | 1     | 281 | SER  |
| 4   | 1     | 283 | MET  |
| 4   | 1     | 287 | ILE  |
| 4   | 1     | 291 | LYS  |
| 4   | 1     | 293 | LEU  |
| 4   | 1     | 297 | ASN  |
| 4   | 1     | 299 | MET  |
| 4   | 1     | 312 | ARG  |
| 4   | 1     | 315 | LYS  |
| 4   | 1     | 318 | THR  |
| 4   | 1     | 320 | LEU  |
| 4   | 1     | 327 | ILE  |
| 4   | 1     | 334 | GLU  |
| 4   | 1     | 349 | LEU  |
| 4   | 1     | 350 | SER  |
| 4   | 1     | 351 | THR  |
| 4   | 1     | 354 | GLN  |
| 4   | 1     | 359 | LYS  |
| 4   | 1     | 360 | GLN  |
| 4   | 1     | 361 | GLU  |
| 4   | 1     | 368 | SER  |
| 4   | 2     | 16  | LEU  |
| 4   | 2     | 33  | SER  |
| 4   | 2     | 34  | ILE  |
| 4   | 2     | 37  | ARG  |
| 4   | 2     | 66  | THR  |
| 4   | 2     | 72  | GLU  |
| 4   | 2     | 80  | ASP  |
| 4   | 2     | 100 | GLU  |
| 4   | 2     | 109 | PRO  |
| 4   | 2     | 116 | ARG  |
| 4   | 2     | 145 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 2     | 153 | LEU  |
| 4   | 2     | 159 | VAL  |
| 4   | 2     | 180 | LEU  |
| 4   | 2     | 191 | LYS  |
| 4   | 2     | 196 | ARG  |
| 4   | 2     | 199 | SER  |
| 4   | 2     | 201 | VAL  |
| 4   | 2     | 206 | ARG  |
| 4   | 2     | 221 | LEU  |
| 4   | 2     | 223 | PHE  |
| 4   | 2     | 229 | THR  |
| 4   | 2     | 239 | SER  |
| 4   | 2     | 242 | LEU  |
| 4   | 2     | 246 | GLN  |
| 4   | 2     | 263 | GLN  |
| 4   | 2     | 281 | SER  |
| 4   | 2     | 283 | MET  |
| 4   | 2     | 287 | ILE  |
| 4   | 2     | 291 | LYS  |
| 4   | 2     | 293 | LEU  |
| 4   | 2     | 297 | ASN  |
| 4   | 2     | 299 | MET  |
| 4   | 2     | 312 | ARG  |
| 4   | 2     | 315 | LYS  |
| 4   | 2     | 318 | THR  |
| 4   | 2     | 320 | LEU  |
| 4   | 2     | 327 | ILE  |
| 4   | 2     | 334 | GLU  |
| 4   | 2     | 349 | LEU  |
| 4   | 2     | 350 | SER  |
| 4   | 2     | 351 | THR  |
| 4   | 2     | 354 | GLN  |
| 4   | 2     | 359 | LYS  |
| 4   | 2     | 360 | GLN  |
| 4   | 2     | 361 | GLU  |
| 4   | 2     | 368 | SER  |
| 4   | 3     | 33  | SER  |
| 4   | 3     | 34  | ILE  |
| 4   | 3     | 37  | ARG  |
| 4   | 3     | 66  | THR  |
| 4   | 3     | 72  | GLU  |
| 4   | 3     | 80  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 3     | 100 | GLU  |
| 4   | 3     | 109 | PRO  |
| 4   | 3     | 116 | ARG  |
| 4   | 3     | 145 | SER  |
| 4   | 3     | 153 | LEU  |
| 4   | 3     | 159 | VAL  |
| 4   | 3     | 180 | LEU  |
| 4   | 3     | 191 | LYS  |
| 4   | 3     | 196 | ARG  |
| 4   | 3     | 199 | SER  |
| 4   | 3     | 201 | VAL  |
| 4   | 3     | 206 | ARG  |
| 4   | 3     | 221 | LEU  |
| 4   | 3     | 223 | PHE  |
| 4   | 3     | 229 | THR  |
| 4   | 3     | 239 | SER  |
| 4   | 3     | 242 | LEU  |
| 4   | 3     | 246 | GLN  |
| 4   | 3     | 263 | GLN  |
| 4   | 3     | 281 | SER  |
| 4   | 3     | 283 | MET  |
| 4   | 3     | 287 | ILE  |
| 4   | 3     | 291 | LYS  |
| 4   | 3     | 293 | LEU  |
| 4   | 3     | 297 | ASN  |
| 4   | 3     | 299 | MET  |
| 4   | 3     | 312 | ARG  |
| 4   | 3     | 315 | LYS  |
| 4   | 3     | 318 | THR  |
| 4   | 3     | 320 | LEU  |
| 4   | 3     | 327 | ILE  |
| 4   | 3     | 334 | GLU  |
| 4   | 3     | 349 | LEU  |
| 4   | 3     | 350 | SER  |
| 4   | 3     | 351 | THR  |
| 4   | 3     | 354 | GLN  |
| 4   | 3     | 359 | LYS  |
| 4   | 3     | 360 | GLN  |
| 4   | 3     | 361 | GLU  |
| 4   | 3     | 368 | SER  |
| 4   | 4     | 33  | SER  |
| 4   | 4     | 34  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 37  | ARG  |
| 4   | 4     | 66  | THR  |
| 4   | 4     | 72  | GLU  |
| 4   | 4     | 80  | ASP  |
| 4   | 4     | 100 | GLU  |
| 4   | 4     | 109 | PRO  |
| 4   | 4     | 116 | ARG  |
| 4   | 4     | 145 | SER  |
| 4   | 4     | 153 | LEU  |
| 4   | 4     | 159 | VAL  |
| 4   | 4     | 180 | LEU  |
| 4   | 4     | 191 | LYS  |
| 4   | 4     | 196 | ARG  |
| 4   | 4     | 199 | SER  |
| 4   | 4     | 201 | VAL  |
| 4   | 4     | 206 | ARG  |
| 4   | 4     | 221 | LEU  |
| 4   | 4     | 223 | PHE  |
| 4   | 4     | 229 | THR  |
| 4   | 4     | 239 | SER  |
| 4   | 4     | 242 | LEU  |
| 4   | 4     | 246 | GLN  |
| 4   | 4     | 263 | GLN  |
| 4   | 4     | 281 | SER  |
| 4   | 4     | 283 | MET  |
| 4   | 4     | 287 | ILE  |
| 4   | 4     | 291 | LYS  |
| 4   | 4     | 293 | LEU  |
| 4   | 4     | 297 | ASN  |
| 4   | 4     | 299 | MET  |
| 4   | 4     | 312 | ARG  |
| 4   | 4     | 315 | LYS  |
| 4   | 4     | 318 | THR  |
| 4   | 4     | 320 | LEU  |
| 4   | 4     | 327 | ILE  |
| 4   | 4     | 334 | GLU  |
| 4   | 4     | 349 | LEU  |
| 4   | 4     | 350 | SER  |
| 4   | 4     | 351 | THR  |
| 4   | 4     | 354 | GLN  |
| 4   | 4     | 359 | LYS  |
| 4   | 4     | 360 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 4     | 361 | GLU  |
| 4   | 4     | 368 | SER  |
| 4   | 5     | 16  | LEU  |
| 4   | 5     | 33  | SER  |
| 4   | 5     | 34  | ILE  |
| 4   | 5     | 37  | ARG  |
| 4   | 5     | 66  | THR  |
| 4   | 5     | 72  | GLU  |
| 4   | 5     | 80  | ASP  |
| 4   | 5     | 100 | GLU  |
| 4   | 5     | 109 | PRO  |
| 4   | 5     | 116 | ARG  |
| 4   | 5     | 145 | SER  |
| 4   | 5     | 153 | LEU  |
| 4   | 5     | 159 | VAL  |
| 4   | 5     | 180 | LEU  |
| 4   | 5     | 191 | LYS  |
| 4   | 5     | 196 | ARG  |
| 4   | 5     | 199 | SER  |
| 4   | 5     | 201 | VAL  |
| 4   | 5     | 206 | ARG  |
| 4   | 5     | 221 | LEU  |
| 4   | 5     | 223 | PHE  |
| 4   | 5     | 229 | THR  |
| 4   | 5     | 239 | SER  |
| 4   | 5     | 242 | LEU  |
| 4   | 5     | 246 | GLN  |
| 4   | 5     | 263 | GLN  |
| 4   | 5     | 281 | SER  |
| 4   | 5     | 283 | MET  |
| 4   | 5     | 287 | ILE  |
| 4   | 5     | 291 | LYS  |
| 4   | 5     | 293 | LEU  |
| 4   | 5     | 297 | ASN  |
| 4   | 5     | 299 | MET  |
| 4   | 5     | 312 | ARG  |
| 4   | 5     | 315 | LYS  |
| 4   | 5     | 318 | THR  |
| 4   | 5     | 320 | LEU  |
| 4   | 5     | 327 | ILE  |
| 4   | 5     | 334 | GLU  |
| 4   | 5     | 349 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 5     | 350 | SER  |
| 4   | 5     | 351 | THR  |
| 4   | 5     | 354 | GLN  |
| 4   | 5     | 359 | LYS  |
| 4   | 5     | 360 | GLN  |
| 4   | 5     | 361 | GLU  |
| 4   | 5     | 368 | SER  |
| 4   | 7     | 33  | SER  |
| 4   | 7     | 34  | ILE  |
| 4   | 7     | 37  | ARG  |
| 4   | 7     | 66  | THR  |
| 4   | 7     | 72  | GLU  |
| 4   | 7     | 80  | ASP  |
| 4   | 7     | 100 | GLU  |
| 4   | 7     | 109 | PRO  |
| 4   | 7     | 116 | ARG  |
| 4   | 7     | 145 | SER  |
| 4   | 7     | 153 | LEU  |
| 4   | 7     | 159 | VAL  |
| 4   | 7     | 180 | LEU  |
| 4   | 7     | 191 | LYS  |
| 4   | 7     | 196 | ARG  |
| 4   | 7     | 199 | SER  |
| 4   | 7     | 201 | VAL  |
| 4   | 7     | 206 | ARG  |
| 4   | 7     | 221 | LEU  |
| 4   | 7     | 223 | PHE  |
| 4   | 7     | 229 | THR  |
| 4   | 7     | 239 | SER  |
| 4   | 7     | 242 | LEU  |
| 4   | 7     | 246 | GLN  |
| 4   | 7     | 263 | GLN  |
| 4   | 7     | 281 | SER  |
| 4   | 7     | 283 | MET  |
| 4   | 7     | 287 | ILE  |
| 4   | 7     | 291 | LYS  |
| 4   | 7     | 293 | LEU  |
| 4   | 7     | 297 | ASN  |
| 4   | 7     | 299 | MET  |
| 4   | 7     | 312 | ARG  |
| 4   | 7     | 315 | LYS  |
| 4   | 7     | 318 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 7     | 320 | LEU  |
| 4   | 7     | 327 | ILE  |
| 4   | 7     | 334 | GLU  |
| 4   | 7     | 349 | LEU  |
| 4   | 7     | 350 | SER  |
| 4   | 7     | 351 | THR  |
| 4   | 7     | 354 | GLN  |
| 4   | 7     | 359 | LYS  |
| 4   | 7     | 360 | GLN  |
| 4   | 7     | 361 | GLU  |
| 4   | 7     | 368 | SER  |
| 4   | 8     | 16  | LEU  |
| 4   | 8     | 33  | SER  |
| 4   | 8     | 34  | ILE  |
| 4   | 8     | 37  | ARG  |
| 4   | 8     | 66  | THR  |
| 4   | 8     | 72  | GLU  |
| 4   | 8     | 80  | ASP  |
| 4   | 8     | 100 | GLU  |
| 4   | 8     | 109 | PRO  |
| 4   | 8     | 116 | ARG  |
| 4   | 8     | 145 | SER  |
| 4   | 8     | 153 | LEU  |
| 4   | 8     | 159 | VAL  |
| 4   | 8     | 180 | LEU  |
| 4   | 8     | 191 | LYS  |
| 4   | 8     | 196 | ARG  |
| 4   | 8     | 199 | SER  |
| 4   | 8     | 201 | VAL  |
| 4   | 8     | 206 | ARG  |
| 4   | 8     | 221 | LEU  |
| 4   | 8     | 223 | PHE  |
| 4   | 8     | 229 | THR  |
| 4   | 8     | 239 | SER  |
| 4   | 8     | 242 | LEU  |
| 4   | 8     | 246 | GLN  |
| 4   | 8     | 263 | GLN  |
| 4   | 8     | 281 | SER  |
| 4   | 8     | 283 | MET  |
| 4   | 8     | 287 | ILE  |
| 4   | 8     | 291 | LYS  |
| 4   | 8     | 293 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 8     | 297 | ASN  |
| 4   | 8     | 299 | MET  |
| 4   | 8     | 312 | ARG  |
| 4   | 8     | 315 | LYS  |
| 4   | 8     | 318 | THR  |
| 4   | 8     | 320 | LEU  |
| 4   | 8     | 327 | ILE  |
| 4   | 8     | 334 | GLU  |
| 4   | 8     | 349 | LEU  |
| 4   | 8     | 350 | SER  |
| 4   | 8     | 351 | THR  |
| 4   | 8     | 354 | GLN  |
| 4   | 8     | 359 | LYS  |
| 4   | 8     | 360 | GLN  |
| 4   | 8     | 361 | GLU  |
| 4   | 8     | 368 | SER  |
| 4   | 9     | 33  | SER  |
| 4   | 9     | 34  | ILE  |
| 4   | 9     | 37  | ARG  |
| 4   | 9     | 66  | THR  |
| 4   | 9     | 72  | GLU  |
| 4   | 9     | 80  | ASP  |
| 4   | 9     | 100 | GLU  |
| 4   | 9     | 109 | PRO  |
| 4   | 9     | 116 | ARG  |
| 4   | 9     | 145 | SER  |
