



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:30 PM GMT

PDB ID : 1XFV  
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin and 3' deoxy-ATP  
Authors : Shen, Q.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.  
Deposited on : 2004-09-15  
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
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/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

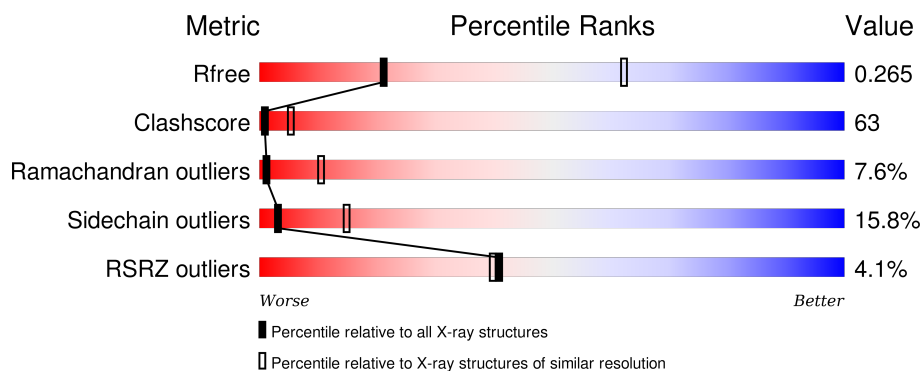
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1005 (3.42-3.30)                                      |
| Clashscore            | 102246                      | 1076 (3.42-3.30)                                      |
| Ramachandran outliers | 100387                      | 1059 (3.42-3.30)                                      |
| Sidechain outliers    | 100360                      | 1058 (3.42-3.30)                                      |
| RSRZ outliers         | 91569                       | 1010 (3.42-3.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain        |
|-----|-------|--------|-------------------------|
| 1   | A     | 777    | <br>5% 23% 55% 15% • 5% |
| 1   | B     | 777    | <br>4% 23% 55% 15% • 5% |
| 1   | C     | 777    | <br>3% 23% 56% 15% • 5% |
| 1   | D     | 777    | <br>4% 23% 56% 15% • 5% |
| 1   | E     | 777    | <br>5% 23% 55% 15% • 5% |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | F     | 777    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%24%55%15%5%</div></div> |
| 2   | O     | 149    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%61%13%</div></div>    |
| 2   | P     | 149    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%22%64%12%</div></div>    |
| 2   | Q     | 149    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%23%62%13%</div></div>    |
| 2   | R     | 149    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%21%63%13%</div></div>    |
| 2   | S     | 149    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%22%63%13%</div></div>   |
| 2   | T     | 149    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%23%62%13%</div></div>   |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 43044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Calmodulin-sensitive adenylate cyclase.

| Mol | Chain | Residues | Atoms |      |     |      |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|---|---------|---------|-------|
| 1   | A     | 735      | Total | C    | N   | O    | S | 0       | 0       | 0     |
|     |       |          | 5992  | 3828 | 995 | 1163 | 6 |         |         |       |
| 1   | B     | 735      | Total | C    | N   | O    | S | 0       | 0       | 0     |
|     |       |          | 5992  | 3828 | 995 | 1163 | 6 |         |         |       |
| 1   | C     | 735      | Total | C    | N   | O    | S | 0       | 0       | 0     |
|     |       |          | 5992  | 3828 | 995 | 1163 | 6 |         |         |       |
| 1   | D     | 735      | Total | C    | N   | O    | S | 0       | 0       | 0     |
|     |       |          | 5992  | 3828 | 995 | 1163 | 6 |         |         |       |
| 1   | E     | 735      | Total | C    | N   | O    | S | 0       | 0       | 0     |
|     |       |          | 5992  | 3828 | 995 | 1163 | 6 |         |         |       |
| 1   | F     | 735      | Total | C    | N   | O    | S | 0       | 0       | 0     |
|     |       |          | 5992  | 3828 | 995 | 1163 | 6 |         |         |       |

There are 54 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 24      | MET      | -      | INITIATING METHIONINE | UNP P40136 |
| A     | 25      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| A     | 26      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| A     | 27      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| A     | 28      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| A     | 29      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| A     | 30      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| A     | 31      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| A     | 32      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| B     | 24      | MET      | -      | INITIATING METHIONINE | UNP P40136 |
| B     | 25      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| B     | 26      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| B     | 27      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| B     | 28      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| B     | 29      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| B     | 30      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| B     | 31      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | 32      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| C     | 24      | MET      | -      | INITIATING METHIONINE | UNP P40136 |
| C     | 25      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| C     | 26      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| C     | 27      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| C     | 28      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| C     | 29      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| C     | 30      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| C     | 31      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| C     | 32      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| D     | 24      | MET      | -      | INITIATING METHIONINE | UNP P40136 |
| D     | 25      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| D     | 26      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| D     | 27      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| D     | 28      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| D     | 29      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| D     | 30      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| D     | 31      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| D     | 32      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| E     | 24      | MET      | -      | INITIATING METHIONINE | UNP P40136 |
| E     | 25      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| E     | 26      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| E     | 27      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| E     | 28      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| E     | 29      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| E     | 30      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| E     | 31      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| E     | 32      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| F     | 24      | MET      | -      | INITIATING METHIONINE | UNP P40136 |
| F     | 25      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| F     | 26      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| F     | 27      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| F     | 28      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| F     | 29      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| F     | 30      | HIS      | -      | EXPRESSION TAG        | UNP P40136 |
| F     | 31      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |
| F     | 32      | ALA      | -      | CLONING ARTIFACT      | UNP P40136 |

- Molecule 2 is a protein called Calmodulin 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | O     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 186 | 249 | 9 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | P     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 186 | 249 | 9 |         |         |       |
| 2   | Q     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 186 | 249 | 9 |         |         |       |
| 2   | R     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 186 | 249 | 9 |         |         |       |
| 2   | S     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 186 | 249 | 9 |         |         |       |
| 2   | T     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1146  | 702 | 186 | 249 | 9 |         |         |       |

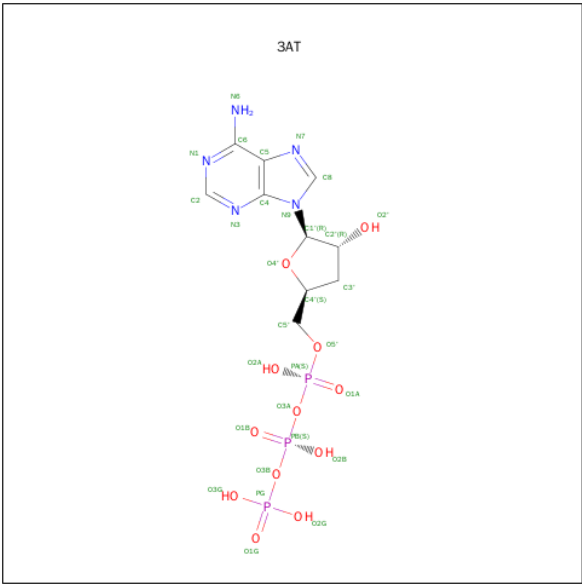
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | P     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 3   | Q     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 3   | T     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 3   | O     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 3   | R     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 3   | S     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | D     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | E     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | B     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | C     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | A     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 4   | F     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 5 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |         |
| 5   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |         |
| 5   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |         |
| 5   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |         |
| 5   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |         |
| 5   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 30    | 10 | 5 | 12 | 3 |         |         |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6   | A     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | B     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | C     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | D     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

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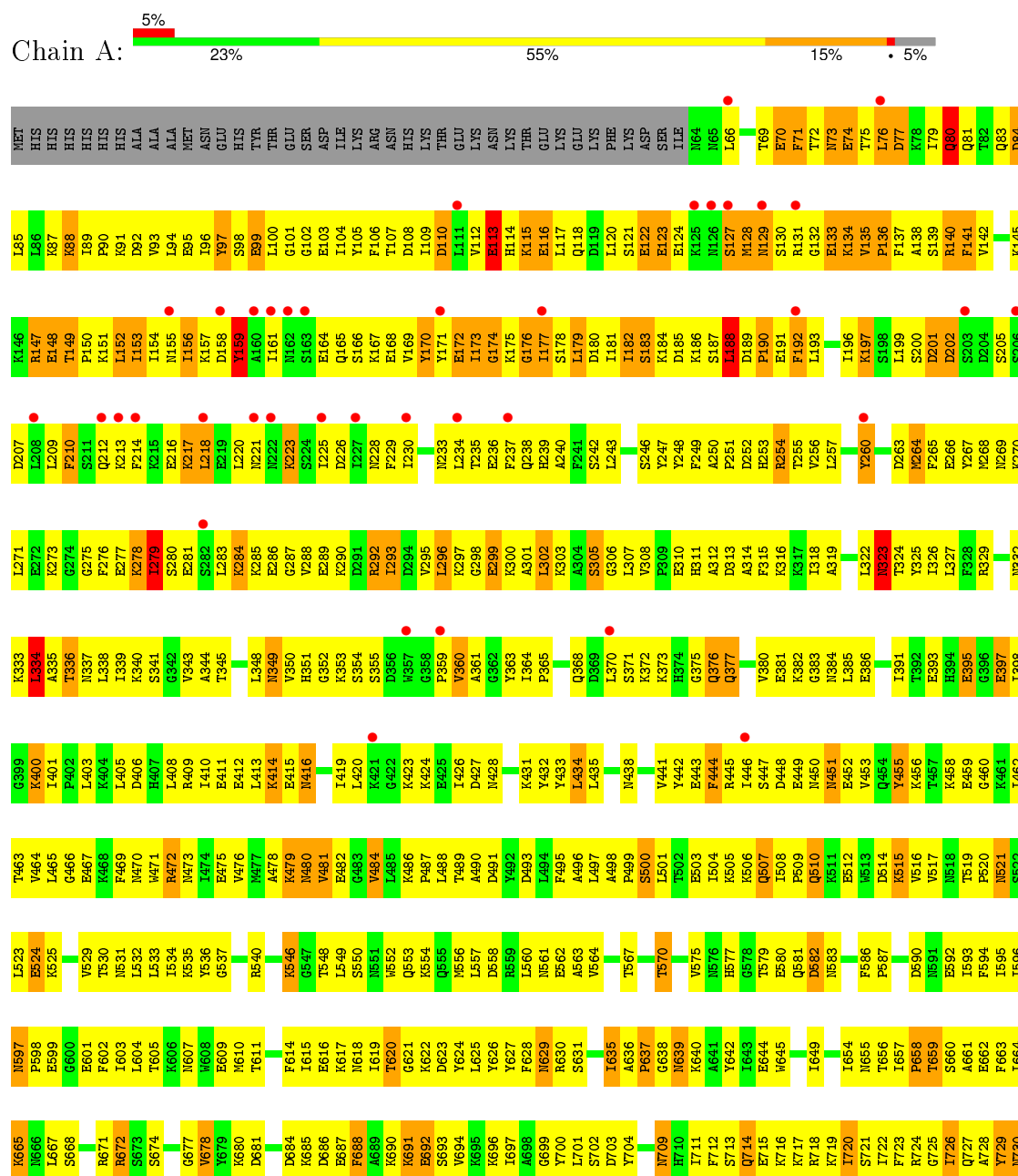
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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6   | E     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | F     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

### 3 Residue-property plots

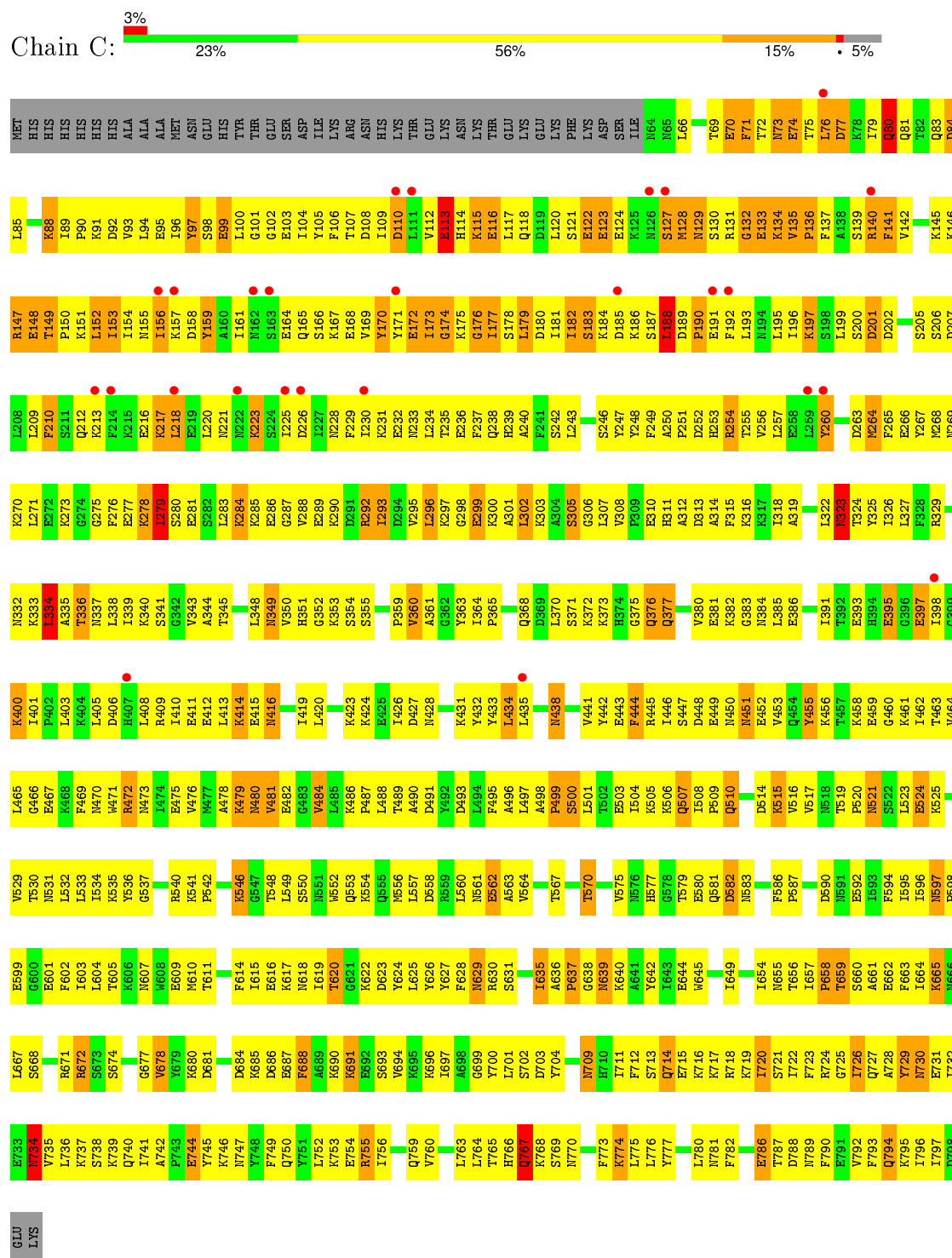
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: Calmodulin-sensitive adenylate cyclase

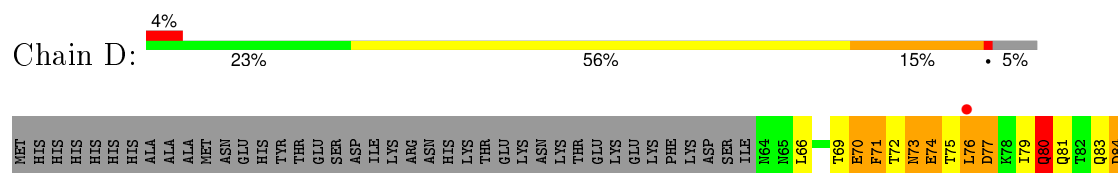




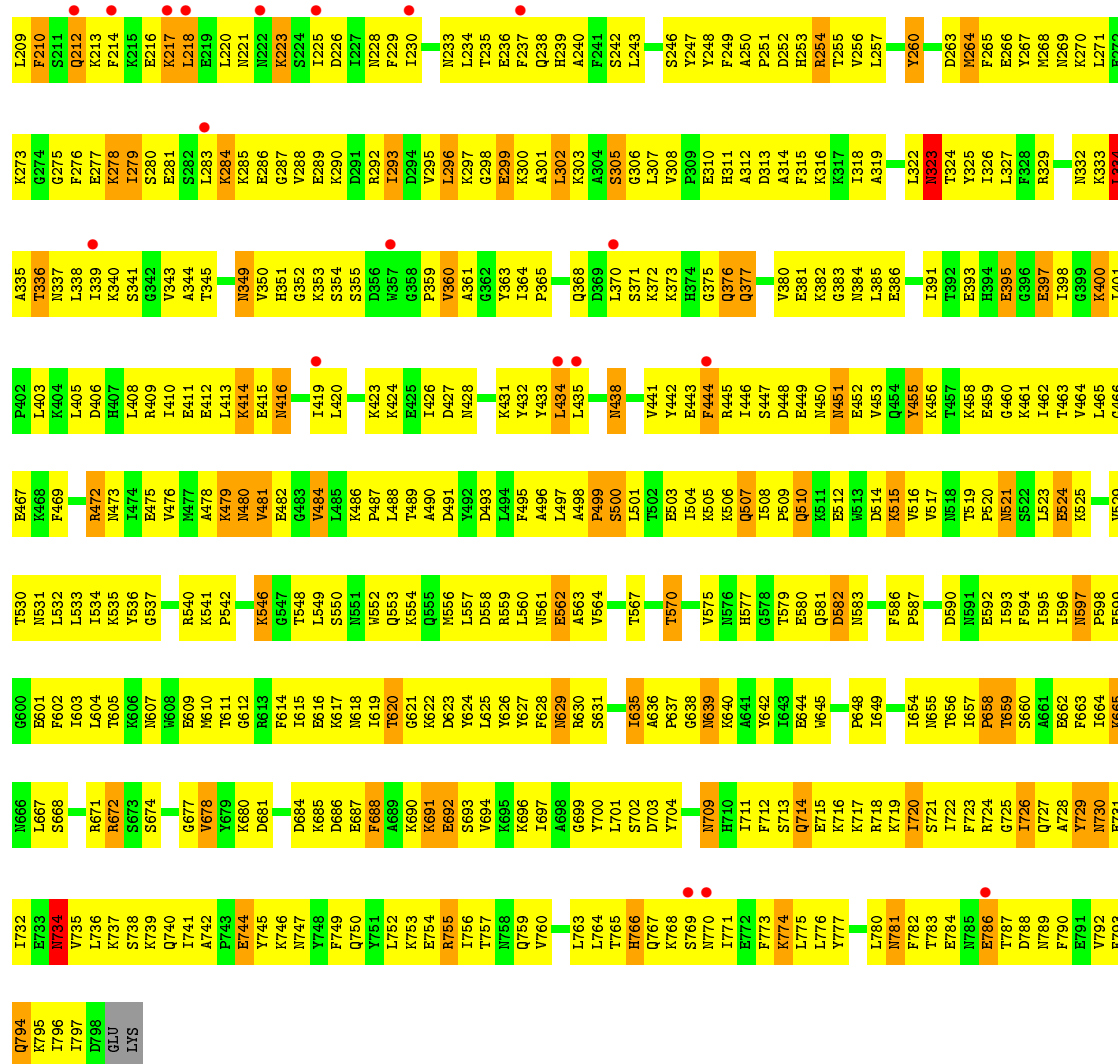
- Molecule 1: Calmodulin-sensitive adenylate cyclase



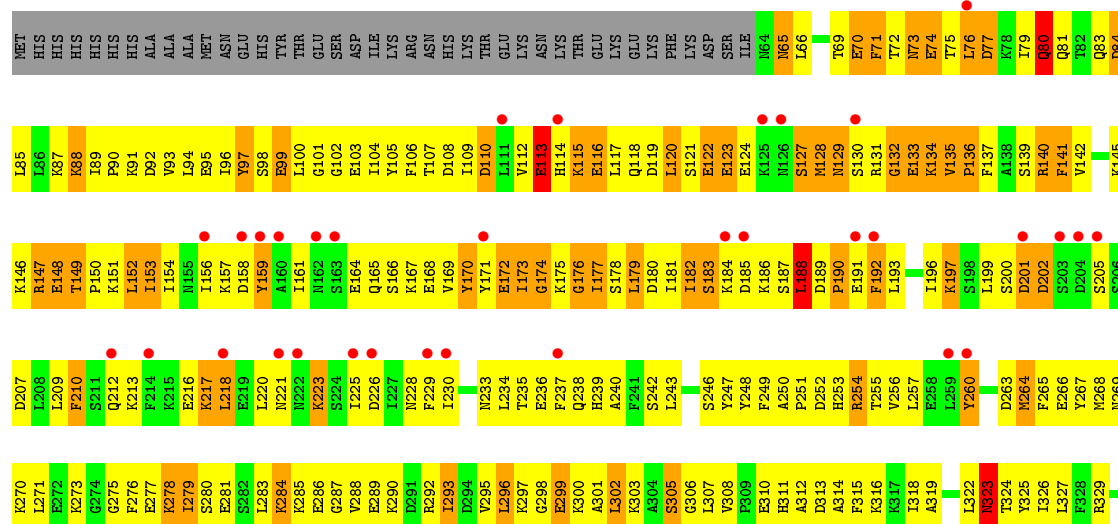
- Molecule 1: Calmodulin-sensitive adenylate cyclase





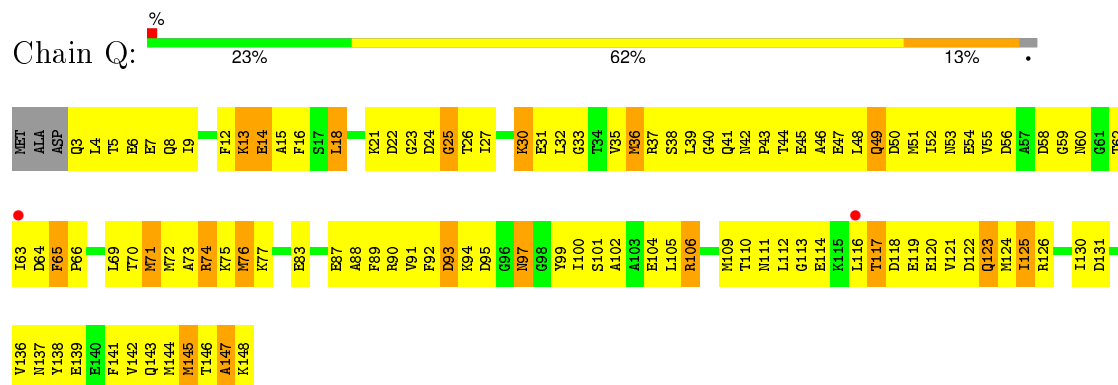


• Molecule 1: Calmodulin-sensitive adenylate cyclase

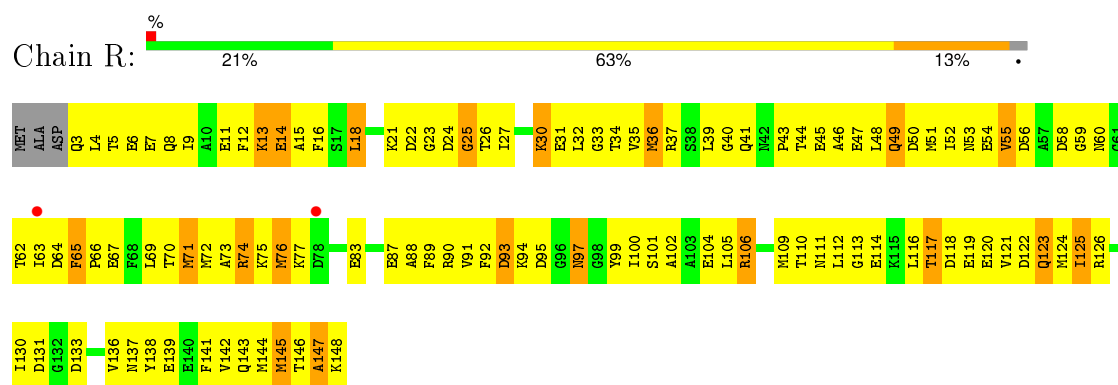




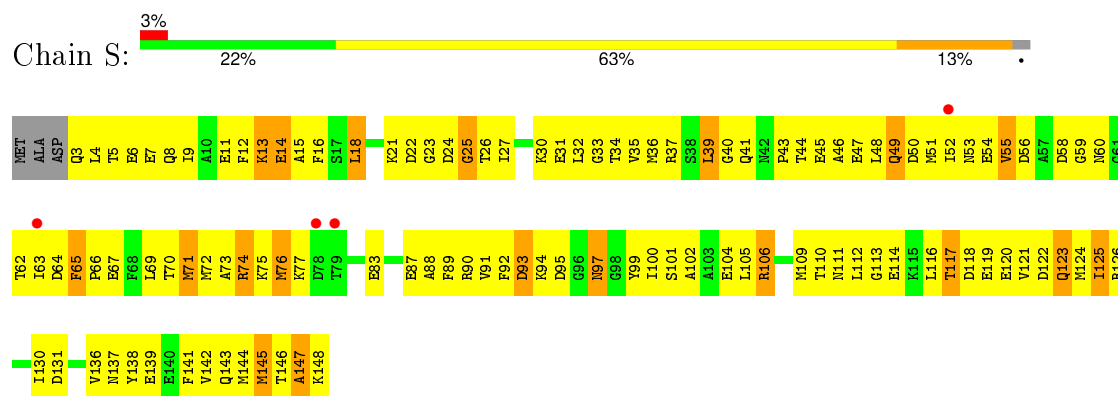
## ● Molecule 2: Calmodulin 2



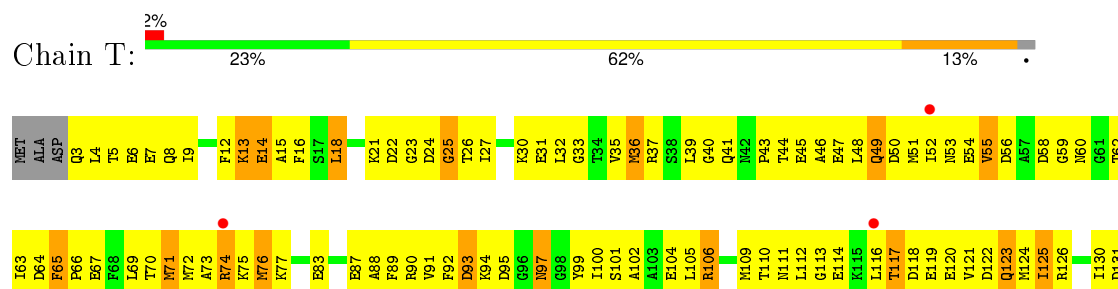
## ● Molecule 2: Calmodulin 2



## ● Molecule 2: Calmodulin 2



## ● Molecule 2: Calmodulin 2



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| V132 | D133 | V136 | M137 | Y138 | E139 | F140 | F141 | V142 | Q143 | M144 | M145 | T146 | A147 | K148 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 184.60Å 319.29Å 142.05Å<br>90.00° 90.22° 90.00°   | Depositor        |
| Resolution (Å)  | 29.57 – 3.35<br>35.51 – 3.35  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.6 (29.57-3.35)<br>91.6 (35.51-3.35)  | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | 0.06  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.04 (at 3.32Å)   | Xtriage          |
| Refinement program  | CNS 1.1   | Depositor        |
| R, $R_{free}$   | 0.263 , 0.282<br>0.250 , 0.265  | Depositor<br>DCC |
| $R_{free}$ test set   | 5479 reflections (5.06%)  | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 97.5  | Xtriage          |
| Anisotropy  | 0.117   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 56.3   | EDS              |
| Estimated twinning fraction   | 0.458 for -1/2*h+1/2*k,3/2*h+1/2*k,-l<br>0.458 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l<br>0.440 for 1/2*h+1/2*k,3/2*h-1/2*k,-l<br>0.447 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l<br>0.439 for -h,-k,l | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$   | Xtriage          |
| Outliers  | 0 of 114975 reflections   | Xtriage          |
| $F_o, F_c$ correlation  | 0.90  | EDS              |
| Total number of atoms   | 43044   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 81.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, 3AT

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  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.53         | 0/6104         | 0.82        | 13/8208 (0.2%)  |
| 1   | B     | 0.54         | 0/6104         | 0.83        | 13/8208 (0.2%)  |
| 1   | C     | 0.56         | 1/6104 (0.0%)  | 0.89        | 22/8208 (0.3%)  |
| 1   | D     | 0.56         | 3/6104 (0.0%)  | 0.85        | 15/8208 (0.2%)  |
| 1   | E     | 0.56         | 2/6104 (0.0%)  | 0.85        | 16/8208 (0.2%)  |
| 1   | F     | 0.54         | 0/6104         | 0.84        | 12/8208 (0.1%)  |
| 2   | O     | 0.53         | 0/1158         | 0.76        | 0/1553          |
| 2   | P     | 0.54         | 0/1158         | 0.76        | 0/1553          |
| 2   | Q     | 0.55         | 0/1158         | 0.75        | 0/1553          |
| 2   | R     | 0.55         | 0/1158         | 0.76        | 0/1553          |
| 2   | S     | 0.56         | 0/1158         | 0.76        | 0/1553          |
| 2   | T     | 0.56         | 0/1158         | 0.76        | 0/1553          |
| All | All   | 0.55         | 6/43572 (0.0%) | 0.83        | 91/58566 (0.2%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 740 | GLN  | C-N   | -5.88 | 1.20        | 1.34     |
| 1   | C     | 766 | HIS  | C-N   | -5.74 | 1.20        | 1.34     |
| 1   | D     | 784 | GLU  | C-N   | 5.50  | 1.46        | 1.34     |
| 1   | D     | 621 | GLY  | C-N   | 5.27  | 1.46        | 1.34     |
| 1   | E     | 784 | GLU  | C-N   | 5.14  | 1.45        | 1.34     |
| 1   | E     | 212 | GLN  | C-N   | -5.03 | 1.22        | 1.34     |

All (91) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | C     | 766 | HIS  | O-C-N      | -15.18 | 98.42       | 122.70   |
| 1   | C     | 767 | GLN  | CA-C-N     | 12.73  | 145.20      | 117.20   |
| 1   | C     | 766 | HIS  | CG-ND1-CE1 | 9.42   | 121.39      | 108.20   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 766 | HIS  | ND1-CG-CD2 | -8.71 | 93.81       | 106.00   |
| 1   | C     | 767 | GLN  | O-C-N      | -7.95 | 109.99      | 122.70   |
| 1   | E     | 188 | LEU  | N-CA-C     | -7.71 | 90.19       | 111.00   |
| 1   | B     | 188 | LEU  | N-CA-C     | -7.61 | 90.44       | 111.00   |
| 1   | E     | 129 | ASN  | N-CA-C     | 7.54  | 131.35      | 111.00   |
| 1   | A     | 188 | LEU  | N-CA-C     | -7.47 | 90.83       | 111.00   |
| 1   | B     | 674 | SER  | N-CA-C     | -7.44 | 90.92       | 111.00   |
| 1   | A     | 674 | SER  | N-CA-C     | -7.43 | 90.94       | 111.00   |
| 1   | D     | 674 | SER  | N-CA-C     | -7.43 | 90.94       | 111.00   |
| 1   | C     | 674 | SER  | N-CA-C     | -7.43 | 90.94       | 111.00   |
| 1   | E     | 674 | SER  | N-CA-C     | -7.42 | 90.96       | 111.00   |
| 1   | F     | 674 | SER  | N-CA-C     | -7.42 | 90.97       | 111.00   |
| 1   | C     | 188 | LEU  | N-CA-C     | -7.29 | 91.31       | 111.00   |
| 1   | C     | 767 | GLN  | CA-C-O     | -7.28 | 104.81      | 120.10   |
| 1   | F     | 134 | LYS  | C-N-CA     | -7.25 | 103.58      | 121.70   |
| 1   | B     | 134 | LYS  | C-N-CA     | -7.24 | 103.59      | 121.70   |
| 1   | E     | 134 | LYS  | C-N-CA     | -7.24 | 103.60      | 121.70   |
| 1   | A     | 134 | LYS  | C-N-CA     | -7.24 | 103.61      | 121.70   |
| 1   | D     | 134 | LYS  | C-N-CA     | -7.24 | 103.61      | 121.70   |
| 1   | C     | 134 | LYS  | C-N-CA     | -7.23 | 103.63      | 121.70   |
| 1   | D     | 147 | ARG  | C-N-CA     | -7.12 | 103.89      | 121.70   |
| 1   | F     | 147 | ARG  | C-N-CA     | -7.11 | 103.93      | 121.70   |
| 1   | A     | 147 | ARG  | C-N-CA     | -7.10 | 103.94      | 121.70   |
| 1   | C     | 147 | ARG  | C-N-CA     | -7.10 | 103.96      | 121.70   |
| 1   | B     | 147 | ARG  | C-N-CA     | -7.09 | 103.97      | 121.70   |
| 1   | E     | 147 | ARG  | C-N-CA     | -7.09 | 103.97      | 121.70   |
| 1   | F     | 188 | LEU  | N-CA-C     | -7.08 | 91.89       | 111.00   |
| 1   | C     | 129 | ASN  | N-CA-C     | 7.08  | 130.11      | 111.00   |
| 1   | F     | 129 | ASN  | N-CA-C     | 7.05  | 130.04      | 111.00   |
| 1   | E     | 159 | TYR  | CA-C-N     | 6.88  | 132.34      | 117.20   |
| 1   | D     | 188 | LEU  | N-CA-C     | -6.72 | 92.85       | 111.00   |
| 1   | D     | 159 | TYR  | CA-C-N     | 6.67  | 131.88      | 117.20   |
| 1   | B     | 129 | ASN  | N-CA-C     | 6.67  | 129.01      | 111.00   |
| 1   | C     | 766 | HIS  | CA-C-N     | 6.53  | 131.57      | 117.20   |
| 1   | A     | 132 | GLY  | N-CA-C     | -6.52 | 96.79       | 113.10   |
| 1   | E     | 132 | GLY  | N-CA-C     | -6.52 | 96.80       | 113.10   |
| 1   | D     | 132 | GLY  | N-CA-C     | -6.52 | 96.80       | 113.10   |
| 1   | C     | 132 | GLY  | N-CA-C     | -6.51 | 96.82       | 113.10   |
| 1   | F     | 132 | GLY  | N-CA-C     | -6.42 | 97.05       | 113.10   |
| 1   | B     | 147 | ARG  | CA-C-N     | 6.41  | 131.30      | 117.20   |
| 1   | A     | 129 | ASN  | N-CA-C     | 6.40  | 128.28      | 111.00   |
| 1   | F     | 147 | ARG  | CA-C-N     | 6.40  | 131.28      | 117.20   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 147 | ARG  | CA-C-N  | 6.40  | 131.27      | 117.20   |
| 1   | A     | 147 | ARG  | CA-C-N  | 6.39  | 131.26      | 117.20   |
| 1   | E     | 147 | ARG  | CA-C-N  | 6.39  | 131.26      | 117.20   |
| 1   | D     | 147 | ARG  | CA-C-N  | 6.38  | 131.24      | 117.20   |
| 1   | F     | 159 | TYR  | CA-C-N  | 6.23  | 130.91      | 117.20   |
| 1   | D     | 129 | ASN  | N-CA-C  | 5.99  | 127.18      | 111.00   |
| 1   | C     | 768 | LYS  | N-CA-C  | -5.99 | 94.83       | 111.00   |
| 1   | B     | 132 | GLY  | N-CA-C  | -5.95 | 98.23       | 113.10   |
| 1   | D     | 188 | LEU  | C-N-CA  | -5.93 | 106.88      | 121.70   |
| 1   | E     | 147 | ARG  | N-CA-C  | 5.79  | 126.63      | 111.00   |
| 1   | C     | 147 | ARG  | N-CA-C  | 5.79  | 126.62      | 111.00   |
| 1   | B     | 147 | ARG  | N-CA-C  | 5.78  | 126.61      | 111.00   |
| 1   | A     | 147 | ARG  | N-CA-C  | 5.78  | 126.60      | 111.00   |
| 1   | D     | 147 | ARG  | N-CA-C  | 5.76  | 126.56      | 111.00   |
| 1   | F     | 147 | ARG  | N-CA-C  | 5.76  | 126.55      | 111.00   |
| 1   | D     | 146 | LYS  | C-N-CA  | -5.75 | 107.33      | 121.70   |
| 1   | B     | 159 | TYR  | CA-C-N  | 5.56  | 129.44      | 117.20   |
| 1   | B     | 188 | LEU  | C-N-CA  | -5.56 | 107.80      | 121.70   |
| 1   | C     | 159 | TYR  | CA-C-N  | 5.56  | 129.42      | 117.20   |
| 1   | A     | 159 | TYR  | CA-C-N  | 5.55  | 129.42      | 117.20   |
| 1   | E     | 146 | LYS  | C-N-CA  | -5.43 | 108.13      | 121.70   |
| 1   | B     | 127 | SER  | N-CA-C  | 5.42  | 125.65      | 111.00   |
| 1   | A     | 188 | LEU  | C-N-CA  | -5.40 | 108.21      | 121.70   |
| 1   | C     | 188 | LEU  | CA-C-N  | 5.39  | 129.07      | 117.20   |
| 1   | E     | 188 | LEU  | CA-C-N  | 5.36  | 128.99      | 117.20   |
| 1   | F     | 190 | PRO  | CB-CA-C | 5.35  | 125.37      | 112.00   |
| 1   | A     | 190 | PRO  | CB-CA-C | 5.31  | 125.28      | 112.00   |
| 1   | E     | 190 | PRO  | CB-CA-C | 5.28  | 125.21      | 112.00   |
| 1   | C     | 188 | LEU  | C-N-CA  | -5.26 | 108.54      | 121.70   |
| 1   | E     | 159 | TYR  | O-C-N   | -5.24 | 114.32      | 122.70   |
| 1   | E     | 147 | ARG  | O-C-N   | -5.20 | 114.38      | 122.70   |
| 1   | C     | 147 | ARG  | O-C-N   | -5.20 | 114.38      | 122.70   |
| 1   | C     | 765 | THR  | CB-CA-C | 5.20  | 125.64      | 111.60   |
| 1   | E     | 188 | LEU  | C-N-CA  | -5.19 | 108.72      | 121.70   |
| 1   | A     | 147 | ARG  | O-C-N   | -5.18 | 114.42      | 122.70   |
| 1   | B     | 147 | ARG  | O-C-N   | -5.17 | 114.42      | 122.70   |
| 1   | F     | 147 | ARG  | O-C-N   | -5.16 | 114.44      | 122.70   |
| 1   | D     | 147 | ARG  | O-C-N   | -5.16 | 114.45      | 122.70   |
| 1   | B     | 190 | PRO  | CB-CA-C | 5.15  | 124.86      | 112.00   |
| 1   | C     | 127 | SER  | N-CA-C  | 5.11  | 124.81      | 111.00   |
| 1   | A     | 127 | SER  | N-CA-C  | 5.11  | 124.79      | 111.00   |
| 1   | D     | 127 | SER  | N-CA-C  | 5.10  | 124.78      | 111.00   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|--------|-------|------------------------|---------------------|
| 1   | E     | 127 | SER  | N-CA-C | 5.10  | 124.77                 | 111.00              |
| 1   | F     | 127 | SER  | N-CA-C | 5.10  | 124.77                 | 111.00              |
| 1   | D     | 188 | LEU  | CA-C-N | 5.05  | 128.31                 | 117.20              |
| 1   | D     | 331 | VAL  | N-CA-C | -5.03 | 97.42                  | 111.00              |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 5992  | 0        | 6010     | 771     | 2            |
| 1   | B     | 5992  | 0        | 6010     | 765     | 2            |
| 1   | C     | 5992  | 0        | 6010     | 770     | 2            |
| 1   | D     | 5992  | 0        | 6009     | 771     | 3            |
| 1   | E     | 5992  | 0        | 6009     | 772     | 3            |
| 1   | F     | 5992  | 0        | 6010     | 755     | 1            |
| 2   | O     | 1146  | 0        | 1071     | 150     | 0            |
| 2   | P     | 1146  | 0        | 1071     | 157     | 0            |
| 2   | Q     | 1146  | 0        | 1071     | 155     | 0            |
| 2   | R     | 1146  | 0        | 1071     | 157     | 0            |
| 2   | S     | 1146  | 0        | 1071     | 162     | 0            |
| 2   | T     | 1146  | 0        | 1071     | 157     | 0            |
| 3   | O     | 3     | 0        | 0        | 0       | 0            |
| 3   | P     | 3     | 0        | 0        | 0       | 0            |
| 3   | Q     | 3     | 0        | 0        | 0       | 0            |
| 3   | R     | 3     | 0        | 0        | 0       | 0            |
| 3   | S     | 3     | 0        | 0        | 0       | 0            |
| 3   | T     | 3     | 0        | 0        | 0       | 0            |
| 4   | A     | 2     | 0        | 0        | 0       | 0            |
| 4   | B     | 2     | 0        | 0        | 0       | 0            |
| 4   | C     | 2     | 0        | 0        | 0       | 0            |
| 4   | D     | 2     | 0        | 0        | 0       | 0            |
| 4   | E     | 2     | 0        | 0        | 0       | 0            |
| 4   | F     | 2     | 0        | 0        | 0       | 0            |
| 5   | A     | 30    | 0        | 12       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | B     | 30    | 0        | 12       | 1       | 0            |
| 5   | C     | 30    | 0        | 12       | 1       | 0            |
| 5   | D     | 30    | 0        | 12       | 1       | 0            |
| 5   | E     | 30    | 0        | 12       | 1       | 0            |
| 5   | F     | 30    | 0        | 12       | 1       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 6   | C     | 1     | 0        | 0        | 0       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | E     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 43044 | 0        | 42556    | 5389    | 8            |

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 63.