| 4   | 9     | 153 | LEU  |
| 4   | 9     | 159 | VAL  |
| 4   | 9     | 180 | LEU  |
| 4   | 9     | 191 | LYS  |
| 4   | 9     | 196 | ARG  |
| 4   | 9     | 199 | SER  |
| 4   | 9     | 201 | VAL  |
| 4   | 9     | 206 | ARG  |
| 4   | 9     | 221 | LEU  |
| 4   | 9     | 223 | PHE  |
| 4   | 9     | 229 | THR  |
| 4   | 9     | 239 | SER  |
| 4   | 9     | 242 | LEU  |
| 4   | 9     | 246 | GLN  |
| 4   | 9     | 263 | GLN  |
| 4   | 9     | 281 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 9     | 283 | MET  |
| 4   | 9     | 287 | ILE  |
| 4   | 9     | 291 | LYS  |
| 4   | 9     | 293 | LEU  |
| 4   | 9     | 297 | ASN  |
| 4   | 9     | 299 | MET  |
| 4   | 9     | 312 | ARG  |
| 4   | 9     | 315 | LYS  |
| 4   | 9     | 318 | THR  |
| 4   | 9     | 320 | LEU  |
| 4   | 9     | 327 | ILE  |
| 4   | 9     | 334 | GLU  |
| 4   | 9     | 349 | LEU  |
| 4   | 9     | 350 | SER  |
| 4   | 9     | 351 | THR  |
| 4   | 9     | 354 | GLN  |
| 4   | 9     | 359 | LYS  |
| 4   | 9     | 360 | GLN  |
| 4   | 9     | 361 | GLU  |
| 4   | 9     | 368 | SER  |
| 4   | V     | 16  | LEU  |
| 4   | V     | 33  | SER  |
| 4   | V     | 34  | ILE  |
| 4   | V     | 37  | ARG  |
| 4   | V     | 66  | THR  |
| 4   | V     | 72  | GLU  |
| 4   | V     | 80  | ASP  |
| 4   | V     | 100 | GLU  |
| 4   | V     | 109 | PRO  |
| 4   | V     | 116 | ARG  |
| 4   | V     | 145 | SER  |
| 4   | V     | 153 | LEU  |
| 4   | V     | 159 | VAL  |
| 4   | V     | 180 | LEU  |
| 4   | V     | 191 | LYS  |
| 4   | V     | 196 | ARG  |
| 4   | V     | 199 | SER  |
| 4   | V     | 201 | VAL  |
| 4   | V     | 206 | ARG  |
| 4   | V     | 221 | LEU  |
| 4   | V     | 223 | PHE  |
| 4   | V     | 229 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | V     | 239 | SER  |
| 4   | V     | 242 | LEU  |
| 4   | V     | 246 | GLN  |
| 4   | V     | 263 | GLN  |
| 4   | V     | 281 | SER  |
| 4   | V     | 283 | MET  |
| 4   | V     | 287 | ILE  |
| 4   | V     | 291 | LYS  |
| 4   | V     | 293 | LEU  |
| 4   | V     | 297 | ASN  |
| 4   | V     | 299 | MET  |
| 4   | V     | 312 | ARG  |
| 4   | V     | 315 | LYS  |
| 4   | V     | 318 | THR  |
| 4   | V     | 320 | LEU  |
| 4   | V     | 327 | ILE  |
| 4   | V     | 334 | GLU  |
| 4   | V     | 349 | LEU  |
| 4   | V     | 350 | SER  |
| 4   | V     | 351 | THR  |
| 4   | V     | 354 | GLN  |
| 4   | V     | 359 | LYS  |
| 4   | V     | 360 | GLN  |
| 4   | V     | 361 | GLU  |
| 4   | V     | 368 | SER  |
| 4   | W     | 33  | SER  |
| 4   | W     | 34  | ILE  |
| 4   | W     | 37  | ARG  |
| 4   | W     | 66  | THR  |
| 4   | W     | 72  | GLU  |
| 4   | W     | 80  | ASP  |
| 4   | W     | 100 | GLU  |
| 4   | W     | 109 | PRO  |
| 4   | W     | 116 | ARG  |
| 4   | W     | 145 | SER  |
| 4   | W     | 153 | LEU  |
| 4   | W     | 159 | VAL  |
| 4   | W     | 180 | LEU  |
| 4   | W     | 191 | LYS  |
| 4   | W     | 196 | ARG  |
| 4   | W     | 199 | SER  |
| 4   | W     | 201 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | W     | 206 | ARG  |
| 4   | W     | 221 | LEU  |
| 4   | W     | 223 | PHE  |
| 4   | W     | 229 | THR  |
| 4   | W     | 239 | SER  |
| 4   | W     | 242 | LEU  |
| 4   | W     | 246 | GLN  |
| 4   | W     | 263 | GLN  |
| 4   | W     | 281 | SER  |
| 4   | W     | 283 | MET  |
| 4   | W     | 287 | ILE  |
| 4   | W     | 291 | LYS  |
| 4   | W     | 293 | LEU  |
| 4   | W     | 297 | ASN  |
| 4   | W     | 299 | MET  |
| 4   | W     | 312 | ARG  |
| 4   | W     | 315 | LYS  |
| 4   | W     | 318 | THR  |
| 4   | W     | 320 | LEU  |
| 4   | W     | 327 | ILE  |
| 4   | W     | 334 | GLU  |
| 4   | W     | 349 | LEU  |
| 4   | W     | 350 | SER  |
| 4   | W     | 351 | THR  |
| 4   | W     | 354 | GLN  |
| 4   | W     | 359 | LYS  |
| 4   | W     | 360 | GLN  |
| 4   | W     | 361 | GLU  |
| 4   | W     | 368 | SER  |
| 4   | X     | 16  | LEU  |
| 4   | X     | 33  | SER  |
| 4   | X     | 34  | ILE  |
| 4   | X     | 37  | ARG  |
| 4   | X     | 66  | THR  |
| 4   | X     | 72  | GLU  |
| 4   | X     | 80  | ASP  |
| 4   | X     | 100 | GLU  |
| 4   | X     | 109 | PRO  |
| 4   | X     | 116 | ARG  |
| 4   | X     | 145 | SER  |
| 4   | X     | 153 | LEU  |
| 4   | X     | 159 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | X     | 180 | LEU  |
| 4   | X     | 191 | LYS  |
| 4   | X     | 196 | ARG  |
| 4   | X     | 199 | SER  |
| 4   | X     | 201 | VAL  |
| 4   | X     | 206 | ARG  |
| 4   | X     | 221 | LEU  |
| 4   | X     | 223 | PHE  |
| 4   | X     | 229 | THR  |
| 4   | X     | 239 | SER  |
| 4   | X     | 242 | LEU  |
| 4   | X     | 246 | GLN  |
| 4   | X     | 263 | GLN  |
| 4   | X     | 281 | SER  |
| 4   | X     | 283 | MET  |
| 4   | X     | 287 | ILE  |
| 4   | X     | 291 | LYS  |
| 4   | X     | 293 | LEU  |
| 4   | X     | 297 | ASN  |
| 4   | X     | 299 | MET  |
| 4   | X     | 312 | ARG  |
| 4   | X     | 315 | LYS  |
| 4   | X     | 318 | THR  |
| 4   | X     | 320 | LEU  |
| 4   | X     | 327 | ILE  |
| 4   | X     | 334 | GLU  |
| 4   | X     | 349 | LEU  |
| 4   | X     | 350 | SER  |
| 4   | X     | 351 | THR  |
| 4   | X     | 354 | GLN  |
| 4   | X     | 359 | LYS  |
| 4   | X     | 360 | GLN  |
| 4   | X     | 361 | GLU  |
| 4   | X     | 368 | SER  |
| 4   | Y     | 16  | LEU  |
| 4   | Y     | 33  | SER  |
| 4   | Y     | 34  | ILE  |
| 4   | Y     | 37  | ARG  |
| 4   | Y     | 66  | THR  |
| 4   | Y     | 72  | GLU  |
| 4   | Y     | 80  | ASP  |
| 4   | Y     | 100 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Y     | 109 | PRO  |
| 4   | Y     | 116 | ARG  |
| 4   | Y     | 145 | SER  |
| 4   | Y     | 153 | LEU  |
| 4   | Y     | 159 | VAL  |
| 4   | Y     | 180 | LEU  |
| 4   | Y     | 191 | LYS  |
| 4   | Y     | 196 | ARG  |
| 4   | Y     | 199 | SER  |
| 4   | Y     | 201 | VAL  |
| 4   | Y     | 206 | ARG  |
| 4   | Y     | 221 | LEU  |
| 4   | Y     | 223 | PHE  |
| 4   | Y     | 229 | THR  |
| 4   | Y     | 239 | SER  |
| 4   | Y     | 242 | LEU  |
| 4   | Y     | 246 | GLN  |
| 4   | Y     | 263 | GLN  |
| 4   | Y     | 281 | SER  |
| 4   | Y     | 283 | MET  |
| 4   | Y     | 287 | ILE  |
| 4   | Y     | 291 | LYS  |
| 4   | Y     | 293 | LEU  |
| 4   | Y     | 297 | ASN  |
| 4   | Y     | 299 | MET  |
| 4   | Y     | 312 | ARG  |
| 4   | Y     | 315 | LYS  |
| 4   | Y     | 318 | THR  |
| 4   | Y     | 320 | LEU  |
| 4   | Y     | 327 | ILE  |
| 4   | Y     | 334 | GLU  |
| 4   | Y     | 349 | LEU  |
| 4   | Y     | 350 | SER  |
| 4   | Y     | 351 | THR  |
| 4   | Y     | 354 | GLN  |
| 4   | Y     | 359 | LYS  |
| 4   | Y     | 360 | GLN  |
| 4   | Y     | 361 | GLU  |
| 4   | Y     | 368 | SER  |
| 4   | Z     | 33  | SER  |
| 4   | Z     | 34  | ILE  |
| 4   | Z     | 37  | ARG  |

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*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Z     | 66  | THR  |
| 4   | Z     | 72  | GLU  |
| 4   | Z     | 80  | ASP  |
| 4   | Z     | 100 | GLU  |
| 4   | Z     | 109 | PRO  |
| 4   | Z     | 116 | ARG  |
| 4   | Z     | 145 | SER  |
| 4   | Z     | 153 | LEU  |
| 4   | Z     | 159 | VAL  |
| 4   | Z     | 180 | LEU  |
| 4   | Z     | 191 | LYS  |
| 4   | Z     | 196 | ARG  |
| 4   | Z     | 199 | SER  |
| 4   | Z     | 201 | VAL  |
| 4   | Z     | 206 | ARG  |
| 4   | Z     | 221 | LEU  |
| 4   | Z     | 223 | PHE  |
| 4   | Z     | 229 | THR  |
| 4   | Z     | 239 | SER  |
| 4   | Z     | 242 | LEU  |
| 4   | Z     | 246 | GLN  |
| 4   | Z     | 263 | GLN  |
| 4   | Z     | 281 | SER  |
| 4   | Z     | 283 | MET  |
| 4   | Z     | 287 | ILE  |
| 4   | Z     | 291 | LYS  |
| 4   | Z     | 293 | LEU  |
| 4   | Z     | 297 | ASN  |
| 4   | Z     | 299 | MET  |
| 4   | Z     | 312 | ARG  |
| 4   | Z     | 315 | LYS  |
| 4   | Z     | 318 | THR  |
| 4   | Z     | 320 | LEU  |
| 4   | Z     | 327 | ILE  |
| 4   | Z     | 334 | GLU  |
| 4   | Z     | 349 | LEU  |
| 4   | Z     | 350 | SER  |
| 4   | Z     | 351 | THR  |
| 4   | Z     | 354 | GLN  |
| 4   | Z     | 359 | LYS  |
| 4   | Z     | 360 | GLN  |
| 4   | Z     | 361 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | Z     | 368 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (237) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | GLN  |
| 1   | A     | 29  | ASN  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 164 | GLN  |
| 1   | A     | 188 | ASN  |
| 1   | A     | 194 | GLN  |
| 1   | A     | 221 | GLN  |
| 1   | A     | 253 | HIS  |
| 1   | A     | 290 | GLN  |
| 1   | A     | 368 | GLN  |
| 1   | A     | 424 | ASN  |
| 1   | A     | 447 | GLN  |
| 1   | A     | 453 | GLN  |
| 1   | A     | 481 | ASN  |
| 1   | A     | 484 | ASN  |
| 1   | A     | 563 | ASN  |
| 1   | A     | 564 | ASN  |
| 1   | A     | 578 | HIS  |
| 1   | A     | 612 | GLN  |
| 1   | A     | 656 | ASN  |
| 1   | A     | 670 | HIS  |
| 1   | A     | 757 | GLN  |
| 1   | A     | 762 | HIS  |
| 1   | A     | 791 | GLN  |
| 2   | B     | 159 | HIS  |
| 3   | C     | 52  | ASN  |
| 1   | D     | 29  | ASN  |
| 1   | D     | 127 | ASN  |
| 1   | D     | 149 | GLN  |
| 1   | D     | 164 | GLN  |
| 1   | D     | 188 | ASN  |
| 1   | D     | 194 | GLN  |
| 1   | D     | 221 | GLN  |
| 1   | D     | 253 | HIS  |
| 1   | D     | 290 | GLN  |
| 1   | D     | 368 | GLN  |
| 1   | D     | 424 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 447 | GLN  |
| 1   | D     | 453 | GLN  |
| 1   | D     | 481 | ASN  |
| 1   | D     | 484 | ASN  |
| 1   | D     | 563 | ASN  |
| 1   | D     | 564 | ASN  |
| 1   | D     | 578 | HIS  |
| 1   | D     | 612 | GLN  |
| 1   | D     | 656 | ASN  |
| 1   | D     | 670 | HIS  |
| 1   | D     | 698 | ASN  |
| 1   | D     | 757 | GLN  |
| 1   | D     | 762 | HIS  |
| 1   | D     | 791 | GLN  |
| 3   | F     | 40  | ASN  |
| 3   | F     | 52  | ASN  |
| 1   | G     | 29  | ASN  |
| 1   | G     | 127 | ASN  |
| 1   | G     | 149 | GLN  |
| 1   | G     | 164 | GLN  |
| 1   | G     | 188 | ASN  |
| 1   | G     | 194 | GLN  |
| 1   | G     | 221 | GLN  |
| 1   | G     | 253 | HIS  |
| 1   | G     | 290 | GLN  |
| 1   | G     | 368 | GLN  |
| 1   | G     | 424 | ASN  |
| 1   | G     | 447 | GLN  |
| 1   | G     | 453 | GLN  |
| 1   | G     | 481 | ASN  |
| 1   | G     | 484 | ASN  |
| 1   | G     | 563 | ASN  |
| 1   | G     | 564 | ASN  |
| 1   | G     | 578 | HIS  |
| 1   | G     | 612 | GLN  |
| 1   | G     | 656 | ASN  |
| 1   | G     | 670 | HIS  |
| 1   | G     | 698 | ASN  |
| 1   | G     | 762 | HIS  |
| 1   | G     | 791 | GLN  |
| 3   | I     | 39  | GLN  |
| 3   | I     | 52  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 81  | GLN  |
| 1   | J     | 29  | ASN  |
| 1   | J     | 127 | ASN  |
| 1   | J     | 164 | GLN  |
| 1   | J     | 188 | ASN  |
| 1   | J     | 194 | GLN  |
| 1   | J     | 221 | GLN  |
| 1   | J     | 253 | HIS  |
| 1   | J     | 290 | GLN  |
| 1   | J     | 368 | GLN  |
| 1   | J     | 424 | ASN  |
| 1   | J     | 447 | GLN  |
| 1   | J     | 453 | GLN  |
| 1   | J     | 481 | ASN  |
| 1   | J     | 484 | ASN  |
| 1   | J     | 563 | ASN  |
| 1   | J     | 564 | ASN  |
| 1   | J     | 578 | HIS  |
| 1   | J     | 612 | GLN  |
| 1   | J     | 656 | ASN  |
| 1   | J     | 670 | HIS  |
| 1   | J     | 698 | ASN  |
| 1   | J     | 762 | HIS  |
| 1   | J     | 791 | GLN  |
| 2   | K     | 159 | HIS  |
| 3   | L     | 52  | ASN  |
| 3   | L     | 81  | GLN  |
| 1   | M     | 29  | ASN  |
| 1   | M     | 127 | ASN  |
| 1   | M     | 164 | GLN  |
| 1   | M     | 188 | ASN  |
| 1   | M     | 194 | GLN  |
| 1   | M     | 221 | GLN  |
| 1   | M     | 253 | HIS  |
| 1   | M     | 290 | GLN  |
| 1   | M     | 368 | GLN  |
| 1   | M     | 424 | ASN  |
| 1   | M     | 447 | GLN  |
| 1   | M     | 453 | GLN  |
| 1   | M     | 481 | ASN  |
| 1   | M     | 484 | ASN  |
| 1   | M     | 563 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 564 | ASN  |
| 1   | M     | 578 | HIS  |
| 1   | M     | 612 | GLN  |
| 1   | M     | 656 | ASN  |
| 1   | M     | 670 | HIS  |
| 1   | M     | 757 | GLN  |
| 1   | M     | 762 | HIS  |
| 2   | N     | 159 | HIS  |
| 3   | O     | 39  | GLN  |
| 3   | O     | 52  | ASN  |
| 1   | P     | 29  | ASN  |
| 1   | P     | 127 | ASN  |
| 1   | P     | 164 | GLN  |
| 1   | P     | 188 | ASN  |
| 1   | P     | 194 | GLN  |
| 1   | P     | 221 | GLN  |
| 1   | P     | 253 | HIS  |
| 1   | P     | 290 | GLN  |
| 1   | P     | 368 | GLN  |
| 1   | P     | 424 | ASN  |
| 1   | P     | 447 | GLN  |
| 1   | P     | 453 | GLN  |
| 1   | P     | 481 | ASN  |
| 1   | P     | 484 | ASN  |
| 1   | P     | 552 | ASN  |
| 1   | P     | 563 | ASN  |
| 1   | P     | 564 | ASN  |
| 1   | P     | 578 | HIS  |
| 1   | P     | 612 | GLN  |
| 1   | P     | 656 | ASN  |
| 1   | P     | 670 | HIS  |
| 1   | P     | 698 | ASN  |
| 1   | P     | 757 | GLN  |
| 1   | P     | 791 | GLN  |
| 2   | Q     | 159 | HIS  |
| 3   | R     | 39  | GLN  |
| 3   | R     | 40  | ASN  |
| 3   | R     | 52  | ASN  |
| 4   | 0     | 41  | GLN  |
| 4   | 0     | 92  | ASN  |
| 4   | 0     | 137 | GLN  |
| 4   | 0     | 252 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 0     | 263 | GLN  |
| 4   | 1     | 41  | GLN  |
| 4   | 1     | 87  | HIS  |
| 4   | 1     | 92  | ASN  |
| 4   | 1     | 137 | GLN  |
| 4   | 1     | 263 | GLN  |
| 4   | 1     | 354 | GLN  |
| 4   | 2     | 41  | GLN  |
| 4   | 2     | 92  | ASN  |
| 4   | 2     | 137 | GLN  |
| 4   | 2     | 252 | ASN  |
| 4   | 2     | 263 | GLN  |
| 4   | 2     | 354 | GLN  |
| 4   | 3     | 41  | GLN  |
| 4   | 3     | 92  | ASN  |
| 4   | 3     | 137 | GLN  |
| 4   | 3     | 252 | ASN  |
| 4   | 3     | 263 | GLN  |
| 4   | 3     | 354 | GLN  |
| 4   | 4     | 41  | GLN  |
| 4   | 4     | 92  | ASN  |
| 4   | 4     | 137 | GLN  |
| 4   | 4     | 252 | ASN  |
| 4   | 4     | 263 | GLN  |
| 4   | 4     | 354 | GLN  |
| 4   | 5     | 41  | GLN  |
| 4   | 5     | 92  | ASN  |
| 4   | 5     | 137 | GLN  |
| 4   | 5     | 252 | ASN  |
| 4   | 5     | 263 | GLN  |
| 4   | 5     | 354 | GLN  |
| 4   | 7     | 41  | GLN  |
| 4   | 7     | 92  | ASN  |
| 4   | 7     | 137 | GLN  |
| 4   | 7     | 252 | ASN  |
| 4   | 7     | 263 | GLN  |
| 4   | 7     | 354 | GLN  |
| 4   | 8     | 41  | GLN  |
| 4   | 8     | 92  | ASN  |
| 4   | 8     | 137 | GLN  |
| 4   | 8     | 252 | ASN  |
| 4   | 8     | 263 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 9     | 41  | GLN  |
| 4   | 9     | 92  | ASN  |
| 4   | 9     | 137 | GLN  |
| 4   | 9     | 252 | ASN  |
| 4   | 9     | 263 | GLN  |
| 4   | V     | 41  | GLN  |
| 4   | V     | 92  | ASN  |
| 4   | V     | 137 | GLN  |
| 4   | V     | 252 | ASN  |
| 4   | V     | 263 | GLN  |
| 4   | W     | 41  | GLN  |
| 4   | W     | 92  | ASN  |
| 4   | W     | 137 | GLN  |
| 4   | W     | 252 | ASN  |
| 4   | W     | 263 | GLN  |
| 4   | X     | 41  | GLN  |
| 4   | X     | 92  | ASN  |
| 4   | X     | 137 | GLN  |
| 4   | X     | 252 | ASN  |
| 4   | X     | 263 | GLN  |
| 4   | X     | 354 | GLN  |
| 4   | Y     | 41  | GLN  |
| 4   | Y     | 92  | ASN  |
| 4   | Y     | 137 | GLN  |
| 4   | Y     | 252 | ASN  |
| 4   | Y     | 263 | GLN  |
| 4   | Y     | 354 | GLN  |
| 4   | Z     | 41  | GLN  |
| 4   | Z     | 92  | ASN  |
| 4   | Z     | 137 | GLN  |
| 4   | Z     | 252 | ASN  |
| 4   | Z     | 263 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

270 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | A     | 107 | 1    | 8,10,11      | 0.43 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | A     | 130 | 1    | 8,10,11      | 0.59 | 0        | 9,11,13     | 1.06 | 1 (11%)  |
| 1   | MLY  | A     | 138 | 1    | 8,10,11      | 1.34 | 1 (12%)  | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | A     | 19  | 1    | 8,10,11      | 1.14 | 1 (12%)  | 9,11,13     | 0.68 | 0        |
| 1   | MLY  | A     | 190 | 1    | 8,10,11      | 1.10 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | A     | 236 | 1    | 8,10,11      | 0.35 | 0        | 9,11,13     | 1.33 | 1 (11%)  |
| 1   | MLY  | A     | 248 | 1    | 8,10,11      | 0.74 | 0        | 9,11,13     | 0.92 | 1 (11%)  |
| 1   | MLY  | A     | 272 | 1    | 8,10,11      | 1.03 | 1 (12%)  | 9,11,13     | 0.57 | 0        |
| 1   | MLY  | A     | 295 | 1    | 8,10,11      | 0.74 | 0        | 9,11,13     | 0.46 | 0        |
| 1   | MLY  | A     | 296 | 1    | 8,10,11      | 0.60 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | A     | 30  | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.82 | 0        |
| 1   | MLY  | A     | 348 | 1    | 8,10,11      | 0.84 | 0        | 9,11,13     | 0.81 | 0        |
| 1   | MLY  | A     | 35  | 1    | 8,10,11      | 0.57 | 0        | 9,11,13     | 0.69 | 0        |
| 1   | MLY  | A     | 353 | 1    | 8,10,11      | 0.89 | 0        | 9,11,13     | 0.79 | 0        |
| 1   | MLY  | A     | 367 | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | A     | 369 | 1    | 8,10,11      | 0.54 | 0        | 9,11,13     | 0.93 | 1 (11%)  |
| 1   | MLY  | A     | 385 | 1    | 8,10,11      | 1.00 | 1 (12%)  | 9,11,13     | 0.55 | 0        |
| 1   | MLY  | A     | 415 | 1    | 8,10,11      | 0.75 | 0        | 9,11,13     | 0.45 | 0        |
| 1   | MLY  | A     | 431 | 1    | 8,10,11      | 0.46 | 0        | 9,11,13     | 0.76 | 0        |
| 1   | MLY  | A     | 436 | 1    | 8,10,11      | 1.10 | 1 (12%)  | 9,11,13     | 0.57 | 0        |
| 1   | MLY  | A     | 486 | 1    | 8,10,11      | 0.35 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | A     | 49  | 1    | 8,10,11      | 1.04 | 1 (12%)  | 9,11,13     | 0.98 | 0        |
| 1   | MLY  | A     | 504 | 1    | 8,10,11      | 0.79 | 0        | 9,11,13     | 0.49 | 0        |
| 1   | MLY  | A     | 505 | 1    | 8,10,11      | 0.90 | 1 (12%)  | 9,11,13     | 0.38 | 0        |
| 1   | MLY  | A     | 528 | 1    | 8,10,11      | 0.80 | 0        | 9,11,13     | 1.17 | 1 (11%)  |
| 1   | MLY  | A     | 55  | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.97 | 0        |
| 1   | MLY  | A     | 551 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.65 | 0        |
| 1   | MLY  | A     | 553 | 1,4  | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | A     | 59  | 1    | 8,10,11      | 0.76 | 0        | 9,11,13     | 0.76 | 0        |
| 1   | MLY  | A     | 598 | 1    | 8,10,11      | 0.85 | 1 (12%)  | 9,11,13     | 0.72 | 0        |
| 1   | MLY  | A     | 600 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.49 | 0        |
| 1   | MLY  | A     | 613 | 1    | 8,10,11      | 0.50 | 0        | 9,11,13     | 0.92 | 0        |