All (5389) 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:E:179:LEU:O    | 1:E:183:SER:CB   | 1.74                     | 1.36              |
| 1:D:179:LEU:O    | 1:D:183:SER:CB   | 1.77                     | 1.30              |
| 1:F:179:LEU:O    | 1:F:183:SER:CB   | 1.80                     | 1.30              |
| 1:C:179:LEU:O    | 1:C:183:SER:CB   | 1.77                     | 1.30              |
| 1:F:188:LEU:H    | 1:F:188:LEU:CD2  | 1.46                     | 1.27              |
| 1:B:179:LEU:O    | 1:B:183:SER:HB2  | 1.18                     | 1.27              |
| 1:E:188:LEU:H    | 1:E:188:LEU:CD2  | 1.46                     | 1.26              |
| 1:A:179:LEU:O    | 1:A:183:SER:CB   | 1.85                     | 1.24              |
| 1:A:188:LEU:HD23 | 1:A:188:LEU:N    | 1.45                     | 1.24              |
| 1:A:188:LEU:CD2  | 1:A:188:LEU:H    | 1.46                     | 1.23              |
| 1:A:296:LEU:N    | 1:A:296:LEU:HD23 | 1.44                     | 1.22              |
| 1:E:296:LEU:HD23 | 1:E:296:LEU:N    | 1.44                     | 1.22              |
| 1:B:296:LEU:HD23 | 1:B:296:LEU:N    | 1.44                     | 1.20              |
| 1:C:188:LEU:CD2  | 1:C:188:LEU:H    | 1.53                     | 1.17              |
| 1:C:186:LYS:HA   | 1:C:190:PRO:HD3  | 1.25                     | 1.16              |
| 1:A:186:LYS:HA   | 1:A:190:PRO:HD3  | 1.25                     | 1.15              |
| 1:D:188:LEU:H    | 1:D:188:LEU:CD2  | 1.54                     | 1.15              |
| 1:A:179:LEU:O    | 1:A:183:SER:HB2  | 0.98                     | 1.15              |
| 1:B:697:ILE:HD13 | 1:B:732:ILE:HD13 | 1.26                     | 1.15              |
| 1:B:179:LEU:O    | 1:B:183:SER:CB   | 1.94                     | 1.14              |
| 1:B:188:LEU:CD2  | 1:B:188:LEU:H    | 1.61                     | 1.14              |
| 1:D:179:LEU:O    | 1:D:183:SER:HB2  | 0.96                     | 1.14              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:182:ILE:O    | 1:F:187:SER:HB2  | 1.47                     | 1.14              |
| 1:A:697:ILE:HD13 | 1:A:732:ILE:HD13 | 1.26                     | 1.14              |
| 1:C:296:LEU:N    | 1:C:296:LEU:HD23 | 1.44                     | 1.14              |
| 1:F:296:LEU:N    | 1:F:296:LEU:HD23 | 1.44                     | 1.13              |
| 1:E:182:ILE:O    | 1:E:187:SER:HB2  | 1.49                     | 1.13              |
| 1:F:179:LEU:O    | 1:F:183:SER:HB2  | 0.97                     | 1.13              |
| 1:E:179:LEU:O    | 1:E:183:SER:HB2  | 0.95                     | 1.12              |
| 1:C:179:LEU:O    | 1:C:183:SER:HB2  | 0.95                     | 1.11              |
| 1:A:89:ILE:HG22  | 1:A:93:VAL:HG11  | 1.13                     | 1.11              |
| 1:D:186:LYS:HA   | 1:D:190:PRO:HD3  | 1.27                     | 1.10              |
| 1:D:296:LEU:N    | 1:D:296:LEU:HD23 | 1.44                     | 1.10              |
| 1:E:697:ILE:HD13 | 1:E:732:ILE:HD13 | 1.28                     | 1.10              |
| 1:B:89:ILE:HG22  | 1:B:93:VAL:HG11  | 1.13                     | 1.10              |
| 1:E:89:ILE:HG22  | 1:E:93:VAL:HG11  | 1.15                     | 1.10              |
| 1:F:186:LYS:HA   | 1:F:190:PRO:HD3  | 1.34                     | 1.10              |
| 1:D:188:LEU:H    | 1:D:188:LEU:HD23 | 0.95                     | 1.10              |
| 1:D:697:ILE:HD13 | 1:D:732:ILE:HD13 | 1.25                     | 1.10              |
| 1:C:697:ILE:HD13 | 1:C:732:ILE:HD13 | 1.27                     | 1.09              |
| 1:F:697:ILE:HD13 | 1:F:732:ILE:HD13 | 1.25                     | 1.09              |
| 2:R:106:ARG:HG3  | 2:R:121:VAL:HG21 | 1.12                     | 1.09              |
| 1:A:183:SER:O    | 1:A:187:SER:CB   | 2.00                     | 1.09              |
| 1:D:89:ILE:HG22  | 1:D:93:VAL:HG11  | 1.14                     | 1.08              |
| 1:F:188:LEU:HD23 | 1:F:188:LEU:N    | 1.66                     | 1.08              |
| 1:F:89:ILE:HG22  | 1:F:93:VAL:HG11  | 1.13                     | 1.08              |
| 2:Q:106:ARG:HG3  | 2:Q:121:VAL:HG21 | 1.10                     | 1.08              |
| 2:P:106:ARG:HG3  | 2:P:121:VAL:HG21 | 1.10                     | 1.08              |
| 1:C:414:LYS:HA   | 1:C:414:LYS:HZ3  | 1.19                     | 1.08              |
| 2:S:106:ARG:HG3  | 2:S:121:VAL:HG21 | 1.10                     | 1.08              |
| 1:E:186:LYS:HA   | 1:E:190:PRO:HD3  | 1.36                     | 1.07              |
| 1:E:188:LEU:N    | 1:E:188:LEU:HD23 | 1.67                     | 1.06              |
| 2:O:106:ARG:HG3  | 2:O:121:VAL:HG21 | 1.12                     | 1.06              |
| 1:C:89:ILE:HG22  | 1:C:93:VAL:HG11  | 1.15                     | 1.05              |
| 1:D:188:LEU:N    | 1:D:188:LEU:HD23 | 1.70                     | 1.05              |
| 1:B:188:LEU:HD23 | 1:B:188:LEU:H    | 0.90                     | 1.05              |
| 2:T:106:ARG:HG3  | 2:T:121:VAL:HG21 | 1.10                     | 1.05              |
| 1:C:188:LEU:HD23 | 1:C:188:LEU:H    | 0.89                     | 1.04              |
| 1:C:188:LEU:HD23 | 1:C:188:LEU:N    | 1.68                     | 1.04              |
| 2:T:3:GLN:N      | 2:T:77:LYS:HE3   | 1.72                     | 1.04              |
| 1:A:414:LYS:HA   | 1:A:414:LYS:HZ3  | 1.22                     | 1.03              |
| 1:C:182:ILE:O    | 1:C:187:SER:HB2  | 1.59                     | 1.03              |
| 1:B:186:LYS:HA   | 1:B:190:PRO:HD3  | 1.41                     | 1.02              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:296:LEU:N    | 1:F:296:LEU:CD2  | 2.19                     | 1.02              |
| 1:D:182:ILE:O    | 1:D:187:SER:HB2  | 1.60                     | 1.02              |
| 1:F:188:LEU:HD23 | 1:F:188:LEU:H    | 0.88                     | 1.02              |
| 1:D:414:LYS:NZ   | 1:D:414:LYS:HA   | 1.75                     | 1.02              |
| 1:D:521:ASN:HB3  | 1:D:524:GLU:HB2  | 1.41                     | 1.02              |
| 1:A:296:LEU:N    | 1:A:296:LEU:CD2  | 2.19                     | 1.01              |
| 1:C:479:LYS:HG2  | 1:C:488:LEU:HD21 | 1.42                     | 1.01              |
| 1:C:521:ASN:HB3  | 1:C:524:GLU:HB2  | 1.41                     | 1.01              |
| 1:E:296:LEU:N    | 1:E:296:LEU:CD2  | 2.19                     | 1.01              |
| 1:A:70:GLU:HB2   | 1:A:107:THR:HG22 | 1.41                     | 1.01              |
| 1:E:414:LYS:NZ   | 1:E:414:LYS:HA   | 1.75                     | 1.01              |
| 1:F:597:ASN:HB2  | 1:F:598:PRO:HD2  | 1.43                     | 1.01              |
| 1:A:597:ASN:HB2  | 1:A:598:PRO:HD2  | 1.43                     | 1.01              |
| 1:D:296:LEU:CD2  | 1:D:296:LEU:N    | 2.19                     | 1.01              |
| 1:F:715:GLU:HA   | 1:F:718:ARG:NH1  | 1.76                     | 1.01              |
| 1:B:296:LEU:CD2  | 1:B:296:LEU:N    | 2.19                     | 1.00              |
| 1:C:296:LEU:CD2  | 1:C:296:LEU:N    | 2.19                     | 1.00              |
| 1:C:414:LYS:HA   | 1:C:414:LYS:NZ   | 1.76                     | 1.00              |
| 1:A:414:LYS:HA   | 1:A:414:LYS:NZ   | 1.76                     | 1.00              |
| 1:B:635:ILE:HD12 | 1:B:635:ILE:H    | 1.27                     | 1.00              |
| 1:C:597:ASN:HB2  | 1:C:598:PRO:HD2  | 1.43                     | 1.00              |
| 1:A:521:ASN:HB3  | 1:A:524:GLU:HB2  | 1.41                     | 1.00              |
| 1:B:550:SER:H    | 1:B:553:GLN:NE2  | 1.59                     | 1.00              |
| 1:C:715:GLU:HA   | 1:C:718:ARG:NH1  | 1.77                     | 1.00              |
| 2:T:100:ILE:HB   | 2:T:136:VAL:HG23 | 1.43                     | 1.00              |
| 1:D:597:ASN:HB2  | 1:D:598:PRO:HD2  | 1.44                     | 1.00              |
| 2:O:100:ILE:HB   | 2:O:136:VAL:HG23 | 1.42                     | 1.00              |
| 1:B:480:ASN:HD22 | 1:B:481:VAL:N    | 1.59                     | 1.00              |
| 1:E:521:ASN:HB3  | 1:E:524:GLU:HB2  | 1.41                     | 1.00              |
| 1:D:142:VAL:HG22 | 1:D:154:ILE:HD12 | 1.44                     | 1.00              |
| 1:B:597:ASN:HB2  | 1:B:598:PRO:HD2  | 1.44                     | 0.99              |
| 2:Q:3:GLN:N      | 2:Q:77:LYS:HE3   | 1.76                     | 0.99              |
| 1:F:521:ASN:HB3  | 1:F:524:GLU:HB2  | 1.41                     | 0.99              |
| 1:B:414:LYS:NZ   | 1:B:414:LYS:HA   | 1.76                     | 0.99              |
| 1:A:550:SER:H    | 1:A:553:GLN:NE2  | 1.60                     | 0.99              |
| 1:B:479:LYS:HG2  | 1:B:488:LEU:HD21 | 1.44                     | 0.99              |
| 1:D:479:LYS:HG2  | 1:D:488:LEU:HD21 | 1.44                     | 0.99              |
| 1:D:480:ASN:HD22 | 1:D:481:VAL:N    | 1.60                     | 0.99              |
| 1:B:715:GLU:HA   | 1:B:718:ARG:NH1  | 1.77                     | 0.99              |
| 1:F:70:GLU:HB2   | 1:F:107:THR:HG22 | 1.44                     | 0.99              |
| 1:A:188:LEU:CD2  | 1:A:188:LEU:N    | 2.08                     | 0.99              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:629:ASN:ND2  | 1:E:631:SER:H    | 1.60                     | 0.99              |
| 1:E:142:VAL:HG22 | 1:E:154:ILE:HD12 | 1.45                     | 0.99              |
| 1:A:635:ILE:HD12 | 1:A:635:ILE:H    | 1.28                     | 0.99              |
| 1:C:629:ASN:ND2  | 1:C:631:SER:H    | 1.61                     | 0.99              |
| 1:E:414:LYS:HA   | 1:E:414:LYS:HZ3  | 1.27                     | 0.99              |
| 1:F:414:LYS:HA   | 1:F:414:LYS:NZ   | 1.76                     | 0.99              |
| 1:B:629:ASN:ND2  | 1:B:631:SER:H    | 1.61                     | 0.99              |
| 2:S:3:GLN:N      | 2:S:77:LYS:HE3   | 1.77                     | 0.99              |
| 2:R:3:GLN:N      | 2:R:77:LYS:HE3   | 1.77                     | 0.99              |
| 1:A:715:GLU:HA   | 1:A:718:ARG:NH1  | 1.77                     | 0.99              |
| 1:E:715:GLU:HA   | 1:E:718:ARG:NH1  | 1.78                     | 0.99              |
| 1:E:188:LEU:H    | 1:E:188:LEU:HD23 | 0.87                     | 0.98              |
| 1:E:597:ASN:HB2  | 1:E:598:PRO:HD2  | 1.43                     | 0.98              |
| 1:C:142:VAL:HG22 | 1:C:154:ILE:HD12 | 1.45                     | 0.98              |
| 2:S:100:ILE:HB   | 2:S:136:VAL:HG23 | 1.43                     | 0.98              |
| 1:C:480:ASN:HD22 | 1:C:481:VAL:N    | 1.60                     | 0.98              |
| 1:E:480:ASN:HD22 | 1:E:481:VAL:N    | 1.60                     | 0.98              |
| 1:E:479:LYS:HG2  | 1:E:488:LEU:HD21 | 1.42                     | 0.98              |
| 1:F:479:LYS:HG2  | 1:F:488:LEU:HD21 | 1.43                     | 0.98              |
| 1:A:629:ASN:ND2  | 1:A:631:SER:H    | 1.60                     | 0.98              |
| 2:P:100:ILE:HB   | 2:P:136:VAL:HG23 | 1.43                     | 0.98              |
| 1:D:550:SER:H    | 1:D:553:GLN:NE2  | 1.59                     | 0.98              |
| 1:A:480:ASN:HD22 | 1:A:481:VAL:N    | 1.59                     | 0.98              |
| 1:A:479:LYS:HG2  | 1:A:488:LEU:HD21 | 1.45                     | 0.98              |
| 1:E:635:ILE:H    | 1:E:635:ILE:HD12 | 1.27                     | 0.98              |
| 1:F:183:SER:O    | 1:F:187:SER:HB3  | 1.63                     | 0.98              |
| 1:B:70:GLU:HB2   | 1:B:107:THR:HG22 | 1.43                     | 0.98              |
| 2:Q:100:ILE:HB   | 2:Q:136:VAL:HG23 | 1.43                     | 0.98              |
| 1:B:521:ASN:HB3  | 1:B:524:GLU:HB2  | 1.41                     | 0.98              |
| 1:D:635:ILE:HD12 | 1:D:635:ILE:H    | 1.27                     | 0.98              |
| 1:C:635:ILE:H    | 1:C:635:ILE:HD12 | 1.28                     | 0.98              |
| 1:D:715:GLU:HA   | 1:D:718:ARG:NH1  | 1.77                     | 0.97              |
| 1:F:629:ASN:ND2  | 1:F:631:SER:H    | 1.61                     | 0.97              |
| 1:F:480:ASN:HD22 | 1:F:481:VAL:N    | 1.60                     | 0.97              |
| 1:F:550:SER:H    | 1:F:553:GLN:NE2  | 1.60                     | 0.97              |
| 1:D:629:ASN:ND2  | 1:D:631:SER:H    | 1.62                     | 0.97              |
| 1:A:142:VAL:HG22 | 1:A:154:ILE:HD12 | 1.46                     | 0.97              |
| 1:B:142:VAL:HG22 | 1:B:154:ILE:HD12 | 1.46                     | 0.97              |
| 1:F:635:ILE:H    | 1:F:635:ILE:HD12 | 1.28                     | 0.97              |
| 1:C:70:GLU:HB2   | 1:C:107:THR:HG22 | 1.47                     | 0.97              |
| 2:O:3:GLN:N      | 2:O:77:LYS:HE3   | 1.78                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:550:SER:H    | 1:C:553:GLN:NE2  | 1.61                     | 0.97              |
| 1:F:142:VAL:HG22 | 1:F:154:ILE:HD12 | 1.46                     | 0.97              |
| 1:F:184:LYS:NZ   | 1:F:191:GLU:HB2  | 1.80                     | 0.96              |
| 1:B:188:LEU:HD23 | 1:B:188:LEU:N    | 1.72                     | 0.96              |
| 1:C:550:SER:H    | 1:C:553:GLN:HE21 | 1.04                     | 0.96              |
| 1:E:550:SER:H    | 1:E:553:GLN:NE2  | 1.61                     | 0.96              |
| 2:R:100:ILE:HB   | 2:R:136:VAL:HG23 | 1.43                     | 0.96              |
| 1:F:188:LEU:N    | 1:F:188:LEU:CD2  | 2.19                     | 0.96              |
| 1:D:414:LYS:HZ3  | 1:D:414:LYS:HA   | 1.29                     | 0.96              |
| 1:E:188:LEU:N    | 1:E:188:LEU:CD2  | 2.18                     | 0.96              |
| 2:P:3:GLN:N      | 2:P:77:LYS:HE3   | 1.80                     | 0.95              |
| 1:E:550:SER:H    | 1:E:553:GLN:HE21 | 1.05                     | 0.95              |
| 1:E:183:SER:O    | 1:E:187:SER:HB3  | 1.64                     | 0.95              |
| 1:A:115:LYS:HZ1  | 1:A:116:GLU:HG2  | 1.31                     | 0.95              |
| 1:A:668:SER:HA   | 2:O:14:GLU:HG3   | 1.48                     | 0.95              |
| 1:E:788:ASP:O    | 1:E:792:VAL:HG23 | 1.67                     | 0.95              |
| 1:D:184:LYS:NZ   | 1:D:191:GLU:HB2  | 1.82                     | 0.94              |
| 1:F:550:SER:H    | 1:F:553:GLN:HE21 | 1.03                     | 0.94              |
| 1:F:414:LYS:HA   | 1:F:414:LYS:HZ3  | 1.31                     | 0.94              |
| 1:F:788:ASP:O    | 1:F:792:VAL:HG23 | 1.67                     | 0.94              |
| 1:B:180:ASP:N    | 1:B:180:ASP:OD1  | 1.95                     | 0.94              |
| 1:E:70:GLU:HB2   | 1:E:107:THR:HG22 | 1.47                     | 0.94              |
| 1:D:550:SER:H    | 1:D:553:GLN:HE21 | 1.03                     | 0.94              |
| 1:A:354:SER:O    | 1:A:371:SER:HB2  | 1.68                     | 0.94              |
| 1:E:354:SER:O    | 1:E:371:SER:HB2  | 1.67                     | 0.94              |
| 1:D:70:GLU:HB2   | 1:D:107:THR:HG22 | 1.47                     | 0.94              |
| 1:D:788:ASP:O    | 1:D:792:VAL:HG23 | 1.68                     | 0.94              |
| 1:F:218:LEU:HD11 | 1:F:225:ILE:HD11 | 1.50                     | 0.94              |
| 1:C:188:LEU:CD2  | 1:C:188:LEU:N    | 2.27                     | 0.94              |
| 1:E:218:LEU:HD11 | 1:E:225:ILE:HD11 | 1.50                     | 0.93              |
| 1:A:296:LEU:HD23 | 1:A:296:LEU:H    | 1.11                     | 0.93              |
| 1:B:414:LYS:HA   | 1:B:414:LYS:HZ3  | 1.30                     | 0.93              |
| 1:F:354:SER:O    | 1:F:371:SER:HB2  | 1.67                     | 0.93              |
| 1:B:550:SER:H    | 1:B:553:GLN:HE21 | 1.03                     | 0.93              |
| 1:B:354:SER:O    | 1:B:371:SER:HB2  | 1.67                     | 0.93              |
| 1:D:354:SER:O    | 1:D:371:SER:HB2  | 1.67                     | 0.93              |
| 1:A:183:SER:O    | 1:A:187:SER:HB3  | 1.66                     | 0.93              |
| 1:B:296:LEU:HD23 | 1:B:296:LEU:H    | 1.11                     | 0.93              |
| 1:C:354:SER:O    | 1:C:371:SER:HB2  | 1.67                     | 0.93              |
| 1:C:668:SER:HA   | 2:Q:14:GLU:HG3   | 1.47                     | 0.93              |
| 1:B:182:ILE:O    | 1:B:187:SER:HB2  | 1.69                     | 0.92              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:182:ILE:C    | 1:F:187:SER:HB2  | 1.90                     | 0.92              |
| 1:B:218:LEU:HD11 | 1:B:225:ILE:HD11 | 1.50                     | 0.92              |
| 1:A:629:ASN:HD22 | 1:A:631:SER:H    | 1.16                     | 0.91              |
| 1:B:715:GLU:HA   | 1:B:718:ARG:HH12 | 1.35                     | 0.91              |
| 1:C:218:LEU:HD11 | 1:C:225:ILE:HD11 | 1.50                     | 0.91              |
| 1:F:173:ILE:HG13 | 1:F:242:SER:HB3  | 1.52                     | 0.91              |
| 1:D:718:ARG:NH1  | 1:D:767:GLN:HE21 | 1.69                     | 0.91              |
| 1:A:463:THR:HG22 | 1:A:465:LEU:H    | 1.36                     | 0.91              |
| 1:A:175:LYS:HB2  | 1:A:175:LYS:NZ   | 1.86                     | 0.91              |
| 1:B:115:LYS:HZ1  | 1:B:116:GLU:HG2  | 1.34                     | 0.91              |
| 1:B:668:SER:HA   | 2:P:14:GLU:HG3   | 1.49                     | 0.91              |
| 1:A:218:LEU:HD11 | 1:A:225:ILE:HD11 | 1.50                     | 0.91              |
| 1:B:89:ILE:CG2   | 1:B:93:VAL:HG11  | 2.01                     | 0.91              |
| 1:C:296:LEU:HD23 | 1:C:296:LEU:H    | 1.11                     | 0.90              |
| 1:A:550:SER:H    | 1:A:553:GLN:HE21 | 1.03                     | 0.90              |
| 2:S:32:LEU:HD22  | 2:S:63:ILE:HD11  | 1.53                     | 0.90              |
| 1:F:296:LEU:H    | 1:F:296:LEU:HD23 | 1.11                     | 0.90              |
| 1:E:183:SER:O    | 1:E:187:SER:CB   | 2.19                     | 0.90              |
| 1:D:173:ILE:HG13 | 1:D:242:SER:HB3  | 1.53                     | 0.90              |
| 1:A:89:ILE:CG2   | 1:A:93:VAL:HG11  | 2.01                     | 0.90              |
| 1:C:115:LYS:HZ3  | 1:C:116:GLU:HG2  | 1.36                     | 0.90              |
| 2:T:117:THR:HG23 | 2:T:120:GLU:HB2  | 1.54                     | 0.90              |
| 1:E:184:LYS:NZ   | 1:E:191:GLU:HB2  | 1.86                     | 0.90              |
| 1:F:463:THR:HG22 | 1:F:465:LEU:H    | 1.36                     | 0.90              |
| 2:T:32:LEU:HD22  | 2:T:63:ILE:HD11  | 1.53                     | 0.90              |
| 1:D:218:LEU:HD11 | 1:D:225:ILE:HD11 | 1.50                     | 0.90              |
| 1:A:173:ILE:HG13 | 1:A:242:SER:HB3  | 1.54                     | 0.90              |
| 1:F:629:ASN:HD22 | 1:F:631:SER:H    | 1.17                     | 0.90              |
| 1:F:668:SER:HA   | 2:T:14:GLU:HG3   | 1.52                     | 0.90              |
| 1:C:788:ASP:O    | 1:C:792:VAL:HG23 | 1.72                     | 0.89              |
| 1:E:191:GLU:O    | 1:E:193:LEU:N    | 2.05                     | 0.89              |
| 1:E:463:THR:HG22 | 1:E:465:LEU:H    | 1.37                     | 0.89              |
| 1:E:179:LEU:O    | 1:E:183:SER:CA   | 2.20                     | 0.89              |
| 1:A:405:LEU:HD13 | 1:A:453:VAL:HG21 | 1.54                     | 0.89              |
| 2:R:117:THR:HG23 | 2:R:120:GLU:HB2  | 1.55                     | 0.89              |
| 1:D:463:THR:HG22 | 1:D:465:LEU:H    | 1.36                     | 0.89              |
| 1:E:629:ASN:HD22 | 1:E:631:SER:H    | 1.15                     | 0.89              |
| 1:D:188:LEU:N    | 1:D:188:LEU:CD2  | 2.28                     | 0.89              |
| 1:A:134:LYS:HG2  | 1:A:136:PRO:HD3  | 1.55                     | 0.89              |
| 1:C:173:ILE:HG13 | 1:C:242:SER:HB3  | 1.53                     | 0.89              |
| 2:P:117:THR:HG23 | 2:P:120:GLU:HB2  | 1.54                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:629:ASN:HD22 | 1:B:631:SER:H    | 1.16                     | 0.89              |
| 1:D:115:LYS:HZ1  | 1:D:116:GLU:HG2  | 1.37                     | 0.89              |
| 1:F:89:ILE:CG2   | 1:F:93:VAL:HG11  | 2.01                     | 0.89              |
| 2:Q:117:THR:HG23 | 2:Q:120:GLU:HB2  | 1.54                     | 0.89              |
| 2:P:58:ASP:C     | 2:P:60:ASN:H     | 1.75                     | 0.89              |
| 1:B:134:LYS:HG2  | 1:B:136:PRO:HD3  | 1.55                     | 0.89              |
| 1:B:173:ILE:HG13 | 1:B:242:SER:HB3  | 1.54                     | 0.89              |
| 1:C:463:THR:HG22 | 1:C:465:LEU:H    | 1.36                     | 0.88              |
| 1:E:296:LEU:HD23 | 1:E:296:LEU:H    | 1.11                     | 0.88              |
| 2:O:58:ASP:C     | 2:O:60:ASN:H     | 1.75                     | 0.88              |
| 2:Q:32:LEU:HD22  | 2:Q:63:ILE:HD11  | 1.55                     | 0.88              |
| 1:B:463:THR:HG22 | 1:B:465:LEU:H    | 1.37                     | 0.88              |
| 1:D:435:LEU:HG   | 1:D:446:ILE:HG22 | 1.55                     | 0.88              |
| 1:E:173:ILE:HG13 | 1:E:242:SER:HB3  | 1.53                     | 0.88              |
| 1:A:180:ASP:N    | 1:A:180:ASP:OD1  | 1.99                     | 0.88              |
| 1:D:296:LEU:HD23 | 1:D:296:LEU:H    | 1.11                     | 0.88              |
| 1:E:715:GLU:HA   | 1:E:718:ARG:HH12 | 1.36                     | 0.88              |
| 1:A:788:ASP:O    | 1:A:792:VAL:HG23 | 1.72                     | 0.88              |
| 1:D:668:SER:HA   | 2:R:14:GLU:HG3   | 1.52                     | 0.88              |
| 1:E:182:ILE:C    | 1:E:187:SER:HB2  | 1.93                     | 0.88              |
| 2:O:117:THR:HG23 | 2:O:120:GLU:HB2  | 1.55                     | 0.88              |
| 1:F:405:LEU:HD13 | 1:F:453:VAL:HG21 | 1.55                     | 0.88              |
| 1:F:175:LYS:HB2  | 1:F:175:LYS:NZ   | 1.88                     | 0.88              |
| 1:F:715:GLU:HA   | 1:F:718:ARG:HH12 | 1.33                     | 0.88              |
| 1:D:629:ASN:HD22 | 1:D:631:SER:H    | 1.18                     | 0.88              |
| 1:B:435:LEU:HG   | 1:B:446:ILE:HG22 | 1.56                     | 0.88              |
| 1:F:678:VAL:HG22 | 1:F:745:TYR:HE2  | 1.37                     | 0.88              |
| 1:C:435:LEU:HG   | 1:C:446:ILE:HG22 | 1.56                     | 0.88              |
| 1:B:175:LYS:HB2  | 1:B:175:LYS:NZ   | 1.89                     | 0.88              |
| 1:A:678:VAL:HG22 | 1:A:745:TYR:HE2  | 1.38                     | 0.88              |
| 1:A:435:LEU:HG   | 1:A:446:ILE:HG22 | 1.56                     | 0.88              |
| 2:S:58:ASP:C     | 2:S:60:ASN:H     | 1.76                     | 0.88              |
| 2:S:117:THR:HG23 | 2:S:120:GLU:HB2  | 1.55                     | 0.88              |
| 1:C:678:VAL:HG22 | 1:C:745:TYR:HE2  | 1.38                     | 0.88              |
| 1:B:405:LEU:HD13 | 1:B:453:VAL:HG21 | 1.54                     | 0.88              |
| 1:E:718:ARG:NH1  | 1:E:767:GLN:HE21 | 1.72                     | 0.87              |
| 1:D:405:LEU:HD13 | 1:D:453:VAL:HG21 | 1.54                     | 0.87              |
| 1:E:435:LEU:HG   | 1:E:446:ILE:HG22 | 1.56                     | 0.87              |
| 1:C:175:LYS:NZ   | 1:C:175:LYS:HB2  | 1.87                     | 0.87              |
| 1:F:115:LYS:HZ1  | 1:F:116:GLU:HG2  | 1.39                     | 0.87              |
| 1:C:134:LYS:HG2  | 1:C:136:PRO:HD3  | 1.55                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:175:LYS:NZ   | 1:E:175:LYS:HB2  | 1.87                     | 0.87              |
| 1:F:182:ILE:O    | 1:F:187:SER:CB   | 2.22                     | 0.87              |
| 1:D:183:SER:O    | 1:D:187:SER:HB3  | 1.75                     | 0.87              |
| 2:O:32:LEU:HD22  | 2:O:63:ILE:HD11  | 1.53                     | 0.87              |
| 1:E:668:SER:HA   | 2:S:14:GLU:HG3   | 1.55                     | 0.87              |
| 1:C:405:LEU:HD13 | 1:C:453:VAL:HG21 | 1.54                     | 0.87              |
| 1:F:122:GLU:OE1  | 1:F:147:ARG:HB2  | 1.75                     | 0.87              |
| 1:D:678:VAL:HG22 | 1:D:745:TYR:HE2  | 1.38                     | 0.87              |
| 2:R:32:LEU:HD22  | 2:R:63:ILE:HD11  | 1.54                     | 0.87              |
| 1:B:678:VAL:HG22 | 1:B:745:TYR:HE2  | 1.39                     | 0.87              |
| 1:F:724:ARG:HG3  | 1:F:724:ARG:HH11 | 1.40                     | 0.86              |
| 1:A:715:GLU:HA   | 1:A:718:ARG:HH12 | 1.35                     | 0.86              |
| 1:C:629:ASN:HD22 | 1:C:631:SER:H    | 1.16                     | 0.86              |
| 1:F:435:LEU:HG   | 1:F:446:ILE:HG22 | 1.56                     | 0.86              |
| 1:E:501:LEU:HD22 | 2:S:112:LEU:HD21 | 1.57                     | 0.86              |
| 1:E:179:LEU:C    | 1:E:183:SER:HB2  | 1.94                     | 0.86              |
| 1:D:89:ILE:CG2   | 1:D:93:VAL:HG11  | 2.02                     | 0.86              |
| 1:F:697:ILE:CD1  | 1:F:732:ILE:HD13 | 2.06                     | 0.86              |
| 1:E:678:VAL:HG22 | 1:E:745:TYR:HE2  | 1.38                     | 0.86              |
| 2:P:32:LEU:HD22  | 2:P:63:ILE:HD11  | 1.55                     | 0.86              |
| 2:O:30:LYS:HD3   | 2:O:30:LYS:H     | 1.40                     | 0.86              |
| 1:E:405:LEU:HD13 | 1:E:453:VAL:HG21 | 1.56                     | 0.86              |
| 2:R:58:ASP:C     | 2:R:60:ASN:H     | 1.75                     | 0.86              |
| 1:D:175:LYS:HB2  | 1:D:175:LYS:NZ   | 1.87                     | 0.86              |
| 1:B:296:LEU:CD2  | 1:B:296:LEU:H    | 1.83                     | 0.86              |
| 1:D:715:GLU:HA   | 1:D:718:ARG:HH12 | 1.35                     | 0.86              |
| 1:A:724:ARG:HH11 | 1:A:724:ARG:HG3  | 1.41                     | 0.86              |
| 1:D:724:ARG:HH11 | 1:D:724:ARG:HG3  | 1.41                     | 0.86              |
| 1:F:718:ARG:NH1  | 1:F:767:GLN:HE21 | 1.73                     | 0.86              |
| 1:D:275:GLY:HA2  | 1:D:278:LYS:HE3  | 1.58                     | 0.86              |
| 2:Q:58:ASP:C     | 2:Q:60:ASN:H     | 1.75                     | 0.86              |
| 1:C:715:GLU:HA   | 1:C:718:ARG:HH12 | 1.35                     | 0.85              |
| 1:E:724:ARG:HG3  | 1:E:724:ARG:HH11 | 1.42                     | 0.85              |
| 2:Q:30:LYS:H     | 2:Q:30:LYS:HD3   | 1.40                     | 0.85              |
| 1:E:89:ILE:CG2   | 1:E:93:VAL:HG11  | 2.02                     | 0.85              |
| 1:D:501:LEU:HD22 | 2:R:112:LEU:HD21 | 1.58                     | 0.85              |
| 1:C:89:ILE:CG2   | 1:C:93:VAL:HG11  | 2.02                     | 0.85              |
| 1:B:788:ASP:O    | 1:B:792:VAL:HG23 | 1.76                     | 0.85              |
| 2:P:30:LYS:HD3   | 2:P:30:LYS:H     | 1.41                     | 0.85              |
| 1:D:447:SER:OG   | 1:D:450:ASN:O    | 1.94                     | 0.85              |
| 1:C:724:ARG:HG3  | 1:C:724:ARG:HH11 | 1.41                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:30:LYS:HD3   | 2:S:30:LYS:H     | 1.41                     | 0.85              |
| 1:C:142:VAL:HG22 | 1:C:154:ILE:HG23 | 1.59                     | 0.85              |
| 1:C:597:ASN:HD21 | 1:C:601:GLU:H    | 1.24                     | 0.85              |
| 1:A:275:GLY:HA2  | 1:A:278:LYS:HE3  | 1.58                     | 0.85              |
| 1:D:183:SER:O    | 1:D:187:SER:CB   | 2.25                     | 0.85              |
| 1:B:564:VAL:O    | 1:B:567:THR:HG22 | 1.77                     | 0.85              |
| 1:D:179:LEU:O    | 1:D:183:SER:CA   | 2.25                     | 0.84              |
| 2:T:30:LYS:H     | 2:T:30:LYS:HD3   | 1.41                     | 0.84              |
| 1:A:183:SER:O    | 1:A:187:SER:HB2  | 1.76                     | 0.84              |
| 1:D:697:ILE:CD1  | 1:D:732:ILE:HD13 | 2.06                     | 0.84              |
| 1:B:597:ASN:HD21 | 1:B:601:GLU:H    | 1.24                     | 0.84              |
| 2:T:37:ARG:HA    | 2:T:41:GLN:O     | 1.77                     | 0.84              |
| 2:R:37:ARG:HA    | 2:R:41:GLN:O     | 1.77                     | 0.84              |
| 1:E:122:GLU:OE1  | 1:E:147:ARG:HB2  | 1.77                     | 0.84              |
| 2:R:30:LYS:H     | 2:R:30:LYS:HD3   | 1.40                     | 0.84              |
| 2:O:37:ARG:HA    | 2:O:41:GLN:O     | 1.77                     | 0.84              |
| 1:D:180:ASP:OD1  | 1:D:180:ASP:N    | 2.08                     | 0.84              |
| 2:Q:37:ARG:HA    | 2:Q:41:GLN:O     | 1.77                     | 0.84              |
| 1:A:564:VAL:O    | 1:A:567:THR:HG22 | 1.78                     | 0.84              |
| 1:C:275:GLY:HA2  | 1:C:278:LYS:HE3  | 1.60                     | 0.84              |
| 1:F:493:ASP:OD2  | 1:F:577:HIS:CE1  | 2.30                     | 0.84              |
| 1:C:564:VAL:O    | 1:C:567:THR:HG22 | 1.77                     | 0.84              |
| 1:A:697:ILE:CD1  | 1:A:732:ILE:HD13 | 2.07                     | 0.84              |
| 1:D:115:LYS:NZ   | 1:D:116:GLU:HG2  | 1.91                     | 0.84              |
| 1:E:447:SER:OG   | 1:E:450:ASN:O    | 1.95                     | 0.84              |
| 1:A:308:VAL:HB   | 1:A:311:HIS:ND1  | 1.93                     | 0.84              |
| 1:F:308:VAL:HB   | 1:F:311:HIS:ND1  | 1.93                     | 0.84              |
| 1:C:697:ILE:CD1  | 1:C:732:ILE:HD13 | 2.07                     | 0.83              |
| 2:P:40:GLY:O     | 2:P:41:GLN:HG3   | 1.78                     | 0.83              |
| 2:P:37:ARG:HA    | 2:P:41:GLN:O     | 1.77                     | 0.83              |
| 1:B:275:GLY:HA2  | 1:B:278:LYS:HE3  | 1.60                     | 0.83              |