| 1   | MLY  | A     | 617 | 1    | 8,10,11      | 0.89 | 1 (12%)  | 9,11,13     | 0.46 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | A     | 63  | 1    | 8,10,11      | 0.82 | 0        | 9,11,13     | 0.94 | 0        |
| 1   | MLY  | A     | 659 | 1    | 8,10,11      | 0.53 | 0        | 9,11,13     | 0.95 | 0        |
| 1   | MLY  | A     | 681 | 1    | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.63 | 0        |
| 1   | MLY  | A     | 764 | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.56 | 0        |
| 1   | MLY  | A     | 768 | 1    | 8,10,11      | 0.64 | 0        | 9,11,13     | 0.86 | 0        |
| 1   | MLY  | A     | 782 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.93 | 1 (11%)  |
| 1   | MLY  | A     | 827 | 1    | 8,10,11      | 0.68 | 0        | 9,11,13     | 0.95 | 1 (11%)  |
| 1   | MLY  | A     | 833 | 1    | 8,10,11      | 0.98 | 1 (12%)  | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | A     | 837 | 1    | 8,10,11      | 0.54 | 0        | 9,11,13     | 0.57 | 0        |
| 1   | MLY  | A     | 839 | 1    | 8,10,11      | 0.68 | 0        | 9,11,13     | 0.79 | 0        |
| 1   | MLY  | A     | 84  | 1    | 8,10,11      | 0.47 | 0        | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | A     | 87  | 1    | 8,10,11      | 1.18 | 1 (12%)  | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | D     | 107 | 1    | 8,10,11      | 0.47 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | D     | 130 | 1    | 8,10,11      | 0.58 | 0        | 9,11,13     | 1.06 | 1 (11%)  |
| 1   | MLY  | D     | 138 | 1    | 8,10,11      | 1.40 | 1 (12%)  | 9,11,13     | 0.82 | 0        |
| 1   | MLY  | D     | 19  | 1    | 8,10,11      | 1.19 | 1 (12%)  | 9,11,13     | 0.69 | 0        |
| 1   | MLY  | D     | 190 | 1    | 8,10,11      | 1.07 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | D     | 236 | 1    | 8,10,11      | 0.36 | 0        | 9,11,13     | 1.32 | 1 (11%)  |
| 1   | MLY  | D     | 248 | 1    | 8,10,11      | 0.74 | 0        | 9,11,13     | 0.92 | 1 (11%)  |
| 1   | MLY  | D     | 272 | 1    | 8,10,11      | 0.99 | 1 (12%)  | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | D     | 295 | 1    | 8,10,11      | 0.70 | 0        | 9,11,13     | 0.48 | 0        |
| 1   | MLY  | D     | 296 | 1    | 8,10,11      | 0.61 | 0        | 9,11,13     | 0.78 | 0        |
| 1   | MLY  | D     | 30  | 1    | 8,10,11      | 0.72 | 0        | 9,11,13     | 0.84 | 1 (11%)  |
| 1   | MLY  | D     | 348 | 1    | 8,10,11      | 0.80 | 0        | 9,11,13     | 0.81 | 0        |
| 1   | MLY  | D     | 35  | 1    | 8,10,11      | 0.59 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | D     | 353 | 1    | 8,10,11      | 0.85 | 0        | 9,11,13     | 0.79 | 0        |
| 1   | MLY  | D     | 367 | 1    | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | D     | 369 | 1    | 8,10,11      | 0.54 | 0        | 9,11,13     | 0.91 | 1 (11%)  |
| 1   | MLY  | D     | 385 | 1    | 8,10,11      | 0.99 | 1 (12%)  | 9,11,13     | 0.56 | 0        |
| 1   | MLY  | D     | 415 | 1    | 8,10,11      | 0.78 | 0        | 9,11,13     | 0.46 | 0        |
| 1   | MLY  | D     | 431 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.78 | 0        |
| 1   | MLY  | D     | 436 | 1    | 8,10,11      | 1.15 | 1 (12%)  | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | D     | 486 | 1    | 8,10,11      | 0.35 | 0        | 9,11,13     | 0.61 | 0        |
| 1   | MLY  | D     | 49  | 1    | 8,10,11      | 1.08 | 1 (12%)  | 9,11,13     | 0.99 | 0        |
| 1   | MLY  | D     | 504 | 1    | 8,10,11      | 0.80 | 0        | 9,11,13     | 0.49 | 0        |
| 1   | MLY  | D     | 505 | 1    | 8,10,11      | 0.85 | 1 (12%)  | 9,11,13     | 0.39 | 0        |
| 1   | MLY  | D     | 528 | 1    | 8,10,11      | 0.82 | 0        | 9,11,13     | 1.17 | 1 (11%)  |
| 1   | MLY  | D     | 55  | 1    | 8,10,11      | 0.65 | 0        | 9,11,13     | 0.98 | 0        |
| 1   | MLY  | D     | 551 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.65 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | D     | 553 | 1,4  | 8,10,11      | 0.64 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | D     | 59  | 1    | 8,10,11      | 0.76 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | D     | 598 | 1    | 8,10,11      | 0.86 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | D     | 600 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.47 | 0        |
| 1   | MLY  | D     | 613 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.92 | 0        |
| 1   | MLY  | D     | 617 | 1    | 8,10,11      | 0.95 | 1 (12%)  | 9,11,13     | 0.46 | 0        |
| 1   | MLY  | D     | 63  | 1    | 8,10,11      | 0.78 | 0        | 9,11,13     | 0.95 | 0        |
| 1   | MLY  | D     | 659 | 1    | 8,10,11      | 0.53 | 0        | 9,11,13     | 0.95 | 0        |
| 1   | MLY  | D     | 681 | 1    | 8,10,11      | 0.60 | 0        | 9,11,13     | 0.65 | 0        |
| 1   | MLY  | D     | 764 | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.57 | 0        |
| 1   | MLY  | D     | 768 | 1    | 8,10,11      | 0.61 | 0        | 9,11,13     | 0.87 | 0        |
| 1   | MLY  | D     | 782 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.93 | 1 (11%)  |
| 1   | MLY  | D     | 827 | 1    | 8,10,11      | 0.64 | 0        | 9,11,13     | 0.95 | 1 (11%)  |
| 1   | MLY  | D     | 833 | 1    | 8,10,11      | 0.95 | 1 (12%)  | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | D     | 837 | 1    | 8,10,11      | 0.56 | 0        | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | D     | 839 | 1    | 8,10,11      | 0.69 | 0        | 9,11,13     | 0.78 | 0        |
| 1   | MLY  | D     | 84  | 1    | 8,10,11      | 0.48 | 0        | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | D     | 87  | 1    | 8,10,11      | 1.16 | 1 (12%)  | 9,11,13     | 0.69 | 0        |
| 1   | MLY  | G     | 107 | 1    | 8,10,11      | 0.44 | 0        | 9,11,13     | 0.66 | 0        |
| 1   | MLY  | G     | 130 | 1    | 8,10,11      | 0.61 | 0        | 9,11,13     | 1.07 | 1 (11%)  |
| 1   | MLY  | G     | 138 | 1    | 8,10,11      | 1.38 | 1 (12%)  | 9,11,13     | 0.81 | 0        |
| 1   | MLY  | G     | 19  | 1    | 8,10,11      | 1.17 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | G     | 190 | 1    | 8,10,11      | 1.09 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | G     | 236 | 1    | 8,10,11      | 0.36 | 0        | 9,11,13     | 1.31 | 1 (11%)  |
| 1   | MLY  | G     | 248 | 1    | 8,10,11      | 0.70 | 0        | 9,11,13     | 0.93 | 1 (11%)  |
| 1   | MLY  | G     | 272 | 1    | 8,10,11      | 1.00 | 1 (12%)  | 9,11,13     | 0.56 | 0        |
| 1   | MLY  | G     | 295 | 1    | 8,10,11      | 0.71 | 0        | 9,11,13     | 0.47 | 0        |
| 1   | MLY  | G     | 296 | 1    | 8,10,11      | 0.61 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | G     | 30  | 1    | 8,10,11      | 0.68 | 0        | 9,11,13     | 0.83 | 1 (11%)  |
| 1   | MLY  | G     | 348 | 1    | 8,10,11      | 0.83 | 0        | 9,11,13     | 0.82 | 0        |
| 1   | MLY  | G     | 35  | 1    | 8,10,11      | 0.59 | 0        | 9,11,13     | 0.68 | 0        |
| 1   | MLY  | G     | 353 | 1    | 8,10,11      | 0.86 | 0        | 9,11,13     | 0.79 | 0        |
| 1   | MLY  | G     | 367 | 1    | 8,10,11      | 0.68 | 0        | 9,11,13     | 0.61 | 0        |
| 1   | MLY  | G     | 369 | 1    | 8,10,11      | 0.55 | 0        | 9,11,13     | 0.92 | 1 (11%)  |
| 1   | MLY  | G     | 385 | 1    | 8,10,11      | 1.00 | 1 (12%)  | 9,11,13     | 0.55 | 0        |
| 1   | MLY  | G     | 415 | 1    | 8,10,11      | 0.78 | 0        | 9,11,13     | 0.44 | 0        |
| 1   | MLY  | G     | 431 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | G     | 436 | 1    | 8,10,11      | 1.07 | 1 (12%)  | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | G     | 486 | 1    | 8,10,11      | 0.34 | 0        | 9,11,13     | 0.60 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | G     | 49  | 1    | 8,10,11      | 1.07 | 1 (12%)  | 9,11,13     | 0.97 | 0        |
| 1   | MLY  | G     | 504 | 1    | 8,10,11      | 0.76 | 0        | 9,11,13     | 0.48 | 0        |
| 1   | MLY  | G     | 505 | 1    | 8,10,11      | 0.90 | 1 (12%)  | 9,11,13     | 0.40 | 0        |
| 1   | MLY  | G     | 528 | 1    | 8,10,11      | 0.80 | 0        | 9,11,13     | 1.17 | 1 (11%)  |
| 1   | MLY  | G     | 55  | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.99 | 0        |
| 1   | MLY  | G     | 551 | 1    | 8,10,11      | 0.50 | 0        | 9,11,13     | 0.65 | 0        |
| 1   | MLY  | G     | 553 | 1,4  | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | G     | 59  | 1    | 8,10,11      | 0.72 | 0        | 9,11,13     | 0.78 | 0        |
| 1   | MLY  | G     | 598 | 1    | 8,10,11      | 0.85 | 1 (12%)  | 9,11,13     | 0.71 | 0        |
| 1   | MLY  | G     | 600 | 1    | 8,10,11      | 0.52 | 0        | 9,11,13     | 0.46 | 0        |
| 1   | MLY  | G     | 613 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.92 | 0        |
| 1   | MLY  | G     | 617 | 1    | 8,10,11      | 0.91 | 1 (12%)  | 9,11,13     | 0.45 | 0        |
| 1   | MLY  | G     | 63  | 1    | 8,10,11      | 0.80 | 0        | 9,11,13     | 0.95 | 0        |