| 2:T:58:ASP:C     | 2:T:60:ASN:H     | 1.75                     | 0.83              |
| 1:A:408:LEU:HD12 | 1:A:408:LEU:H    | 1.43                     | 0.83              |
| 1:E:597:ASN:HD21 | 1:E:601:GLU:H    | 1.25                     | 0.83              |
| 1:B:115:LYS:NZ   | 1:B:116:GLU:HG2  | 1.93                     | 0.83              |
| 1:C:497:LEU:HD13 | 1:C:556:MET:HG2  | 1.60                     | 0.83              |
| 1:E:275:GLY:HA2  | 1:E:278:LYS:HE3  | 1.59                     | 0.83              |
| 1:C:296:LEU:CD2  | 1:C:296:LEU:H    | 1.84                     | 0.83              |
| 1:B:718:ARG:NH1  | 1:B:767:GLN:HE21 | 1.74                     | 0.83              |
| 1:B:308:VAL:HB   | 1:B:311:HIS:ND1  | 1.93                     | 0.83              |
| 1:B:697:ILE:CD1  | 1:B:732:ILE:HD13 | 2.07                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:142:VAL:HG22 | 1:F:154:ILE:HG23 | 1.59                     | 0.83              |
| 1:E:115:LYS:NZ   | 1:E:116:GLU:HG2  | 1.93                     | 0.83              |
| 1:D:564:VAL:O    | 1:D:567:THR:HG22 | 1.77                     | 0.83              |
| 1:C:184:LYS:NZ   | 1:C:191:GLU:HB2  | 1.94                     | 0.83              |
| 1:C:297:LYS:HZ1  | 1:C:601:GLU:HB3  | 1.44                     | 0.83              |
| 1:C:308:VAL:HB   | 1:C:311:HIS:ND1  | 1.93                     | 0.83              |
| 1:E:334:LEU:H    | 1:E:334:LEU:HD12 | 1.43                     | 0.83              |
| 1:F:597:ASN:HD21 | 1:F:601:GLU:H    | 1.24                     | 0.83              |
| 1:C:408:LEU:HD12 | 1:C:408:LEU:H    | 1.43                     | 0.83              |
| 1:A:501:LEU:HD22 | 2:O:112:LEU:HD21 | 1.59                     | 0.83              |
| 1:C:493:ASP:OD2  | 1:C:577:HIS:CE1  | 2.31                     | 0.83              |
| 1:F:275:GLY:HA2  | 1:F:278:LYS:HE3  | 1.59                     | 0.83              |
| 1:E:308:VAL:HB   | 1:E:311:HIS:ND1  | 1.93                     | 0.83              |
| 1:A:217:LYS:HB3  | 1:A:217:LYS:HZ3  | 1.42                     | 0.83              |
| 1:B:724:ARG:HG3  | 1:B:724:ARG:HH11 | 1.43                     | 0.83              |
| 1:D:334:LEU:HD12 | 1:D:334:LEU:H    | 1.43                     | 0.83              |
| 1:E:697:ILE:CD1  | 1:E:732:ILE:HD13 | 2.09                     | 0.83              |
| 1:E:142:VAL:HG22 | 1:E:154:ILE:HG23 | 1.59                     | 0.83              |
| 1:D:308:VAL:HB   | 1:D:311:HIS:ND1  | 1.93                     | 0.83              |
| 1:F:173:ILE:HD12 | 1:F:243:LEU:HD23 | 1.61                     | 0.83              |
| 1:A:115:LYS:NZ   | 1:A:116:GLU:HG2  | 1.94                     | 0.83              |
| 1:D:597:ASN:HD21 | 1:D:601:GLU:H    | 1.26                     | 0.83              |
| 1:D:122:GLU:OE1  | 1:D:147:ARG:HB2  | 1.79                     | 0.82              |
| 1:F:183:SER:O    | 1:F:187:SER:CB   | 2.26                     | 0.82              |
| 1:B:175:LYS:HZ1  | 1:B:175:LYS:HB2  | 1.44                     | 0.82              |
| 1:A:597:ASN:HD21 | 1:A:601:GLU:H    | 1.25                     | 0.82              |
| 1:A:122:GLU:OE1  | 1:A:147:ARG:HB2  | 1.77                     | 0.82              |
| 2:S:37:ARG:HA    | 2:S:41:GLN:O     | 1.79                     | 0.82              |
| 1:F:564:VAL:O    | 1:F:567:THR:HG22 | 1.78                     | 0.82              |
| 1:C:501:LEU:HD22 | 2:Q:112:LEU:HD21 | 1.61                     | 0.82              |
| 1:A:493:ASP:OD2  | 1:A:577:HIS:CE1  | 2.31                     | 0.82              |
| 1:C:122:GLU:OE1  | 1:C:147:ARG:HB2  | 1.80                     | 0.82              |
| 1:F:597:ASN:HD21 | 1:F:601:GLU:N    | 1.78                     | 0.82              |
| 1:D:142:VAL:HG22 | 1:D:154:ILE:HG23 | 1.61                     | 0.82              |
| 2:Q:40:GLY:O     | 2:Q:41:GLN:HG3   | 1.79                     | 0.82              |
| 1:D:408:LEU:H    | 1:D:408:LEU:HD12 | 1.43                     | 0.82              |
| 2:O:40:GLY:O     | 2:O:41:GLN:HG3   | 1.78                     | 0.82              |
| 1:A:334:LEU:H    | 1:A:334:LEU:HD12 | 1.45                     | 0.82              |
| 1:E:597:ASN:HD21 | 1:E:601:GLU:N    | 1.78                     | 0.82              |
| 1:B:142:VAL:HG22 | 1:B:154:ILE:HG23 | 1.61                     | 0.82              |
| 1:C:115:LYS:NZ   | 1:C:116:GLU:HG2  | 1.93                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:493:ASP:OD2  | 1:D:577:HIS:CE1  | 2.33                     | 0.82              |
| 1:B:334:LEU:H    | 1:B:334:LEU:HD12 | 1.44                     | 0.82              |
| 1:B:182:ILE:O    | 1:B:187:SER:CB   | 2.27                     | 0.82              |
| 1:B:597:ASN:HD21 | 1:B:601:GLU:N    | 1.78                     | 0.82              |
| 1:E:325:TYR:HB2  | 1:E:498:ALA:HB3  | 1.61                     | 0.82              |
| 1:B:493:ASP:OD2  | 1:B:577:HIS:CE1  | 2.32                     | 0.82              |
| 1:B:408:LEU:H    | 1:B:408:LEU:HD12 | 1.44                     | 0.82              |
| 1:E:173:ILE:HD12 | 1:E:243:LEU:HD23 | 1.62                     | 0.82              |
| 1:B:182:ILE:C    | 1:B:187:SER:HB2  | 2.00                     | 0.82              |
| 1:F:697:ILE:HD13 | 1:F:732:ILE:CD1  | 2.09                     | 0.82              |
| 1:E:564:VAL:O    | 1:E:567:THR:HG22 | 1.78                     | 0.82              |
| 1:B:217:LYS:HZ3  | 1:B:217:LYS:HB3  | 1.44                     | 0.82              |
| 1:A:718:ARG:NH1  | 1:A:767:GLN:HE21 | 1.77                     | 0.82              |
| 1:E:493:ASP:OD2  | 1:E:577:HIS:CE1  | 2.33                     | 0.81              |
| 1:C:597:ASN:HD21 | 1:C:601:GLU:N    | 1.78                     | 0.81              |
| 1:F:115:LYS:NZ   | 1:F:116:GLU:HG2  | 1.94                     | 0.81              |
| 1:B:122:GLU:OE1  | 1:B:147:ARG:HB2  | 1.80                     | 0.81              |
| 1:D:173:ILE:HD12 | 1:D:243:LEU:HD23 | 1.62                     | 0.81              |
| 1:F:180:ASP:OD1  | 1:F:180:ASP:N    | 2.06                     | 0.81              |
| 1:A:184:LYS:NZ   | 1:A:191:GLU:HB2  | 1.94                     | 0.81              |
| 1:A:173:ILE:HD12 | 1:A:243:LEU:HD23 | 1.63                     | 0.81              |
| 1:C:334:LEU:H    | 1:C:334:LEU:HD12 | 1.45                     | 0.81              |
| 1:F:408:LEU:H    | 1:F:408:LEU:HD12 | 1.43                     | 0.81              |
| 1:E:408:LEU:H    | 1:E:408:LEU:HD12 | 1.43                     | 0.81              |
| 1:A:597:ASN:HD21 | 1:A:601:GLU:N    | 1.79                     | 0.81              |
| 1:F:334:LEU:HD12 | 1:F:334:LEU:H    | 1.46                     | 0.81              |
| 1:F:447:SER:OG   | 1:F:450:ASN:O    | 1.97                     | 0.81              |
| 1:D:546:LYS:HD2  | 1:D:554:LYS:HE3  | 1.62                     | 0.81              |
| 1:A:546:LYS:HD2  | 1:A:554:LYS:HE3  | 1.62                     | 0.81              |
| 1:B:135:VAL:O    | 1:B:135:VAL:HG22 | 1.81                     | 0.81              |
| 1:B:173:ILE:HD12 | 1:B:243:LEU:HD23 | 1.62                     | 0.81              |
| 1:F:629:ASN:C    | 1:F:629:ASN:HD22 | 1.84                     | 0.81              |
| 1:A:497:LEU:HD13 | 1:A:556:MET:HG2  | 1.62                     | 0.81              |
| 1:B:497:LEU:HD13 | 1:B:556:MET:HG2  | 1.63                     | 0.81              |
| 2:S:106:ARG:HG3  | 2:S:121:VAL:CG2  | 2.05                     | 0.80              |
| 1:A:135:VAL:O    | 1:A:135:VAL:HG22 | 1.81                     | 0.80              |
| 1:A:697:ILE:HD13 | 1:A:732:ILE:CD1  | 2.11                     | 0.80              |
| 1:D:597:ASN:HD21 | 1:D:601:GLU:N    | 1.80                     | 0.80              |
| 1:F:736:LEU:HD21 | 1:F:750:GLN:NE2  | 1.96                     | 0.80              |
| 2:T:40:GLY:O     | 2:T:41:GLN:HG3   | 1.80                     | 0.80              |
| 2:R:40:GLY:O     | 2:R:41:GLN:HG3   | 1.81                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:501:LEU:HD22 | 2:P:112:LEU:HD21 | 1.61                     | 0.80              |
| 1:F:134:LYS:HG2  | 1:F:136:PRO:HD3  | 1.62                     | 0.80              |
| 1:A:142:VAL:HG22 | 1:A:154:ILE:HG23 | 1.60                     | 0.80              |
| 1:E:736:LEU:HD21 | 1:E:750:GLN:NE2  | 1.96                     | 0.80              |
| 1:D:497:LEU:HD13 | 1:D:556:MET:HG2  | 1.62                     | 0.80              |
| 1:C:173:ILE:HD12 | 1:C:243:LEU:HD23 | 1.63                     | 0.80              |
| 1:D:325:TYR:HB2  | 1:D:498:ALA:HB3  | 1.64                     | 0.80              |
| 2:S:40:GLY:O     | 2:S:41:GLN:HG3   | 1.80                     | 0.80              |
| 1:E:191:GLU:O    | 1:E:192:PHE:C    | 2.16                     | 0.80              |
| 1:C:182:ILE:C    | 1:C:187:SER:HB2  | 2.01                     | 0.80              |
| 1:B:184:LYS:NZ   | 1:B:191:GLU:HB2  | 1.97                     | 0.80              |
| 1:E:629:ASN:C    | 1:E:629:ASN:HD22 | 1.85                     | 0.80              |
| 1:F:161:ILE:HA   | 1:F:167:LYS:HD2  | 1.64                     | 0.80              |
| 1:E:180:ASP:N    | 1:E:180:ASP:OD1  | 2.15                     | 0.80              |
| 1:B:297:LYS:HZ1  | 1:B:601:GLU:HB3  | 1.47                     | 0.80              |
| 1:B:179:LEU:O    | 1:B:183:SER:CA   | 2.30                     | 0.80              |
| 1:E:546:LYS:HD2  | 1:E:554:LYS:HE3  | 1.62                     | 0.80              |
| 2:O:9:ILE:HD12   | 2:O:69:LEU:HD11  | 1.64                     | 0.80              |
| 1:D:90:PRO:O     | 1:D:93:VAL:HG12  | 1.82                     | 0.80              |
| 1:D:296:LEU:CD2  | 1:D:296:LEU:H    | 1.83                     | 0.80              |
| 1:F:325:TYR:HB2  | 1:F:498:ALA:HB3  | 1.63                     | 0.80              |
| 1:B:325:TYR:HB2  | 1:B:498:ALA:HB3  | 1.64                     | 0.80              |
| 1:C:135:VAL:HG22 | 1:C:135:VAL:O    | 1.81                     | 0.80              |
| 1:D:697:ILE:HD13 | 1:D:732:ILE:CD1  | 2.09                     | 0.80              |
| 2:Q:106:ARG:HG3  | 2:Q:121:VAL:CG2  | 2.05                     | 0.80              |
| 1:B:107:THR:HG21 | 1:B:115:LYS:HE3  | 1.62                     | 0.80              |
| 1:A:182:ILE:O    | 1:A:187:SER:HB2  | 1.82                     | 0.79              |
| 2:T:51:MET:HB3   | 2:T:71:MET:HG3   | 1.65                     | 0.79              |
| 2:S:9:ILE:HD12   | 2:S:69:LEU:HD11  | 1.62                     | 0.79              |
| 1:C:183:SER:O    | 1:C:187:SER:HB3  | 1.82                     | 0.79              |
| 1:C:629:ASN:C    | 1:C:629:ASN:HD22 | 1.86                     | 0.79              |
| 1:B:736:LEU:HD21 | 1:B:750:GLN:NE2  | 1.96                     | 0.79              |
| 1:C:447:SER:OG   | 1:C:450:ASN:O    | 2.00                     | 0.79              |
| 1:F:373:LYS:HD3  | 1:F:376:GLN:NE2  | 1.97                     | 0.79              |
| 1:B:183:SER:O    | 1:B:187:SER:HB3  | 1.83                     | 0.79              |
| 1:D:629:ASN:C    | 1:D:629:ASN:HD22 | 1.86                     | 0.79              |
| 1:F:497:LEU:HD13 | 1:F:556:MET:HG2  | 1.62                     | 0.79              |
| 1:E:135:VAL:O    | 1:E:135:VAL:HG22 | 1.81                     | 0.79              |
| 1:B:697:ILE:HD13 | 1:B:732:ILE:CD1  | 2.10                     | 0.79              |
| 1:C:736:LEU:HD21 | 1:C:750:GLN:NE2  | 1.97                     | 0.79              |
| 1:D:736:LEU:HD21 | 1:D:750:GLN:NE2  | 1.97                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:184:LYS:NZ   | 1:B:193:LEU:HD12 | 1.96                     | 0.79              |
| 1:C:325:TYR:HB2  | 1:C:498:ALA:HB3  | 1.64                     | 0.79              |
| 1:A:629:ASN:HD22 | 1:A:629:ASN:C    | 1.85                     | 0.79              |
| 1:F:135:VAL:O    | 1:F:135:VAL:HG22 | 1.81                     | 0.79              |
| 1:D:135:VAL:HG22 | 1:D:135:VAL:O    | 1.81                     | 0.79              |
| 1:F:179:LEU:O    | 1:F:183:SER:CA   | 2.30                     | 0.79              |
| 1:F:90:PRO:O     | 1:F:93:VAL:HG12  | 1.82                     | 0.79              |
| 1:A:736:LEU:HD21 | 1:A:750:GLN:NE2  | 1.96                     | 0.79              |
| 1:F:501:LEU:HD22 | 2:T:112:LEU:HD21 | 1.63                     | 0.79              |
| 1:B:546:LYS:HD2  | 1:B:554:LYS:HE3  | 1.65                     | 0.79              |
| 1:B:373:LYS:HD3  | 1:B:376:GLN:NE2  | 1.98                     | 0.79              |
| 1:B:90:PRO:O     | 1:B:93:VAL:HG12  | 1.83                     | 0.79              |
| 1:A:90:PRO:O     | 1:A:93:VAL:HG12  | 1.82                     | 0.79              |
| 1:E:497:LEU:HD13 | 1:E:556:MET:HG2  | 1.62                     | 0.79              |
| 1:E:90:PRO:O     | 1:E:93:VAL:HG12  | 1.83                     | 0.79              |
| 1:C:179:LEU:O    | 1:C:183:SER:CA   | 2.30                     | 0.79              |
| 2:O:51:MET:HB3   | 2:O:71:MET:HG3   | 1.65                     | 0.79              |
| 1:C:546:LYS:HD2  | 1:C:554:LYS:HE3  | 1.64                     | 0.79              |
| 2:R:94:LYS:NZ    | 2:R:94:LYS:HB3   | 1.97                     | 0.79              |
| 1:E:115:LYS:HZ1  | 1:E:116:GLU:N    | 1.80                     | 0.79              |
| 2:S:94:LYS:HB3   | 2:S:94:LYS:NZ    | 1.97                     | 0.79              |
| 2:P:51:MET:HB3   | 2:P:71:MET:HG3   | 1.65                     | 0.78              |
| 1:C:373:LYS:HD3  | 1:C:376:GLN:NE2  | 1.98                     | 0.78              |
| 1:E:318:ILE:H    | 1:E:318:ILE:HD12 | 1.49                     | 0.78              |
| 1:C:152:LEU:HD22 | 1:C:154:ILE:HD11 | 1.65                     | 0.78              |
| 2:P:9:ILE:HD12   | 2:P:69:LEU:HD11  | 1.64                     | 0.78              |
| 1:C:180:ASP:CG   | 1:C:181:ILE:H    | 1.86                     | 0.78              |
| 1:B:629:ASN:HD22 | 1:B:629:ASN:C    | 1.87                     | 0.78              |
| 2:T:94:LYS:NZ    | 2:T:94:LYS:HB3   | 1.98                     | 0.78              |
| 2:P:94:LYS:HB3   | 2:P:94:LYS:NZ    | 1.98                     | 0.78              |
| 1:E:373:LYS:HD3  | 1:E:376:GLN:NE2  | 1.98                     | 0.78              |
| 2:O:94:LYS:NZ    | 2:O:94:LYS:HB3   | 1.98                     | 0.78              |
| 1:A:373:LYS:HD3  | 1:A:376:GLN:NE2  | 1.98                     | 0.78              |
| 1:A:325:TYR:HB2  | 1:A:498:ALA:HB3  | 1.64                     | 0.78              |
| 2:Q:51:MET:HB3   | 2:Q:71:MET:HG3   | 1.66                     | 0.78              |
| 2:R:51:MET:HB3   | 2:R:71:MET:HG3   | 1.66                     | 0.78              |
| 1:F:546:LYS:HD2  | 1:F:554:LYS:HE3  | 1.63                     | 0.78              |
| 1:C:180:ASP:OD1  | 1:C:180:ASP:N    | 2.16                     | 0.78              |
| 1:E:697:ILE:HD13 | 1:E:732:ILE:CD1  | 2.12                     | 0.78              |
| 1:B:179:LEU:O    | 1:B:183:SER:N    | 2.17                     | 0.78              |
| 1:E:728:ALA:O    | 1:E:732:ILE:HG12 | 1.84                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:728:ALA:O    | 1:D:732:ILE:HG12 | 1.84                     | 0.78              |
| 1:D:581:GLN:NE2  | 1:D:629:ASN:H    | 1.82                     | 0.78              |
| 1:E:443:GLU:HG2  | 1:E:458:LYS:NZ   | 1.99                     | 0.78              |
| 1:C:184:LYS:NZ   | 1:C:193:LEU:HD12 | 1.98                     | 0.78              |
| 1:B:581:GLN:NE2  | 1:B:629:ASN:H    | 1.82                     | 0.78              |
| 1:F:443:GLU:HG2  | 1:F:458:LYS:NZ   | 1.99                     | 0.78              |
| 2:Q:94:LYS:HB3   | 2:Q:94:LYS:NZ    | 1.98                     | 0.78              |
| 2:T:9:ILE:HD12   | 2:T:69:LEU:HD11  | 1.65                     | 0.78              |
| 1:D:179:LEU:C    | 1:D:183:SER:HB2  | 2.01                     | 0.77              |
| 2:R:106:ARG:HG3  | 2:R:121:VAL:CG2  | 2.06                     | 0.77              |
| 2:R:9:ILE:HD12   | 2:R:69:LEU:HD11  | 1.65                     | 0.77              |
| 1:F:184:LYS:NZ   | 1:F:193:LEU:HD12 | 1.99                     | 0.77              |
| 1:D:180:ASP:CG   | 1:D:181:ILE:H    | 1.88                     | 0.77              |
| 1:D:182:ILE:C    | 1:D:187:SER:HB2  | 2.04                     | 0.77              |
| 1:C:90:PRO:O     | 1:C:93:VAL:HG12  | 1.84                     | 0.77              |
| 2:P:106:ARG:HG3  | 2:P:121:VAL:CG2  | 2.05                     | 0.77              |
| 1:C:581:GLN:NE2  | 1:C:629:ASN:H    | 1.83                     | 0.77              |
| 1:A:152:LEU:HD22 | 1:A:154:ILE:HD11 | 1.64                     | 0.77              |
| 2:S:51:MET:HB3   | 2:S:71:MET:HG3   | 1.66                     | 0.77              |
| 1:A:540:ARG:NH2  | 2:O:87:GLU:OE1   | 2.17                     | 0.77              |
| 1:D:373:LYS:HD3  | 1:D:376:GLN:NE2  | 1.99                     | 0.77              |
| 1:D:161:ILE:HA   | 1:D:167:LYS:HD2  | 1.66                     | 0.77              |
| 1:E:625:LEU:HD12 | 1:E:626:TYR:N    | 2.00                     | 0.77              |
| 1:B:152:LEU:HD22 | 1:B:154:ILE:HD11 | 1.65                     | 0.77              |
| 1:E:115:LYS:HZ1  | 1:E:116:GLU:HG2  | 1.49                     | 0.77              |
| 1:A:318:ILE:H    | 1:A:318:ILE:HD12 | 1.48                     | 0.77              |
| 1:C:443:GLU:HG2  | 1:C:458:LYS:NZ   | 2.00                     | 0.77              |
| 1:F:318:ILE:HD12 | 1:F:318:ILE:H    | 1.50                     | 0.77              |
| 1:A:184:LYS:NZ   | 1:A:193:LEU:HD12 | 1.99                     | 0.77              |
| 1:B:90:PRO:HD3   | 1:B:249:PHE:CE2  | 2.19                     | 0.77              |
| 1:C:697:ILE:HD13 | 1:C:732:ILE:CD1  | 2.11                     | 0.77              |
| 1:B:480:ASN:HD22 | 1:B:481:VAL:H    | 1.30                     | 0.77              |
| 1:E:152:LEU:HD22 | 1:E:154:ILE:HD11 | 1.65                     | 0.77              |
| 2:S:33:GLY:O     | 2:S:37:ARG:HG3   | 1.85                     | 0.77              |
| 1:B:443:GLU:HG2  | 1:B:458:LYS:HZ1  | 1.47                     | 0.77              |
| 1:C:161:ILE:HA   | 1:C:167:LYS:HD2  | 1.64                     | 0.77              |
| 1:F:254:ARG:HG2  | 1:F:255:THR:H    | 1.50                     | 0.77              |
| 1:E:182:ILE:O    | 1:E:187:SER:CB   | 2.30                     | 0.76              |
| 1:E:581:GLN:NE2  | 1:E:629:ASN:H    | 1.83                     | 0.76              |
| 1:B:254:ARG:HG2  | 1:B:255:THR:H    | 1.50                     | 0.76              |
| 1:D:625:LEU:HD12 | 1:D:626:TYR:N    | 2.00                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:581:GLN:NE2  | 1:F:629:ASN:H    | 1.83                     | 0.76              |
| 1:B:443:GLU:HG2  | 1:B:458:LYS:NZ   | 2.00                     | 0.76              |
| 1:E:540:ARG:NH2  | 2:S:87:GLU:OE1   | 2.18                     | 0.76              |
| 2:O:93:ASP:OD1   | 2:O:97:ASN:ND2   | 2.19                     | 0.76              |
| 1:D:318:ILE:HD12 | 1:D:318:ILE:H    | 1.50                     | 0.76              |
| 1:A:66:LEU:HD11  | 1:A:104:ILE:HG13 | 1.67                     | 0.76              |
| 1:B:728:ALA:O    | 1:B:732:ILE:HG12 | 1.84                     | 0.76              |
| 1:D:152:LEU:HD22 | 1:D:154:ILE:HD11 | 1.66                     | 0.76              |
| 1:A:480:ASN:HD22 | 1:A:481:VAL:H    | 1.30                     | 0.76              |
| 1:C:540:ARG:NH2  | 2:Q:87:GLU:OE1   | 2.18                     | 0.76              |
| 1:F:540:ARG:NH2  | 2:T:87:GLU:OE1   | 2.19                     | 0.76              |
| 1:D:540:ARG:NH2  | 2:R:87:GLU:OE1   | 2.19                     | 0.76              |
| 1:E:480:ASN:HD22 | 1:E:481:VAL:H    | 1.31                     | 0.76              |
| 1:F:480:ASN:ND2  | 1:F:481:VAL:N    | 2.34                     | 0.76              |
| 1:F:152:LEU:HD22 | 1:F:154:ILE:HD11 | 1.66                     | 0.76              |
| 2:Q:9:ILE:HD12   | 2:Q:69:LEU:HD11  | 1.65                     | 0.76              |
| 1:B:169:VAL:O    | 1:B:173:ILE:HG22 | 1.86                     | 0.76              |
| 1:C:728:ALA:O    | 1:C:732:ILE:HG12 | 1.85                     | 0.76              |
| 2:O:97:ASN:H     | 2:O:97:ASN:ND2   | 1.84                     | 0.76              |
| 1:F:297:LYS:HZ1  | 1:F:601:GLU:HB3  | 1.51                     | 0.76              |
| 2:O:33:GLY:O     | 2:O:37:ARG:HG3   | 1.86                     | 0.76              |
| 1:B:318:ILE:H    | 1:B:318:ILE:HD12 | 1.50                     | 0.76              |
| 1:F:625:LEU:HD12 | 1:F:626:TYR:N    | 2.01                     | 0.76              |
| 1:D:184:LYS:NZ   | 1:D:193:LEU:HD12 | 1.99                     | 0.76              |
| 1:C:169:VAL:O    | 1:C:173:ILE:HG22 | 1.86                     | 0.76              |
| 1:A:728:ALA:O    | 1:A:732:ILE:HG12 | 1.84                     | 0.76              |
| 2:P:33:GLY:O     | 2:P:37:ARG:HG3   | 1.86                     | 0.76              |
| 1:F:169:VAL:O    | 1:F:173:ILE:HG22 | 1.86                     | 0.75              |
| 1:A:480:ASN:ND2  | 1:A:481:VAL:N    | 2.34                     | 0.75              |
| 1:A:161:ILE:HA   | 1:A:167:LYS:HD2  | 1.66                     | 0.75              |
| 1:C:472:ARG:HH11 | 1:C:472:ARG:HB3  | 1.52                     | 0.75              |
| 1:B:625:LEU:HD12 | 1:B:626:TYR:N    | 2.01                     | 0.75              |
| 1:A:443:GLU:HG2  | 1:A:458:LYS:NZ   | 2.01                     | 0.75              |
| 1:A:128:MET:HB2  | 1:A:239:HIS:CE1  | 2.22                     | 0.75              |
| 1:C:711:ILE:HG13 | 1:C:712:PHE:CD2  | 2.22                     | 0.75              |
| 1:E:297:LYS:HZ1  | 1:E:601:GLU:HB3  | 1.51                     | 0.75              |
| 1:E:711:ILE:HG13 | 1:E:712:PHE:CD2  | 2.21                     | 0.75              |
| 1:F:472:ARG:HH11 | 1:F:472:ARG:HB3  | 1.52                     | 0.75              |
| 1:F:728:ALA:O    | 1:F:732:ILE:HG12 | 1.86                     | 0.75              |
| 1:A:581:GLN:NE2  | 1:A:629:ASN:H    | 1.82                     | 0.75              |
| 2:T:33:GLY:O     | 2:T:37:ARG:HG3   | 1.87                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:164:GLU:O    | 1:F:167:LYS:HG2  | 1.87                     | 0.75              |
| 2:Q:97:ASN:H     | 2:Q:97:ASN:ND2   | 1.84                     | 0.75              |
| 1:D:443:GLU:HG2  | 1:D:458:LYS:NZ   | 2.00                     | 0.75              |
| 1:E:254:ARG:HG2  | 1:E:255:THR:H    | 1.50                     | 0.75              |
| 1:E:184:LYS:NZ   | 1:E:193:LEU:HD12 | 2.01                     | 0.75              |
| 1:D:711:ILE:HG13 | 1:D:712:PHE:CD2  | 2.22                     | 0.75              |
| 1:D:254:ARG:HG2  | 1:D:255:THR:H    | 1.51                     | 0.75              |
| 1:E:305:SER:HB2  | 1:E:594:PHE:CD1  | 2.22                     | 0.75              |
| 1:F:794:GLN:O    | 1:F:797:ILE:HG12 | 1.87                     | 0.75              |
| 1:E:169:VAL:O    | 1:E:173:ILE:HG22 | 1.86                     | 0.75              |
| 1:A:169:VAL:O    | 1:A:173:ILE:HG22 | 1.86                     | 0.75              |
| 1:A:188:LEU:HD23 | 1:A:188:LEU:H    | 0.62                     | 0.75              |
| 1:E:480:ASN:ND2  | 1:E:481:VAL:N    | 2.34                     | 0.75              |
| 1:C:625:LEU:HD12 | 1:C:626:TYR:N    | 2.02                     | 0.75              |
| 1:D:472:ARG:HB3  | 1:D:472:ARG:HH11 | 1.52                     | 0.75              |
| 1:A:164:GLU:O    | 1:A:167:LYS:HG2  | 1.86                     | 0.75              |
| 1:A:254:ARG:HG2  | 1:A:255:THR:H    | 1.50                     | 0.75              |
| 1:C:301:ALA:O    | 1:C:303:LYS:N    | 2.20                     | 0.75              |
| 1:B:711:ILE:HG13 | 1:B:712:PHE:CD2  | 2.22                     | 0.75              |
| 1:C:179:LEU:C    | 1:C:183:SER:HB2  | 2.01                     | 0.75              |
| 1:D:301:ALA:O    | 1:D:303:LYS:N    | 2.20                     | 0.75              |
| 2:R:100:ILE:HB   | 2:R:136:VAL:CG2  | 2.17                     | 0.75              |
| 1:D:164:GLU:O    | 1:D:167:LYS:HG2  | 1.86                     | 0.75              |
| 1:C:254:ARG:HG2  | 1:C:255:THR:H    | 1.50                     | 0.75              |
| 1:D:443:GLU:CG   | 1:D:458:LYS:HG2  | 2.17                     | 0.75              |
| 1:B:66:LEU:HD11  | 1:B:104:ILE:HG13 | 1.68                     | 0.75              |
| 1:F:66:LEU:HD11  | 1:F:104:ILE:HG13 | 1.69                     | 0.75              |
| 2:T:106:ARG:HG3  | 2:T:121:VAL:CG2  | 2.05                     | 0.75              |
| 1:A:297:LYS:HZ1  | 1:A:601:GLU:HB3  | 1.52                     | 0.75              |
| 2:O:100:ILE:HB   | 2:O:136:VAL:CG2  | 2.16                     | 0.75              |
| 1:B:480:ASN:ND2  | 1:B:481:VAL:N    | 2.34                     | 0.75              |
| 1:B:792:VAL:O    | 1:B:796:ILE:HG12 | 1.87                     | 0.75              |
| 2:R:94:LYS:HB3   | 2:R:94:LYS:HZ2   | 1.51                     | 0.75              |
| 1:B:161:ILE:HA   | 1:B:167:LYS:HD2  | 1.67                     | 0.75              |
| 1:D:123:GLU:HG2  | 1:D:124:GLU:N    | 2.02                     | 0.75              |
| 1:A:184:LYS:HZ3  | 1:A:193:LEU:HD12 | 1.52                     | 0.74              |
| 2:Q:100:ILE:HB   | 2:Q:136:VAL:CG2  | 2.17                     | 0.74              |
| 1:F:443:GLU:CG   | 1:F:458:LYS:HG2  | 2.17                     | 0.74              |
| 1:E:164:GLU:O    | 1:E:167:LYS:HG2  | 1.87                     | 0.74              |
| 1:A:625:LEU:HD12 | 1:A:626:TYR:N    | 2.02                     | 0.74              |
| 1:E:180:ASP:CG   | 1:E:181:ILE:H    | 1.88                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:480:ASN:HD22 | 1:D:481:VAL:H    | 1.32                     | 0.74              |
| 1:D:134:LYS:C    | 1:D:136:PRO:HD3  | 2.07                     | 0.74              |
| 1:C:318:ILE:HD12 | 1:C:318:ILE:H    | 1.51                     | 0.74              |
| 1:A:472:ARG:HB3  | 1:A:472:ARG:HH11 | 1.52                     | 0.74              |
| 1:D:275:GLY:HA2  | 1:D:278:LYS:CE   | 2.18                     | 0.74              |
| 1:B:443:GLU:CG   | 1:B:458:LYS:HG2  | 2.16                     | 0.74              |
| 1:A:443:GLU:HG2  | 1:A:458:LYS:HZ1  | 1.51                     | 0.74              |
| 1:E:161:ILE:HA   | 1:E:167:LYS:HD2  | 1.68                     | 0.74              |
| 1:C:217:LYS:HZ3  | 1:C:217:LYS:HB3  | 1.51                     | 0.74              |
| 1:A:305:SER:HB2  | 1:A:594:PHE:CD1  | 2.23                     | 0.74              |
| 1:F:173:ILE:HD12 | 1:F:243:LEU:CD2  | 2.18                     | 0.74              |
| 1:B:305:SER:HB2  | 1:B:594:PHE:CD1  | 2.22                     | 0.74              |
| 1:F:123:GLU:HG2  | 1:F:124:GLU:N    | 2.02                     | 0.74              |
| 1:A:107:THR:HG21 | 1:A:115:LYS:HE3  | 1.67                     | 0.74              |
| 1:D:199:LEU:C    | 1:D:201:ASP:H    | 1.91                     | 0.74              |
| 1:B:301:ALA:O    | 1:B:303:LYS:N    | 2.20                     | 0.74              |
| 1:A:711:ILE:HG13 | 1:A:712:PHE:CD2  | 2.23                     | 0.74              |
| 1:C:794:GLN:O    | 1:C:797:ILE:HG12 | 1.87                     | 0.74              |
| 1:B:447:SER:OG   | 1:B:450:ASN:O    | 2.03                     | 0.74              |
| 2:Q:33:GLY:O     | 2:Q:37:ARG:HG3   | 1.87                     | 0.74              |
| 1:E:308:VAL:O    | 1:E:311:HIS:HB2  | 1.88                     | 0.74              |
| 1:E:443:GLU:CG   | 1:E:458:LYS:HG2  | 2.17                     | 0.74              |
| 1:A:794:GLN:O    | 1:A:797:ILE:HG12 | 1.88                     | 0.74              |
| 1:B:188:LEU:CD2  | 1:B:188:LEU:N    | 2.32                     | 0.74              |
| 1:C:443:GLU:CG   | 1:C:458:LYS:HG2  | 2.17                     | 0.74              |
| 1:E:794:GLN:O    | 1:E:797:ILE:HG12 | 1.87                     | 0.74              |
| 1:F:301:ALA:O    | 1:F:303:LYS:N    | 2.20                     | 0.74              |
| 2:P:100:ILE:HB   | 2:P:136:VAL:CG2  | 2.16                     | 0.74              |
| 1:D:792:VAL:O    | 1:D:796:ILE:HG12 | 1.87                     | 0.74              |
| 1:A:134:LYS:HG2  | 1:A:136:PRO:CD   | 2.17                     | 0.74              |
| 1:A:792:VAL:O    | 1:A:796:ILE:HG12 | 1.88                     | 0.74              |
| 1:D:308:VAL:O    | 1:D:311:HIS:HB2  | 1.87                     | 0.74              |
| 1:D:794:GLN:O    | 1:D:797:ILE:HG12 | 1.87                     | 0.74              |
| 1:C:480:ASN:ND2  | 1:C:481:VAL:N    | 2.35                     | 0.74              |
| 1:F:480:ASN:HD22 | 1:F:481:VAL:H    | 1.30                     | 0.74              |
| 1:C:199:LEU:C    | 1:C:201:ASP:H    | 1.91                     | 0.74              |
| 1:F:711:ILE:HG13 | 1:F:712:PHE:CD2  | 2.22                     | 0.74              |
| 1:B:472:ARG:HB3  | 1:B:472:ARG:HH11 | 1.52                     | 0.74              |
| 1:D:480:ASN:ND2  | 1:D:481:VAL:N    | 2.35                     | 0.74              |
| 1:C:164:GLU:O    | 1:C:167:LYS:HG2  | 1.87                     | 0.74              |
| 1:D:175:LYS:HB2  | 1:D:175:LYS:HZ2  | 1.50                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:794:GLN:O    | 1:B:797:ILE:HG12 | 1.87                     | 0.73              |
| 1:E:66:LEU:HD11  | 1:E:104:ILE:HG13 | 1.69                     | 0.73              |
| 1:C:480:ASN:HD22 | 1:C:481:VAL:H    | 1.31                     | 0.73              |
| 1:D:678:VAL:HG22 | 1:D:745:TYR:CE2  | 2.23                     | 0.73              |