| 1   | MLY  | G     | 659 | 1    | 8,10,11      | 0.54 | 0        | 9,11,13     | 0.94 | 0        |
| 1   | MLY  | G     | 681 | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.64 | 0        |
| 1   | MLY  | G     | 764 | 1    | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.57 | 0        |
| 1   | MLY  | G     | 768 | 1    | 8,10,11      | 0.60 | 0        | 9,11,13     | 0.88 | 0        |
| 1   | MLY  | G     | 782 | 1    | 8,10,11      | 0.47 | 0        | 9,11,13     | 0.92 | 1 (11%)  |
| 1   | MLY  | G     | 827 | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.96 | 1 (11%)  |
| 1   | MLY  | G     | 833 | 1    | 8,10,11      | 0.96 | 1 (12%)  | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | G     | 837 | 1    | 8,10,11      | 0.53 | 0        | 9,11,13     | 0.55 | 0        |
| 1   | MLY  | G     | 839 | 1    | 8,10,11      | 0.71 | 0        | 9,11,13     | 0.79 | 0        |
| 1   | MLY  | G     | 84  | 1    | 8,10,11      | 0.46 | 0        | 9,11,13     | 0.81 | 0        |
| 1   | MLY  | G     | 87  | 1    | 8,10,11      | 1.17 | 1 (12%)  | 9,11,13     | 0.69 | 0        |
| 1   | MLY  | J     | 107 | 1    | 8,10,11      | 0.45 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | J     | 130 | 1    | 8,10,11      | 0.55 | 0        | 9,11,13     | 1.06 | 1 (11%)  |
| 1   | MLY  | J     | 138 | 1    | 8,10,11      | 1.35 | 1 (12%)  | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | J     | 19  | 1    | 8,10,11      | 1.20 | 1 (12%)  | 9,11,13     | 0.71 | 0        |
| 1   | MLY  | J     | 190 | 1    | 8,10,11      | 1.12 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | J     | 236 | 1    | 8,10,11      | 0.36 | 0        | 9,11,13     | 1.32 | 1 (11%)  |
| 1   | MLY  | J     | 248 | 1    | 8,10,11      | 0.74 | 0        | 9,11,13     | 0.94 | 1 (11%)  |
| 1   | MLY  | J     | 272 | 1    | 8,10,11      | 1.04 | 1 (12%)  | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | J     | 295 | 1    | 8,10,11      | 0.69 | 0        | 9,11,13     | 0.48 | 0        |
| 1   | MLY  | J     | 296 | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | J     | 30  | 1    | 8,10,11      | 0.68 | 0        | 9,11,13     | 0.82 | 0        |
| 1   | MLY  | J     | 348 | 1    | 8,10,11      | 0.76 | 0        | 9,11,13     | 0.81 | 0        |
| 1   | MLY  | J     | 35  | 1    | 8,10,11      | 0.58 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | J     | 353 | 1    | 8,10,11      | 0.86 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | J     | 367 | 1    | 8,10,11      | 0.64 | 0        | 9,11,13     | 0.60 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | J     | 369 | 1    | 8,10,11      | 0.54 | 0        | 9,11,13     | 0.93 | 1 (11%)  |
| 1   | MLY  | J     | 385 | 1    | 8,10,11      | 1.02 | 1 (12%)  | 9,11,13     | 0.54 | 0        |
| 1   | MLY  | J     | 415 | 1    | 8,10,11      | 0.79 | 0        | 9,11,13     | 0.44 | 0        |
| 1   | MLY  | J     | 431 | 1    | 8,10,11      | 0.43 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | J     | 436 | 1    | 8,10,11      | 1.10 | 1 (12%)  | 9,11,13     | 0.56 | 0        |
| 1   | MLY  | J     | 486 | 1    | 8,10,11      | 0.32 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | J     | 49  | 1    | 8,10,11      | 1.08 | 1 (12%)  | 9,11,13     | 0.99 | 0        |
| 1   | MLY  | J     | 504 | 1    | 8,10,11      | 0.75 | 0        | 9,11,13     | 0.49 | 0        |
| 1   | MLY  | J     | 505 | 1    | 8,10,11      | 0.92 | 1 (12%)  | 9,11,13     | 0.39 | 0        |
| 1   | MLY  | J     | 528 | 1    | 8,10,11      | 0.81 | 0        | 9,11,13     | 1.16 | 1 (11%)  |
| 1   | MLY  | J     | 55  | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.98 | 0        |
| 1   | MLY  | J     | 551 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.66 | 0        |
| 1   | MLY  | J     | 553 | 1    | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | J     | 59  | 1    | 8,10,11      | 0.77 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | J     | 598 | 1    | 8,10,11      | 0.84 | 1 (12%)  | 9,11,13     | 0.71 | 0        |
| 1   | MLY  | J     | 600 | 1    | 8,10,11      | 0.53 | 0        | 9,11,13     | 0.47 | 0        |
| 1   | MLY  | J     | 613 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.93 | 0        |
| 1   | MLY  | J     | 617 | 1    | 8,10,11      | 0.92 | 1 (12%)  | 9,11,13     | 0.45 | 0        |
| 1   | MLY  | J     | 63  | 1    | 8,10,11      | 0.81 | 0        | 9,11,13     | 0.95 | 0        |
| 1   | MLY  | J     | 659 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.93 | 0        |
| 1   | MLY  | J     | 681 | 1    | 8,10,11      | 0.61 | 0        | 9,11,13     | 0.64 | 0        |
| 1   | MLY  | J     | 764 | 1    | 8,10,11      | 0.64 | 0        | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | J     | 768 | 1    | 8,10,11      | 0.64 | 0        | 9,11,13     | 0.85 | 0        |
| 1   | MLY  | J     | 782 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.94 | 1 (11%)  |
| 1   | MLY  | J     | 827 | 1    | 8,10,11      | 0.70 | 0        | 9,11,13     | 0.94 | 1 (11%)  |
| 1   | MLY  | J     | 833 | 1    | 8,10,11      | 1.03 | 1 (12%)  | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | J     | 837 | 1    | 8,10,11      | 0.55 | 0        | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | J     | 839 | 1    | 8,10,11      | 0.70 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | J     | 84  | 1    | 8,10,11      | 0.46 | 0        | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | J     | 87  | 1    | 8,10,11      | 1.18 | 1 (12%)  | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | M     | 107 | 1    | 8,10,11      | 0.46 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | M     | 130 | 1    | 8,10,11      | 0.59 | 0        | 9,11,13     | 1.07 | 1 (11%)  |
| 1   | MLY  | M     | 138 | 1    | 8,10,11      | 1.35 | 1 (12%)  | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | M     | 19  | 1    | 8,10,11      | 1.18 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | M     | 190 | 1    | 8,10,11      | 1.11 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | M     | 236 | 1    | 8,10,11      | 0.38 | 0        | 9,11,13     | 1.31 | 1 (11%)  |
| 1   | MLY  | M     | 248 | 1    | 8,10,11      | 0.73 | 0        | 9,11,13     | 0.93 | 1 (11%)  |
| 1   | MLY  | M     | 272 | 1    | 8,10,11      | 1.03 | 1 (12%)  | 9,11,13     | 0.57 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | M     | 295 | 1    | 8,10,11      | 0.70 | 0        | 9,11,13     | 0.48 | 0        |
| 1   | MLY  | M     | 296 | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | M     | 30  | 1    | 8,10,11      | 0.69 | 0        | 9,11,13     | 0.82 | 1 (11%)  |
| 1   | MLY  | M     | 348 | 1    | 8,10,11      | 0.78 | 0        | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | M     | 35  | 1    | 8,10,11      | 0.59 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | M     | 353 | 1    | 8,10,11      | 0.86 | 0        | 9,11,13     | 0.78 | 0        |
| 1   | MLY  | M     | 367 | 1    | 8,10,11      | 0.65 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | M     | 369 | 1    | 8,10,11      | 0.54 | 0        | 9,11,13     | 0.92 | 1 (11%)  |
| 1   | MLY  | M     | 385 | 1    | 8,10,11      | 1.02 | 1 (12%)  | 9,11,13     | 0.55 | 0        |
| 1   | MLY  | M     | 415 | 1    | 8,10,11      | 0.79 | 0        | 9,11,13     | 0.44 | 0        |
| 1   | MLY  | M     | 431 | 1    | 8,10,11      | 0.45 | 0        | 9,11,13     | 0.78 | 0        |
| 1   | MLY  | M     | 436 | 1    | 8,10,11      | 1.11 | 1 (12%)  | 9,11,13     | 0.56 | 0        |
| 1   | MLY  | M     | 486 | 1    | 8,10,11      | 0.32 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | M     | 49  | 1    | 8,10,11      | 1.09 | 1 (12%)  | 9,11,13     | 1.00 | 0        |
| 1   | MLY  | M     | 504 | 1    | 8,10,11      | 0.74 | 0        | 9,11,13     | 0.47 | 0        |
| 1   | MLY  | M     | 505 | 1    | 8,10,11      | 0.93 | 1 (12%)  | 9,11,13     | 0.38 | 0        |
| 1   | MLY  | M     | 528 | 1    | 8,10,11      | 0.80 | 0        | 9,11,13     | 1.16 | 1 (11%)  |
| 1   | MLY  | M     | 55  | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.99 | 0        |
| 1   | MLY  | M     | 551 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | M     | 553 | 1,4  | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | M     | 59  | 1    | 8,10,11      | 0.78 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | M     | 598 | 1    | 8,10,11      | 0.83 | 1 (12%)  | 9,11,13     | 0.71 | 0        |
| 1   | MLY  | M     | 600 | 1    | 8,10,11      | 0.52 | 0        | 9,11,13     | 0.47 | 0        |
| 1   | MLY  | M     | 613 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.93 | 0        |
| 1   | MLY  | M     | 617 | 1    | 8,10,11      | 0.92 | 1 (12%)  | 9,11,13     | 0.46 | 0        |
| 1   | MLY  | M     | 63  | 1    | 8,10,11      | 0.81 | 0        | 9,11,13     | 0.95 | 0        |
| 1   | MLY  | M     | 659 | 1    | 8,10,11      | 0.52 | 0        | 9,11,13     | 0.93 | 0        |
| 1   | MLY  | M     | 681 | 1    | 8,10,11      | 0.60 | 0        | 9,11,13     | 0.63 | 0        |