| 1:E:275:GLY:HA2  | 1:E:278:LYS:CE   | 2.18                     | 0.73              |
| 1:C:123:GLU:HG2  | 1:C:124:GLU:N    | 2.03                     | 0.73              |
| 1:A:301:ALA:O    | 1:A:303:LYS:N    | 2.20                     | 0.73              |
| 1:F:305:SER:HB2  | 1:F:594:PHE:CD1  | 2.23                     | 0.73              |
| 1:F:180:ASP:CG   | 1:F:181:ILE:H    | 1.91                     | 0.73              |
| 1:A:180:ASP:CG   | 1:A:181:ILE:H    | 1.92                     | 0.73              |
| 1:C:718:ARG:NH1  | 1:C:767:GLN:HE21 | 1.85                     | 0.73              |
| 2:T:100:ILE:HB   | 2:T:136:VAL:CG2  | 2.17                     | 0.73              |
| 1:D:66:LEU:HD11  | 1:D:104:ILE:HG13 | 1.69                     | 0.73              |
| 1:C:107:THR:HG21 | 1:C:115:LYS:HE3  | 1.69                     | 0.73              |
| 1:C:275:GLY:HA2  | 1:C:278:LYS:CE   | 2.18                     | 0.73              |
| 1:A:123:GLU:HG2  | 1:A:124:GLU:N    | 2.03                     | 0.73              |
| 1:D:169:VAL:O    | 1:D:173:ILE:HG22 | 1.87                     | 0.73              |
| 1:C:90:PRO:HD3   | 1:C:249:PHE:CE2  | 2.22                     | 0.73              |
| 1:A:354:SER:HA   | 1:A:364:ILE:HD13 | 1.70                     | 0.73              |
| 1:F:354:SER:HA   | 1:F:364:ILE:HD13 | 1.68                     | 0.73              |
| 1:E:134:LYS:HG2  | 1:E:136:PRO:HD3  | 1.69                     | 0.73              |
| 1:B:164:GLU:O    | 1:B:167:LYS:HG2  | 1.87                     | 0.73              |
| 1:A:443:GLU:CG   | 1:A:458:LYS:HG2  | 2.17                     | 0.73              |
| 1:F:90:PRO:HD3   | 1:F:249:PHE:CE2  | 2.23                     | 0.73              |
| 1:B:107:THR:HG21 | 1:B:115:LYS:CE   | 2.18                     | 0.73              |
| 1:F:792:VAL:O    | 1:F:796:ILE:HG12 | 1.87                     | 0.73              |
| 1:B:134:LYS:HG2  | 1:B:136:PRO:CD   | 2.17                     | 0.73              |
| 1:E:329:ARG:HD2  | 1:E:590:ASP:OD2  | 1.88                     | 0.73              |
| 1:F:657:ILE:HG13 | 1:F:756:ILE:CD1  | 2.18                     | 0.73              |
| 1:C:134:LYS:HG2  | 1:C:136:PRO:CD   | 2.17                     | 0.73              |
| 2:R:33:GLY:O     | 2:R:37:ARG:HG3   | 1.88                     | 0.73              |
| 1:C:329:ARG:HD2  | 1:C:590:ASP:OD2  | 1.89                     | 0.73              |
| 1:A:173:ILE:HD12 | 1:A:243:LEU:CD2  | 2.19                     | 0.73              |
| 1:B:154:ILE:HG13 | 1:B:171:TYR:CE1  | 2.23                     | 0.73              |
| 2:S:100:ILE:HB   | 2:S:136:VAL:CG2  | 2.17                     | 0.73              |
| 1:E:354:SER:HA   | 1:E:364:ILE:HD13 | 1.70                     | 0.73              |
| 1:B:275:GLY:HA2  | 1:B:278:LYS:CE   | 2.18                     | 0.73              |
| 1:D:354:SER:HA   | 1:D:364:ILE:HD13 | 1.69                     | 0.73              |
| 1:C:792:VAL:O    | 1:C:796:ILE:HG12 | 1.87                     | 0.73              |
| 1:E:678:VAL:HG22 | 1:E:745:TYR:CE2  | 2.23                     | 0.73              |
| 1:B:123:GLU:HG2  | 1:B:124:GLU:N    | 2.03                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:97:ASN:ND2   | 2:T:97:ASN:H     | 1.86                     | 0.73              |
| 1:E:472:ARG:HB3  | 1:E:472:ARG:HH11 | 1.52                     | 0.73              |
| 1:D:305:SER:HB2  | 1:D:594:PHE:CD1  | 2.23                     | 0.73              |
| 1:C:175:LYS:HZ2  | 1:C:175:LYS:HB2  | 1.53                     | 0.72              |
| 1:C:66:LEU:HD11  | 1:C:104:ILE:HG13 | 1.69                     | 0.72              |
| 1:A:329:ARG:HD2  | 1:A:590:ASP:OD2  | 1.89                     | 0.72              |
| 1:A:199:LEU:C    | 1:A:201:ASP:H    | 1.91                     | 0.72              |
| 1:C:154:ILE:HG13 | 1:C:171:TYR:CE1  | 2.24                     | 0.72              |
| 1:D:657:ILE:HG13 | 1:D:756:ILE:CD1  | 2.19                     | 0.72              |
| 1:B:354:SER:HA   | 1:B:364:ILE:HD13 | 1.70                     | 0.72              |
| 1:C:354:SER:HA   | 1:C:364:ILE:HD13 | 1.70                     | 0.72              |
| 1:B:329:ARG:HD2  | 1:B:590:ASP:OD2  | 1.88                     | 0.72              |
| 1:E:301:ALA:O    | 1:E:303:LYS:N    | 2.21                     | 0.72              |
| 1:C:735:VAL:HG12 | 1:C:741:ILE:CD1  | 2.19                     | 0.72              |
| 1:E:217:LYS:HB3  | 1:E:217:LYS:NZ   | 2.04                     | 0.72              |
| 1:E:123:GLU:HG2  | 1:E:124:GLU:N    | 2.02                     | 0.72              |
| 1:E:173:ILE:HD12 | 1:E:243:LEU:CD2  | 2.19                     | 0.72              |
| 1:D:173:ILE:HD12 | 1:D:243:LEU:CD2  | 2.19                     | 0.72              |
| 1:C:657:ILE:HG13 | 1:C:756:ILE:CD1  | 2.19                     | 0.72              |
| 1:B:370:LEU:HD11 | 1:B:455:TYR:CE1  | 2.24                     | 0.72              |
| 1:D:329:ARG:HD2  | 1:D:590:ASP:OD2  | 1.90                     | 0.72              |
| 2:P:97:ASN:ND2   | 2:P:97:ASN:H     | 1.85                     | 0.72              |
| 1:F:217:LYS:HB3  | 1:F:217:LYS:HZ3  | 1.52                     | 0.72              |
| 2:R:97:ASN:ND2   | 2:R:97:ASN:H     | 1.86                     | 0.72              |
| 1:A:90:PRO:HD3   | 1:A:249:PHE:CE2  | 2.23                     | 0.72              |
| 1:D:297:LYS:HZ1  | 1:D:601:GLU:HB3  | 1.54                     | 0.72              |
| 1:F:199:LEU:C    | 1:F:201:ASP:H    | 1.91                     | 0.72              |
| 1:A:447:SER:OG   | 1:A:450:ASN:O    | 2.01                     | 0.72              |
| 2:Q:93:ASP:OD1   | 2:Q:97:ASN:ND2   | 2.22                     | 0.72              |
| 1:F:130:SER:HB2  | 1:F:170:TYR:CZ   | 2.24                     | 0.72              |
| 1:F:185:ASP:O    | 1:F:190:PRO:HG3  | 1.90                     | 0.72              |
| 1:C:173:ILE:HD12 | 1:C:243:LEU:CD2  | 2.20                     | 0.72              |
| 1:B:295:VAL:C    | 1:B:296:LEU:HD23 | 2.10                     | 0.72              |
| 1:F:293:ILE:HD11 | 1:F:617:LYS:HD3  | 1.72                     | 0.72              |
| 1:E:792:VAL:O    | 1:E:796:ILE:HG12 | 1.89                     | 0.72              |
| 1:A:275:GLY:HA2  | 1:A:278:LYS:CE   | 2.17                     | 0.72              |
| 1:C:305:SER:HB2  | 1:C:594:PHE:CD1  | 2.23                     | 0.72              |
| 1:C:185:ASP:O    | 1:C:190:PRO:HG3  | 1.89                     | 0.72              |
| 1:B:391:ILE:HG23 | 1:B:398:ILE:O    | 1.89                     | 0.72              |
| 1:A:462:ILE:HG12 | 1:A:463:THR:N    | 2.05                     | 0.72              |
| 1:A:308:VAL:O    | 1:A:311:HIS:HB2  | 1.90                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:13:LYS:NZ    | 2:O:65:PHE:HB3   | 2.05                     | 0.72              |
| 1:A:735:VAL:HG12 | 1:A:741:ILE:CD1  | 2.20                     | 0.72              |
| 1:B:173:ILE:HD12 | 1:B:243:LEU:CD2  | 2.19                     | 0.72              |
| 1:A:657:ILE:HG13 | 1:A:756:ILE:CD1  | 2.19                     | 0.72              |
| 1:A:154:ILE:HG13 | 1:A:171:TYR:CE1  | 2.25                     | 0.72              |
| 1:F:275:GLY:HA2  | 1:F:278:LYS:CE   | 2.18                     | 0.72              |
| 1:F:370:LEU:HD11 | 1:F:455:TYR:CE1  | 2.25                     | 0.72              |
| 1:D:217:LYS:HB3  | 1:D:217:LYS:NZ   | 2.04                     | 0.72              |
| 1:E:90:PRO:HD3   | 1:E:249:PHE:CE2  | 2.25                     | 0.72              |
| 1:C:107:THR:HG21 | 1:C:115:LYS:CE   | 2.20                     | 0.72              |
| 1:F:154:ILE:HG13 | 1:F:171:TYR:CE1  | 2.25                     | 0.72              |
| 1:C:308:VAL:O    | 1:C:311:HIS:HB2  | 1.89                     | 0.72              |
| 2:O:92:PHE:O     | 2:O:94:LYS:N     | 2.23                     | 0.72              |
| 1:A:370:LEU:HD11 | 1:A:455:TYR:CE1  | 2.25                     | 0.72              |
| 1:E:217:LYS:HZ2  | 1:E:236:GLU:HG3  | 1.55                     | 0.72              |
| 2:S:97:ASN:ND2   | 2:S:97:ASN:H     | 1.86                     | 0.72              |
| 1:B:735:VAL:HG12 | 1:B:741:ILE:CD1  | 2.19                     | 0.72              |
| 1:F:142:VAL:HG13 | 1:F:154:ILE:CD1  | 2.20                     | 0.72              |
| 1:F:678:VAL:HG22 | 1:F:745:TYR:CE2  | 2.23                     | 0.72              |
| 2:T:93:ASP:OD1   | 2:T:97:ASN:ND2   | 2.23                     | 0.72              |
| 1:D:182:ILE:O    | 1:D:187:SER:CB   | 2.35                     | 0.71              |
| 1:D:90:PRO:HD3   | 1:D:249:PHE:CE2  | 2.25                     | 0.71              |
| 1:C:182:ILE:O    | 1:C:187:SER:CB   | 2.35                     | 0.71              |
| 2:P:92:PHE:O     | 2:P:94:LYS:N     | 2.23                     | 0.71              |
| 1:B:183:SER:O    | 1:B:187:SER:CB   | 2.37                     | 0.71              |
| 1:A:295:VAL:C    | 1:A:296:LEU:HD23 | 2.10                     | 0.71              |
| 1:C:411:GLU:HA   | 1:C:414:LYS:HG3  | 1.72                     | 0.71              |
| 1:A:678:VAL:HG22 | 1:A:745:TYR:CE2  | 2.23                     | 0.71              |
| 1:E:199:LEU:C    | 1:E:201:ASP:H    | 1.91                     | 0.71              |
| 2:O:32:LEU:HD22  | 2:O:63:ILE:CD1   | 2.20                     | 0.71              |
| 1:E:134:LYS:C    | 1:E:136:PRO:HD3  | 2.09                     | 0.71              |
| 2:Q:46:ALA:HA    | 2:Q:49:GLN:HE22  | 1.55                     | 0.71              |
| 2:P:13:LYS:NZ    | 2:P:65:PHE:HB3   | 2.05                     | 0.71              |
| 1:C:462:ILE:HG12 | 1:C:463:THR:N    | 2.05                     | 0.71              |
| 2:T:92:PHE:O     | 2:T:94:LYS:N     | 2.23                     | 0.71              |
| 2:O:46:ALA:HA    | 2:O:49:GLN:HE22  | 1.55                     | 0.71              |
| 1:B:540:ARG:NH2  | 2:P:87:GLU:OE1   | 2.23                     | 0.71              |
| 1:A:660:SER:HB2  | 1:A:702:SER:HB3  | 1.72                     | 0.71              |
| 1:E:130:SER:HB2  | 1:E:170:TYR:CZ   | 2.25                     | 0.71              |
| 1:E:391:ILE:HG23 | 1:E:398:ILE:O    | 1.90                     | 0.71              |
| 1:E:115:LYS:HZ1  | 1:E:116:GLU:H    | 1.38                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:462:ILE:HG12 | 1:B:463:THR:N    | 2.05                     | 0.71              |
| 1:F:696:LYS:HE2  | 1:F:731:GLU:HG3  | 1.73                     | 0.71              |
| 2:O:6:GLU:HG3    | 2:O:7:GLU:N      | 2.06                     | 0.71              |
| 1:E:187:SER:C    | 1:E:188:LEU:O    | 2.25                     | 0.71              |
| 1:B:180:ASP:CG   | 1:B:181:ILE:H    | 1.90                     | 0.71              |
| 1:D:462:ILE:HG12 | 1:D:463:THR:N    | 2.05                     | 0.71              |
| 1:F:308:VAL:O    | 1:F:311:HIS:HB2  | 1.90                     | 0.71              |
| 1:C:217:LYS:NZ   | 1:C:217:LYS:HB3  | 2.04                     | 0.71              |
| 2:R:46:ALA:HA    | 2:R:49:GLN:HE22  | 1.54                     | 0.71              |
| 2:T:46:ALA:HA    | 2:T:49:GLN:HE22  | 1.55                     | 0.71              |
| 1:E:184:LYS:HZ2  | 1:E:191:GLU:HB2  | 1.55                     | 0.71              |
| 1:C:186:LYS:HE3  | 1:C:234:LEU:HD12 | 1.72                     | 0.71              |
| 1:D:142:VAL:HG13 | 1:D:154:ILE:CD1  | 2.20                     | 0.71              |
| 1:A:391:ILE:HG23 | 1:A:398:ILE:O    | 1.91                     | 0.71              |
| 1:E:370:LEU:HD11 | 1:E:455:TYR:CE1  | 2.26                     | 0.71              |
| 2:T:13:LYS:NZ    | 2:T:65:PHE:HB3   | 2.06                     | 0.71              |
| 1:E:735:VAL:HG12 | 1:E:741:ILE:CD1  | 2.20                     | 0.71              |
| 1:B:411:GLU:HA   | 1:B:414:LYS:HG3  | 1.73                     | 0.71              |
| 1:E:142:VAL:HG13 | 1:E:154:ILE:CD1  | 2.20                     | 0.71              |
| 1:B:308:VAL:O    | 1:B:311:HIS:HB2  | 1.90                     | 0.71              |
| 1:C:370:LEU:HD11 | 1:C:455:TYR:CE1  | 2.26                     | 0.71              |
| 1:C:776:LEU:HD23 | 1:C:776:LEU:O    | 1.91                     | 0.71              |
| 1:F:329:ARG:HD2  | 1:F:590:ASP:OD2  | 1.89                     | 0.71              |
| 1:D:391:ILE:HG23 | 1:D:398:ILE:O    | 1.90                     | 0.71              |
| 1:D:115:LYS:HZ1  | 1:D:116:GLU:N    | 1.89                     | 0.71              |
| 1:F:199:LEU:O    | 1:F:201:ASP:N    | 2.22                     | 0.71              |
| 1:B:443:GLU:HG2  | 1:B:458:LYS:CE   | 2.21                     | 0.71              |
| 1:C:324:THR:HB   | 1:C:499:PRO:HA   | 1.73                     | 0.71              |
| 1:D:694:VAL:CG2  | 2:R:18:LEU:HD21  | 2.20                     | 0.71              |
| 1:D:411:GLU:HA   | 1:D:414:LYS:HG3  | 1.73                     | 0.71              |
| 2:Q:92:PHE:O     | 2:Q:94:LYS:N     | 2.23                     | 0.71              |
| 1:A:165:GLN:NE2  | 1:A:252:ASP:HB3  | 2.06                     | 0.71              |
| 1:F:217:LYS:NZ   | 1:F:217:LYS:HB3  | 2.04                     | 0.71              |
| 1:D:735:VAL:HG12 | 1:D:741:ILE:CD1  | 2.21                     | 0.71              |
| 1:E:184:LYS:CE   | 1:E:191:GLU:HB2  | 2.20                     | 0.71              |
| 1:C:293:ILE:HD11 | 1:C:617:LYS:HD3  | 1.73                     | 0.71              |
| 2:O:106:ARG:HG3  | 2:O:121:VAL:CG2  | 2.07                     | 0.71              |
| 1:E:411:GLU:HA   | 1:E:414:LYS:HG3  | 1.72                     | 0.71              |
| 1:A:142:VAL:HG13 | 1:A:154:ILE:CD1  | 2.20                     | 0.71              |
| 1:B:142:VAL:HG13 | 1:B:154:ILE:CD1  | 2.20                     | 0.71              |
| 2:S:32:LEU:HD22  | 2:S:63:ILE:CD1   | 2.21                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:293:ILE:HD11 | 1:B:617:LYS:HD3  | 1.73                     | 0.70              |
| 1:F:295:VAL:C    | 1:F:296:LEU:HD23 | 2.10                     | 0.70              |
| 1:A:411:GLU:HA   | 1:A:414:LYS:HG3  | 1.73                     | 0.70              |
| 1:F:134:LYS:C    | 1:F:136:PRO:HD3  | 2.10                     | 0.70              |
| 1:F:324:THR:HB   | 1:F:499:PRO:HA   | 1.73                     | 0.70              |
| 2:R:13:LYS:NZ    | 2:R:65:PHE:HB3   | 2.05                     | 0.70              |
| 2:P:6:GLU:HG3    | 2:P:7:GLU:N      | 2.06                     | 0.70              |
| 1:D:776:LEU:O    | 1:D:776:LEU:HD23 | 1.91                     | 0.70              |
| 2:S:6:GLU:HG3    | 2:S:7:GLU:N      | 2.05                     | 0.70              |
| 1:C:187:SER:C    | 1:C:188:LEU:O    | 2.26                     | 0.70              |
| 1:D:293:ILE:HD11 | 1:D:617:LYS:HD3  | 1.72                     | 0.70              |
| 1:A:107:THR:HG21 | 1:A:115:LYS:CE   | 2.21                     | 0.70              |
| 1:E:629:ASN:HD22 | 1:E:630:ARG:N    | 1.89                     | 0.70              |
| 1:E:776:LEU:HD23 | 1:E:776:LEU:O    | 1.91                     | 0.70              |
| 1:C:391:ILE:HG23 | 1:C:398:ILE:O    | 1.91                     | 0.70              |
| 2:O:94:LYS:HB3   | 2:O:94:LYS:HZ2   | 1.54                     | 0.70              |
| 1:F:443:GLU:HG2  | 1:F:458:LYS:HZ1  | 1.56                     | 0.70              |
| 1:A:175:LYS:HZ2  | 1:A:175:LYS:HB2  | 1.55                     | 0.70              |
| 1:B:657:ILE:HG13 | 1:B:756:ILE:CD1  | 2.21                     | 0.70              |
| 1:F:115:LYS:HZ1  | 1:F:116:GLU:N    | 1.90                     | 0.70              |
| 1:F:411:GLU:HA   | 1:F:414:LYS:HG3  | 1.73                     | 0.70              |
| 2:T:32:LEU:HD22  | 2:T:63:ILE:CD1   | 2.21                     | 0.70              |
| 2:R:32:LEU:HD22  | 2:R:63:ILE:CD1   | 2.21                     | 0.70              |
| 1:F:493:ASP:OD2  | 1:F:577:HIS:HE1  | 1.74                     | 0.70              |
| 1:B:217:LYS:HB3  | 1:B:217:LYS:NZ   | 2.04                     | 0.70              |
| 2:S:92:PHE:O     | 2:S:94:LYS:N     | 2.23                     | 0.70              |
| 1:B:660:SER:HB2  | 1:B:702:SER:HB3  | 1.72                     | 0.70              |
| 2:R:6:GLU:HG3    | 2:R:7:GLU:N      | 2.05                     | 0.70              |
| 2:T:6:GLU:HG3    | 2:T:7:GLU:N      | 2.05                     | 0.70              |
| 1:A:191:GLU:O    | 1:A:193:LEU:N    | 2.24                     | 0.70              |
| 1:D:550:SER:N    | 1:D:553:GLN:HE21 | 1.85                     | 0.70              |
| 1:F:462:ILE:HG12 | 1:F:463:THR:N    | 2.05                     | 0.70              |
| 2:O:97:ASN:H     | 2:O:97:ASN:HD22  | 1.39                     | 0.70              |
| 1:A:443:GLU:HG2  | 1:A:458:LYS:CE   | 2.21                     | 0.70              |
| 2:O:49:GLN:HA    | 2:O:52:ILE:HG22  | 1.73                     | 0.70              |
| 2:P:73:ALA:O     | 2:P:76:MET:N     | 2.23                     | 0.70              |
| 1:E:293:ILE:HD11 | 1:E:617:LYS:HD3  | 1.73                     | 0.70              |
| 1:C:142:VAL:HG13 | 1:C:154:ILE:CD1  | 2.20                     | 0.70              |
| 1:A:217:LYS:HB3  | 1:A:217:LYS:NZ   | 2.04                     | 0.70              |
| 1:A:324:THR:HB   | 1:A:499:PRO:HA   | 1.73                     | 0.70              |
| 2:R:93:ASP:OD1   | 2:R:97:ASN:ND2   | 2.24                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:186:LYS:HE3  | 1:E:234:LEU:HD12 | 1.71                     | 0.70              |
| 1:C:184:LYS:HE2  | 1:C:193:LEU:HB2  | 1.74                     | 0.70              |
| 1:B:128:MET:HB2  | 1:B:239:HIS:CE1  | 2.26                     | 0.70              |
| 1:B:199:LEU:O    | 1:B:201:ASP:N    | 2.22                     | 0.70              |
| 1:D:443:GLU:HG2  | 1:D:458:LYS:CE   | 2.22                     | 0.70              |
| 1:F:797:ILE:O    | 1:F:797:ILE:HG13 | 1.91                     | 0.70              |
| 1:F:735:VAL:HG12 | 1:F:741:ILE:CD1  | 2.21                     | 0.70              |
| 1:E:696:LYS:HE2  | 1:E:731:GLU:HG3  | 1.74                     | 0.70              |
| 1:D:660:SER:HB2  | 1:D:702:SER:HB3  | 1.73                     | 0.70              |
| 1:A:776:LEU:O    | 1:A:776:LEU:HD23 | 1.92                     | 0.70              |
| 1:D:187:SER:C    | 1:D:188:LEU:O    | 2.26                     | 0.70              |
| 1:B:550:SER:N    | 1:B:553:GLN:HE21 | 1.86                     | 0.70              |
| 1:C:797:ILE:HG13 | 1:C:797:ILE:O    | 1.92                     | 0.70              |
| 2:R:49:GLN:HA    | 2:R:52:ILE:HG22  | 1.73                     | 0.70              |
| 1:F:776:LEU:HD23 | 1:F:776:LEU:O    | 1.91                     | 0.70              |
| 1:C:493:ASP:OD2  | 1:C:577:HIS:HE1  | 1.75                     | 0.70              |
| 1:B:408:LEU:N    | 1:B:408:LEU:HD12 | 2.07                     | 0.70              |
| 1:F:443:GLU:HG2  | 1:F:458:LYS:CE   | 2.21                     | 0.70              |
| 1:A:368:GLN:HG3  | 1:A:383:GLY:HA3  | 1.74                     | 0.70              |
| 1:D:370:LEU:HD11 | 1:D:455:TYR:CE1  | 2.27                     | 0.70              |
| 2:P:93:ASP:OD1   | 2:P:97:ASN:ND2   | 2.24                     | 0.70              |
| 2:P:46:ALA:HA    | 2:P:49:GLN:HE22  | 1.55                     | 0.70              |
| 1:E:694:VAL:CG2  | 2:S:18:LEU:HD21  | 2.21                     | 0.70              |
| 1:E:462:ILE:HG12 | 1:E:463:THR:N    | 2.05                     | 0.70              |
| 2:R:92:PHE:O     | 2:R:94:LYS:N     | 2.23                     | 0.70              |
| 1:E:660:SER:HB2  | 1:E:702:SER:HB3  | 1.73                     | 0.70              |
| 1:E:295:VAL:C    | 1:E:296:LEU:HD23 | 2.10                     | 0.69              |
| 1:F:629:ASN:HD22 | 1:F:630:ARG:N    | 1.90                     | 0.69              |
| 1:C:678:VAL:HG22 | 1:C:745:TYR:CE2  | 2.24                     | 0.69              |
| 2:R:58:ASP:C     | 2:R:60:ASN:N     | 2.46                     | 0.69              |
| 1:E:408:LEU:N    | 1:E:408:LEU:HD12 | 2.07                     | 0.69              |
| 1:F:165:GLN:NE2  | 1:F:252:ASP:HB3  | 2.07                     | 0.69              |
| 1:D:324:THR:HB   | 1:D:499:PRO:HA   | 1.74                     | 0.69              |
| 1:D:797:ILE:HG13 | 1:D:797:ILE:O    | 1.92                     | 0.69              |
| 2:P:49:GLN:HA    | 2:P:52:ILE:HG22  | 1.73                     | 0.69              |
| 2:Q:6:GLU:HG3    | 2:Q:7:GLU:N      | 2.06                     | 0.69              |
| 2:S:13:LYS:NZ    | 2:S:65:PHE:HB3   | 2.06                     | 0.69              |
| 1:A:296:LEU:CD2  | 1:A:296:LEU:H    | 1.83                     | 0.69              |
| 1:E:657:ILE:HG13 | 1:E:756:ILE:CD1  | 2.22                     | 0.69              |
| 2:Q:32:LEU:HD22  | 2:Q:63:ILE:CD1   | 2.21                     | 0.69              |
| 1:C:408:LEU:HD12 | 1:C:408:LEU:N    | 2.06                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:443:GLU:HG2  | 1:E:458:LYS:CE   | 2.21                     | 0.69              |
| 1:C:443:GLU:HG2  | 1:C:458:LYS:CE   | 2.22                     | 0.69              |
| 2:Q:97:ASN:HD22  | 2:Q:97:ASN:H     | 1.39                     | 0.69              |
| 1:D:154:ILE:HG13 | 1:D:171:TYR:CE1  | 2.28                     | 0.69              |
| 1:F:368:GLN:HG3  | 1:F:383:GLY:HA3  | 1.74                     | 0.69              |
| 1:C:694:VAL:CG2  | 2:Q:18:LEU:HD21  | 2.22                     | 0.69              |
| 1:D:199:LEU:O    | 1:D:201:ASP:N    | 2.22                     | 0.69              |
| 1:D:311:HIS:CD2  | 1:D:564:VAL:HB   | 2.28                     | 0.69              |
| 1:D:165:GLN:NE2  | 1:D:252:ASP:HB3  | 2.07                     | 0.69              |
| 1:D:368:GLN:HG3  | 1:D:383:GLY:HA3  | 1.73                     | 0.69              |
| 2:S:93:ASP:OD1   | 2:S:97:ASN:ND2   | 2.25                     | 0.69              |
| 2:T:49:GLN:HA    | 2:T:52:ILE:HG22  | 1.73                     | 0.69              |
| 1:F:660:SER:HB2  | 1:F:702:SER:HB3  | 1.73                     | 0.69              |
| 2:S:46:ALA:HA    | 2:S:49:GLN:HE22  | 1.55                     | 0.69              |
| 1:A:715:GLU:HA   | 1:A:718:ARG:CZ   | 2.22                     | 0.69              |
| 1:F:478:ALA:HB1  | 1:F:486:LYS:O    | 1.93                     | 0.69              |
| 1:D:722:ILE:HD11 | 1:D:763:LEU:O    | 1.91                     | 0.69              |
| 1:D:629:ASN:HD22 | 1:D:630:ARG:N    | 1.90                     | 0.69              |
| 1:D:408:LEU:N    | 1:D:408:LEU:HD12 | 2.07                     | 0.69              |
| 2:Q:49:GLN:HA    | 2:Q:52:ILE:HG22  | 1.73                     | 0.69              |
| 1:B:478:ALA:HB1  | 1:B:486:LYS:O    | 1.93                     | 0.69              |
| 1:F:391:ILE:HG23 | 1:F:398:ILE:O    | 1.93                     | 0.69              |
| 2:S:58:ASP:C     | 2:S:60:ASN:N     | 2.46                     | 0.69              |
| 1:A:493:ASP:OD2  | 1:A:577:HIS:HE1  | 1.75                     | 0.69              |
| 1:C:660:SER:HB2  | 1:C:702:SER:HB3  | 1.73                     | 0.69              |
| 1:B:776:LEU:HD23 | 1:B:776:LEU:O    | 1.91                     | 0.69              |
| 1:B:199:LEU:C    | 1:B:201:ASP:H    | 1.95                     | 0.69              |
| 1:A:89:ILE:HG22  | 1:A:93:VAL:CG1   | 2.08                     | 0.69              |
| 1:E:797:ILE:HG13 | 1:E:797:ILE:O    | 1.92                     | 0.69              |
| 1:A:293:ILE:O    | 1:A:295:VAL:HG22 | 1.92                     | 0.69              |
| 1:D:295:VAL:C    | 1:D:296:LEU:HD23 | 2.10                     | 0.69              |
| 1:C:718:ARG:O    | 1:C:722:ILE:HG13 | 1.93                     | 0.69              |
| 2:O:58:ASP:C     | 2:O:60:ASN:N     | 2.45                     | 0.69              |
| 2:P:32:LEU:HD22  | 2:P:63:ILE:CD1   | 2.22                     | 0.69              |
| 1:A:408:LEU:HD12 | 1:A:408:LEU:N    | 2.06                     | 0.69              |
| 1:E:334:LEU:HD12 | 1:E:334:LEU:N    | 2.08                     | 0.69              |
| 1:D:334:LEU:HD12 | 1:D:334:LEU:N    | 2.08                     | 0.69              |
| 1:D:134:LYS:HG2  | 1:D:136:PRO:HD3  | 1.73                     | 0.69              |
| 1:B:368:GLN:HG3  | 1:B:383:GLY:HA3  | 1.73                     | 0.69              |
| 1:B:165:GLN:NE2  | 1:B:252:ASP:HB3  | 2.08                     | 0.69              |
| 2:P:97:ASN:HD22  | 2:P:97:ASN:H     | 1.41                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:696:LYS:HE2  | 1:B:731:GLU:HG3  | 1.75                     | 0.69              |
| 2:S:49:GLN:HA    | 2:S:52:ILE:HG22  | 1.73                     | 0.69              |
| 2:Q:13:LYS:NZ    | 2:Q:65:PHE:HB3   | 2.07                     | 0.69              |
| 1:F:548:THR:O    | 5:F:908:3AT:N6   | 2.26                     | 0.69              |
| 1:F:715:GLU:HA   | 1:F:718:ARG:CZ   | 2.22                     | 0.69              |
| 1:D:715:GLU:HA   | 1:D:718:ARG:CZ   | 2.23                     | 0.69              |
| 2:P:58:ASP:C     | 2:P:60:ASN:N     | 2.45                     | 0.69              |
| 1:C:165:GLN:NE2  | 1:C:252:ASP:HB3  | 2.08                     | 0.69              |
| 1:E:165:GLN:NE2  | 1:E:252:ASP:HB3  | 2.07                     | 0.69              |
| 1:B:715:GLU:HA   | 1:B:718:ARG:CZ   | 2.23                     | 0.69              |
| 1:C:311:HIS:CD2  | 1:C:564:VAL:HB   | 2.27                     | 0.69              |
| 1:A:550:SER:N    | 1:A:553:GLN:HE21 | 1.86                     | 0.68              |
| 1:A:311:HIS:CD2  | 1:A:564:VAL:HB   | 2.28                     | 0.68              |
| 1:E:311:HIS:CD2  | 1:E:564:VAL:HB   | 2.28                     | 0.68              |
| 1:E:324:THR:HB   | 1:E:499:PRO:HA   | 1.74                     | 0.68              |
| 1:E:188:LEU:HD22 | 1:E:188:LEU:N    | 2.07                     | 0.68              |
| 1:F:408:LEU:N    | 1:F:408:LEU:HD12 | 2.07                     | 0.68              |
| 1:C:368:GLN:HG3  | 1:C:383:GLY:HA3  | 1.73                     | 0.68              |
| 1:B:324:THR:HB   | 1:B:499:PRO:HA   | 1.73                     | 0.68              |
| 1:A:797:ILE:HG13 | 1:A:797:ILE:O    | 1.92                     | 0.68              |
| 1:E:123:GLU:HG2  | 1:E:124:GLU:H    | 1.57                     | 0.68              |
| 1:D:735:VAL:O    | 1:D:738:SER:HB2  | 1.94                     | 0.68              |
| 1:B:197:LYS:HD2  | 1:B:197:LYS:O    | 1.93                     | 0.68              |
| 1:D:184:LYS:HE2  | 1:D:193:LEU:HB2  | 1.74                     | 0.68              |
| 1:C:722:ILE:HG23 | 1:C:760:VAL:HG13 | 1.74                     | 0.68              |
| 1:D:334:LEU:CD1  | 1:D:334:LEU:H    | 2.06                     | 0.68              |
| 1:B:694:VAL:CG2  | 2:P:18:LEU:HD21  | 2.24                     | 0.68              |
| 1:E:186:LYS:CE   | 1:E:234:LEU:HD12 | 2.24                     | 0.68              |
| 1:A:597:ASN:ND2  | 1:A:601:GLU:H    | 1.92                     | 0.68              |
| 1:D:759:GLN:HE21 | 1:D:763:LEU:HD11 | 1.57                     | 0.68              |
| 1:E:334:LEU:H    | 1:E:334:LEU:CD1  | 2.06                     | 0.68              |
| 1:B:123:GLU:HG2  | 1:B:124:GLU:H    | 1.58                     | 0.68              |
| 2:T:97:ASN:H     | 2:T:97:ASN:HD22  | 1.42                     | 0.68              |
| 1:D:197:LYS:O    | 1:D:197:LYS:HD2  | 1.93                     | 0.68              |
| 1:E:128:MET:HB2  | 1:E:239:HIS:CE1  | 2.28                     | 0.68              |
| 1:D:186:LYS:HE3  | 1:D:234:LEU:HD12 | 1.74                     | 0.68              |
| 1:F:184:LYS:HE2  | 1:F:193:LEU:HB2  | 1.74                     | 0.68              |
| 1:C:183:SER:O    | 1:C:187:SER:CB   | 2.41                     | 0.68              |
| 1:B:184:LYS:HE2  | 1:B:193:LEU:HB2  | 1.76                     | 0.68              |
| 1:C:295:VAL:C    | 1:C:296:LEU:HD23 | 2.10                     | 0.68              |
| 1:C:715:GLU:HA   | 1:C:718:ARG:CZ   | 2.22                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:134:LYS:C    | 1:B:136:PRO:HD3  | 2.14                     | 0.68              |
| 1:F:128:MET:HB2  | 1:F:239:HIS:CE1  | 2.29                     | 0.68              |
| 1:F:175:LYS:HB2  | 1:F:175:LYS:HZ2  | 1.59                     | 0.68              |
| 1:C:597:ASN:ND2  | 1:C:601:GLU:H    | 1.92                     | 0.68              |
| 1:E:478:ALA:HB1  | 1:E:486:LYS:O    | 1.93                     | 0.68              |
| 1:C:134:LYS:C    | 1:C:136:PRO:HD3  | 2.14                     | 0.68              |
| 1:F:134:LYS:HG2  | 1:F:136:PRO:CD   | 2.24                     | 0.68              |
| 1:C:629:ASN:HD22 | 1:C:630:ARG:N    | 1.90                     | 0.68              |
| 1:E:597:ASN:HB2  | 1:E:598:PRO:CD   | 2.23                     | 0.68              |
| 1:A:478:ALA:HB1  | 1:A:486:LYS:O    | 1.94                     | 0.68              |
| 1:D:718:ARG:O    | 1:D:722:ILE:HG13 | 1.94                     | 0.68              |
| 1:F:550:SER:N    | 1:F:553:GLN:HE21 | 1.86                     | 0.68              |
| 1:A:134:LYS:C    | 1:A:136:PRO:HD3  | 2.14                     | 0.68              |
| 2:O:97:ASN:N     | 2:O:97:ASN:HD22  | 1.92                     | 0.68              |
| 1:F:123:GLU:HG2  | 1:F:124:GLU:H    | 1.58                     | 0.68              |
| 1:F:197:LYS:HD2  | 1:F:197:LYS:O    | 1.93                     | 0.68              |
| 1:E:286:GLU:O    | 1:E:290:LYS:HE3  | 1.94                     | 0.68              |
| 1:F:286:GLU:O    | 1:F:290:LYS:HE3  | 1.94                     | 0.68              |