| 1   | MLY  | M     | 764 | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | M     | 768 | 1    | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.87 | 0        |
| 1   | MLY  | M     | 782 | 1    | 8,10,11      | 0.50 | 0        | 9,11,13     | 0.94 | 1 (11%)  |
| 1   | MLY  | M     | 827 | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.95 | 1 (11%)  |
| 1   | MLY  | M     | 833 | 1    | 8,10,11      | 1.05 | 1 (12%)  | 9,11,13     | 0.59 | 0        |
| 1   | MLY  | M     | 837 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | M     | 839 | 1    | 8,10,11      | 0.68 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | M     | 84  | 1    | 8,10,11      | 0.47 | 0        | 9,11,13     | 0.80 | 0        |
| 1   | MLY  | M     | 87  | 1    | 8,10,11      | 1.17 | 1 (12%)  | 9,11,13     | 0.68 | 0        |
| 1   | MLY  | P     | 107 | 1    | 8,10,11      | 0.46 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | P     | 130 | 1    | 8,10,11      | 0.57 | 0        | 9,11,13     | 1.06 | 1 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | P     | 138 | 1    | 8,10,11      | 1.35 | 1 (12%)  | 9,11,13     | 0.81 | 0        |
| 1   | MLY  | P     | 19  | 1    | 8,10,11      | 1.20 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | P     | 190 | 1    | 8,10,11      | 1.11 | 1 (12%)  | 9,11,13     | 0.70 | 0        |
| 1   | MLY  | P     | 236 | 1    | 8,10,11      | 0.38 | 0        | 9,11,13     | 1.32 | 1 (11%)  |
| 1   | MLY  | P     | 248 | 1    | 8,10,11      | 0.73 | 0        | 9,11,13     | 0.94 | 1 (11%)  |
| 1   | MLY  | P     | 272 | 1    | 8,10,11      | 1.05 | 1 (12%)  | 9,11,13     | 0.57 | 0        |
| 1   | MLY  | P     | 295 | 1    | 8,10,11      | 0.71 | 0        | 9,11,13     | 0.47 | 0        |
| 1   | MLY  | P     | 296 | 1    | 8,10,11      | 0.63 | 0        | 9,11,13     | 0.79 | 1 (11%)  |
| 1   | MLY  | P     | 30  | 1    | 8,10,11      | 0.69 | 0        | 9,11,13     | 0.82 | 1 (11%)  |
| 1   | MLY  | P     | 348 | 1    | 8,10,11      | 0.81 | 0        | 9,11,13     | 0.81 | 0        |
| 1   | MLY  | P     | 35  | 1    | 8,10,11      | 0.59 | 0        | 9,11,13     | 0.67 | 0        |
| 1   | MLY  | P     | 353 | 1    | 8,10,11      | 0.86 | 0        | 9,11,13     | 0.78 | 0        |
| 1   | MLY  | P     | 367 | 1    | 8,10,11      | 0.65 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | P     | 369 | 1    | 8,10,11      | 0.54 | 0        | 9,11,13     | 0.92 | 1 (11%)  |
| 1   | MLY  | P     | 385 | 1    | 8,10,11      | 1.02 | 1 (12%)  | 9,11,13     | 0.54 | 0        |
| 1   | MLY  | P     | 415 | 1    | 8,10,11      | 0.78 | 0        | 9,11,13     | 0.44 | 0        |
| 1   | MLY  | P     | 431 | 1    | 8,10,11      | 0.43 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | P     | 436 | 1    | 8,10,11      | 1.11 | 1 (12%)  | 9,11,13     | 0.57 | 0        |
| 1   | MLY  | P     | 486 | 1    | 8,10,11      | 0.33 | 0        | 9,11,13     | 0.60 | 0        |
| 1   | MLY  | P     | 49  | 1    | 8,10,11      | 1.13 | 1 (12%)  | 9,11,13     | 0.99 | 0        |
| 1   | MLY  | P     | 504 | 1    | 8,10,11      | 0.74 | 0        | 9,11,13     | 0.48 | 0        |
| 1   | MLY  | P     | 505 | 1    | 8,10,11      | 0.92 | 1 (12%)  | 9,11,13     | 0.38 | 0        |
| 1   | MLY  | P     | 528 | 1    | 8,10,11      | 0.81 | 0        | 9,11,13     | 1.16 | 1 (11%)  |
| 1   | MLY  | P     | 55  | 1    | 8,10,11      | 0.66 | 0        | 9,11,13     | 0.99 | 0        |
| 1   | MLY  | P     | 551 | 1    | 8,10,11      | 0.51 | 0        | 9,11,13     | 0.66 | 0        |
| 1   | MLY  | P     | 553 | 1    | 8,10,11      | 0.62 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | P     | 59  | 1    | 8,10,11      | 0.79 | 0        | 9,11,13     | 0.77 | 0        |
| 1   | MLY  | P     | 598 | 1    | 8,10,11      | 0.85 | 1 (12%)  | 9,11,13     | 0.71 | 0        |
| 1   | MLY  | P     | 600 | 1    | 8,10,11      | 0.52 | 0        | 9,11,13     | 0.47 | 0        |
| 1   | MLY  | P     | 613 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.93 | 0        |
| 1   | MLY  | P     | 617 | 1    | 8,10,11      | 0.93 | 1 (12%)  | 9,11,13     | 0.46 | 0        |
| 1   | MLY  | P     | 63  | 1    | 8,10,11      | 0.79 | 0        | 9,11,13     | 0.94 | 0        |
| 1   | MLY  | P     | 659 | 1    | 8,10,11      | 0.55 | 0        | 9,11,13     | 0.94 | 0        |
| 1   | MLY  | P     | 681 | 1    | 8,10,11      | 0.63 | 0        | 9,11,13     | 0.64 | 0        |
| 1   | MLY  | P     | 764 | 1    | 8,10,11      | 0.64 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | P     | 768 | 1    | 8,10,11      | 0.67 | 0        | 9,11,13     | 0.87 | 0        |
| 1   | MLY  | P     | 782 | 1    | 8,10,11      | 0.49 | 0        | 9,11,13     | 0.96 | 1 (11%)  |
| 1   | MLY  | P     | 827 | 1    | 8,10,11      | 0.68 | 0        | 9,11,13     | 0.95 | 1 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 1   | MLY  | P     | 833 | 1    | 8,10,11      | 1.02 | 1 (12%)  | 9,11,13     | 0.56 | 0        |
| 1   | MLY  | P     | 837 | 1    | 8,10,11      | 0.52 | 0        | 9,11,13     | 0.58 | 0        |
| 1   | MLY  | P     | 839 | 1    | 8,10,11      | 0.69 | 0        | 9,11,13     | 0.76 | 0        |
| 1   | MLY  | P     | 84  | 1    | 8,10,11      | 0.47 | 0        | 9,11,13     | 0.79 | 0        |
| 1   | MLY  | P     | 87  | 1    | 8,10,11      | 1.21 | 1 (12%)  | 9,11,13     | 0.68 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | A     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | A     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | A     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | D     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | D     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | G     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | G     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | J     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 553 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | J     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | M     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 553 | 1,4  | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | M     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 107 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 130 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 138 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 19  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 190 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 236 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 248 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 272 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 295 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 296 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 30  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 348 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 35  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 353 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 367 | 1    | -       | 0/7/9/11 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings   |
|-----|------|-------|-----|------|---------|----------|---------|
| 1   | MLY  | P     | 369 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 385 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 415 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 431 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 436 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 486 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 49  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 504 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 505 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 528 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 55  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 551 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 553 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 59  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 598 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 600 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 613 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 617 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 63  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 659 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 681 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 764 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 768 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 782 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 827 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 833 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 837 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 839 | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 84  | 1    | -       | 0/7/9/11 | 0/0/0/0 |
| 1   | MLY  | P     | 87  | 1    | -       | 0/7/9/11 | 0/0/0/0 |

All (72) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 138 | MLY  | CB-CA | -3.68 | 1.48        | 1.53     |
| 1   | G     | 138 | MLY  | CB-CA | -3.63 | 1.48        | 1.53     |
| 1   | P     | 138 | MLY  | CB-CA | -3.56 | 1.48        | 1.53     |
| 1   | J     | 138 | MLY  | CB-CA | -3.53 | 1.48        | 1.53     |