| 1:D:478:ALA:HB1  | 1:D:486:LYS:O    | 1.94                     | 0.68              |
| 2:T:58:ASP:C     | 2:T:60:ASN:N     | 2.46                     | 0.68              |
| 2:S:73:ALA:O     | 2:S:76:MET:N     | 2.27                     | 0.68              |
| 1:B:179:LEU:C    | 1:B:183:SER:HB2  | 2.10                     | 0.68              |
| 1:A:184:LYS:HE2  | 1:A:193:LEU:HB2  | 1.74                     | 0.68              |
| 1:F:718:ARG:O    | 1:F:722:ILE:HG13 | 1.94                     | 0.68              |
| 1:C:334:LEU:N    | 1:C:334:LEU:HD12 | 2.09                     | 0.68              |
| 1:E:368:GLN:HG3  | 1:E:383:GLY:HA3  | 1.75                     | 0.68              |
| 1:B:797:ILE:HG13 | 1:B:797:ILE:O    | 1.92                     | 0.68              |
| 1:A:696:LYS:HE2  | 1:A:731:GLU:HG3  | 1.74                     | 0.68              |
| 2:Q:18:LEU:HD22  | 2:Q:18:LEU:O     | 1.94                     | 0.68              |
| 1:E:310:GLU:OE2  | 1:E:340:LYS:HD2  | 1.94                     | 0.68              |
| 1:B:286:GLU:O    | 1:B:290:LYS:HE3  | 1.94                     | 0.68              |
| 1:F:107:THR:HG21 | 1:F:115:LYS:HE3  | 1.74                     | 0.68              |
| 1:C:77:ASP:O     | 1:C:81:GLN:HB2   | 1.94                     | 0.68              |
| 1:E:77:ASP:O     | 1:E:81:GLN:HB2   | 1.94                     | 0.68              |
| 1:F:694:VAL:CG2  | 2:T:18:LEU:HD21  | 2.23                     | 0.68              |
| 1:D:414:LYS:HZ2  | 1:D:414:LYS:HA   | 1.59                     | 0.67              |
| 1:F:597:ASN:ND2  | 1:F:601:GLU:H    | 1.91                     | 0.67              |
| 1:E:715:GLU:HA   | 1:E:718:ARG:CZ   | 2.24                     | 0.67              |
| 1:A:629:ASN:HD22 | 1:A:630:ARG:N    | 1.91                     | 0.67              |
| 1:D:718:ARG:HH12 | 1:D:767:GLN:HE21 | 1.42                     | 0.67              |
| 1:A:334:LEU:N    | 1:A:334:LEU:HD12 | 2.09                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:493:ASP:OD2  | 1:E:577:HIS:HE1  | 1.77                     | 0.67              |
| 1:B:77:ASP:O     | 1:B:81:GLN:HB2   | 1.94                     | 0.67              |
| 1:C:286:GLU:O    | 1:C:290:LYS:HE3  | 1.94                     | 0.67              |
| 1:E:184:LYS:HE2  | 1:E:193:LEU:HB2  | 1.76                     | 0.67              |
| 1:E:597:ASN:ND2  | 1:E:601:GLU:H    | 1.92                     | 0.67              |
| 1:D:722:ILE:HG23 | 1:D:760:VAL:HG13 | 1.76                     | 0.67              |
| 1:A:254:ARG:H    | 1:A:254:ARG:HD2  | 1.60                     | 0.67              |
| 1:A:123:GLU:HG2  | 1:A:124:GLU:H    | 1.59                     | 0.67              |
| 1:D:217:LYS:HZ2  | 1:D:236:GLU:HG3  | 1.59                     | 0.67              |
| 1:A:197:LYS:O    | 1:A:197:LYS:HD2  | 1.94                     | 0.67              |
| 1:A:77:ASP:O     | 1:A:81:GLN:HB2   | 1.94                     | 0.67              |
| 1:C:130:SER:HB2  | 1:C:170:TYR:CZ   | 2.29                     | 0.67              |
| 1:D:115:LYS:HZ1  | 1:D:116:GLU:H    | 1.43                     | 0.67              |
| 1:A:278:LYS:O    | 1:A:281:GLU:N    | 2.27                     | 0.67              |
| 1:B:311:HIS:CD2  | 1:B:564:VAL:HB   | 2.29                     | 0.67              |
| 1:A:334:LEU:H    | 1:A:334:LEU:CD1  | 2.07                     | 0.67              |
| 1:D:123:GLU:HG2  | 1:D:124:GLU:H    | 1.58                     | 0.67              |
| 1:C:696:LYS:HE2  | 1:C:731:GLU:HG3  | 1.75                     | 0.67              |
| 1:E:735:VAL:O    | 1:E:738:SER:HB2  | 1.95                     | 0.67              |
| 1:D:696:LYS:HE2  | 1:D:731:GLU:HG3  | 1.76                     | 0.67              |
| 2:P:18:LEU:HD22  | 2:P:18:LEU:O     | 1.94                     | 0.67              |
| 1:D:77:ASP:O     | 1:D:81:GLN:HB2   | 1.94                     | 0.67              |
| 1:D:548:THR:O    | 5:D:906:3AT:N6   | 2.28                     | 0.67              |
| 1:F:189:ASP:O    | 1:F:190:PRO:C    | 2.31                     | 0.67              |
| 1:B:293:ILE:O    | 1:B:295:VAL:HG22 | 1.94                     | 0.67              |
| 1:D:105:TYR:N    | 1:D:152:LEU:O    | 2.26                     | 0.67              |
| 1:B:414:LYS:HA   | 1:B:414:LYS:HZ2  | 1.59                     | 0.67              |
| 1:B:630:ARG:CZ   | 2:P:83:GLU:HG2   | 2.24                     | 0.67              |
| 1:E:718:ARG:O    | 1:E:722:ILE:HG13 | 1.94                     | 0.67              |
| 1:B:334:LEU:N    | 1:B:334:LEU:HD12 | 2.09                     | 0.67              |
| 1:F:184:LYS:HZ2  | 1:F:191:GLU:HB2  | 1.58                     | 0.67              |
| 1:C:478:ALA:HB1  | 1:C:486:LYS:O    | 1.94                     | 0.67              |
| 1:B:629:ASN:HD22 | 1:B:630:ARG:N    | 1.91                     | 0.67              |
| 1:A:630:ARG:CZ   | 2:O:83:GLU:HG2   | 2.25                     | 0.67              |
| 1:B:678:VAL:HG22 | 1:B:745:TYR:CE2  | 2.25                     | 0.67              |
| 1:F:311:HIS:CD2  | 1:F:564:VAL:HB   | 2.29                     | 0.67              |
| 2:S:94:LYS:HB3   | 2:S:94:LYS:HZ2   | 1.56                     | 0.67              |
| 2:Q:73:ALA:O     | 2:Q:76:MET:N     | 2.26                     | 0.67              |
| 1:A:286:GLU:O    | 1:A:290:LYS:HE3  | 1.95                     | 0.67              |
| 1:A:694:VAL:CG2  | 2:O:18:LEU:HD21  | 2.24                     | 0.67              |
| 1:C:213:LYS:HD2  | 1:C:240:ALA:HB1  | 1.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:278:LYS:O    | 1:C:281:GLU:N    | 2.28                     | 0.67              |
| 1:B:278:LYS:O    | 1:B:281:GLU:N    | 2.28                     | 0.67              |
| 1:C:334:LEU:CD1  | 1:C:334:LEU:H    | 2.07                     | 0.67              |
| 2:O:9:ILE:CD1    | 2:O:69:LEU:HD11  | 2.25                     | 0.67              |
| 2:P:94:LYS:HB3   | 2:P:94:LYS:HZ2   | 1.59                     | 0.67              |
| 2:Q:94:LYS:HB3   | 2:Q:94:LYS:HZ2   | 1.59                     | 0.67              |
| 2:S:137:ASN:OD1  | 2:S:139:GLU:HB2  | 1.95                     | 0.67              |
| 1:D:128:MET:HB2  | 1:D:239:HIS:CE1  | 2.30                     | 0.67              |
| 1:A:199:LEU:O    | 1:A:201:ASP:N    | 2.22                     | 0.67              |
| 1:B:718:ARG:O    | 1:B:722:ILE:HG13 | 1.94                     | 0.67              |
| 2:Q:58:ASP:C     | 2:Q:60:ASN:N     | 2.46                     | 0.67              |
| 1:F:334:LEU:HD12 | 1:F:334:LEU:N    | 2.09                     | 0.67              |
| 2:S:9:ILE:CD1    | 2:S:69:LEU:HD11  | 2.25                     | 0.67              |
| 2:P:137:ASN:OD1  | 2:P:139:GLU:HB2  | 1.95                     | 0.67              |
| 1:C:310:GLU:OE2  | 1:C:340:LYS:HD2  | 1.95                     | 0.67              |
| 1:F:310:GLU:OE2  | 1:F:340:LYS:HD2  | 1.95                     | 0.67              |
| 1:D:184:LYS:HZ3  | 1:D:193:LEU:HD12 | 1.58                     | 0.67              |
| 1:A:175:LYS:O    | 1:A:177:ILE:N    | 2.28                     | 0.67              |
| 1:E:154:ILE:HG13 | 1:E:171:TYR:CE1  | 2.29                     | 0.67              |
| 1:B:254:ARG:HD2  | 1:B:254:ARG:H    | 1.60                     | 0.67              |
| 2:P:97:ASN:N     | 2:P:97:ASN:HD22  | 1.92                     | 0.67              |
| 2:T:73:ALA:O     | 2:T:76:MET:N     | 2.27                     | 0.67              |
| 1:B:310:GLU:OE2  | 1:B:340:LYS:HD2  | 1.94                     | 0.67              |
| 1:B:186:LYS:HE3  | 1:B:234:LEU:HD12 | 1.77                     | 0.67              |
| 1:C:115:LYS:HZ3  | 1:C:116:GLU:N    | 1.92                     | 0.67              |
| 1:E:550:SER:N    | 1:E:553:GLN:HE21 | 1.88                     | 0.67              |
| 1:D:107:THR:HG21 | 1:D:115:LYS:HE3  | 1.74                     | 0.67              |
| 1:B:334:LEU:H    | 1:B:334:LEU:CD1  | 2.07                     | 0.67              |
| 1:F:254:ARG:HD2  | 1:F:254:ARG:H    | 1.60                     | 0.67              |
| 2:T:94:LYS:HB3   | 2:T:94:LYS:HZ2   | 1.56                     | 0.67              |
| 1:C:254:ARG:H    | 1:C:254:ARG:HD2  | 1.60                     | 0.67              |
| 2:S:97:ASN:HD22  | 2:S:97:ASN:H     | 1.42                     | 0.67              |
| 2:O:73:ALA:O     | 2:O:76:MET:N     | 2.27                     | 0.67              |
| 1:D:286:GLU:O    | 1:D:290:LYS:HE3  | 1.94                     | 0.67              |
| 1:E:185:ASP:O    | 1:E:190:PRO:HG3  | 1.95                     | 0.67              |
| 1:B:175:LYS:O    | 1:B:177:ILE:N    | 2.28                     | 0.67              |
| 1:B:213:LYS:HD2  | 1:B:240:ALA:HB1  | 1.77                     | 0.67              |
| 1:A:183:SER:C    | 1:A:187:SER:HB2  | 2.14                     | 0.67              |
| 1:A:718:ARG:O    | 1:A:722:ILE:HG13 | 1.95                     | 0.67              |
| 1:D:107:THR:HG21 | 1:D:115:LYS:CE   | 2.25                     | 0.67              |
| 1:C:123:GLU:HG2  | 1:C:124:GLU:H    | 1.58                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:179:LEU:O    | 1:E:183:SER:N    | 2.27                     | 0.66              |
| 1:B:187:SER:C    | 1:B:188:LEU:O    | 2.31                     | 0.66              |
| 1:B:597:ASN:ND2  | 1:B:601:GLU:H    | 1.91                     | 0.66              |
| 1:E:105:TYR:N    | 1:E:152:LEU:O    | 2.25                     | 0.66              |
| 1:C:463:THR:HG22 | 1:C:465:LEU:N    | 2.10                     | 0.66              |
| 1:F:334:LEU:CD1  | 1:F:334:LEU:H    | 2.08                     | 0.66              |
| 1:E:443:GLU:HG3  | 1:E:458:LYS:HG2  | 1.76                     | 0.66              |
| 2:R:137:ASN:OD1  | 2:R:139:GLU:HB2  | 1.95                     | 0.66              |
| 1:D:443:GLU:HG3  | 1:D:458:LYS:HG2  | 1.76                     | 0.66              |
| 1:E:197:LYS:O    | 1:E:197:LYS:HD2  | 1.95                     | 0.66              |
| 2:Q:137:ASN:OD1  | 2:Q:139:GLU:HB2  | 1.95                     | 0.66              |
| 1:F:175:LYS:O    | 1:F:177:ILE:N    | 2.28                     | 0.66              |
| 1:C:186:LYS:CE   | 1:C:234:LEU:HD12 | 2.25                     | 0.66              |
| 1:A:191:GLU:O    | 1:A:192:PHE:C    | 2.31                     | 0.66              |
| 1:A:186:LYS:HE3  | 1:A:234:LEU:HD12 | 1.77                     | 0.66              |
| 1:E:254:ARG:HD2  | 1:E:254:ARG:H    | 1.60                     | 0.66              |
| 1:B:225:ILE:HG12 | 1:B:229:PHE:HE2  | 1.60                     | 0.66              |
| 1:A:293:ILE:HD11 | 1:A:617:LYS:HD3  | 1.78                     | 0.66              |
| 2:P:117:THR:O    | 2:P:119:GLU:N    | 2.29                     | 0.66              |
| 1:D:597:ASN:HB2  | 1:D:598:PRO:CD   | 2.23                     | 0.66              |
| 1:E:107:THR:HG21 | 1:E:115:LYS:HE3  | 1.76                     | 0.66              |
| 1:D:540:ARG:NH1  | 1:D:627:TYR:CE1  | 2.62                     | 0.66              |
| 1:C:105:TYR:N    | 1:C:152:LEU:O    | 2.26                     | 0.66              |
| 1:B:115:LYS:HZ1  | 1:B:116:GLU:N    | 1.92                     | 0.66              |
| 1:E:225:ILE:HG12 | 1:E:229:PHE:CE2  | 2.31                     | 0.66              |
| 2:P:9:ILE:CD1    | 2:P:69:LEU:HD11  | 2.26                     | 0.66              |
| 1:B:548:THR:O    | 5:B:904:3AT:N6   | 2.28                     | 0.66              |
| 1:B:89:ILE:HG22  | 1:B:93:VAL:CG1   | 2.08                     | 0.66              |
| 1:A:225:ILE:HG12 | 1:A:229:PHE:HE2  | 1.60                     | 0.66              |
| 1:A:630:ARG:NH1  | 2:O:83:GLU:HG2   | 2.11                     | 0.66              |
| 1:F:225:ILE:HG12 | 1:F:229:PHE:CE2  | 2.31                     | 0.66              |
| 1:C:225:ILE:HG12 | 1:C:229:PHE:CE2  | 2.31                     | 0.66              |
| 1:C:225:ILE:HG12 | 1:C:229:PHE:HE2  | 1.60                     | 0.66              |
| 1:D:225:ILE:HG12 | 1:D:229:PHE:CE2  | 2.31                     | 0.66              |
| 1:D:278:LYS:O    | 1:D:281:GLU:N    | 2.28                     | 0.66              |
| 1:A:310:GLU:OE2  | 1:A:340:LYS:HD2  | 1.94                     | 0.66              |
| 1:D:310:GLU:OE2  | 1:D:340:LYS:HD2  | 1.95                     | 0.66              |
| 1:D:225:ILE:HG12 | 1:D:229:PHE:HE2  | 1.60                     | 0.66              |
| 1:D:359:PRO:HG2  | 1:D:360:VAL:H    | 1.61                     | 0.66              |
| 2:R:73:ALA:O     | 2:R:76:MET:N     | 2.28                     | 0.66              |
| 1:A:628:PHE:HE2  | 2:O:90:ARG:HD2   | 1.61                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:186:LYS:HE3  | 1:F:234:LEU:HD12 | 1.76                     | 0.66              |
| 1:D:597:ASN:ND2  | 1:D:601:GLU:H    | 1.94                     | 0.66              |
| 1:F:278:LYS:O    | 1:F:281:GLU:N    | 2.28                     | 0.66              |
| 1:A:443:GLU:HG3  | 1:A:458:LYS:HG2  | 1.77                     | 0.66              |
| 1:F:296:LEU:H    | 1:F:296:LEU:CD2  | 1.83                     | 0.66              |
| 1:F:414:LYS:HA   | 1:F:414:LYS:HZ2  | 1.59                     | 0.66              |
| 1:E:225:ILE:HG12 | 1:E:229:PHE:HE2  | 1.60                     | 0.66              |
| 1:F:187:SER:C    | 1:F:188:LEU:O    | 2.28                     | 0.66              |
| 1:A:179:LEU:O    | 1:A:183:SER:CA   | 2.42                     | 0.66              |
| 1:A:182:ILE:O    | 1:A:187:SER:CB   | 2.43                     | 0.66              |
| 1:A:540:ARG:NH1  | 1:A:627:TYR:CE1  | 2.64                     | 0.66              |
| 2:R:97:ASN:HD22  | 2:R:97:ASN:H     | 1.43                     | 0.66              |
| 1:C:197:LYS:O    | 1:C:197:LYS:HD2  | 1.94                     | 0.66              |
| 1:D:175:LYS:O    | 1:D:177:ILE:N    | 2.29                     | 0.65              |
| 1:A:597:ASN:HB2  | 1:A:598:PRO:CD   | 2.22                     | 0.65              |
| 1:E:540:ARG:NH1  | 1:E:627:TYR:CE1  | 2.64                     | 0.65              |
| 1:C:540:ARG:NH1  | 1:C:627:TYR:CE1  | 2.63                     | 0.65              |
| 2:T:18:LEU:HD22  | 2:T:18:LEU:O     | 1.96                     | 0.65              |
| 1:F:107:THR:HG21 | 1:F:115:LYS:CE   | 2.26                     | 0.65              |
| 1:F:630:ARG:CZ   | 2:T:83:GLU:HG2   | 2.27                     | 0.65              |
| 2:R:18:LEU:O     | 2:R:18:LEU:HD22  | 1.96                     | 0.65              |
| 2:S:18:LEU:O     | 2:S:18:LEU:HD22  | 1.97                     | 0.65              |
| 1:C:515:LYS:HE2  | 1:C:515:LYS:O    | 1.96                     | 0.65              |
| 1:C:548:THR:O    | 5:C:905:3AT:N6   | 2.28                     | 0.65              |
| 1:E:175:LYS:O    | 1:E:177:ILE:N    | 2.29                     | 0.65              |
| 1:B:597:ASN:HB2  | 1:B:598:PRO:CD   | 2.24                     | 0.65              |
| 1:A:635:ILE:CD1  | 1:A:635:ILE:H    | 2.00                     | 0.65              |
| 1:C:630:ARG:CZ   | 2:Q:83:GLU:HG2   | 2.25                     | 0.65              |
| 1:C:550:SER:HB3  | 1:C:553:GLN:HB2  | 1.78                     | 0.65              |
| 1:E:107:THR:HG21 | 1:E:115:LYS:CE   | 2.26                     | 0.65              |
| 1:E:199:LEU:O    | 1:E:201:ASP:N    | 2.22                     | 0.65              |
| 1:D:254:ARG:HD2  | 1:D:254:ARG:H    | 1.61                     | 0.65              |
| 1:B:443:GLU:HG3  | 1:B:458:LYS:HG2  | 1.77                     | 0.65              |
| 1:F:77:ASP:O     | 1:F:81:GLN:HB2   | 1.94                     | 0.65              |
| 1:D:213:LYS:HD2  | 1:D:240:ALA:HB1  | 1.77                     | 0.65              |
| 1:B:225:ILE:HG12 | 1:B:229:PHE:CE2  | 2.31                     | 0.65              |
| 2:Q:117:THR:O    | 2:Q:119:GLU:N    | 2.29                     | 0.65              |
| 2:O:117:THR:O    | 2:O:119:GLU:N    | 2.30                     | 0.65              |
| 1:A:412:GLU:O    | 1:A:416:ASN:HB2  | 1.96                     | 0.65              |
| 2:T:9:ILE:CD1    | 2:T:69:LEU:HD11  | 2.27                     | 0.65              |
| 1:F:625:LEU:HD12 | 1:F:625:LEU:C    | 2.17                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:65:PHE:HB2   | 2:T:66:PRO:HD3   | 1.78                     | 0.65              |
| 1:B:686:ASP:HB3  | 1:B:739:LYS:HD2  | 1.79                     | 0.65              |
| 1:A:128:MET:HB2  | 1:A:239:HIS:NE2  | 2.11                     | 0.65              |
| 1:C:199:LEU:O    | 1:C:201:ASP:N    | 2.22                     | 0.65              |
| 1:C:443:GLU:HG3  | 1:C:458:LYS:HG2  | 1.77                     | 0.65              |
| 2:P:13:LYS:HZ3   | 2:P:65:PHE:HB3   | 1.59                     | 0.65              |
| 1:F:709:ASN:HB2  | 2:T:130:ILE:HG23 | 1.78                     | 0.65              |
| 2:T:137:ASN:OD1  | 2:T:139:GLU:HB2  | 1.95                     | 0.65              |
| 1:E:548:THR:O    | 5:E:907:3AT:N6   | 2.30                     | 0.65              |
| 1:D:628:PHE:HE2  | 2:R:90:ARG:HD2   | 1.60                     | 0.65              |
| 1:C:175:LYS:O    | 1:C:177:ILE:N    | 2.29                     | 0.65              |
| 1:A:225:ILE:HG12 | 1:A:229:PHE:CE2  | 2.31                     | 0.65              |
| 1:A:550:SER:HB3  | 1:A:553:GLN:HB2  | 1.78                     | 0.65              |
| 1:C:630:ARG:NH1  | 2:Q:83:GLU:HG2   | 2.11                     | 0.65              |
| 1:B:630:ARG:NH1  | 2:P:83:GLU:HG2   | 2.12                     | 0.65              |
| 1:D:718:ARG:NH1  | 1:D:767:GLN:NE2  | 2.44                     | 0.65              |
| 1:C:724:ARG:HG3  | 1:C:724:ARG:NH1  | 2.11                     | 0.65              |
| 1:D:493:ASP:OD2  | 1:D:577:HIS:HE1  | 1.77                     | 0.65              |
| 2:Q:9:ILE:CD1    | 2:Q:69:LEU:HD11  | 2.26                     | 0.65              |
| 1:F:115:LYS:HZ1  | 1:F:116:GLU:H    | 1.45                     | 0.65              |
| 1:F:412:GLU:O    | 1:F:416:ASN:HB2  | 1.96                     | 0.65              |
| 1:B:105:TYR:N    | 1:B:152:LEU:O    | 2.25                     | 0.65              |
| 1:D:625:LEU:C    | 1:D:625:LEU:HD12 | 2.16                     | 0.65              |
| 1:A:515:LYS:O    | 1:A:515:LYS:HE2  | 1.97                     | 0.65              |
| 2:O:137:ASN:OD1  | 2:O:139:GLU:HB2  | 1.96                     | 0.65              |
| 1:D:141:PHE:CD1  | 1:D:141:PHE:N    | 2.65                     | 0.65              |
| 1:B:130:SER:HB2  | 1:B:170:TYR:CZ   | 2.32                     | 0.65              |
| 1:E:722:ILE:HG23 | 1:E:760:VAL:HG13 | 1.79                     | 0.65              |
| 1:B:463:THR:HG22 | 1:B:465:LEU:N    | 2.11                     | 0.65              |
| 2:Q:88:ALA:O     | 2:Q:91:VAL:HB    | 1.97                     | 0.65              |
| 2:S:65:PHE:HB2   | 2:S:66:PRO:HD3   | 1.78                     | 0.65              |
| 1:E:427:ASP:O    | 1:E:428:ASN:HB2  | 1.96                     | 0.65              |
| 1:D:186:LYS:CE   | 1:D:234:LEU:HD12 | 2.26                     | 0.65              |
| 1:C:359:PRO:HG2  | 1:C:360:VAL:H    | 1.62                     | 0.65              |
| 1:F:427:ASP:O    | 1:F:428:ASN:HB2  | 1.96                     | 0.65              |
| 1:D:427:ASP:O    | 1:D:428:ASN:HB2  | 1.96                     | 0.65              |
| 1:E:184:LYS:HE3  | 1:E:191:GLU:HB2  | 1.79                     | 0.65              |
| 1:E:412:GLU:O    | 1:E:416:ASN:HB2  | 1.97                     | 0.65              |
| 1:B:724:ARG:NH1  | 1:B:724:ARG:HG3  | 2.12                     | 0.65              |
| 2:O:18:LEU:O     | 2:O:18:LEU:HD22  | 1.96                     | 0.65              |
| 1:D:345:THR:HB   | 1:D:491:ASP:HB3  | 1.79                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:188:LEU:HD22 | 1:F:188:LEU:H    | 1.55                     | 0.64              |
| 1:A:176:GLY:C    | 1:A:178:SER:H    | 2.00                     | 0.64              |
| 2:R:117:THR:O    | 2:R:119:GLU:N    | 2.30                     | 0.64              |
| 2:S:117:THR:O    | 2:S:119:GLU:N    | 2.30                     | 0.64              |
| 1:B:550:SER:HB3  | 1:B:553:GLN:HB2  | 1.78                     | 0.64              |
| 1:B:345:THR:HG22 | 1:B:490:ALA:O    | 1.98                     | 0.64              |
| 1:F:550:SER:HB3  | 1:F:553:GLN:HB2  | 1.79                     | 0.64              |
| 1:A:463:THR:HG22 | 1:A:465:LEU:N    | 2.10                     | 0.64              |
| 1:E:278:LYS:O    | 1:E:281:GLU:N    | 2.29                     | 0.64              |
| 1:E:408:LEU:H    | 1:E:408:LEU:CD1  | 2.09                     | 0.64              |
| 1:B:515:LYS:O    | 1:B:515:LYS:HE2  | 1.97                     | 0.64              |
| 1:A:686:ASP:HB3  | 1:A:739:LYS:HD2  | 1.79                     | 0.64              |
| 1:C:345:THR:HB   | 1:C:491:ASP:HB3  | 1.79                     | 0.64              |
| 1:C:628:PHE:HE2  | 2:Q:90:ARG:HD2   | 1.62                     | 0.64              |
| 1:E:515:LYS:O    | 1:E:515:LYS:HE2  | 1.97                     | 0.64              |
| 1:F:722:ILE:HG23 | 1:F:760:VAL:HG13 | 1.78                     | 0.64              |
| 1:B:412:GLU:O    | 1:B:416:ASN:HB2  | 1.97                     | 0.64              |
| 1:E:760:VAL:O    | 1:E:764:LEU:HG   | 1.98                     | 0.64              |
| 1:A:153:ILE:O    | 1:A:154:ILE:HD13 | 1.97                     | 0.64              |
| 2:S:48:LEU:HA    | 2:S:51:MET:HE1   | 1.79                     | 0.64              |
| 2:R:9:ILE:CD1    | 2:R:69:LEU:HD11  | 2.27                     | 0.64              |
| 1:D:550:SER:HB3  | 1:D:553:GLN:HB2  | 1.78                     | 0.64              |
| 1:F:724:ARG:NH1  | 1:F:724:ARG:HG3  | 2.10                     | 0.64              |
| 1:F:443:GLU:HG3  | 1:F:458:LYS:HG2  | 1.77                     | 0.64              |
| 1:F:540:ARG:NH1  | 1:F:627:TYR:CE1  | 2.66                     | 0.64              |
| 1:C:472:ARG:NH1  | 1:C:472:ARG:HB3  | 2.13                     | 0.64              |
| 1:A:345:THR:HB   | 1:A:491:ASP:HB3  | 1.78                     | 0.64              |
| 1:B:628:PHE:HE2  | 2:P:90:ARG:HD2   | 1.62                     | 0.64              |
| 1:C:427:ASP:O    | 1:C:428:ASN:HB2  | 1.96                     | 0.64              |
| 1:D:630:ARG:NH1  | 2:R:83:GLU:HG2   | 2.12                     | 0.64              |
| 1:D:408:LEU:H    | 1:D:408:LEU:CD1  | 2.10                     | 0.64              |
| 1:E:625:LEU:C    | 1:E:625:LEU:HD12 | 2.17                     | 0.64              |
| 1:D:472:ARG:HB3  | 1:D:472:ARG:NH1  | 2.13                     | 0.64              |
| 1:F:345:THR:HG22 | 1:F:490:ALA:O    | 1.97                     | 0.64              |
| 1:A:427:ASP:O    | 1:A:428:ASN:HB2  | 1.96                     | 0.64              |
| 1:C:223:LYS:NZ   | 1:C:228:ASN:HB3  | 2.13                     | 0.64              |
| 1:E:609:GLU:N    | 1:E:609:GLU:OE2  | 2.30                     | 0.64              |
| 1:D:184:LYS:HZ1  | 1:D:191:GLU:HB2  | 1.59                     | 0.64              |
| 1:B:722:ILE:HG23 | 1:B:760:VAL:HG13 | 1.78                     | 0.64              |
| 1:E:142:VAL:CG2  | 1:E:154:ILE:HD12 | 2.26                     | 0.64              |
| 1:F:105:TYR:N    | 1:F:152:LEU:O    | 2.25                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:550:SER:HB3  | 1:E:553:GLN:HB2  | 1.78                     | 0.64              |
| 2:O:48:LEU:HA    | 2:O:51:MET:HE1   | 1.80                     | 0.64              |
| 1:A:268:MET:O    | 1:A:271:LEU:HB2  | 1.97                     | 0.64              |
| 1:E:472:ARG:HB3  | 1:E:472:ARG:NH1  | 2.13                     | 0.64              |
| 1:E:628:PHE:HE2  | 2:S:90:ARG:HD2   | 1.60                     | 0.64              |
| 1:F:628:PHE:HE2  | 2:T:90:ARG:HD2   | 1.63                     | 0.64              |
| 2:T:117:THR:O    | 2:T:119:GLU:N    | 2.30                     | 0.64              |
| 1:C:408:LEU:H    | 1:C:408:LEU:CD1  | 2.10                     | 0.64              |
| 1:C:625:LEU:C    | 1:C:625:LEU:HD12 | 2.17                     | 0.64              |
| 2:R:13:LYS:HZ3   | 2:R:65:PHE:HB3   | 1.61                     | 0.64              |
| 1:D:609:GLU:OE2  | 1:D:609:GLU:N    | 2.30                     | 0.64              |
| 1:B:90:PRO:O     | 1:B:92:ASP:N     | 2.31                     | 0.64              |
| 2:P:117:THR:C    | 2:P:119:GLU:H    | 2.00                     | 0.64              |
| 1:D:412:GLU:O    | 1:D:416:ASN:HB2  | 1.97                     | 0.64              |
| 1:F:630:ARG:NH1  | 2:T:83:GLU:HG2   | 2.13                     | 0.64              |
| 1:F:225:ILE:HG12 | 1:F:229:PHE:HE2  | 1.60                     | 0.64              |
| 2:S:32:LEU:HD21  | 2:S:71:MET:CE    | 2.28                     | 0.64              |
| 1:E:359:PRO:HG2  | 1:E:360:VAL:H    | 1.62                     | 0.64              |
| 1:B:625:LEU:HD12 | 1:B:625:LEU:C    | 2.17                     | 0.64              |
| 1:D:223:LYS:NZ   | 1:D:228:ASN:HB3  | 2.13                     | 0.64              |
| 1:C:412:GLU:O    | 1:C:416:ASN:HB2  | 1.97                     | 0.64              |
| 2:O:117:THR:C    | 2:O:119:GLU:H    | 2.01                     | 0.64              |
| 1:A:722:ILE:HG23 | 1:A:760:VAL:HG13 | 1.77                     | 0.64              |
| 1:F:153:ILE:O    | 1:F:154:ILE:HD13 | 1.97                     | 0.64              |
| 2:T:88:ALA:O     | 2:T:91:VAL:HB    | 1.98                     | 0.64              |
| 1:B:472:ARG:HB3  | 1:B:472:ARG:NH1  | 2.13                     | 0.64              |
| 2:P:65:PHE:HB2   | 2:P:66:PRO:HD3   | 1.78                     | 0.64              |
| 1:F:345:THR:HB   | 1:F:491:ASP:HB3  | 1.79                     | 0.64              |
| 1:B:400:LYS:HE2  | 1:B:475:GLU:OE2  | 1.98                     | 0.64              |
| 1:F:184:LYS:HZ1  | 1:F:191:GLU:HB2  | 1.59                     | 0.64              |
| 1:E:718:ARG:HH12 | 1:E:767:GLN:HE21 | 1.45                     | 0.64              |
| 1:D:630:ARG:CZ   | 2:R:83:GLU:HG2   | 2.28                     | 0.64              |
| 2:R:70:THR:O     | 2:R:72:MET:N     | 2.31                     | 0.64              |
| 2:P:48:LEU:HA    | 2:P:51:MET:HE1   | 1.80                     | 0.64              |
| 1:E:724:ARG:HG3  | 1:E:724:ARG:NH1  | 2.11                     | 0.64              |
| 1:C:268:MET:O    | 1:C:271:LEU:HB2  | 1.98                     | 0.64              |
| 1:F:268:MET:O    | 1:F:271:LEU:HB2  | 1.98                     | 0.64              |
| 1:A:400:LYS:HE2  | 1:A:475:GLU:OE2  | 1.98                     | 0.64              |
| 1:F:515:LYS:O    | 1:F:515:LYS:HE2  | 1.98                     | 0.64              |
| 1:B:223:LYS:NZ   | 1:B:228:ASN:HB3  | 2.13                     | 0.64              |
| 1:D:515:LYS:O    | 1:D:515:LYS:HE2  | 1.97                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:709:ASN:HB2  | 2:R:130:ILE:HG23 | 1.80                     | 0.64              |
| 1:F:141:PHE:CD1  | 1:F:141:PHE:N    | 2.66                     | 0.64              |
| 1:C:141:PHE:CD1  | 1:C:141:PHE:N    | 2.65                     | 0.64              |
| 1:B:191:GLU:O    | 1:B:192:PHE:C    | 2.33                     | 0.64              |
| 1:F:760:VAL:O    | 1:F:764:LEU:HG   | 1.98                     | 0.64              |
| 1:E:153:ILE:O    | 1:E:154:ILE:HD13 | 1.98                     | 0.64              |
| 1:E:268:MET:O    | 1:E:271:LEU:HB2  | 1.97                     | 0.64              |
| 2:Q:44:THR:C     | 2:Q:46:ALA:H     | 2.01                     | 0.64              |
| 1:D:400:LYS:HE2  | 1:D:475:GLU:OE2  | 1.98                     | 0.64              |
| 1:C:173:ILE:O    | 1:C:175:LYS:N    | 2.30                     | 0.63              |
| 2:T:70:THR:O     | 2:T:72:MET:N     | 2.31                     | 0.63              |
| 1:B:359:PRO:HG2  | 1:B:360:VAL:H    | 1.63                     | 0.63              |
| 2:Q:97:ASN:HD22  | 2:Q:97:ASN:N     | 1.92                     | 0.63              |
| 1:A:625:LEU:HD12 | 1:A:625:LEU:C    | 2.18                     | 0.63              |
| 1:B:540:ARG:HD3  | 1:B:627:TYR:CZ   | 2.34                     | 0.63              |
| 1:C:375:GLY:HA2  | 1:C:464:VAL:HG11 | 1.80                     | 0.63              |
| 1:A:548:THR:O    | 5:A:903:3AT:N6   | 2.30                     | 0.63              |
| 1:E:141:PHE:N    | 1:E:141:PHE:CD1  | 2.66                     | 0.63              |
| 1:E:296:LEU:CD2  | 1:E:296:LEU:H    | 1.83                     | 0.63              |
| 1:F:759:GLN:HE21 | 1:F:763:LEU:HD11 | 1.64                     | 0.63              |
| 1:C:597:ASN:HB2  | 1:C:598:PRO:CD   | 2.23                     | 0.63              |
| 1:D:142:VAL:CG2  | 1:D:154:ILE:HD12 | 2.25                     | 0.63              |
| 1:F:408:LEU:H    | 1:F:408:LEU:CD1  | 2.10                     | 0.63              |
| 1:B:540:ARG:NH1  | 1:B:627:TYR:CE1  | 2.65                     | 0.63              |
| 2:Q:65:PHE:HB2   | 2:Q:66:PRO:HD3   | 1.79                     | 0.63              |
| 2:O:88:ALA:O     | 2:O:91:VAL:HB    | 1.97                     | 0.63              |
| 1:B:709:ASN:HB2  | 2:P:130:ILE:HG23 | 1.80                     | 0.63              |
| 1:D:189:ASP:O    | 1:D:190:PRO:C    | 2.33                     | 0.63              |
| 1:D:96:ILE:HG22  | 1:D:100:LEU:HD11 | 1.80                     | 0.63              |
| 2:T:117:THR:C    | 2:T:119:GLU:H    | 2.02                     | 0.63              |
| 1:A:70:GLU:CB    | 1:A:107:THR:HG22 | 2.24                     | 0.63              |
| 1:F:325:TYR:CE1  | 1:F:598:PRO:HD3  | 2.34                     | 0.63              |
| 2:T:32:LEU:HD21  | 2:T:71:MET:CE    | 2.28                     | 0.63              |