| 1   | M     | 138 | MLY  | CB-CA | -3.53 | 1.48        | 1.53     |
| 1   | A     | 138 | MLY  | CB-CA | -3.51 | 1.48        | 1.53     |
| 1   | P     | 87  | MLY  | CB-CA | -3.12 | 1.49        | 1.53     |
| 1   | J     | 19  | MLY  | CB-CA | -3.09 | 1.49        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | P     | 19  | MLY  | CB-CA | -3.08 | 1.49        | 1.53     |
| 1   | G     | 87  | MLY  | CB-CA | -3.07 | 1.49        | 1.53     |
| 1   | A     | 87  | MLY  | CB-CA | -3.06 | 1.49        | 1.53     |
| 1   | D     | 19  | MLY  | CB-CA | -3.06 | 1.49        | 1.53     |
| 1   | M     | 19  | MLY  | CB-CA | -3.05 | 1.49        | 1.53     |
| 1   | J     | 87  | MLY  | CB-CA | -3.05 | 1.49        | 1.53     |
| 1   | M     | 87  | MLY  | CB-CA | -3.03 | 1.49        | 1.53     |
| 1   | D     | 87  | MLY  | CB-CA | -3.02 | 1.49        | 1.53     |
| 1   | D     | 436 | MLY  | CB-CA | -3.01 | 1.49        | 1.53     |
| 1   | G     | 19  | MLY  | CB-CA | -2.97 | 1.49        | 1.53     |
| 1   | M     | 436 | MLY  | CB-CA | -2.90 | 1.49        | 1.53     |
| 1   | P     | 436 | MLY  | CB-CA | -2.90 | 1.49        | 1.53     |
| 1   | A     | 19  | MLY  | CB-CA | -2.90 | 1.49        | 1.53     |
| 1   | P     | 49  | MLY  | CB-CA | -2.88 | 1.49        | 1.53     |
| 1   | J     | 436 | MLY  | CB-CA | -2.87 | 1.49        | 1.53     |
| 1   | A     | 436 | MLY  | CB-CA | -2.84 | 1.49        | 1.53     |
| 1   | G     | 436 | MLY  | CB-CA | -2.78 | 1.49        | 1.53     |
| 1   | M     | 49  | MLY  | CB-CA | -2.78 | 1.49        | 1.53     |
| 1   | J     | 49  | MLY  | CB-CA | -2.75 | 1.49        | 1.53     |
| 1   | D     | 49  | MLY  | CB-CA | -2.73 | 1.49        | 1.53     |
| 1   | P     | 272 | MLY  | CB-CA | -2.71 | 1.49        | 1.53     |
| 1   | G     | 49  | MLY  | CB-CA | -2.68 | 1.49        | 1.53     |
| 1   | J     | 272 | MLY  | CB-CA | -2.68 | 1.49        | 1.53     |
| 1   | M     | 272 | MLY  | CB-CA | -2.68 | 1.49        | 1.53     |
| 1   | A     | 272 | MLY  | CB-CA | -2.66 | 1.49        | 1.53     |
| 1   | A     | 49  | MLY  | CB-CA | -2.60 | 1.50        | 1.53     |
| 1   | J     | 190 | MLY  | CB-CA | -2.58 | 1.50        | 1.53     |
| 1   | G     | 272 | MLY  | CB-CA | -2.57 | 1.50        | 1.53     |
| 1   | D     | 272 | MLY  | CB-CA | -2.54 | 1.50        | 1.53     |
| 1   | M     | 190 | MLY  | CB-CA | -2.53 | 1.50        | 1.53     |
| 1   | P     | 190 | MLY  | CB-CA | -2.52 | 1.50        | 1.53     |
| 1   | A     | 190 | MLY  | CB-CA | -2.47 | 1.50        | 1.53     |
| 1   | M     | 385 | MLY  | CB-CA | -2.47 | 1.50        | 1.53     |
| 1   | G     | 190 | MLY  | CB-CA | -2.46 | 1.50        | 1.53     |
| 1   | M     | 833 | MLY  | CB-CA | -2.46 | 1.50        | 1.53     |
| 1   | J     | 385 | MLY  | CB-CA | -2.46 | 1.50        | 1.53     |
| 1   | P     | 385 | MLY  | CB-CA | -2.44 | 1.50        | 1.53     |
| 1   | J     | 833 | MLY  | CB-CA | -2.42 | 1.50        | 1.53     |
| 1   | P     | 833 | MLY  | CB-CA | -2.40 | 1.50        | 1.53     |
| 1   | D     | 190 | MLY  | CB-CA | -2.40 | 1.50        | 1.53     |
| 1   | A     | 385 | MLY  | CB-CA | -2.38 | 1.50        | 1.53     |
| 1   | G     | 385 | MLY  | CB-CA | -2.35 | 1.50        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 385 | MLY  | CB-CA | -2.34 | 1.50        | 1.53     |
| 1   | D     | 617 | MLY  | CB-CA | -2.31 | 1.50        | 1.53     |
| 1   | M     | 505 | MLY  | CB-CA | -2.27 | 1.50        | 1.53     |
| 1   | J     | 505 | MLY  | CB-CA | -2.24 | 1.50        | 1.53     |
| 1   | D     | 598 | MLY  | CB-CA | -2.22 | 1.50        | 1.53     |
| 1   | P     | 617 | MLY  | CB-CA | -2.22 | 1.50        | 1.53     |
| 1   | G     | 505 | MLY  | CB-CA | -2.21 | 1.50        | 1.53     |
| 1   | G     | 598 | MLY  | CB-CA | -2.21 | 1.50        | 1.53     |
| 1   | P     | 505 | MLY  | CB-CA | -2.21 | 1.50        | 1.53     |
| 1   | A     | 833 | MLY  | CB-CA | -2.20 | 1.50        | 1.53     |
| 1   | A     | 598 | MLY  | CB-CA | -2.20 | 1.50        | 1.53     |
| 1   | P     | 598 | MLY  | CB-CA | -2.19 | 1.50        | 1.53     |
| 1   | A     | 505 | MLY  | CB-CA | -2.18 | 1.50        | 1.53     |
| 1   | J     | 617 | MLY  | CB-CA | -2.18 | 1.50        | 1.53     |
| 1   | M     | 617 | MLY  | CB-CA | -2.17 | 1.50        | 1.53     |
| 1   | J     | 598 | MLY  | CB-CA | -2.16 | 1.50        | 1.53     |
| 1   | G     | 617 | MLY  | CB-CA | -2.15 | 1.50        | 1.53     |
| 1   | G     | 833 | MLY  | CB-CA | -2.15 | 1.50        | 1.53     |
| 1   | M     | 598 | MLY  | CB-CA | -2.12 | 1.50        | 1.53     |
| 1   | D     | 833 | MLY  | CB-CA | -2.12 | 1.50        | 1.53     |
| 1   | A     | 617 | MLY  | CB-CA | -2.11 | 1.50        | 1.53     |
| 1   | D     | 505 | MLY  | CB-CA | -2.04 | 1.50        | 1.53     |

All (47) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 236 | MLY  | O-C-CA | -3.25 | 117.02      | 125.72   |
| 1   | P     | 236 | MLY  | O-C-CA | -3.24 | 117.03      | 125.72   |
| 1   | D     | 236 | MLY  | O-C-CA | -3.23 | 117.07      | 125.72   |
| 1   | J     | 236 | MLY  | O-C-CA | -3.22 | 117.09      | 125.72   |
| 1   | M     | 236 | MLY  | O-C-CA | -3.21 | 117.10      | 125.72   |
| 1   | G     | 236 | MLY  | O-C-CA | -3.20 | 117.14      | 125.72   |
| 1   | D     | 528 | MLY  | O-C-CA | -3.10 | 117.40      | 125.72   |
| 1   | G     | 528 | MLY  | O-C-CA | -3.09 | 117.43      | 125.72   |
| 1   | A     | 528 | MLY  | O-C-CA | -3.07 | 117.49      | 125.72   |
| 1   | M     | 528 | MLY  | O-C-CA | -3.05 | 117.55      | 125.72   |
| 1   | J     | 528 | MLY  | O-C-CA | -3.04 | 117.56      | 125.72   |
| 1   | P     | 528 | MLY  | O-C-CA | -3.04 | 117.57      | 125.72   |
| 1   | A     | 827 | MLY  | O-C-CA | -2.56 | 118.85      | 125.72   |
| 1   | D     | 827 | MLY  | O-C-CA | -2.55 | 118.88      | 125.72   |
| 1   | G     | 827 | MLY  | O-C-CA | -2.55 | 118.90      | 125.72   |
| 1   | P     | 827 | MLY  | O-C-CA | -2.53 | 118.93      | 125.72   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 827 | MLY  | O-C-CA  | -2.53 | 118.93      | 125.72   |
| 1   | J     | 827 | MLY  | O-C-CA  | -2.51 | 118.99      | 125.72   |
| 1   | G     | 130 | MLY  | O-C-CA  | -2.49 | 119.04      | 125.72   |
| 1   | M     | 130 | MLY  | O-C-CA  | -2.49 | 119.04      | 125.72   |
| 1   | D     | 130 | MLY  | O-C-CA  | -2.48 | 119.07      | 125.72   |
| 1   | P     | 130 | MLY  | O-C-CA  | -2.46 | 119.12      | 125.72   |
| 1   | A     | 130 | MLY  | O-C-CA  | -2.46 | 119.13      | 125.72   |
| 1   | J     | 130 | MLY  | O-C-CA  | -2.46 | 119.14      | 125.72   |
| 1   | J     | 248 | MLY  | O-C-CA  | -2.23 | 119.75      | 125.72   |
| 1   | P     | 248 | MLY  | O-C-CA  | -2.22 | 119.76      | 125.72   |
| 1   | J     | 369 | MLY  | O-C-CA  | -2.21 | 119.79      | 125.72   |
| 1   | M     | 248 | MLY  | O-C-CA  | -2.21 | 119.81      | 125.72   |
| 1   | G     | 248 | MLY  | O-C-CA  | -2.20 | 119.82      | 125.72   |
| 1   | A     | 248 | MLY  | O-C-CA  | -2.20 | 119.83      | 125.72   |
| 1   | A     | 369 | MLY  | O-C-CA  | -2.19 | 119.84      | 125.72   |
| 1   | M     | 369 | MLY  | O-C-CA  | -2.19 | 119.85      | 125.72   |
| 1   | D     | 369 | MLY  | O-C-CA  | -2.18 | 119.87      | 125.72   |
| 1   | P     | 369 | MLY  | O-C-CA  | -2.18 | 119.87      | 125.72   |
| 1   | G     | 369 | MLY  | O-C-CA  | -2.18 | 119.87      | 125.72   |
| 1   | D     | 248 | MLY  | O-C-CA  | -2.18 | 119.89      | 125.72   |
| 1   | D     | 30  | MLY  | O-C-CA  | -2.05 | 120.22      | 125.72   |
| 1   | P     | 296 | MLY  | O-C-CA  | -2.04 | 120.25      | 125.72   |
| 1   | G     | 30  | MLY  | O-C-CA  | -2.03 | 120.28      | 125.72   |
| 1   | P     | 30  | MLY  | O-C-CA  | -2.00 | 120.35      | 125.72   |
| 1   | M     | 30  | MLY  | O-C-CA  | -2.00 | 120.36      | 125.72   |
| 1   | G     | 782 | MLY  | CB-CA-N | 2.07  | 116.35      | 110.54   |
| 1   | D     | 782 | MLY  | CB-CA-N | 2.07  | 116.37      | 110.54   |
| 1   | A     | 782 | MLY  | CB-CA-N | 2.08  | 116.38      | 110.54   |
| 1   | J     | 782 | MLY  | CB-CA-N | 2.08  | 116.39      | 110.54   |
| 1   | M     | 782 | MLY  | CB-CA-N | 2.08  | 116.39      | 110.54   |
| 1   | P     | 782 | MLY  | CB-CA-N | 2.10  | 116.45      | 110.54   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

184 monomers are involved in 814 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | A     | 107 | MLY  | 2       | 0            |
| 1   | A     | 138 | MLY  | 1       | 0            |
| 1   | A     | 190 | MLY  | 2       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | A     | 248 | MLY  | 2       | 0            |
| 1   | A     | 272 | MLY  | 1       | 0            |
| 1   | A     | 295 | MLY  | 6       | 0            |
| 1   | A     | 296 | MLY  | 2       | 0            |
| 1   | A     | 30  | MLY  | 1       | 0            |
| 1   | A     | 348 | MLY  | 5       | 0            |
| 1   | A     | 369 | MLY  | 1       | 0            |
| 1   | A     | 415 | MLY  | 1       | 0            |
| 1   | A     | 436 | MLY  | 2       | 0            |
| 1   | A     | 486 | MLY  | 3       | 0            |
| 1   | A     | 49  | MLY  | 3       | 0            |
| 1   | A     | 504 | MLY  | 2       | 0            |