| 1:C:136:PRO:HG2  | 1:C:139:SER:OG   | 1.99                     | 0.63              |
| 2:R:48:LEU:HA    | 2:R:51:MET:HE1   | 1.80                     | 0.63              |
| 1:F:400:LYS:HE2  | 1:F:475:GLU:OE2  | 1.98                     | 0.63              |
| 1:E:223:LYS:NZ   | 1:E:228:ASN:HB3  | 2.13                     | 0.63              |
| 1:E:175:LYS:HB2  | 1:E:175:LYS:HZ2  | 1.60                     | 0.63              |
| 2:R:117:THR:C    | 2:R:119:GLU:H    | 2.02                     | 0.63              |
| 1:A:325:TYR:CE1  | 1:A:598:PRO:HD3  | 2.34                     | 0.63              |
| 1:F:463:THR:HG22 | 1:F:465:LEU:N    | 2.10                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:724:ARG:HG3  | 1:A:724:ARG:NH1  | 2.11                     | 0.63              |
| 1:A:408:LEU:H    | 1:A:408:LEU:CD1  | 2.09                     | 0.63              |
| 1:F:472:ARG:NH1  | 1:F:472:ARG:HB3  | 2.13                     | 0.63              |
| 1:B:301:ALA:C    | 1:B:303:LYS:H    | 2.02                     | 0.63              |
| 2:R:65:PHE:HB2   | 2:R:66:PRO:HD3   | 1.78                     | 0.63              |
| 1:E:230:ILE:HG13 | 1:E:237:PHE:CE2  | 2.34                     | 0.63              |
| 1:E:345:THR:HG22 | 1:E:490:ALA:O    | 1.98                     | 0.63              |
| 1:F:96:ILE:HG22  | 1:F:100:LEU:HD11 | 1.80                     | 0.63              |
| 1:B:184:LYS:HZ3  | 1:B:193:LEU:HD12 | 1.63                     | 0.63              |
| 1:E:409:ARG:NE   | 1:E:413:LEU:HD21 | 2.14                     | 0.63              |
| 1:C:115:LYS:HZ3  | 1:C:116:GLU:H    | 1.46                     | 0.63              |
| 2:S:70:THR:O     | 2:S:72:MET:N     | 2.31                     | 0.63              |
| 2:O:32:LEU:HD21  | 2:O:71:MET:CE    | 2.29                     | 0.63              |
| 1:B:712:PHE:CD1  | 1:B:716:LYS:HG2  | 2.34                     | 0.63              |
| 2:R:97:ASN:HD22  | 2:R:97:ASN:N     | 1.94                     | 0.63              |
| 1:D:560:LEU:O    | 1:D:563:ALA:HB3  | 1.99                     | 0.63              |
| 1:C:128:MET:HB2  | 1:C:239:HIS:CE1  | 2.33                     | 0.63              |
| 1:D:409:ARG:NE   | 1:D:413:LEU:HD21 | 2.14                     | 0.63              |
| 2:Q:48:LEU:HA    | 2:Q:51:MET:HE1   | 1.81                     | 0.63              |
| 1:B:493:ASP:OD2  | 1:B:577:HIS:HE1  | 1.77                     | 0.63              |
| 1:C:400:LYS:HE2  | 1:C:475:GLU:OE2  | 1.98                     | 0.63              |
| 1:A:517:VAL:HB   | 1:A:525:LYS:NZ   | 2.13                     | 0.63              |
| 1:D:184:LYS:CE   | 1:D:191:GLU:HB2  | 2.28                     | 0.63              |
| 1:E:301:ALA:C    | 1:E:303:LYS:H    | 2.02                     | 0.63              |
| 2:Q:117:THR:C    | 2:Q:119:GLU:H    | 2.01                     | 0.63              |
| 2:R:32:LEU:HD21  | 2:R:71:MET:CE    | 2.29                     | 0.63              |
| 1:B:499:PRO:CG   | 1:B:504:ILE:HD11 | 2.29                     | 0.63              |
| 1:F:735:VAL:O    | 1:F:738:SER:HB2  | 1.99                     | 0.63              |
| 1:B:517:VAL:HB   | 1:B:525:LYS:NZ   | 2.14                     | 0.63              |
| 1:C:709:ASN:HB2  | 2:Q:130:ILE:HG23 | 1.81                     | 0.63              |
| 1:F:191:GLU:O    | 1:F:192:PHE:C    | 2.36                     | 0.63              |
| 1:A:185:ASP:O    | 1:A:190:PRO:HG3  | 1.99                     | 0.63              |
| 1:A:760:VAL:O    | 1:A:764:LEU:HG   | 1.98                     | 0.63              |
| 2:R:88:ALA:O     | 2:R:91:VAL:HB    | 1.99                     | 0.63              |
| 1:F:712:PHE:CD1  | 1:F:716:LYS:HG2  | 2.34                     | 0.63              |
| 2:O:65:PHE:HB2   | 2:O:66:PRO:HD3   | 1.79                     | 0.63              |
| 1:B:427:ASP:O    | 1:B:428:ASN:HB2  | 1.96                     | 0.63              |
| 1:F:375:GLY:HA2  | 1:F:464:VAL:HG11 | 1.81                     | 0.63              |
| 1:E:96:ILE:HG22  | 1:E:100:LEU:HD11 | 1.81                     | 0.63              |
| 1:B:760:VAL:O    | 1:B:764:LEU:HG   | 1.98                     | 0.63              |
| 1:E:718:ARG:NH1  | 1:E:767:GLN:NE2  | 2.47                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:32:LEU:HD21  | 2:P:71:MET:CE    | 2.29                     | 0.63              |
| 2:P:88:ALA:O     | 2:P:91:VAL:HB    | 1.99                     | 0.63              |
| 1:E:173:ILE:O    | 1:E:175:LYS:N    | 2.32                     | 0.62              |
| 1:F:191:GLU:O    | 1:F:193:LEU:N    | 2.32                     | 0.62              |
| 1:B:173:ILE:O    | 1:B:175:LYS:N    | 2.32                     | 0.62              |
| 2:S:117:THR:C    | 2:S:119:GLU:H    | 2.02                     | 0.62              |
| 1:A:115:LYS:HZ1  | 1:A:116:GLU:N    | 1.97                     | 0.62              |
| 1:B:409:ARG:NE   | 1:B:413:LEU:HD21 | 2.14                     | 0.62              |
| 1:F:70:GLU:CB    | 1:F:107:THR:HG22 | 2.26                     | 0.62              |
| 1:B:153:ILE:O    | 1:B:154:ILE:HD13 | 1.99                     | 0.62              |
| 1:E:712:PHE:CD1  | 1:E:716:LYS:HG2  | 2.34                     | 0.62              |
| 1:C:301:ALA:C    | 1:C:303:LYS:H    | 2.02                     | 0.62              |
| 1:F:217:LYS:HZ2  | 1:F:236:GLU:HG3  | 1.62                     | 0.62              |
| 2:T:13:LYS:HZ3   | 2:T:65:PHE:HB3   | 1.63                     | 0.62              |
| 1:E:76:LEU:O     | 1:E:80:GLN:HB2   | 1.98                     | 0.62              |
| 1:C:76:LEU:O     | 1:C:80:GLN:HB2   | 1.99                     | 0.62              |
| 1:C:517:VAL:HB   | 1:C:525:LYS:NZ   | 2.14                     | 0.62              |
| 1:E:709:ASN:HB2  | 2:S:130:ILE:HG23 | 1.81                     | 0.62              |
| 1:F:173:ILE:O    | 1:F:175:LYS:N    | 2.32                     | 0.62              |
| 1:F:213:LYS:HD2  | 1:F:240:ALA:HB1  | 1.80                     | 0.62              |
| 1:F:89:ILE:HG22  | 1:F:93:VAL:CG1   | 2.08                     | 0.62              |
| 1:A:173:ILE:O    | 1:A:175:LYS:N    | 2.32                     | 0.62              |
| 1:D:325:TYR:CE1  | 1:D:598:PRO:HD3  | 2.34                     | 0.62              |
| 1:E:630:ARG:NH1  | 2:S:83:GLU:HG2   | 2.14                     | 0.62              |
| 1:A:635:ILE:HD12 | 1:A:635:ILE:N    | 2.09                     | 0.62              |
| 1:C:153:ILE:O    | 1:C:154:ILE:HD13 | 1.99                     | 0.62              |
| 1:F:635:ILE:N    | 1:F:635:ILE:HD12 | 2.09                     | 0.62              |
| 1:A:359:PRO:HG2  | 1:A:360:VAL:H    | 1.63                     | 0.62              |
| 2:Q:32:LEU:HD21  | 2:Q:71:MET:CE    | 2.29                     | 0.62              |
| 1:A:345:THR:HG22 | 1:A:490:ALA:O    | 1.99                     | 0.62              |
| 1:A:560:LEU:O    | 1:A:563:ALA:HB3  | 1.98                     | 0.62              |
| 1:B:345:THR:HB   | 1:B:491:ASP:HB3  | 1.79                     | 0.62              |
| 2:P:70:THR:O     | 2:P:72:MET:N     | 2.32                     | 0.62              |
| 1:D:268:MET:O    | 1:D:271:LEU:HB2  | 1.98                     | 0.62              |
| 1:B:408:LEU:CD1  | 1:B:408:LEU:H    | 2.10                     | 0.62              |
| 1:A:443:GLU:HG2  | 1:A:458:LYS:HE3  | 1.81                     | 0.62              |
| 1:B:742:ALA:HB1  | 1:B:744:GLU:OE1  | 2.00                     | 0.62              |
| 1:D:76:LEU:O     | 1:D:80:GLN:HB2   | 1.99                     | 0.62              |
| 1:A:375:GLY:HA2  | 1:A:464:VAL:HG11 | 1.81                     | 0.62              |
| 1:B:375:GLY:HA2  | 1:B:464:VAL:HG11 | 1.80                     | 0.62              |
| 1:E:189:ASP:O    | 1:E:190:PRO:C    | 2.36                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:722:ILE:HD11 | 1:B:763:LEU:O    | 1.99                     | 0.62              |
| 1:E:630:ARG:CZ   | 2:S:83:GLU:HG2   | 2.30                     | 0.62              |
| 1:E:325:TYR:CE1  | 1:E:598:PRO:HD3  | 2.34                     | 0.62              |
| 1:A:105:TYR:N    | 1:A:152:LEU:O    | 2.25                     | 0.62              |
| 1:D:463:THR:HG22 | 1:D:465:LEU:N    | 2.10                     | 0.62              |
| 2:O:70:THR:O     | 2:O:72:MET:N     | 2.32                     | 0.62              |
| 1:E:499:PRO:CG   | 1:E:504:ILE:HD11 | 2.29                     | 0.62              |
| 1:A:223:LYS:NZ   | 1:A:228:ASN:HB3  | 2.13                     | 0.62              |
| 1:D:375:GLY:HA2  | 1:D:464:VAL:HG11 | 1.81                     | 0.62              |
| 1:E:560:LEU:O    | 1:E:563:ALA:HB3  | 1.99                     | 0.62              |
| 1:F:76:LEU:O     | 1:F:80:GLN:HB2   | 1.98                     | 0.62              |
| 1:A:88:LYS:NZ    | 1:A:172:GLU:OE1  | 2.32                     | 0.62              |
| 1:F:301:ALA:C    | 1:F:303:LYS:H    | 2.03                     | 0.62              |
| 1:D:153:ILE:O    | 1:D:154:ILE:HD13 | 1.99                     | 0.62              |
| 1:D:332:ASN:HD21 | 1:D:334:LEU:HD13 | 1.65                     | 0.62              |
| 1:A:540:ARG:HD3  | 1:A:627:TYR:CZ   | 2.35                     | 0.62              |
| 1:A:76:LEU:O     | 1:A:80:GLN:HB2   | 1.98                     | 0.62              |
| 1:C:345:THR:HG22 | 1:C:490:ALA:O    | 1.99                     | 0.62              |
| 1:B:560:LEU:O    | 1:B:563:ALA:HB3  | 1.99                     | 0.62              |
| 1:E:375:GLY:HA2  | 1:E:464:VAL:HG11 | 1.81                     | 0.62              |
| 1:F:223:LYS:NZ   | 1:F:228:ASN:HB3  | 2.13                     | 0.62              |
| 1:B:69:THR:HA    | 1:B:106:PHE:O    | 1.99                     | 0.62              |
| 1:D:301:ALA:C    | 1:D:303:LYS:N    | 2.53                     | 0.62              |
| 1:C:712:PHE:CD1  | 1:C:716:LYS:HG2  | 2.35                     | 0.62              |
| 2:T:48:LEU:HA    | 2:T:51:MET:HE1   | 1.81                     | 0.62              |
| 1:E:463:THR:HG22 | 1:E:465:LEU:N    | 2.11                     | 0.62              |
| 1:F:359:PRO:HG2  | 1:F:360:VAL:H    | 1.63                     | 0.62              |
| 1:B:268:MET:O    | 1:B:271:LEU:HB2  | 1.99                     | 0.62              |
| 1:A:472:ARG:NH1  | 1:A:472:ARG:HB3  | 2.13                     | 0.62              |
| 1:A:712:PHE:CD1  | 1:A:716:LYS:HG2  | 2.35                     | 0.62              |
| 1:A:742:ALA:HB1  | 1:A:744:GLU:OE1  | 2.00                     | 0.62              |
| 1:E:400:LYS:HE2  | 1:E:475:GLU:OE2  | 1.98                     | 0.62              |
| 1:D:173:ILE:O    | 1:D:175:LYS:N    | 2.32                     | 0.62              |
| 1:F:90:PRO:O     | 1:F:92:ASP:N     | 2.33                     | 0.62              |
| 1:B:239:HIS:O    | 1:B:243:LEU:HG   | 2.00                     | 0.62              |
| 1:A:213:LYS:HD2  | 1:A:240:ALA:HB1  | 1.80                     | 0.62              |
| 1:B:325:TYR:CE1  | 1:B:598:PRO:HD3  | 2.34                     | 0.62              |
| 1:D:760:VAL:O    | 1:D:764:LEU:HG   | 1.99                     | 0.62              |
| 1:D:540:ARG:HD3  | 1:D:627:TYR:CZ   | 2.35                     | 0.62              |
| 1:E:345:THR:HB   | 1:E:491:ASP:HB3  | 1.80                     | 0.62              |
| 1:B:182:ILE:O    | 1:B:187:SER:OG   | 2.17                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:GLY:HA2  | 1:A:150:PRO:O    | 2.00                     | 0.62              |
| 1:A:182:ILE:C    | 1:A:187:SER:HB2  | 2.19                     | 0.62              |
| 1:F:301:ALA:C    | 1:F:303:LYS:N    | 2.53                     | 0.62              |
| 1:A:409:ARG:NE   | 1:A:413:LEU:HD21 | 2.15                     | 0.62              |
| 1:C:657:ILE:HG23 | 1:C:657:ILE:O    | 1.98                     | 0.62              |
| 1:F:409:ARG:NE   | 1:F:413:LEU:HD21 | 2.14                     | 0.62              |
| 2:S:88:ALA:O     | 2:S:91:VAL:HB    | 1.99                     | 0.62              |
| 2:S:44:THR:C     | 2:S:46:ALA:H     | 2.01                     | 0.62              |
| 1:D:102:GLY:HA2  | 1:D:150:PRO:O    | 2.00                     | 0.62              |
| 1:C:293:ILE:O    | 1:C:295:VAL:HG22 | 1.99                     | 0.62              |
| 1:C:409:ARG:NE   | 1:C:413:LEU:HD21 | 2.14                     | 0.62              |
| 1:B:115:LYS:HZ1  | 1:B:116:GLU:H    | 1.47                     | 0.62              |
| 2:Q:70:THR:O     | 2:Q:72:MET:N     | 2.33                     | 0.62              |
| 1:C:540:ARG:HD3  | 1:C:627:TYR:CZ   | 2.35                     | 0.62              |
| 2:R:44:THR:C     | 2:R:46:ALA:H     | 2.02                     | 0.62              |
| 2:T:44:THR:C     | 2:T:46:ALA:H     | 2.02                     | 0.62              |
| 1:B:672:ARG:O    | 1:B:672:ARG:HD2  | 2.00                     | 0.62              |
| 1:B:141:PHE:N    | 1:B:141:PHE:CD1  | 2.66                     | 0.62              |
| 1:F:179:LEU:C    | 1:F:183:SER:HB2  | 2.06                     | 0.62              |
| 1:C:325:TYR:CE1  | 1:C:598:PRO:HD3  | 2.34                     | 0.62              |
| 1:A:722:ILE:HD11 | 1:A:763:LEU:O    | 2.00                     | 0.62              |
| 1:D:712:PHE:CD1  | 1:D:716:LYS:HG2  | 2.35                     | 0.62              |
| 2:P:44:THR:C     | 2:P:46:ALA:H     | 2.02                     | 0.62              |
| 1:C:672:ARG:O    | 1:C:672:ARG:HD2  | 2.00                     | 0.62              |
| 1:F:672:ARG:O    | 1:F:672:ARG:HD2  | 2.00                     | 0.62              |
| 1:C:560:LEU:O    | 1:C:563:ALA:HB3  | 2.00                     | 0.62              |
| 1:F:186:LYS:CE   | 1:F:234:LEU:HD12 | 2.30                     | 0.61              |
| 1:C:96:ILE:HG22  | 1:C:100:LEU:HD11 | 1.81                     | 0.61              |
| 1:C:239:HIS:O    | 1:C:243:LEU:HG   | 1.99                     | 0.61              |
| 1:C:90:PRO:O     | 1:C:92:ASP:N     | 2.33                     | 0.61              |
| 1:A:189:ASP:O    | 1:A:190:PRO:C    | 2.36                     | 0.61              |
| 1:C:118:GLN:HA   | 1:C:118:GLN:OE1  | 2.00                     | 0.61              |
| 1:F:742:ALA:HB1  | 1:F:744:GLU:OE1  | 2.00                     | 0.61              |
| 1:A:141:PHE:N    | 1:A:141:PHE:CD1  | 2.66                     | 0.61              |
| 1:E:90:PRO:O     | 1:E:92:ASP:N     | 2.33                     | 0.61              |
| 1:F:297:LYS:NZ   | 1:F:297:LYS:HB3  | 2.15                     | 0.61              |
| 1:C:301:ALA:C    | 1:C:303:LYS:N    | 2.53                     | 0.61              |
| 2:O:44:THR:C     | 2:O:46:ALA:H     | 2.01                     | 0.61              |
| 1:D:345:THR:HG22 | 1:D:490:ALA:O    | 2.00                     | 0.61              |
| 1:A:672:ARG:O    | 1:A:672:ARG:HD2  | 2.00                     | 0.61              |
| 1:D:239:HIS:O    | 1:D:243:LEU:HG   | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:297:LYS:NZ   | 1:A:297:LYS:HB3  | 2.15                     | 0.61              |
| 1:C:722:ILE:HD11 | 1:C:763:LEU:O    | 2.00                     | 0.61              |
| 1:C:499:PRO:CG   | 1:C:504:ILE:HD11 | 2.29                     | 0.61              |
| 1:A:499:PRO:CG   | 1:A:504:ILE:HD11 | 2.29                     | 0.61              |
| 2:S:97:ASN:N     | 2:S:97:ASN:HD22  | 1.94                     | 0.61              |
| 1:E:742:ALA:HB1  | 1:E:744:GLU:OE1  | 1.99                     | 0.61              |
| 1:B:76:LEU:O     | 1:B:80:GLN:HB2   | 2.00                     | 0.61              |
| 1:E:213:LYS:HD2  | 1:E:240:ALA:HB1  | 1.81                     | 0.61              |
| 1:D:185:ASP:O    | 1:D:190:PRO:HG3  | 1.99                     | 0.61              |
| 1:C:189:ASP:O    | 1:C:191:GLU:N    | 2.33                     | 0.61              |
| 1:B:102:GLY:CA   | 1:B:150:PRO:HG2  | 2.30                     | 0.61              |
| 1:A:96:ILE:HG22  | 1:A:100:LEU:HD11 | 1.80                     | 0.61              |
| 1:F:293:ILE:O    | 1:F:295:VAL:HG22 | 2.01                     | 0.61              |
| 1:B:297:LYS:HB3  | 1:B:297:LYS:NZ   | 2.15                     | 0.61              |
| 1:F:540:ARG:HD3  | 1:F:627:TYR:CZ   | 2.36                     | 0.61              |
| 1:C:324:THR:CB   | 1:C:499:PRO:HA   | 2.31                     | 0.61              |
| 1:F:377:GLN:O    | 1:F:381:GLU:HB2  | 2.01                     | 0.61              |
| 1:F:607:ASN:HB3  | 1:F:609:GLU:OE2  | 2.00                     | 0.61              |
| 1:E:517:VAL:HB   | 1:E:525:LYS:NZ   | 2.14                     | 0.61              |
| 1:E:672:ARG:HD2  | 1:E:672:ARG:O    | 2.00                     | 0.61              |
| 1:E:184:LYS:NZ   | 1:E:191:GLU:CB   | 2.60                     | 0.61              |
| 1:A:90:PRO:O     | 1:A:92:ASP:N     | 2.33                     | 0.61              |
| 2:T:106:ARG:CG   | 2:T:121:VAL:HG21 | 2.06                     | 0.61              |
| 1:F:722:ILE:HD11 | 1:F:763:LEU:O    | 2.00                     | 0.61              |
| 1:B:718:ARG:HH12 | 1:B:767:GLN:HE21 | 1.46                     | 0.61              |
| 1:D:724:ARG:HG3  | 1:D:724:ARG:NH1  | 2.11                     | 0.61              |
| 1:B:443:GLU:HG2  | 1:B:458:LYS:HE3  | 1.83                     | 0.61              |
| 1:E:69:THR:HA    | 1:E:106:PHE:O    | 2.00                     | 0.61              |
| 1:C:88:LYS:NZ    | 1:C:172:GLU:OE1  | 2.33                     | 0.61              |
| 1:A:607:ASN:HB3  | 1:A:609:GLU:OE2  | 2.00                     | 0.61              |
| 1:A:609:GLU:OE2  | 1:A:609:GLU:N    | 2.31                     | 0.61              |
| 1:C:735:VAL:O    | 1:C:738:SER:HB2  | 2.01                     | 0.61              |
| 2:O:13:LYS:HZ1   | 2:O:65:PHE:CB    | 2.14                     | 0.61              |
| 1:E:607:ASN:HB3  | 1:E:609:GLU:OE2  | 2.00                     | 0.61              |
| 1:F:560:LEU:O    | 1:F:563:ALA:HB3  | 2.00                     | 0.61              |
| 1:D:672:ARG:O    | 1:D:672:ARG:HD2  | 2.00                     | 0.61              |
| 1:D:179:LEU:O    | 1:D:183:SER:N    | 2.33                     | 0.61              |
| 1:D:90:PRO:O     | 1:D:92:ASP:N     | 2.34                     | 0.61              |
| 1:B:102:GLY:HA2  | 1:B:150:PRO:O    | 1.99                     | 0.61              |
| 1:C:297:LYS:NZ   | 1:C:297:LYS:HB3  | 2.15                     | 0.61              |
| 1:F:116:GLU:HG3  | 1:F:117:LEU:CD2  | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:759:GLN:HE21 | 1:E:763:LEU:HD11 | 1.65                     | 0.61              |
| 1:D:377:GLN:O    | 1:D:381:GLU:HB2  | 2.01                     | 0.61              |
| 1:E:377:GLN:O    | 1:E:381:GLU:HB2  | 2.01                     | 0.61              |
| 1:E:102:GLY:HA2  | 1:E:150:PRO:O    | 2.01                     | 0.61              |
| 1:F:102:GLY:HA2  | 1:F:150:PRO:O    | 2.00                     | 0.61              |
| 1:F:83:GLN:O     | 1:F:85:LEU:N     | 2.34                     | 0.61              |
| 1:B:191:GLU:O    | 1:B:193:LEU:N    | 2.34                     | 0.61              |
| 1:A:175:LYS:CB   | 1:A:175:LYS:NZ   | 2.62                     | 0.61              |
| 1:E:722:ILE:HD11 | 1:E:763:LEU:O    | 2.00                     | 0.61              |
| 1:C:142:VAL:CG2  | 1:C:154:ILE:HD12 | 2.26                     | 0.61              |
| 1:A:142:VAL:CG2  | 1:A:154:ILE:HD12 | 2.27                     | 0.61              |
| 1:E:122:GLU:OE1  | 1:E:147:ARG:CB   | 2.48                     | 0.61              |
| 2:S:21:LYS:C     | 2:S:21:LYS:HD3   | 2.21                     | 0.61              |
| 1:C:609:GLU:N    | 1:C:609:GLU:OE2  | 2.32                     | 0.61              |
| 1:E:175:LYS:NZ   | 1:E:175:LYS:CB   | 2.63                     | 0.61              |
| 1:D:176:GLY:C    | 1:D:178:SER:H    | 2.03                     | 0.61              |
| 1:F:188:LEU:HD22 | 1:F:188:LEU:N    | 2.12                     | 0.61              |
| 1:B:128:MET:HB2  | 1:B:239:HIS:NE2  | 2.15                     | 0.61              |
| 1:F:657:ILE:HG23 | 1:F:657:ILE:O    | 2.01                     | 0.61              |
| 1:C:759:GLN:HE21 | 1:C:763:LEU:HD11 | 1.66                     | 0.61              |
| 1:B:657:ILE:O    | 1:B:657:ILE:HG23 | 2.01                     | 0.61              |
| 1:B:118:GLN:HA   | 1:B:118:GLN:OE1  | 2.00                     | 0.61              |
| 2:O:32:LEU:HD21  | 2:O:71:MET:HE1   | 1.82                     | 0.61              |
| 1:F:499:PRO:CG   | 1:F:504:ILE:HD11 | 2.30                     | 0.61              |
| 1:B:301:ALA:C    | 1:B:303:LYS:N    | 2.52                     | 0.61              |
| 2:O:13:LYS:NZ    | 2:O:65:PHE:CB    | 2.64                     | 0.61              |
| 2:S:13:LYS:HZ3   | 2:S:65:PHE:HB3   | 1.65                     | 0.61              |
| 1:C:607:ASN:HB3  | 1:C:609:GLU:OE2  | 2.01                     | 0.61              |
| 1:C:69:THR:HA    | 1:C:106:PHE:O    | 2.00                     | 0.61              |
| 1:D:301:ALA:C    | 1:D:303:LYS:H    | 2.02                     | 0.61              |
| 1:C:412:GLU:C    | 1:C:414:LYS:H    | 2.04                     | 0.61              |
| 1:E:118:GLN:HA   | 1:E:118:GLN:OE1  | 2.01                     | 0.61              |
| 1:B:332:ASN:HD21 | 1:B:334:LEU:HD13 | 1.65                     | 0.61              |
| 1:D:499:PRO:CG   | 1:D:504:ILE:HD11 | 2.30                     | 0.61              |
| 1:A:377:GLN:O    | 1:A:381:GLU:HB2  | 2.01                     | 0.61              |
| 1:E:83:GLN:O     | 1:E:85:LEU:N     | 2.35                     | 0.60              |
| 1:D:88:LYS:NZ    | 1:D:172:GLU:OE1  | 2.33                     | 0.60              |
| 1:F:102:GLY:CA   | 1:F:150:PRO:HG2  | 2.31                     | 0.60              |
| 1:C:597:ASN:HD21 | 1:C:601:GLU:CB   | 2.14                     | 0.60              |
| 1:C:760:VAL:O    | 1:C:764:LEU:HG   | 2.00                     | 0.60              |
| 1:E:635:ILE:N    | 1:E:635:ILE:HD12 | 2.08                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:116:GLU:HG3  | 1:C:117:LEU:CD2  | 2.31                     | 0.60              |
| 1:E:279:ILE:O    | 1:E:283:LEU:HD13 | 2.01                     | 0.60              |
| 1:B:442:TYR:O    | 1:B:458:LYS:NZ   | 2.34                     | 0.60              |
| 1:B:609:GLU:N    | 1:B:609:GLU:OE2  | 2.31                     | 0.60              |
| 1:D:517:VAL:HB   | 1:D:525:LYS:NZ   | 2.15                     | 0.60              |
| 1:A:69:THR:HA    | 1:A:106:PHE:O    | 2.00                     | 0.60              |
| 1:D:395:GLU:O    | 1:D:395:GLU:OE1  | 2.19                     | 0.60              |
| 1:E:102:GLY:CA   | 1:E:150:PRO:HG2  | 2.32                     | 0.60              |
| 1:B:96:ILE:HG22  | 1:B:100:LEU:HD11 | 1.82                     | 0.60              |
| 1:D:116:GLU:HG3  | 1:D:117:LEU:CD2  | 2.31                     | 0.60              |
| 1:B:668:SER:CA   | 2:P:14:GLU:HG3   | 2.30                     | 0.60              |
| 1:A:301:ALA:C    | 1:A:303:LYS:H    | 2.02                     | 0.60              |
| 1:F:349:ASN:HD22 | 1:F:350:VAL:HG23 | 1.66                     | 0.60              |
| 1:B:349:ASN:HD22 | 1:B:350:VAL:HG23 | 1.66                     | 0.60              |
| 2:P:89:PHE:HD1   | 2:P:141:PHE:CD2  | 2.18                     | 0.60              |
| 1:D:230:ILE:HG13 | 1:D:237:PHE:CE2  | 2.36                     | 0.60              |
| 1:F:176:GLY:C    | 1:F:178:SER:H    | 2.04                     | 0.60              |
| 1:C:176:GLY:C    | 1:C:178:SER:H    | 2.03                     | 0.60              |
| 1:B:186:LYS:CE   | 1:B:234:LEU:HD12 | 2.31                     | 0.60              |
| 2:R:102:ALA:CB   | 2:R:125:ILE:HG13 | 2.31                     | 0.60              |
| 1:A:629:ASN:HD22 | 1:A:631:SER:N    | 1.95                     | 0.60              |
| 1:F:142:VAL:CG2  | 1:F:154:ILE:HD12 | 2.26                     | 0.60              |
| 1:D:118:GLN:HA   | 1:D:118:GLN:OE1  | 1.99                     | 0.60              |
| 1:E:332:ASN:HD21 | 1:E:334:LEU:HD13 | 1.66                     | 0.60              |
| 1:E:134:LYS:HG2  | 1:E:136:PRO:CD   | 2.31                     | 0.60              |
| 1:E:324:THR:CB   | 1:E:499:PRO:HA   | 2.31                     | 0.60              |
| 1:C:443:GLU:HG2  | 1:C:458:LYS:HE3  | 1.83                     | 0.60              |
| 1:B:324:THR:CB   | 1:B:499:PRO:HA   | 2.31                     | 0.60              |
| 1:A:442:TYR:O    | 1:A:458:LYS:NZ   | 2.34                     | 0.60              |
| 1:B:377:GLN:O    | 1:B:381:GLU:HB2  | 2.02                     | 0.60              |
| 1:F:69:THR:HA    | 1:F:106:PHE:O    | 2.00                     | 0.60              |
| 2:R:89:PHE:HD1   | 2:R:141:PHE:CD2  | 2.20                     | 0.60              |
| 1:B:102:GLY:HA3  | 1:B:150:PRO:HG2  | 1.84                     | 0.60              |
| 1:A:116:GLU:HG3  | 1:A:117:LEU:CD2  | 2.32                     | 0.60              |
| 1:F:597:ASN:HB2  | 1:F:598:PRO:CD   | 2.23                     | 0.60              |
| 1:B:759:GLN:HE21 | 1:B:763:LEU:HD11 | 1.67                     | 0.60              |
| 1:D:324:THR:CB   | 1:D:499:PRO:HA   | 2.32                     | 0.60              |
| 1:F:517:VAL:HB   | 1:F:525:LYS:NZ   | 2.15                     | 0.60              |
| 1:E:239:HIS:O    | 1:E:243:LEU:HG   | 2.00                     | 0.60              |
| 1:C:102:GLY:HA2  | 1:C:150:PRO:O    | 2.01                     | 0.60              |
| 1:B:189:ASP:O    | 1:B:190:PRO:C    | 2.35                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:102:GLY:CA   | 1:A:150:PRO:HG2  | 2.31                     | 0.60              |
| 1:A:759:GLN:HE21 | 1:A:763:LEU:HD11 | 1.67                     | 0.60              |
| 1:E:540:ARG:HD3  | 1:E:627:TYR:CZ   | 2.36                     | 0.60              |
| 2:R:13:LYS:NZ    | 2:R:65:PHE:CB    | 2.65                     | 0.60              |
| 1:D:141:PHE:HD1  | 1:D:141:PHE:N    | 2.00                     | 0.60              |
| 1:D:69:THR:HA    | 1:D:106:PHE:O    | 2.00                     | 0.60              |
| 1:B:176:GLY:C    | 1:B:178:SER:H    | 2.05                     | 0.60              |
| 1:A:102:GLY:HA3  | 1:A:150:PRO:HG2  | 1.84                     | 0.60              |
| 1:A:239:HIS:O    | 1:A:243:LEU:HG   | 2.01                     | 0.60              |
| 1:A:412:GLU:C    | 1:A:414:LYS:H    | 2.05                     | 0.60              |
| 1:B:635:ILE:HD12 | 1:B:635:ILE:N    | 2.08                     | 0.60              |
| 1:D:297:LYS:NZ   | 1:D:297:LYS:HB3  | 2.15                     | 0.60              |
| 1:C:550:SER:N    | 1:C:553:GLN:HE21 | 1.87                     | 0.60              |
| 1:A:668:SER:CA   | 2:O:14:GLU:HG3   | 2.29                     | 0.60              |
| 1:F:332:ASN:HD21 | 1:F:334:LEU:HD13 | 1.65                     | 0.60              |
| 1:B:472:ARG:HH11 | 1:B:472:ARG:CB   | 2.15                     | 0.60              |
| 2:T:97:ASN:N     | 2:T:97:ASN:HD22  | 1.93                     | 0.60              |
| 1:F:73:ASN:HD22  | 1:F:74:GLU:CD    | 2.05                     | 0.60              |
| 1:D:102:GLY:CA   | 1:D:150:PRO:HG2  | 2.32                     | 0.60              |
| 1:F:597:ASN:HD21 | 1:F:601:GLU:CA   | 2.14                     | 0.60              |
| 1:A:520:PRO:HG2  | 1:A:521:ASN:H    | 1.67                     | 0.60              |
| 1:E:297:LYS:NZ   | 1:E:297:LYS:HB3  | 2.16                     | 0.60              |
| 1:D:279:ILE:O    | 1:D:283:LEU:HD13 | 2.02                     | 0.60              |
| 1:C:279:ILE:H    | 1:C:279:ILE:HD13 | 1.67                     | 0.60              |
| 1:D:122:GLU:OE1  | 1:D:147:ARG:CB   | 2.49                     | 0.60              |
| 1:F:472:ARG:CB   | 1:F:472:ARG:HH11 | 2.15                     | 0.60              |
| 1:A:628:PHE:CE2  | 2:O:90:ARG:CZ    | 2.85                     | 0.60              |
| 1:A:118:GLN:HA   | 1:A:118:GLN:OE1  | 2.00                     | 0.60              |
| 1:F:412:GLU:C    | 1:F:414:LYS:H    | 2.04                     | 0.60              |
| 1:B:116:GLU:HG3  | 1:B:117:LEU:CD2  | 2.31                     | 0.60              |
| 1:F:279:ILE:O    | 1:F:283:LEU:HD13 | 2.02                     | 0.60              |
| 1:E:395:GLU:O    | 1:E:395:GLU:OE1  | 2.19                     | 0.60              |
| 1:F:395:GLU:O    | 1:F:395:GLU:OE1  | 2.19                     | 0.60              |
| 1:F:239:HIS:O    | 1:F:243:LEU:HG   | 2.00                     | 0.60              |
| 1:C:102:GLY:CA   | 1:C:150:PRO:HG2  | 2.32                     | 0.60              |
| 1:D:520:PRO:HG2  | 1:D:521:ASN:H    | 1.66                     | 0.60              |
| 1:A:597:ASN:HD21 | 1:A:601:GLU:CA   | 2.15                     | 0.60              |
| 1:F:118:GLN:HA   | 1:F:118:GLN:OE1  | 2.00                     | 0.60              |
| 1:C:629:ASN:HD22 | 1:C:631:SER:N    | 1.96                     | 0.60              |
| 1:C:332:ASN:HD21 | 1:C:334:LEU:HD13 | 1.66                     | 0.60              |
| 1:F:443:GLU:HG2  | 1:F:458:LYS:HE3  | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:324:THR:CB   | 1:F:499:PRO:HA   | 2.30                     | 0.60              |
| 1:E:66:LEU:HD12  | 1:E:103:GLU:HA   | 1.84                     | 0.60              |
| 1:D:607:ASN:HB3  | 1:D:609:GLU:OE2  | 2.02                     | 0.60              |
| 2:S:89:PHE:HD1   | 2:S:141:PHE:CD2  | 2.19                     | 0.60              |
| 2:R:21:LYS:HD3   | 2:R:21:LYS:C     | 2.22                     | 0.60              |
| 1:A:709:ASN:HB2  | 2:O:130:ILE:HG23 | 1.83                     | 0.60              |