| 1   | A     | 505 | MLY  | 35      | 0            |
| 1   | A     | 528 | MLY  | 2       | 0            |
| 1   | A     | 55  | MLY  | 1       | 0            |
| 1   | A     | 551 | MLY  | 2       | 0            |
| 1   | A     | 553 | MLY  | 19      | 3            |
| 1   | A     | 59  | MLY  | 2       | 0            |
| 1   | A     | 598 | MLY  | 1       | 0            |
| 1   | A     | 600 | MLY  | 1       | 0            |
| 1   | A     | 617 | MLY  | 1       | 0            |
| 1   | A     | 63  | MLY  | 3       | 0            |
| 1   | A     | 659 | MLY  | 2       | 0            |
| 1   | A     | 764 | MLY  | 9       | 0            |
| 1   | A     | 768 | MLY  | 18      | 0            |
| 1   | A     | 782 | MLY  | 7       | 0            |
| 1   | A     | 837 | MLY  | 4       | 0            |
| 1   | A     | 839 | MLY  | 8       | 0            |
| 1   | A     | 87  | MLY  | 3       | 0            |
| 1   | D     | 107 | MLY  | 2       | 0            |
| 1   | D     | 138 | MLY  | 1       | 0            |
| 1   | D     | 190 | MLY  | 2       | 0            |
| 1   | D     | 248 | MLY  | 2       | 0            |
| 1   | D     | 272 | MLY  | 1       | 0            |
| 1   | D     | 295 | MLY  | 6       | 0            |
| 1   | D     | 296 | MLY  | 3       | 0            |
| 1   | D     | 30  | MLY  | 1       | 0            |
| 1   | D     | 348 | MLY  | 6       | 0            |
| 1   | D     | 415 | MLY  | 1       | 0            |
| 1   | D     | 436 | MLY  | 2       | 0            |
| 1   | D     | 486 | MLY  | 3       | 0            |
| 1   | D     | 49  | MLY  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | D     | 528 | MLY  | 3       | 0            |
| 1   | D     | 55  | MLY  | 1       | 0            |
| 1   | D     | 551 | MLY  | 1       | 0            |
| 1   | D     | 553 | MLY  | 16      | 1            |
| 1   | D     | 59  | MLY  | 2       | 0            |
| 1   | D     | 598 | MLY  | 1       | 0            |
| 1   | D     | 600 | MLY  | 1       | 0            |
| 1   | D     | 617 | MLY  | 1       | 0            |
| 1   | D     | 63  | MLY  | 3       | 0            |
| 1   | D     | 659 | MLY  | 2       | 0            |
| 1   | D     | 764 | MLY  | 9       | 0            |
| 1   | D     | 768 | MLY  | 11      | 0            |
| 1   | D     | 782 | MLY  | 87      | 0            |
| 1   | D     | 827 | MLY  | 2       | 0            |
| 1   | D     | 837 | MLY  | 1       | 0            |
| 1   | D     | 839 | MLY  | 4       | 0            |
| 1   | D     | 87  | MLY  | 3       | 0            |
| 1   | G     | 107 | MLY  | 2       | 0            |
| 1   | G     | 138 | MLY  | 1       | 0            |
| 1   | G     | 190 | MLY  | 2       | 0            |
| 1   | G     | 248 | MLY  | 2       | 0            |
| 1   | G     | 272 | MLY  | 1       | 0            |
| 1   | G     | 295 | MLY  | 5       | 0            |
| 1   | G     | 296 | MLY  | 2       | 0            |
| 1   | G     | 30  | MLY  | 1       | 0            |
| 1   | G     | 348 | MLY  | 4       | 0            |
| 1   | G     | 369 | MLY  | 1       | 0            |
| 1   | G     | 415 | MLY  | 1       | 0            |
| 1   | G     | 436 | MLY  | 2       | 0            |
| 1   | G     | 486 | MLY  | 3       | 0            |
| 1   | G     | 49  | MLY  | 2       | 0            |
| 1   | G     | 505 | MLY  | 1       | 0            |
| 1   | G     | 528 | MLY  | 3       | 0            |
| 1   | G     | 55  | MLY  | 1       | 0            |
| 1   | G     | 553 | MLY  | 27      | 0            |
| 1   | G     | 59  | MLY  | 3       | 0            |
| 1   | G     | 598 | MLY  | 1       | 0            |
| 1   | G     | 600 | MLY  | 1       | 0            |
| 1   | G     | 617 | MLY  | 1       | 0            |
| 1   | G     | 63  | MLY  | 4       | 0            |
| 1   | G     | 659 | MLY  | 2       | 0            |
| 1   | G     | 764 | MLY  | 22      | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | G     | 768 | MLY  | 7       | 0            |
| 1   | G     | 782 | MLY  | 1       | 0            |
| 1   | G     | 837 | MLY  | 1       | 0            |
| 1   | G     | 839 | MLY  | 4       | 0            |
| 1   | G     | 84  | MLY  | 18      | 0            |
| 1   | G     | 87  | MLY  | 3       | 0            |
| 1   | J     | 107 | MLY  | 3       | 0            |
| 1   | J     | 138 | MLY  | 1       | 0            |
| 1   | J     | 190 | MLY  | 2       | 0            |
| 1   | J     | 248 | MLY  | 2       | 0            |
| 1   | J     | 272 | MLY  | 1       | 0            |
| 1   | J     | 295 | MLY  | 6       | 0            |
| 1   | J     | 296 | MLY  | 3       | 0            |
| 1   | J     | 30  | MLY  | 1       | 0            |
| 1   | J     | 348 | MLY  | 5       | 0            |
| 1   | J     | 415 | MLY  | 1       | 0            |
| 1   | J     | 436 | MLY  | 2       | 0            |
| 1   | J     | 486 | MLY  | 3       | 0            |
| 1   | J     | 49  | MLY  | 2       | 0            |
| 1   | J     | 505 | MLY  | 9       | 0            |
| 1   | J     | 528 | MLY  | 3       | 0            |
| 1   | J     | 55  | MLY  | 1       | 0            |
| 1   | J     | 553 | MLY  | 11      | 0            |
| 1   | J     | 59  | MLY  | 2       | 0            |
| 1   | J     | 598 | MLY  | 1       | 0            |
| 1   | J     | 600 | MLY  | 1       | 0            |
| 1   | J     | 617 | MLY  | 1       | 0            |
| 1   | J     | 63  | MLY  | 4       | 0            |
| 1   | J     | 659 | MLY  | 2       | 0            |
| 1   | J     | 764 | MLY  | 2       | 0            |
| 1   | J     | 768 | MLY  | 4       | 0            |
| 1   | J     | 782 | MLY  | 1       | 0            |
| 1   | J     | 837 | MLY  | 1       | 0            |
| 1   | J     | 839 | MLY  | 8       | 0            |
| 1   | J     | 84  | MLY  | 23      | 0            |
| 1   | J     | 87  | MLY  | 3       | 0            |
| 1   | M     | 107 | MLY  | 3       | 0            |
| 1   | M     | 138 | MLY  | 1       | 0            |
| 1   | M     | 190 | MLY  | 2       | 0            |
| 1   | M     | 248 | MLY  | 2       | 0            |
| 1   | M     | 272 | MLY  | 1       | 0            |
| 1   | M     | 295 | MLY  | 6       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | M     | 296 | MLY  | 3       | 0            |
| 1   | M     | 30  | MLY  | 1       | 0            |
| 1   | M     | 348 | MLY  | 5       | 0            |
| 1   | M     | 35  | MLY  | 12      | 0            |
| 1   | M     | 369 | MLY  | 1       | 0            |
| 1   | M     | 415 | MLY  | 1       | 0            |
| 1   | M     | 436 | MLY  | 2       | 0            |
| 1   | M     | 486 | MLY  | 3       | 0            |
| 1   | M     | 49  | MLY  | 3       | 0            |
| 1   | M     | 505 | MLY  | 12      | 0            |
| 1   | M     | 528 | MLY  | 3       | 0            |
| 1   | M     | 55  | MLY  | 1       | 0            |
| 1   | M     | 551 | MLY  | 3       | 0            |
| 1   | M     | 553 | MLY  | 27      | 0            |
| 1   | M     | 59  | MLY  | 2       | 0            |
| 1   | M     | 598 | MLY  | 1       | 0            |
| 1   | M     | 600 | MLY  | 1       | 0            |
| 1   | M     | 617 | MLY  | 1       | 0            |
| 1   | M     | 63  | MLY  | 3       | 0            |
| 1   | M     | 659 | MLY  | 2       | 0            |
| 1   | M     | 764 | MLY  | 6       | 0            |
| 1   | M     | 768 | MLY  | 1       | 0            |
| 1   | M     | 782 | MLY  | 9       | 0            |
| 1   | M     | 837 | MLY  | 1       | 0            |
| 1   | M     | 839 | MLY  | 11      | 0            |
| 1   | M     | 84  | MLY  | 37      | 0            |
| 1   | M     | 87  | MLY  | 3       | 0            |
| 1   | P     | 107 | MLY  | 3       | 0            |
| 1   | P     | 138 | MLY  | 1       | 0            |
| 1   | P     | 190 | MLY  | 2       | 0            |
| 1   | P     | 248 | MLY  | 2       | 0            |
| 1   | P     | 272 | MLY  | 1       | 0            |
| 1   | P     | 295 | MLY  | 6       | 0            |
| 1   | P     | 296 | MLY  | 3       | 0            |
| 1   | P     | 30  | MLY  | 1       | 0            |
| 1   | P     | 348 | MLY  | 5       | 0            |
| 1   | P     | 415 | MLY  | 1       | 0            |
| 1   | P     | 436 | MLY  | 2       | 0            |
| 1   | P     | 486 | MLY  | 3       | 0            |
| 1   | P     | 49  | MLY  | 3       | 0            |
| 1   | P     | 528 | MLY  | 2       | 0            |
| 1   | P     | 55  | MLY  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1   | P     | 553 | MLY  | 2       | 0            |
| 1   | P     | 59  | MLY  | 2       | 0            |
| 1   | P     | 598 | MLY  | 1       | 0            |
| 1   | P     | 600 | MLY  | 1       | 0            |
| 1   | P     | 617 | MLY  | 1       | 0            |
| 1   | P     | 63  | MLY  | 3       | 0            |
| 1   | P     | 659 | MLY  | 1       | 0            |
| 1   | P     | 764 | MLY  | 9       | 0            |
| 1   | P     | 782 | MLY  | 2       | 0            |
| 1   | P     | 837 | MLY  | 1       | 0            |
| 1   | P     | 839 | MLY  | 12      | 0            |
| 1   | P     | 84  | MLY  | 5       | 0            |
| 1   | P     | 87  | MLY  | 3       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.