| 2:O:89:PHE:HD1   | 2:O:141:PHE:CD2  | 2.19                     | 0.60              |
| 1:B:395:GLU:OE1  | 1:B:395:GLU:O    | 2.19                     | 0.60              |
| 1:C:395:GLU:OE1  | 1:C:395:GLU:O    | 2.20                     | 0.60              |
| 2:S:102:ALA:CB   | 2:S:125:ILE:HG13 | 2.32                     | 0.60              |
| 1:F:597:ASN:HD21 | 1:F:601:GLU:CB   | 2.15                     | 0.60              |
| 1:E:597:ASN:HD21 | 1:E:601:GLU:CA   | 2.15                     | 0.60              |
| 1:C:377:GLN:O    | 1:C:381:GLU:HB2  | 2.01                     | 0.60              |
| 1:D:739:LYS:HG2  | 1:D:740:GLN:H    | 1.67                     | 0.60              |
| 1:B:73:ASN:HD22  | 1:B:74:GLU:CD    | 2.05                     | 0.60              |
| 1:D:89:ILE:HG22  | 1:D:90:PRO:HD2   | 1.84                     | 0.59              |
| 2:Q:106:ARG:CG   | 2:Q:121:VAL:HG21 | 2.06                     | 0.59              |
| 1:A:597:ASN:HD21 | 1:A:601:GLU:CB   | 2.15                     | 0.59              |
| 1:D:297:LYS:HB3  | 1:D:297:LYS:HZ2  | 1.66                     | 0.59              |
| 1:B:520:PRO:HG2  | 1:B:521:ASN:H    | 1.67                     | 0.59              |
| 1:F:122:GLU:OE1  | 1:F:147:ARG:CB   | 2.48                     | 0.59              |
| 1:C:279:ILE:O    | 1:C:283:LEU:HD13 | 2.01                     | 0.59              |
| 1:F:442:TYR:O    | 1:F:458:LYS:NZ   | 2.35                     | 0.59              |
| 1:E:739:LYS:HG2  | 1:E:740:GLN:H    | 1.67                     | 0.59              |
| 2:Q:89:PHE:HD1   | 2:Q:141:PHE:CD2  | 2.19                     | 0.59              |
| 1:D:83:GLN:O     | 1:D:85:LEU:N     | 2.35                     | 0.59              |
| 1:B:88:LYS:NZ    | 1:B:172:GLU:OE1  | 2.35                     | 0.59              |
| 1:A:186:LYS:CE   | 1:A:234:LEU:HD12 | 2.32                     | 0.59              |
| 2:P:102:ALA:CB   | 2:P:125:ILE:HG13 | 2.32                     | 0.59              |
| 1:E:116:GLU:HG3  | 1:E:117:LEU:CD2  | 2.32                     | 0.59              |
| 1:A:332:ASN:HD21 | 1:A:334:LEU:HD13 | 1.66                     | 0.59              |
| 1:F:66:LEU:HD12  | 1:F:103:GLU:HA   | 1.84                     | 0.59              |
| 1:A:324:THR:CB   | 1:A:499:PRO:HA   | 2.31                     | 0.59              |
| 1:A:173:ILE:C    | 1:A:175:LYS:N    | 2.55                     | 0.59              |
| 1:A:184:LYS:CE   | 1:A:191:GLU:HB2  | 2.31                     | 0.59              |
| 1:C:520:PRO:HG2  | 1:C:521:ASN:H    | 1.67                     | 0.59              |
| 1:C:597:ASN:HD21 | 1:C:601:GLU:CA   | 2.15                     | 0.59              |
| 1:E:520:PRO:HG2  | 1:E:521:ASN:H    | 1.67                     | 0.59              |
| 1:B:597:ASN:HD21 | 1:B:601:GLU:CA   | 2.15                     | 0.59              |
| 1:B:412:GLU:C    | 1:B:414:LYS:H    | 2.04                     | 0.59              |
| 1:E:443:GLU:HG2  | 1:E:458:LYS:HE3  | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:44:THR:OG1   | 2:T:47:GLU:N     | 2.34                     | 0.59              |
| 1:D:742:ALA:HB1  | 1:D:744:GLU:OE1  | 2.01                     | 0.59              |
| 1:C:141:PHE:N    | 1:C:141:PHE:HD1  | 2.00                     | 0.59              |
| 1:C:739:LYS:HG2  | 1:C:740:GLN:H    | 1.67                     | 0.59              |
| 2:O:21:LYS:HD3   | 2:O:21:LYS:C     | 2.22                     | 0.59              |
| 1:E:414:LYS:HA   | 1:E:414:LYS:HZ2  | 1.61                     | 0.59              |
| 1:D:431:LYS:O    | 1:D:432:TYR:HD2  | 1.85                     | 0.59              |
| 1:D:451:ASN:N    | 1:D:451:ASN:OD1  | 2.29                     | 0.59              |
| 1:C:122:GLU:OE1  | 1:C:147:ARG:CB   | 2.50                     | 0.59              |
| 1:F:134:LYS:HG2  | 1:F:136:PRO:HG3  | 1.85                     | 0.59              |
| 1:D:443:GLU:HG2  | 1:D:458:LYS:HE3  | 1.83                     | 0.59              |
| 1:D:306:GLY:O    | 1:D:336:THR:HG23 | 2.02                     | 0.59              |
| 1:C:742:ALA:HB1  | 1:C:744:GLU:OE1  | 2.01                     | 0.59              |
| 2:T:13:LYS:NZ    | 2:T:65:PHE:CB    | 2.65                     | 0.59              |
| 1:E:235:THR:O    | 1:E:238:GLN:HB2  | 2.03                     | 0.59              |
| 1:E:88:LYS:NZ    | 1:E:172:GLU:OE1  | 2.35                     | 0.59              |
| 1:D:597:ASN:HD21 | 1:D:601:GLU:CB   | 2.15                     | 0.59              |
| 1:A:279:ILE:O    | 1:A:283:LEU:HD13 | 2.02                     | 0.59              |
| 1:A:517:VAL:HB   | 1:A:525:LYS:HZ1  | 1.68                     | 0.59              |
| 2:Q:21:LYS:C     | 2:Q:21:LYS:HD3   | 2.22                     | 0.59              |
| 2:T:21:LYS:C     | 2:T:21:LYS:HD3   | 2.22                     | 0.59              |
| 1:F:102:GLY:HA3  | 1:F:150:PRO:HG2  | 1.84                     | 0.59              |
| 1:F:88:LYS:NZ    | 1:F:172:GLU:OE1  | 2.35                     | 0.59              |
| 1:C:83:GLN:O     | 1:C:85:LEU:N     | 2.36                     | 0.59              |
| 2:O:102:ALA:CB   | 2:O:125:ILE:HG13 | 2.32                     | 0.59              |
| 1:A:414:LYS:HA   | 1:A:414:LYS:HZ2  | 1.67                     | 0.59              |
| 1:E:412:GLU:C    | 1:E:414:LYS:H    | 2.04                     | 0.59              |
| 1:B:597:ASN:HD21 | 1:B:601:GLU:CB   | 2.15                     | 0.59              |
| 1:D:635:ILE:H    | 1:D:635:ILE:CD1  | 1.99                     | 0.59              |
| 1:B:306:GLY:O    | 1:B:336:THR:HG23 | 2.02                     | 0.59              |
| 1:F:349:ASN:ND2  | 1:F:350:VAL:HG23 | 2.17                     | 0.59              |
| 1:B:349:ASN:ND2  | 1:B:350:VAL:HG23 | 2.17                     | 0.59              |
| 1:C:686:ASP:HB3  | 1:C:739:LYS:HD2  | 1.83                     | 0.59              |
| 1:A:349:ASN:HD22 | 1:A:350:VAL:HG23 | 1.67                     | 0.59              |
| 1:E:73:ASN:HD22  | 1:E:74:GLU:CD    | 2.05                     | 0.59              |
| 1:C:349:ASN:HD22 | 1:C:350:VAL:HG23 | 1.68                     | 0.59              |
| 1:D:349:ASN:HD22 | 1:D:350:VAL:HG23 | 1.68                     | 0.59              |
| 1:D:412:GLU:C    | 1:D:414:LYS:H    | 2.04                     | 0.59              |
| 1:A:657:ILE:O    | 1:A:657:ILE:HG23 | 2.02                     | 0.59              |
| 1:F:218:LEU:HD11 | 1:F:225:ILE:CD1  | 2.29                     | 0.59              |
| 1:C:368:GLN:HB2  | 1:C:380:VAL:HG13 | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:472:ARG:HH11 | 1:D:472:ARG:CB   | 2.15                     | 0.59              |
| 1:E:472:ARG:HH11 | 1:E:472:ARG:CB   | 2.15                     | 0.59              |
| 1:B:739:LYS:HG2  | 1:B:740:GLN:H    | 1.67                     | 0.59              |
| 1:F:686:ASP:HB3  | 1:F:739:LYS:HD2  | 1.83                     | 0.59              |
| 1:F:130:SER:HB2  | 1:F:170:TYR:CE2  | 2.37                     | 0.59              |
| 1:F:235:THR:O    | 1:F:238:GLN:HB2  | 2.03                     | 0.59              |
| 1:D:295:VAL:HB   | 1:D:603:ILE:HG23 | 1.84                     | 0.59              |
| 1:B:142:VAL:CG2  | 1:B:154:ILE:HD12 | 2.27                     | 0.59              |
| 1:B:279:ILE:O    | 1:B:283:LEU:HD13 | 2.02                     | 0.59              |
| 1:E:136:PRO:HG2  | 1:E:139:SER:OG   | 2.01                     | 0.59              |
| 1:C:306:GLY:O    | 1:C:336:THR:HG23 | 2.03                     | 0.59              |
| 1:E:529:VAL:O    | 1:E:532:LEU:HB2  | 2.03                     | 0.59              |
| 1:A:349:ASN:ND2  | 1:A:350:VAL:HG23 | 2.18                     | 0.59              |
| 1:F:739:LYS:HG2  | 1:F:740:GLN:H    | 1.67                     | 0.59              |
| 1:C:73:ASN:HD22  | 1:C:74:GLU:CD    | 2.05                     | 0.59              |
| 2:P:21:LYS:C     | 2:P:21:LYS:HD3   | 2.22                     | 0.59              |
| 1:D:173:ILE:C    | 1:D:175:LYS:N    | 2.55                     | 0.59              |
| 1:A:235:THR:O    | 1:A:238:GLN:HB2  | 2.02                     | 0.59              |
| 2:Q:106:ARG:O    | 2:Q:110:THR:HG23 | 2.03                     | 0.59              |
| 1:C:218:LEU:HD11 | 1:C:225:ILE:CD1  | 2.29                     | 0.59              |
| 2:P:58:ASP:O     | 2:P:60:ASN:N     | 2.36                     | 0.59              |
| 1:D:136:PRO:HG2  | 1:D:139:SER:OG   | 2.03                     | 0.59              |
| 1:A:529:VAL:O    | 1:A:532:LEU:HB2  | 2.02                     | 0.59              |
| 1:B:529:VAL:O    | 1:B:532:LEU:HB2  | 2.02                     | 0.59              |
| 1:C:529:VAL:O    | 1:C:532:LEU:HB2  | 2.01                     | 0.59              |
| 1:B:141:PHE:N    | 1:B:141:PHE:HD1  | 2.00                     | 0.59              |
| 1:F:609:GLU:N    | 1:F:609:GLU:OE2  | 2.32                     | 0.59              |
| 1:F:529:VAL:O    | 1:F:532:LEU:HB2  | 2.03                     | 0.59              |
| 1:E:188:LEU:HD22 | 1:E:188:LEU:H    | 1.55                     | 0.59              |
| 1:D:188:LEU:HD22 | 1:D:188:LEU:H    | 1.61                     | 0.59              |
| 1:F:175:LYS:CB   | 1:F:175:LYS:NZ   | 2.64                     | 0.59              |
| 1:E:629:ASN:HD22 | 1:E:631:SER:N    | 1.95                     | 0.59              |
| 1:E:70:GLU:CB    | 1:E:107:THR:HG22 | 2.28                     | 0.59              |
| 1:C:746:LYS:O    | 1:C:750:GLN:HG2  | 2.03                     | 0.59              |
| 1:A:134:LYS:HG2  | 1:A:136:PRO:HG3  | 1.85                     | 0.59              |
| 1:F:75:THR:C     | 1:F:77:ASP:H     | 2.07                     | 0.59              |
| 1:B:607:ASN:HB3  | 1:B:609:GLU:OE2  | 2.02                     | 0.59              |
| 1:A:395:GLU:O    | 1:A:395:GLU:OE1  | 2.20                     | 0.59              |
| 1:C:718:ARG:NH1  | 1:C:767:GLN:NE2  | 2.51                     | 0.58              |
| 1:E:431:LYS:O    | 1:E:432:TYR:HD2  | 1.86                     | 0.58              |
| 1:E:442:TYR:O    | 1:E:458:LYS:NZ   | 2.35                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:49:GLN:HA    | 2:O:52:ILE:CG2   | 2.33                     | 0.58              |
| 1:A:739:LYS:HG2  | 1:A:740:GLN:H    | 1.67                     | 0.58              |
| 2:O:138:TYR:O    | 2:O:142:VAL:HG23 | 2.03                     | 0.58              |
| 1:C:530:THR:HG21 | 2:Q:145:MET:HE3  | 1.84                     | 0.58              |
| 1:A:73:ASN:HD22  | 1:A:74:GLU:CD    | 2.05                     | 0.58              |
| 1:E:301:ALA:C    | 1:E:303:LYS:N    | 2.53                     | 0.58              |
| 1:A:115:LYS:HB3  | 1:A:115:LYS:HZ3  | 1.68                     | 0.58              |
| 2:T:32:LEU:HD21  | 2:T:71:MET:HE2   | 1.85                     | 0.58              |
| 1:B:431:LYS:O    | 1:B:432:TYR:HD2  | 1.86                     | 0.58              |
| 1:C:442:TYR:O    | 1:C:458:LYS:NZ   | 2.36                     | 0.58              |
| 2:P:13:LYS:NZ    | 2:P:65:PHE:CB    | 2.65                     | 0.58              |
| 1:B:776:LEU:O    | 1:B:780:LEU:HD22 | 2.03                     | 0.58              |
| 1:A:75:THR:C     | 1:A:77:ASP:H     | 2.06                     | 0.58              |
| 2:Q:138:TYR:O    | 2:Q:142:VAL:HG23 | 2.03                     | 0.58              |
| 1:B:570:THR:O    | 1:B:570:THR:OG1  | 2.21                     | 0.58              |
| 1:A:326:ILE:C    | 1:A:327:LEU:HD12 | 2.24                     | 0.58              |
| 1:F:136:PRO:HG2  | 1:F:139:SER:OG   | 2.03                     | 0.58              |
| 1:A:472:ARG:CB   | 1:A:472:ARG:HH11 | 2.15                     | 0.58              |
| 1:F:288:VAL:HG23 | 1:F:289:GLU:H    | 1.67                     | 0.58              |
| 1:D:288:VAL:HG23 | 1:D:289:GLU:H    | 1.68                     | 0.58              |
| 1:D:343:VAL:HG13 | 1:D:487:PRO:O    | 2.03                     | 0.58              |
| 1:F:326:ILE:C    | 1:F:327:LEU:HD12 | 2.24                     | 0.58              |
| 1:B:173:ILE:C    | 1:B:175:LYS:N    | 2.55                     | 0.58              |
| 2:P:106:ARG:CG   | 2:P:121:VAL:HG21 | 2.06                     | 0.58              |
| 1:F:597:ASN:ND2  | 1:F:601:GLU:N    | 2.51                     | 0.58              |
| 1:E:199:LEU:C    | 1:E:201:ASP:N    | 2.57                     | 0.58              |
| 1:A:136:PRO:HG2  | 1:A:139:SER:OG   | 2.02                     | 0.58              |
| 1:B:134:LYS:HG2  | 1:B:136:PRO:HG3  | 1.85                     | 0.58              |
| 1:D:432:TYR:HD1  | 1:D:445:ARG:HD2  | 1.68                     | 0.58              |
| 1:A:318:ILE:HG23 | 1:A:322:LEU:HD12 | 1.86                     | 0.58              |
| 1:F:318:ILE:HG23 | 1:F:322:LEU:HD12 | 1.86                     | 0.58              |
| 1:B:368:GLN:HB2  | 1:B:380:VAL:HG13 | 1.85                     | 0.58              |
| 1:A:368:GLN:HB2  | 1:A:380:VAL:HG13 | 1.86                     | 0.58              |
| 1:E:75:THR:C     | 1:E:77:ASP:H     | 2.07                     | 0.58              |
| 1:B:517:VAL:HB   | 1:B:525:LYS:HZ1  | 1.68                     | 0.58              |
| 1:E:517:VAL:HB   | 1:E:525:LYS:HZ1  | 1.69                     | 0.58              |
| 1:D:109:ILE:HD13 | 1:D:157:LYS:NZ   | 2.19                     | 0.58              |
| 1:D:73:ASN:HD22  | 1:D:74:GLU:CD    | 2.05                     | 0.58              |
| 1:E:326:ILE:C    | 1:E:327:LEU:HD12 | 2.23                     | 0.58              |
| 1:C:235:THR:O    | 1:C:238:GLN:HB2  | 2.03                     | 0.58              |
| 1:D:199:LEU:C    | 1:D:201:ASP:N    | 2.57                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:472:ARG:HH11 | 1:C:472:ARG:CB   | 2.15                     | 0.58              |
| 1:D:442:TYR:O    | 1:D:458:LYS:NZ   | 2.36                     | 0.58              |
| 1:E:288:VAL:HG23 | 1:E:289:GLU:H    | 1.69                     | 0.58              |
| 1:E:349:ASN:HD22 | 1:E:350:VAL:HG23 | 1.69                     | 0.58              |
| 2:T:89:PHE:HD1   | 2:T:141:PHE:CD2  | 2.20                     | 0.58              |
| 1:E:173:ILE:C    | 1:E:175:LYS:N    | 2.55                     | 0.58              |
| 1:C:184:LYS:HZ2  | 1:C:191:GLU:HB2  | 1.68                     | 0.58              |
| 1:B:218:LEU:HD11 | 1:B:225:ILE:CD1  | 2.29                     | 0.58              |
| 2:O:117:THR:C    | 2:O:119:GLU:N    | 2.57                     | 0.58              |
| 2:T:106:ARG:O    | 2:T:110:THR:HG23 | 2.04                     | 0.58              |
| 1:E:495:PHE:O    | 1:E:496:ALA:HB2  | 2.03                     | 0.58              |
| 1:C:107:THR:HG21 | 1:C:115:LYS:HD2  | 1.86                     | 0.58              |
| 2:O:58:ASP:O     | 2:O:60:ASN:N     | 2.37                     | 0.58              |
| 1:E:746:LYS:O    | 1:E:750:GLN:HG2  | 2.04                     | 0.58              |
| 1:F:306:GLY:O    | 1:F:336:THR:HG23 | 2.02                     | 0.58              |
| 1:C:66:LEU:HD12  | 1:C:103:GLU:HA   | 1.85                     | 0.58              |
| 1:D:735:VAL:O    | 1:D:738:SER:CB   | 2.52                     | 0.58              |
| 2:Q:13:LYS:NZ    | 2:Q:65:PHE:CB    | 2.67                     | 0.58              |
| 1:F:343:VAL:HG13 | 1:F:487:PRO:O    | 2.03                     | 0.58              |
| 1:F:141:PHE:N    | 1:F:141:PHE:HD1  | 2.01                     | 0.58              |
| 1:D:349:ASN:ND2  | 1:D:350:VAL:HG23 | 2.18                     | 0.58              |
| 1:E:420:LEU:O    | 1:E:420:LEU:HD13 | 2.04                     | 0.58              |
| 2:Q:102:ALA:CB   | 2:Q:125:ILE:HG13 | 2.34                     | 0.58              |
| 1:B:343:VAL:HG13 | 1:B:487:PRO:O    | 2.02                     | 0.58              |
| 1:D:657:ILE:O    | 1:D:657:ILE:HG23 | 2.02                     | 0.58              |
| 1:A:431:LYS:O    | 1:A:432:TYR:HD2  | 1.85                     | 0.58              |
| 1:A:776:LEU:O    | 1:A:780:LEU:HD22 | 2.04                     | 0.58              |
| 1:C:343:VAL:HG13 | 1:C:487:PRO:O    | 2.03                     | 0.58              |
| 1:D:517:VAL:HB   | 1:D:525:LYS:HZ1  | 1.69                     | 0.58              |
| 2:O:22:ASP:O     | 2:O:24:ASP:N     | 2.37                     | 0.58              |
| 1:C:109:ILE:HD13 | 1:C:157:LYS:NZ   | 2.19                     | 0.58              |
| 1:D:351:HIS:HB2  | 1:D:386:GLU:HG2  | 1.86                     | 0.58              |
| 1:A:218:LEU:HD11 | 1:A:225:ILE:CD1  | 2.29                     | 0.58              |
| 2:Q:117:THR:C    | 2:Q:119:GLU:N    | 2.57                     | 0.58              |
| 1:F:414:LYS:NZ   | 1:F:419:ILE:O    | 2.37                     | 0.58              |
| 1:D:107:THR:HG21 | 1:D:115:LYS:HD2  | 1.86                     | 0.58              |
| 2:R:58:ASP:O     | 2:R:60:ASN:N     | 2.37                     | 0.58              |
| 2:S:13:LYS:NZ    | 2:S:65:PHE:CB    | 2.66                     | 0.58              |
| 2:T:22:ASP:O     | 2:T:24:ASP:N     | 2.37                     | 0.58              |
| 1:D:530:THR:HG21 | 2:R:145:MET:HE3  | 1.84                     | 0.58              |
| 1:E:109:ILE:HD13 | 1:E:157:LYS:NZ   | 2.19                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:230:ILE:HG13 | 1:F:237:PHE:CE2  | 2.39                     | 0.58              |
| 2:P:138:TYR:O    | 2:P:142:VAL:HG23 | 2.03                     | 0.58              |
| 1:E:102:GLY:HA3  | 1:E:150:PRO:HG2  | 1.84                     | 0.58              |
| 1:B:83:GLN:O     | 1:B:85:LEU:N     | 2.37                     | 0.58              |
| 1:A:199:LEU:C    | 1:A:201:ASP:N    | 2.57                     | 0.58              |
| 2:O:106:ARG:O    | 2:O:110:THR:HG23 | 2.03                     | 0.58              |
| 2:T:102:ALA:CB   | 2:T:125:ILE:HG13 | 2.34                     | 0.58              |
| 1:E:414:LYS:NZ   | 1:E:419:ILE:O    | 2.36                     | 0.58              |
| 1:D:597:ASN:HD21 | 1:D:601:GLU:CA   | 2.15                     | 0.58              |
| 1:F:520:PRO:HG2  | 1:F:521:ASN:H    | 1.67                     | 0.58              |
| 1:C:495:PHE:O    | 1:C:496:ALA:HB2  | 2.04                     | 0.58              |
| 1:D:635:ILE:N    | 1:D:635:ILE:HD12 | 2.08                     | 0.58              |
| 1:F:746:LYS:O    | 1:F:750:GLN:HG2  | 2.04                     | 0.58              |
| 2:T:58:ASP:O     | 2:T:60:ASN:N     | 2.37                     | 0.58              |
| 1:B:318:ILE:HG23 | 1:B:322:LEU:HD12 | 1.86                     | 0.58              |
| 1:E:686:ASP:HB3  | 1:E:739:LYS:HD2  | 1.85                     | 0.58              |
| 1:F:351:HIS:HB2  | 1:F:386:GLU:HG2  | 1.86                     | 0.58              |
| 1:A:420:LEU:O    | 1:A:420:LEU:HD13 | 2.04                     | 0.58              |
| 1:E:176:GLY:C    | 1:E:178:SER:H    | 2.05                     | 0.58              |
| 1:D:235:THR:O    | 1:D:238:GLN:HB2  | 2.04                     | 0.58              |
| 1:D:66:LEU:HD12  | 1:D:103:GLU:HA   | 1.84                     | 0.58              |
| 1:C:134:LYS:HG2  | 1:C:136:PRO:HG3  | 1.85                     | 0.58              |
| 2:Q:58:ASP:O     | 2:Q:60:ASN:N     | 2.37                     | 0.58              |
| 1:A:279:ILE:HD13 | 1:A:279:ILE:H    | 1.69                     | 0.58              |
| 1:C:318:ILE:HG23 | 1:C:322:LEU:HD12 | 1.85                     | 0.58              |
| 1:C:66:LEU:HD12  | 1:C:66:LEU:O     | 2.04                     | 0.58              |
| 1:B:288:VAL:HG23 | 1:B:289:GLU:H    | 1.68                     | 0.58              |
| 1:C:288:VAL:HG23 | 1:C:289:GLU:H    | 1.68                     | 0.58              |
| 2:P:22:ASP:O     | 2:P:24:ASP:N     | 2.37                     | 0.58              |
| 1:F:65:ASN:N     | 1:F:65:ASN:HD22  | 2.02                     | 0.58              |
| 1:C:175:LYS:NZ   | 1:C:175:LYS:CB   | 2.63                     | 0.57              |
| 1:C:175:LYS:O    | 1:C:178:SER:N    | 2.37                     | 0.57              |
| 1:B:175:LYS:O    | 1:B:178:SER:N    | 2.37                     | 0.57              |
| 1:A:83:GLN:O     | 1:A:85:LEU:N     | 2.36                     | 0.57              |
| 2:P:117:THR:C    | 2:P:119:GLU:N    | 2.56                     | 0.57              |
| 1:B:326:ILE:C    | 1:B:327:LEU:HD12 | 2.24                     | 0.57              |
| 1:C:115:LYS:HZ2  | 1:C:115:LYS:HB3  | 1.68                     | 0.57              |
| 1:E:107:THR:HG21 | 1:E:115:LYS:HD2  | 1.86                     | 0.57              |
| 1:E:115:LYS:C    | 1:E:117:LEU:H    | 2.07                     | 0.57              |
| 1:B:746:LYS:O    | 1:B:750:GLN:HG2  | 2.04                     | 0.57              |
| 1:B:66:LEU:HD12  | 1:B:103:GLU:HA   | 1.85                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:301:ALA:C    | 1:A:303:LYS:N    | 2.53                     | 0.57              |
| 2:R:46:ALA:CA    | 2:R:49:GLN:HE22  | 2.17                     | 0.57              |
| 1:F:776:LEU:O    | 1:F:780:LEU:HD22 | 2.03                     | 0.57              |
| 1:C:184:LYS:HZ3  | 1:C:193:LEU:HD12 | 1.68                     | 0.57              |
| 1:C:704:TYR:OH   | 1:C:759:GLN:NE2  | 2.37                     | 0.57              |
| 1:E:597:ASN:HD21 | 1:E:601:GLU:CB   | 2.16                     | 0.57              |
| 1:B:70:GLU:CB    | 1:B:107:THR:HG22 | 2.26                     | 0.57              |
| 1:D:495:PHE:O    | 1:D:496:ALA:HB2  | 2.04                     | 0.57              |
| 1:C:135:VAL:O    | 1:C:135:VAL:CG2  | 2.53                     | 0.57              |
| 1:F:324:THR:CG2  | 1:F:499:PRO:HA   | 2.34                     | 0.57              |
| 2:S:44:THR:OG1   | 2:S:47:GLU:N     | 2.34                     | 0.57              |
| 1:A:628:PHE:CZ   | 2:O:90:ARG:CZ    | 2.87                     | 0.57              |
| 1:C:628:PHE:CE2  | 2:Q:90:ARG:CZ    | 2.87                     | 0.57              |
| 1:F:628:PHE:CE2  | 2:T:90:ARG:CZ    | 2.88                     | 0.57              |
| 1:D:615:ILE:HG23 | 1:D:619:ILE:HB   | 1.86                     | 0.57              |
| 1:B:351:HIS:HB2  | 1:B:386:GLU:HG2  | 1.86                     | 0.57              |
| 2:S:138:TYR:O    | 2:S:142:VAL:HG23 | 2.04                     | 0.57              |
| 1:B:307:LEU:H    | 1:B:307:LEU:HD12 | 1.70                     | 0.57              |
| 1:E:89:ILE:HG22  | 1:E:90:PRO:HD2   | 1.86                     | 0.57              |
| 1:F:89:ILE:HG22  | 1:F:90:PRO:HD2   | 1.86                     | 0.57              |
| 1:B:175:LYS:NZ   | 1:B:175:LYS:CB   | 2.65                     | 0.57              |
| 1:E:293:ILE:O    | 1:E:295:VAL:HG22 | 2.04                     | 0.57              |
| 1:B:115:LYS:NZ   | 1:B:116:GLU:N    | 2.53                     | 0.57              |
| 1:E:667:LEU:HD13 | 1:E:678:VAL:HG21 | 1.86                     | 0.57              |
| 1:E:324:THR:CG2  | 1:E:499:PRO:HA   | 2.34                     | 0.57              |
| 1:D:776:LEU:O    | 1:D:780:LEU:HD22 | 2.03                     | 0.57              |
| 1:D:75:THR:C     | 1:D:77:ASP:H     | 2.07                     | 0.57              |
| 1:F:79:ILE:C     | 1:F:81:GLN:H     | 2.08                     | 0.57              |
| 1:E:343:VAL:HG13 | 1:E:487:PRO:O    | 2.03                     | 0.57              |
| 1:A:141:PHE:N    | 1:A:141:PHE:HD1  | 2.01                     | 0.57              |
| 2:S:22:ASP:O     | 2:S:24:ASP:N     | 2.37                     | 0.57              |
| 1:A:615:ILE:HG23 | 1:A:619:ILE:HB   | 1.86                     | 0.57              |
| 1:B:109:ILE:HD13 | 1:B:157:LYS:NZ   | 2.19                     | 0.57              |
| 2:T:117:THR:C    | 2:T:119:GLU:N    | 2.57                     | 0.57              |
| 1:D:657:ILE:HG21 | 1:D:704:TYR:CD1  | 2.40                     | 0.57              |
| 1:D:579:THR:O    | 1:D:581:GLN:N    | 2.38                     | 0.57              |
| 1:E:279:ILE:HD13 | 1:E:279:ILE:H    | 1.70                     | 0.57              |
| 1:D:134:LYS:HG2  | 1:D:136:PRO:CD   | 2.34                     | 0.57              |
| 1:E:368:GLN:HB2  | 1:E:380:VAL:HG13 | 1.85                     | 0.57              |
| 2:T:46:ALA:CA    | 2:T:49:GLN:HE22  | 2.18                     | 0.57              |
| 1:E:776:LEU:O    | 1:E:780:LEU:HD22 | 2.03                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:628:PHE:CE2  | 2:P:90:ARG:CZ    | 2.87                     | 0.57              |
| 1:C:349:ASN:ND2  | 1:C:350:VAL:HG23 | 2.18                     | 0.57              |
| 1:F:128:MET:HB2  | 1:F:239:HIS:NE2  | 2.20                     | 0.57              |
| 1:C:89:ILE:HG22  | 1:C:90:PRO:HD2   | 1.86                     | 0.57              |
| 1:C:579:THR:O    | 1:C:581:GLN:N    | 2.38                     | 0.57              |
| 1:E:657:ILE:O    | 1:E:657:ILE:HG23 | 2.02                     | 0.57              |
| 1:E:597:ASN:H    | 1:E:597:ASN:HD22 | 1.50                     | 0.57              |
| 1:A:495:PHE:O    | 1:A:496:ALA:HB2  | 2.03                     | 0.57              |
| 1:E:218:LEU:HD11 | 1:E:225:ILE:CD1  | 2.29                     | 0.57              |
| 1:D:667:LEU:HD13 | 1:D:678:VAL:HG21 | 1.86                     | 0.57              |
| 1:D:134:LYS:HG2  | 1:D:136:PRO:HG3  | 1.86                     | 0.57              |
| 1:D:368:GLN:HB2  | 1:D:380:VAL:HG13 | 1.86                     | 0.57              |
| 1:C:324:THR:CG2  | 1:C:499:PRO:HA   | 2.35                     | 0.57              |
| 1:C:735:VAL:HG12 | 1:C:741:ILE:HD11 | 1.87                     | 0.57              |
| 1:C:776:LEU:O    | 1:C:780:LEU:HD22 | 2.04                     | 0.57              |
| 1:B:75:THR:C     | 1:B:77:ASP:H     | 2.07                     | 0.57              |
| 2:T:138:TYR:O    | 2:T:142:VAL:HG23 | 2.04                     | 0.57              |
| 1:C:230:ILE:HG13 | 1:C:237:PHE:CE2  | 2.39                     | 0.57              |
| 1:F:109:ILE:HD13 | 1:F:157:LYS:HZ3  | 1.69                     | 0.57              |
| 1:C:351:HIS:HB2  | 1:C:386:GLU:HG2  | 1.87                     | 0.57              |
| 1:D:420:LEU:O    | 1:D:420:LEU:HD13 | 2.05                     | 0.57              |
| 1:C:173:ILE:C    | 1:C:175:LYS:N    | 2.54                     | 0.57              |
| 1:A:89:ILE:HG22  | 1:A:90:PRO:HD2   | 1.87                     | 0.57              |
| 1:E:295:VAL:HB   | 1:E:603:ILE:HG23 | 1.86                     | 0.57              |
| 1:F:597:ASN:HD22 | 1:F:597:ASN:H    | 1.52                     | 0.57              |
| 1:C:70:GLU:CB    | 1:C:107:THR:HG22 | 2.27                     | 0.57              |
| 1:B:432:TYR:HD1  | 1:B:445:ARG:HD2  | 1.70                     | 0.57              |
| 1:F:368:GLN:HB2  | 1:F:380:VAL:HG13 | 1.86                     | 0.57              |
| 2:O:95:ASP:OD2   | 2:O:97:ASN:CG    | 2.43                     | 0.57              |
| 1:B:324:THR:CG2  | 1:B:499:PRO:HA   | 2.35                     | 0.57              |
| 2:T:8:GLN:NE2    | 2:T:76:MET:SD    | 2.77                     | 0.57              |
| 1:A:343:VAL:HG13 | 1:A:487:PRO:O    | 2.04                     | 0.57              |
| 1:E:141:PHE:N    | 1:E:141:PHE:HD1  | 2.01                     | 0.57              |
| 1:C:517:VAL:HB   | 1:C:525:LYS:HZ1  | 1.68                     | 0.57              |
| 1:D:529:VAL:O    | 1:D:532:LEU:HB2  | 2.03                     | 0.57              |
| 1:E:618:ASN:O    | 1:E:622:LYS:HB3  | 2.04                     | 0.57              |
| 1:D:181:ILE:HB   | 1:D:238:GLN:OE1  | 2.05                     | 0.57              |
| 1:A:188:LEU:HD22 | 1:A:188:LEU:N    | 2.13                     | 0.57              |
| 1:C:597:ASN:OD1  | 1:C:599:GLU:HB2  | 2.05                     | 0.57              |
| 1:B:718:ARG:NH1  | 1:B:767:GLN:NE2  | 2.48                     | 0.57              |
| 2:Q:46:ALA:CA    | 2:Q:49:GLN:HE22  | 2.18                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:46:ALA:HA    | 2:T:49:GLN:NE2   | 2.20                     | 0.57              |
| 1:E:735:VAL:O    | 1:E:738:SER:CB   | 2.53                     | 0.57              |
| 2:P:46:ALA:CA    | 2:P:49:GLN:HE22  | 2.18                     | 0.57              |
| 1:C:102:GLY:HA3  | 1:C:150:PRO:HG2  | 1.86                     | 0.57              |
| 1:A:629:ASN:ND2  | 1:A:631:SER:N    | 2.44                     | 0.57              |
| 1:B:115:LYS:HB3  | 1:B:115:LYS:HZ3  | 1.68                     | 0.57              |
| 2:R:46:ALA:HA    | 2:R:49:GLN:NE2   | 2.19                     | 0.57              |
| 1:D:628:PHE:CZ   | 2:R:90:ARG:CZ    | 2.88                     | 0.57              |
| 1:C:628:PHE:CZ   | 2:Q:90:ARG:CZ    | 2.88                     | 0.57              |
| 1:D:686:ASP:HB3  | 1:D:739:LYS:HD2  | 1.86                     | 0.57              |
| 1:B:530:THR:HG21 | 2:P:145:MET:HE3  | 1.87                     | 0.57              |
| 1:D:505:LYS:HD2  | 1:D:505:LYS:O    | 2.04                     | 0.57              |
| 1:A:597:ASN:H    | 1:A:597:ASN:HD22 | 1.53                     | 0.57              |
| 1:F:718:ARG:HH12 | 1:F:767:GLN:HE21 | 1.48                     | 0.57              |
| 1:A:718:ARG:HH12 | 1:A:767:GLN:HE21 | 1.50                     | 0.57              |
| 1:A:746:LYS:O    | 1:A:750:GLN:HG2  | 2.05                     | 0.57              |
| 1:D:746:LYS:O    | 1:D:750:GLN:HG2  | 2.04                     | 0.57              |
| 1:B:275:GLY:HA2  | 1:B:278:LYS:CD   | 2.35                     | 0.57              |
| 1:B:279:ILE:HD13 | 1:B:279:ILE:H    | 1.69                     | 0.57              |
| 2:T:49:GLN:HA    | 2:T:52:ILE:CG2   | 2.35                     | 0.57              |
| 2:S:46:ALA:CA    | 2:S:49:GLN:HE22  | 2.17                     | 0.57              |
| 1:A:79:ILE:C     | 1:A:81:GLN:H     | 2.08                     | 0.57              |
| 1:F:109:ILE:HD13 | 1:F:157:LYS:NZ   | 2.19                     | 0.57              |
| 1:A:109:ILE:HD13 | 1:A:157:LYS:NZ   | 2.19                     | 0.57              |
| 1:F:505:LYS:HD2  | 1:F:505:LYS:O    | 2.04                     | 0.57              |
| 2:T:120:GLU:HA   | 2:T:123:GLN:HB2  | 1.87                     | 0.57              |
| 1:D:66:LEU:O     | 1:D:66:LEU:HD12  | 2.05                     | 0.57              |
| 1:A:630:ARG:HH11 | 1:A:630:ARG:HG3  | 1.70                     | 0.57              |
| 1:C:115:LYS:NZ   | 1:C:116:GLU:N    | 2.53                     | 0.57              |
| 1:D:115:LYS:C    | 1:D:117:LEU:H    | 2.08                     | 0.57              |
| 1:C:432:TYR:HD1  | 1:C:445:ARG:HD2  | 1.70                     | 0.57              |
| 1:F:432:TYR:HD1  | 1:F:445:ARG:HD2  | 1.68                     | 0.57              |
| 1:A:66:LEU:HD12  | 1:A:103:GLU:HA   | 1.85                     | 0.57              |
| 1:A:66:LEU:HD12  | 1:A:66:LEU:O     | 2.05                     | 0.57              |
| 2:S:46:ALA:HA    | 2:S:49:GLN:NE2   | 2.20                     | 0.57              |
| 1:E:79:ILE:C     | 1:E:81:GLN:H     | 2.08                     | 0.57              |
| 1:A:288:VAL:HG23 | 1:A:289:GLU:H    | 1.68                     | 0.57              |
| 1:E:349:ASN:ND2  | 1:E:350:VAL:HG23 | 2.19                     | 0.57              |
| 1:D:326:ILE:C    | 1:D:327:LEU:HD12 | 2.25                     | 0.57              |
| 1:C:615:ILE:HG23 | 1:C:619:ILE:HB   | 1.86                     | 0.57              |
| 1:D:102:GLY:HA3  | 1:D:150:PRO:HG2  | 1.85                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:235:THR:O    | 1:B:238:GLN:HB2  | 2.05                     | 0.56              |
| 2:R:106:ARG:O    | 2:R:110:THR:HG23 | 2.05                     | 0.56              |
| 2:S:117:THR:C    | 2:S:119:GLU:N    | 2.57                     | 0.56              |
| 1:B:115:LYS:C    | 1:B:117:LEU:H    | 2.08                     | 0.56              |
| 2:S:58:ASP:O     | 2:S:60:ASN:N     | 2.37                     | 0.56              |
| 1:A:217:LYS:HZ2  | 1:A:236:GLU:HG3  | 1.70                     | 0.56              |
| 1:A:351:HIS:HB2  | 1:A:386:GLU:HG2  | 1.87                     | 0.56              |
| 1:F:420:LEU:HD13 | 1:F:420:LEU:O    | 2.05                     | 0.56              |
| 1:B:112:VAL:O    | 1:B:114:HIS:N    | 2.35                     | 0.56              |
| 1:F:175:LYS:O    | 1:F:178:SER:N    | 2.38                     | 0.56              |
| 1:A:657:ILE:HG21 | 1:A:704:TYR:CD1  | 2.40                     | 0.56              |
| 1:D:764:LEU:C    | 1:D:766:HIS:H    | 2.09                     | 0.56              |
| 1:C:431:LYS:O    | 1:C:432:TYR:HD2  | 1.87                     | 0.56              |
| 1:F:431:LYS:O    | 1:F:432:TYR:HD2  | 1.87                     | 0.56              |
| 1:E:318:ILE:HG23 | 1:E:322:LEU:HD12 | 1.86                     | 0.56              |
| 2:Q:49:GLN:HA    | 2:Q:52:ILE:CG2   | 2.35                     | 0.56              |
| 1:B:628:PHE:CZ   | 2:P:90:ARG:CZ    | 2.88                     | 0.56              |
| 1:D:175:LYS:CB   | 1:D:175:LYS:NZ   | 2.64                     | 0.56              |
| 1:C:337:ASN:O    | 1:C:341:SER:N    | 2.29                     | 0.56              |
| 2:O:120:GLU:HA   | 2:O:123:GLN:HB2  | 1.88                     | 0.56              |
| 1:B:414:LYS:NZ   | 1:B:419:ILE:O    | 2.37                     | 0.56              |
| 1:F:116:GLU:HG3  | 1:F:117:LEU:HD22 | 1.87                     | 0.56              |
| 1:C:326:ILE:C    | 1:C:327:LEU:HD12 | 2.25                     | 0.56              |
| 1:C:115:LYS:C    | 1:C:117:LEU:H    | 2.09                     | 0.56              |
| 1:F:199:LEU:C    | 1:F:201:ASP:N    | 2.57                     | 0.56              |
| 2:O:97:ASN:ND2   | 2:O:97:ASN:N     | 2.48                     | 0.56              |
| 1:E:306:GLY:O    | 1:E:336:THR:HG23 | 2.04                     | 0.56              |
| 1:F:66:LEU:HD12  | 1:F:66:LEU:O     | 2.06                     | 0.56              |
| 1:C:217:LYS:HZ2  | 1:C:236:GLU:HG3  | 1.69                     | 0.56              |
| 2:Q:44:THR:OG1   | 2:Q:47:GLU:N     | 2.34                     | 0.56              |
| 2:T:65:PHE:CB    | 2:T:66:PRO:HD3   | 2.36                     | 0.56              |
| 2:S:65:PHE:CB    | 2:S:66:PRO:HD3   | 2.36                     | 0.56              |
| 1:C:75:THR:C     | 1:C:77:ASP:H     | 2.07                     | 0.56              |
| 1:B:79:ILE:C     | 1:B:81:GLN:H     | 2.08                     | 0.56              |
| 1:D:79:ILE:C     | 1:D:81:GLN:H     | 2.08                     | 0.56              |
| 1:E:351:HIS:HB2  | 1:E:386:GLU:HG2  | 1.87                     | 0.56              |
| 1:F:615:ILE:HG23 | 1:F:619:ILE:HB   | 1.87                     | 0.56              |
| 1:F:535:LYS:HD2  | 1:F:536:TYR:CD2  | 2.40                     | 0.56              |
| 1:A:535:LYS:HD2  | 1:A:536:TYR:CD2  | 2.41                     | 0.56              |
| 1:C:420:LEU:HD13 | 1:C:420:LEU:O    | 2.04                     | 0.56              |
| 1:E:531:ASN:O    | 1:E:535:LYS:HB2  | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:618:ASN:O    | 1:F:622:LYS:HB3  | 2.04                     | 0.56              |
| 1:F:530:THR:HG21 | 2:T:145:MET:HE3  | 1.87                     | 0.56              |
| 1:B:335:ALA:O    | 1:B:339:ILE:HG13 | 2.06                     | 0.56              |
| 1:B:615:ILE:HG23 | 1:B:619:ILE:HB   | 1.87                     | 0.56              |
| 1:F:179:LEU:O    | 1:F:183:SER:N    | 2.38                     | 0.56              |
| 1:B:92:ASP:C     | 1:B:94:LEU:N     | 2.57                     | 0.56              |
| 2:S:120:GLU:HA   | 2:S:123:GLN:HB2  | 1.88                     | 0.56              |
| 1:D:302:LEU:HD22 | 1:D:602:PHE:HE1  | 1.71                     | 0.56              |
| 1:E:635:ILE:CD1  | 1:E:635:ILE:H    | 1.99                     | 0.56              |
| 1:B:435:LEU:H    | 1:B:445:ARG:HA   | 1.70                     | 0.56              |
| 1:C:134:LYS:HG2  | 1:C:136:PRO:CG   | 2.36                     | 0.56              |
| 1:D:324:THR:CG2  | 1:D:499:PRO:HA   | 2.35                     | 0.56              |
| 2:P:65:PHE:CB    | 2:P:66:PRO:HD3   | 2.36                     | 0.56              |
| 1:D:628:PHE:CE2  | 2:R:90:ARG:CZ    | 2.88                     | 0.56              |
| 1:F:531:ASN:O    | 1:F:535:LYS:HB2  | 2.05                     | 0.56              |
| 1:E:615:ILE:HG23 | 1:E:619:ILE:HB   | 1.88                     | 0.56              |
| 1:A:570:THR:O    | 1:A:570:THR:OG1  | 2.23                     | 0.56              |
| 1:C:295:VAL:HB   | 1:C:603:ILE:HG23 | 1.87                     | 0.56              |
| 1:D:293:ILE:O    | 1:D:295:VAL:HG22 | 2.05                     | 0.56              |
| 2:S:106:ARG:O    | 2:S:110:THR:HG23 | 2.05                     | 0.56              |
| 1:A:116:GLU:HG3  | 1:A:117:LEU:HD22 | 1.88                     | 0.56              |
| 1:C:711:ILE:HG13 | 1:C:712:PHE:CE2  | 2.41                     | 0.56              |
| 1:C:635:ILE:HD12 | 1:C:635:ILE:N    | 2.09                     | 0.56              |
| 1:D:115:LYS:NZ   | 1:D:116:GLU:N    | 2.53                     | 0.56              |
| 1:E:451:ASN:OD1  | 1:E:451:ASN:N    | 2.29                     | 0.56              |
| 1:B:711:ILE:HG13 | 1:B:712:PHE:CE2  | 2.41                     | 0.56              |
| 1:A:306:GLY:O    | 1:A:336:THR:HG23 | 2.04                     | 0.56              |
| 2:R:49:GLN:HA    | 2:R:52:ILE:CG2   | 2.35                     | 0.56              |
| 2:Q:22:ASP:O     | 2:Q:24:ASP:N     | 2.38                     | 0.56              |
| 1:F:592:GLU:HB3  | 1:F:604:LEU:HD11 | 1.87                     | 0.56              |
| 1:A:505:LYS:HD2  | 1:A:505:LYS:O    | 2.05                     | 0.56              |
| 1:E:175:LYS:HB2  | 1:E:175:LYS:HZ3  | 1.71                     | 0.56              |
| 1:E:175:LYS:O    | 1:E:178:SER:N    | 2.38                     | 0.56              |
| 1:A:187:SER:C    | 1:A:188:LEU:O    | 2.36                     | 0.56              |
| 1:A:115:LYS:HZ1  | 1:A:116:GLU:H    | 1.52                     | 0.56              |
| 1:F:667:LEU:HD13 | 1:F:678:VAL:HG21 | 1.88                     | 0.56              |
| 1:F:747:ASN:O    | 1:F:750:GLN:HB2  | 2.06                     | 0.56              |
| 1:B:134:LYS:HG2  | 1:B:136:PRO:CG   | 2.36                     | 0.56              |
| 1:A:432:TYR:HD1  | 1:A:445:ARG:HD2  | 1.69                     | 0.56              |
| 1:E:735:VAL:HG12 | 1:E:741:ILE:HD11 | 1.87                     | 0.56              |
| 1:F:628:PHE:CZ   | 2:T:90:ARG:CZ    | 2.89                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:106:ARG:O    | 2:P:110:THR:HG23 | 2.04                     | 0.56              |
| 1:F:115:LYS:HB3  | 1:F:115:LYS:HZ3  | 1.69                     | 0.56              |
| 1:E:657:ILE:HG21 | 1:E:704:TYR:CD1  | 2.41                     | 0.56              |
| 1:A:431:LYS:C    | 1:A:432:TYR:HD2  | 2.09                     | 0.56              |
| 1:A:735:VAL:O    | 1:A:738:SER:HB2  | 2.06                     | 0.56              |
| 1:B:735:VAL:HG12 | 1:B:741:ILE:HD11 | 1.87                     | 0.56              |
| 1:B:727:GLN:O    | 1:B:730:ASN:HB3  | 2.05                     | 0.56              |
| 1:E:592:GLU:HB3  | 1:E:604:LEU:HD11 | 1.88                     | 0.56              |
| 1:F:184:LYS:HZ3  | 1:F:193:LEU:HD12 | 1.68                     | 0.56              |
| 1:F:92:ASP:C     | 1:F:94:LEU:N     | 2.57                     | 0.56              |
| 1:B:181:ILE:HB   | 1:B:238:GLN:OE1  | 2.06                     | 0.56              |
| 1:B:96:ILE:HG22  | 1:B:100:LEU:CD1  | 2.36                     | 0.56              |
| 2:R:120:GLU:HA   | 2:R:123:GLN:HB2  | 1.88                     | 0.56              |
| 1:C:718:ARG:HH12 | 1:C:767:GLN:HE21 | 1.50                     | 0.56              |
| 1:A:704:TYR:OH   | 1:A:759:GLN:NE2  | 2.39                     | 0.56              |
| 1:C:451:ASN:N    | 1:C:451:ASN:OD1  | 2.29                     | 0.56              |
| 1:E:134:LYS:HG2  | 1:E:136:PRO:HG3  | 1.87                     | 0.56              |
| 2:P:49:GLN:HA    | 2:P:52:ILE:CG2   | 2.35                     | 0.56              |
| 1:D:531:ASN:O    | 1:D:535:LYS:HB2  | 2.05                     | 0.56              |
| 1:C:186:LYS:HA   | 1:C:190:PRO:CD   | 2.16                     | 0.56              |
| 1:C:181:ILE:HB   | 1:C:238:GLN:OE1  | 2.06                     | 0.56              |
| 1:A:629:ASN:C    | 1:A:629:ASN:ND2  | 2.58                     | 0.56              |
| 1:B:136:PRO:HG2  | 1:B:139:SER:OG   | 2.04                     | 0.56              |
| 1:F:360:VAL:HG21 | 1:F:365:PRO:HB3  | 1.88                     | 0.56              |
| 1:E:432:TYR:HD1  | 1:E:445:ARG:HD2  | 1.70                     | 0.56              |
| 2:P:32:LEU:HD21  | 2:P:71:MET:HE1   | 1.87                     | 0.56              |
| 1:A:324:THR:CG2  | 1:A:499:PRO:HA   | 2.35                     | 0.56              |
| 1:E:66:LEU:O     | 1:E:66:LEU:HD12  | 2.06                     | 0.56              |
| 1:C:335:ALA:O    | 1:C:339:ILE:HG13 | 2.06                     | 0.56              |
| 1:A:688:PHE:C    | 1:A:688:PHE:CD2  | 2.80                     | 0.56              |
| 1:B:420:LEU:HD13 | 1:B:420:LEU:O    | 2.06                     | 0.56              |
| 1:D:96:ILE:HG22  | 1:D:100:LEU:CD1  | 2.36                     | 0.56              |
| 1:A:181:ILE:HB   | 1:A:238:GLN:OE1  | 2.06                     | 0.56              |
| 2:R:117:THR:C    | 2:R:119:GLU:N    | 2.57                     | 0.56              |
| 1:A:115:LYS:C    | 1:A:117:LEU:H    | 2.09                     | 0.56              |
| 1:C:601:GLU:C    | 1:C:602:PHE:HD2  | 2.09                     | 0.56              |
| 1:D:601:GLU:C    | 1:D:602:PHE:HD2  | 2.10                     | 0.56              |
| 1:B:597:ASN:H    | 1:B:597:ASN:HD22 | 1.54                     | 0.56              |
| 1:B:495:PHE:O    | 1:B:496:ALA:HB2  | 2.05                     | 0.56              |
| 1:E:435:LEU:CG   | 1:E:446:ILE:HG22 | 2.34                     | 0.56              |
| 2:P:64:ASP:OD1   | 2:P:66:PRO:HD2   | 2.06                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:79:ILE:C     | 1:C:81:GLN:H     | 2.08                     | 0.56              |
| 1:F:517:VAL:HB   | 1:F:525:LYS:HZ1  | 1.69                     | 0.56              |
| 2:R:138:TYR:O    | 2:R:142:VAL:HG23 | 2.05                     | 0.56              |
| 1:A:335:ALA:O    | 1:A:339:ILE:HG13 | 2.06                     | 0.56              |
| 1:C:505:LYS:HD2  | 1:C:505:LYS:O    | 2.05                     | 0.56              |
| 1:D:184:LYS:HZ2  | 1:D:191:GLU:HB2  | 1.68                     | 0.55              |
| 1:C:92:ASP:C     | 1:C:94:LEU:N     | 2.57                     | 0.55              |
| 1:A:184:LYS:HE3  | 1:A:191:GLU:HB2  | 1.88                     | 0.55              |
| 1:C:338:LEU:O    | 1:C:341:SER:HB3  | 2.06                     | 0.55              |
| 1:C:414:LYS:NZ   | 1:C:419:ILE:O    | 2.37                     | 0.55              |
| 1:D:337:ASN:O    | 1:D:341:SER:N    | 2.29                     | 0.55              |
| 1:A:115:LYS:NZ   | 1:A:116:GLU:N    | 2.54                     | 0.55              |
| 1:B:431:LYS:C    | 1:B:432:TYR:HD2  | 2.09                     | 0.55              |
| 1:A:122:GLU:OE1  | 1:A:147:ARG:CB   | 2.52                     | 0.55              |
| 2:Q:46:ALA:HA    | 2:Q:49:GLN:NE2   | 2.20                     | 0.55              |
| 1:E:628:PHE:CZ   | 2:S:90:ARG:CZ    | 2.89                     | 0.55              |
| 1:B:531:ASN:O    | 1:B:535:LYS:HB2  | 2.06                     | 0.55              |
| 1:D:335:ALA:O    | 1:D:339:ILE:HG13 | 2.06                     | 0.55              |
| 1:C:307:LEU:HD12 | 1:C:307:LEU:H    | 1.71                     | 0.55              |
| 1:A:96:ILE:HG22  | 1:A:100:LEU:CD1  | 2.35                     | 0.55              |
| 2:Q:120:GLU:HA   | 2:Q:123:GLN:HB2  | 1.88                     | 0.55              |
| 1:F:597:ASN:OD1  | 1:F:599:GLU:HB2  | 2.06                     | 0.55              |
| 1:F:718:ARG:NH1  | 1:F:767:GLN:NE2  | 2.49                     | 0.55              |
| 1:E:579:THR:O    | 1:E:581:GLN:N    | 2.39                     | 0.55              |
| 1:F:495:PHE:O    | 1:F:496:ALA:HB2  | 2.05                     | 0.55              |
| 1:E:462:ILE:HD11 | 1:E:466:GLY:HA2  | 1.88                     | 0.55              |
| 1:D:318:ILE:HG23 | 1:D:322:LEU:HD12 | 1.87                     | 0.55              |
| 1:B:66:LEU:HD12  | 1:B:66:LEU:O     | 2.06                     | 0.55              |
| 2:O:65:PHE:CB    | 2:O:66:PRO:HD3   | 2.37                     | 0.55              |
| 1:A:531:ASN:O    | 1:A:535:LYS:HB2  | 2.06                     | 0.55              |
| 1:B:535:LYS:HD2  | 1:B:536:TYR:CD2  | 2.41                     | 0.55              |
| 1:A:112:VAL:O    | 1:A:114:HIS:N    | 2.37                     | 0.55              |
| 1:B:688:PHE:C    | 1:B:688:PHE:CD2  | 2.79                     | 0.55              |
| 1:E:181:ILE:HB   | 1:E:238:GLN:OE1  | 2.06                     | 0.55              |
| 1:F:181:ILE:HB   | 1:F:238:GLN:OE1  | 2.06                     | 0.55              |
| 1:C:130:SER:HB2  | 1:C:170:TYR:CE2  | 2.42                     | 0.55              |
| 1:B:89:ILE:HG22  | 1:B:90:PRO:HD2   | 1.86                     | 0.55              |
| 2:P:120:GLU:HA   | 2:P:123:GLN:HB2  | 1.88                     | 0.55              |
| 1:A:414:LYS:NZ   | 1:A:419:ILE:O    | 2.36                     | 0.55              |
| 1:F:629:ASN:ND2  | 1:F:631:SER:N    | 2.45                     | 0.55              |
| 1:D:70:GLU:CB    | 1:D:107:THR:HG22 | 2.27                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:279:ILE:HD13 | 1:F:279:ILE:H    | 1.70                     | 0.55              |
| 1:C:592:GLU:HB3  | 1:C:604:LEU:HD11 | 1.88                     | 0.55              |
| 1:E:184:LYS:HZ2  | 1:E:191:GLU:CB   | 2.19                     | 0.55              |
| 1:F:173:ILE:C    | 1:F:175:LYS:N    | 2.55                     | 0.55              |
| 1:B:199:LEU:C    | 1:B:201:ASP:N    | 2.58                     | 0.55              |
| 2:R:106:ARG:CG   | 2:R:121:VAL:HG21 | 2.08                     | 0.55              |
| 1:A:297:LYS:HB3  | 1:A:297:LYS:HZ2  | 1.70                     | 0.55              |
| 1:D:597:ASN:OD1  | 1:D:599:GLU:HB2  | 2.07                     | 0.55              |
| 1:C:668:SER:CA   | 2:Q:14:GLU:HG3   | 2.28                     | 0.55              |
| 1:A:134:LYS:HG2  | 1:A:136:PRO:CG   | 2.36                     | 0.55              |
| 1:F:451:ASN:N    | 1:F:451:ASN:OD1  | 2.29                     | 0.55              |
| 1:D:275:GLY:HA2  | 1:D:278:LYS:CD   | 2.36                     | 0.55              |
| 2:O:46:ALA:CA    | 2:O:49:GLN:HE22  | 2.18                     | 0.55              |
| 1:B:307:LEU:N    | 1:B:307:LEU:HD12 | 2.20                     | 0.55              |
| 1:A:307:LEU:HD12 | 1:A:307:LEU:H    | 1.71                     | 0.55              |
| 1:E:505:LYS:HD2  | 1:E:505:LYS:O    | 2.05                     | 0.55              |
| 1:E:128:MET:HB2  | 1:E:239:HIS:NE2  | 2.22                     | 0.55              |
| 1:E:96:ILE:HG22  | 1:E:100:LEU:CD1  | 2.36                     | 0.55              |
| 1:F:184:LYS:CE   | 1:F:191:GLU:HB2  | 2.36                     | 0.55              |
| 1:F:96:ILE:HG22  | 1:F:100:LEU:CD1  | 2.35                     | 0.55              |
| 1:B:180:ASP:O    | 1:B:183:SER:N    | 2.36                     | 0.55              |
| 1:A:601:GLU:C    | 1:A:602:PHE:HD2  | 2.09                     | 0.55              |
| 1:B:597:ASN:OD1  | 1:B:599:GLU:HB2  | 2.07                     | 0.55              |
| 1:E:629:ASN:ND2  | 1:E:631:SER:N    | 2.44                     | 0.55              |
| 1:D:462:ILE:HD11 | 1:D:466:GLY:HA2  | 1.89                     | 0.55              |
| 1:D:279:ILE:H    | 1:D:279:ILE:HD13 | 1.70                     | 0.55              |
| 2:R:44:THR:OG1   | 2:R:47:GLU:N     | 2.34                     | 0.55              |
| 2:R:65:PHE:CB    | 2:R:66:PRO:HD3   | 2.36                     | 0.55              |
| 1:D:592:GLU:HB3  | 1:D:604:LEU:HD11 | 1.88                     | 0.55              |
| 1:C:535:LYS:HD2  | 1:C:536:TYR:CD2  | 2.41                     | 0.55              |
| 1:E:335:ALA:O    | 1:E:339:ILE:HG13 | 2.06                     | 0.55              |
| 1:D:92:ASP:C     | 1:D:94:LEU:N     | 2.59                     | 0.55              |
| 1:C:186:LYS:HG2  | 1:C:186:LYS:O    | 2.06                     | 0.55              |
| 1:B:186:LYS:HG2  | 1:B:186:LYS:O    | 2.06                     | 0.55              |
| 1:C:414:LYS:HZ2  | 1:C:414:LYS:HA   | 1.71                     | 0.55              |
| 1:C:297:LYS:HZ2  | 1:C:297:LYS:HB3  | 1.70                     | 0.55              |
| 1:B:302:LEU:HD22 | 1:B:602:PHE:HE1  | 1.70                     | 0.55              |
| 1:B:116:GLU:HG3  | 1:B:117:LEU:HD22 | 1.87                     | 0.55              |
| 1:B:446:ILE:HG13 | 1:B:452:GLU:O    | 2.06                     | 0.55              |
| 2:S:76:MET:HG3   | 2:S:76:MET:O     | 2.04                     | 0.55              |
| 2:Q:64:ASP:OD1   | 2:Q:66:PRO:HD2   | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:73:ASN:HB3   | 1:F:74:GLU:OE1   | 2.07                     | 0.55              |
| 1:F:115:LYS:NZ   | 1:F:116:GLU:N    | 2.53                     | 0.55              |
| 1:D:704:TYR:OH   | 1:D:759:GLN:NE2  | 2.39                     | 0.55              |
| 1:D:711:ILE:HG13 | 1:D:712:PHE:CE2  | 2.41                     | 0.55              |
| 1:D:629:ASN:C    | 1:D:629:ASN:ND2  | 2.59                     | 0.55              |
| 1:E:115:LYS:HZ2  | 1:E:116:GLU:HG2  | 1.69                     | 0.55              |
| 1:C:667:LEU:HD13 | 1:C:678:VAL:HG21 | 1.89                     | 0.55              |
| 1:C:199:LEU:HD21 | 1:C:226:ASP:OD2  | 2.07                     | 0.55              |
| 1:E:431:LYS:C    | 1:E:432:TYR:HD2  | 2.10                     | 0.55              |
| 1:E:747:ASN:O    | 1:E:750:GLN:HB2  | 2.07                     | 0.55              |
| 1:E:711:ILE:HG13 | 1:E:712:PHE:CE2  | 2.41                     | 0.55              |
| 2:R:64:ASP:OD1   | 2:R:66:PRO:HD2   | 2.06                     | 0.55              |
| 2:R:22:ASP:O     | 2:R:24:ASP:N     | 2.39                     | 0.55              |
| 1:B:510:GLN:O    | 1:B:514:ASP:HB2  | 2.06                     | 0.55              |
| 1:F:307:LEU:N    | 1:F:307:LEU:HD12 | 2.21                     | 0.55              |
| 1:D:97:TYR:HA    | 1:D:100:LEU:HD12 | 1.89                     | 0.55              |
| 1:C:96:ILE:HG22  | 1:C:100:LEU:CD1  | 2.36                     | 0.55              |
| 1:C:302:LEU:HD22 | 1:C:602:PHE:HE1  | 1.72                     | 0.55              |
| 1:B:601:GLU:C    | 1:B:602:PHE:HD2  | 2.10                     | 0.55              |
| 1:B:629:ASN:HD22 | 1:B:631:SER:N    | 1.95                     | 0.55              |
| 1:A:504:ILE:O    | 1:A:507:GLN:HB3  | 2.07                     | 0.55              |
| 1:A:711:ILE:HG13 | 1:A:712:PHE:CE2  | 2.42                     | 0.55              |
| 1:D:735:VAL:HG12 | 1:D:741:ILE:HD11 | 1.89                     | 0.55              |
| 2:T:76:MET:HG3   | 2:T:76:MET:O     | 2.04                     | 0.55              |
| 2:S:49:GLN:HA    | 2:S:52:ILE:CG2   | 2.35                     | 0.55              |
| 1:F:335:ALA:O    | 1:F:339:ILE:HG13 | 2.07                     | 0.55              |
| 1:A:639:ASN:HD22 | 1:A:639:ASN:H    | 1.55                     | 0.55              |
| 1:C:737:LYS:HE2  | 1:C:737:LYS:HA   | 1.89                     | 0.55              |
| 1:E:97:TYR:HA    | 1:E:100:LEU:HD12 | 1.88                     | 0.55              |
| 1:E:180:ASP:CG   | 1:E:181:ILE:N    | 2.59                     | 0.55              |
| 1:D:89:ILE:HG22  | 1:D:93:VAL:CG1   | 2.10                     | 0.55              |
| 1:A:184:LYS:HZ1  | 1:A:191:GLU:HB2  | 1.69                     | 0.55              |
| 1:D:412:GLU:C    | 1:D:414:LYS:N    | 2.61                     | 0.55              |
| 1:D:597:ASN:HD22 | 1:D:597:ASN:H    | 1.53                     | 0.55              |
| 1:B:411:GLU:O    | 1:B:414:LYS:HB2  | 2.07                     | 0.55              |
| 1:F:115:LYS:C    | 1:F:117:LEU:H    | 2.08                     | 0.55              |
| 1:E:302:LEU:HD22 | 1:E:602:PHE:HE1  | 1.72                     | 0.55              |
| 1:E:597:ASN:OD1  | 1:E:599:GLU:HB2  | 2.06                     | 0.55              |
| 1:F:579:THR:O    | 1:F:581:GLN:N    | 2.39                     | 0.55              |
| 1:C:116:GLU:HG3  | 1:C:117:LEU:HD22 | 1.87                     | 0.55              |
| 1:D:116:GLU:HG3  | 1:D:117:LEU:HD22 | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:218:LEU:HD11 | 1:D:225:ILE:CD1  | 2.29                     | 0.55              |
| 1:C:275:GLY:HA2  | 1:C:278:LYS:CD   | 2.37                     | 0.55              |
| 1:F:275:GLY:HA2  | 1:F:278:LYS:CD   | 2.36                     | 0.55              |
| 1:E:318:ILE:N    | 1:E:318:ILE:HD12 | 2.21                     | 0.55              |
| 1:F:711:ILE:HG13 | 1:F:712:PHE:CE2  | 2.41                     | 0.55              |
| 1:F:735:VAL:HG12 | 1:F:741:ILE:HD11 | 1.89                     | 0.55              |
| 1:A:307:LEU:HD12 | 1:A:307:LEU:N    | 2.21                     | 0.55              |
| 1:A:510:GLN:O    | 1:A:514:ASP:HB2  | 2.07                     | 0.55              |
| 1:E:727:GLN:O    | 1:E:730:ASN:HB3  | 2.07                     | 0.55              |
| 1:D:570:THR:O    | 1:D:570:THR:OG1  | 2.22                     | 0.55              |
| 1:F:570:THR:OG1  | 1:F:570:THR:O    | 2.24                     | 0.55              |
| 1:B:85:LEU:O     | 1:B:88:LYS:HE3   | 2.07                     | 0.55              |
| 1:B:337:ASN:O    | 1:B:341:SER:N    | 2.29                     | 0.55              |
| 1:E:115:LYS:NZ   | 1:E:116:GLU:N    | 2.53                     | 0.55              |
| 1:F:435:LEU:H    | 1:F:445:ARG:HA   | 1.72                     | 0.55              |
| 1:A:275:GLY:HA2  | 1:A:278:LYS:CD   | 2.37                     | 0.55              |
| 1:D:223:LYS:NZ   | 1:D:228:ASN:CB   | 2.70                     | 0.55              |
| 1:F:223:LYS:NZ   | 1:F:228:ASN:CB   | 2.70                     | 0.55              |
| 1:E:525:LYS:HE3  | 2:S:114:GLU:HG2  | 1.89                     | 0.55              |
| 1:D:307:LEU:HD12 | 1:D:307:LEU:H    | 1.72                     | 0.55              |
| 1:F:688:PHE:CD2  | 1:F:688:PHE:C    | 2.80                     | 0.55              |
| 1:B:325:TYR:CD1  | 1:B:598:PRO:HD3  | 2.42                     | 0.54              |
| 1:B:704:TYR:OH   | 1:B:759:GLN:NE2  | 2.40                     | 0.54              |
| 1:B:107:THR:HG21 | 1:B:115:LYS:HD2  | 1.90                     | 0.54              |
| 1:B:667:LEU:HD13 | 1:B:678:VAL:HG21 | 1.88                     | 0.54              |
| 1:C:504:ILE:O    | 1:C:507:GLN:HB3  | 2.07                     | 0.54              |
| 1:D:349:ASN:HD22 | 1:D:350:VAL:N    | 2.05                     | 0.54              |
| 1:E:131:ARG:HG2  | 1:E:131:ARG:HH11 | 1.72                     | 0.54              |
| 1:A:175:LYS:O    | 1:A:178:SER:N    | 2.40                     | 0.54              |
| 1:A:597:ASN:OD1  | 1:A:599:GLU:HB2  | 2.07                     | 0.54              |
| 1:E:704:TYR:OH   | 1:E:759:GLN:NE2  | 2.40                     | 0.54              |
| 1:E:601:GLU:C    | 1:E:602:PHE:HD2  | 2.10                     | 0.54              |
| 1:E:199:LEU:HD21 | 1:E:226:ASP:OD2  | 2.07                     | 0.54              |
| 1:A:462:ILE:HD11 | 1:A:466:GLY:HA2  | 1.88                     | 0.54              |
| 1:D:199:LEU:HD21 | 1:D:226:ASP:OD2  | 2.07                     | 0.54              |
| 1:A:360:VAL:HG21 | 1:A:365:PRO:HB3  | 1.89                     | 0.54              |
| 1:E:275:GLY:HA2  | 1:E:278:LYS:CD   | 2.36                     | 0.54              |
| 2:Q:65:PHE:CB    | 2:Q:66:PRO:HD3   | 2.36                     | 0.54              |
| 1:B:223:LYS:NZ   | 1:B:228:ASN:CB   | 2.70                     | 0.54              |
| 1:E:312:ALA:O    | 1:E:315:PHE:HB2  | 2.08                     | 0.54              |
| 1:E:73:ASN:HB3   | 1:E:74:GLU:OE1   | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:73:ASN:HB3   | 1:A:74:GLU:OE1   | 2.08                     | 0.54              |
| 1:E:535:LYS:HD2  | 1:E:536:TYR:CD2  | 2.42                     | 0.54              |
| 1:C:307:LEU:N    | 1:C:307:LEU:HD12 | 2.21                     | 0.54              |
| 1:C:531:ASN:O    | 1:C:535:LYS:HB2  | 2.06                     | 0.54              |
| 1:F:307:LEU:H    | 1:F:307:LEU:HD12 | 1.72                     | 0.54              |
| 1:D:307:LEU:HD12 | 1:D:307:LEU:N    | 2.21                     | 0.54              |
| 1:B:592:GLU:HB3  | 1:B:604:LEU:HD11 | 1.89                     | 0.54              |
| 1:A:592:GLU:HB3  | 1:A:604:LEU:HD11 | 1.89                     | 0.54              |
| 1:C:210:PHE:N    | 1:C:210:PHE:CD2  | 2.74                     | 0.54              |
| 1:D:688:PHE:C    | 1:D:688:PHE:CD2  | 2.80                     | 0.54              |
| 1:E:130:SER:HB2  | 1:E:170:TYR:OH   | 2.08                     | 0.54              |
| 1:A:199:LEU:HD21 | 1:A:226:ASP:OD2  | 2.07                     | 0.54              |
| 2:O:109:MET:HG3  | 2:O:116:LEU:HD11 | 1.90                     | 0.54              |
| 1:F:325:TYR:CD1  | 1:F:598:PRO:HD3  | 2.43                     | 0.54              |
| 1:F:657:ILE:HG21 | 1:F:704:TYR:CD1  | 2.42                     | 0.54              |
| 1:C:199:LEU:C    | 1:C:201:ASP:N    | 2.57                     | 0.54              |
| 1:C:165:GLN:C    | 1:C:167:LYS:H    | 2.11                     | 0.54              |
| 1:C:223:LYS:NZ   | 1:C:228:ASN:CB   | 2.70                     | 0.54              |
| 1:A:223:LYS:NZ   | 1:A:228:ASN:CB   | 2.70                     | 0.54              |
| 1:E:639:ASN:HD22 | 1:E:639:ASN:H    | 1.55                     | 0.54              |
| 1:F:727:GLN:O    | 1:F:730:ASN:HB3  | 2.07                     | 0.54              |
| 1:A:618:ASN:O    | 1:A:622:LYS:HB3  | 2.07                     | 0.54              |
| 1:C:510:GLN:O    | 1:C:514:ASP:HB2  | 2.07                     | 0.54              |
| 1:C:570:THR:O    | 1:C:570:THR:OG1  | 2.22                     | 0.54              |
| 1:B:90:PRO:C     | 1:B:92:ASP:H     | 2.10                     | 0.54              |
| 1:F:412:GLU:C    | 1:F:414:LYS:N    | 2.60                     | 0.54              |
| 1:E:116:GLU:HG3  | 1:E:117:LEU:HD22 | 1.88                     | 0.54              |
| 1:F:199:LEU:HD21 | 1:F:226:ASP:OD2  | 2.07                     | 0.54              |
| 1:A:360:VAL:O    | 1:A:363:TYR:HB2  | 2.07                     | 0.54              |
| 1:A:135:VAL:CG2  | 1:A:135:VAL:O    | 2.53                     | 0.54              |
| 1:A:435:LEU:H    | 1:A:445:ARG:HA   | 1.72                     | 0.54              |
| 1:F:431:LYS:C    | 1:F:432:TYR:HD2  | 2.10                     | 0.54              |
| 1:A:247:TYR:HE2  | 1:A:256:VAL:HG11 | 1.72                     | 0.54              |
| 1:B:504:ILE:O    | 1:B:507:GLN:HB3  | 2.07                     | 0.54              |
| 2:P:95:ASP:OD2   | 2:P:97:ASN:CG    | 2.46                     | 0.54              |
| 1:E:628:PHE:CE2  | 2:S:90:ARG:CZ    | 2.90                     | 0.54              |
| 1:E:223:LYS:NZ   | 1:E:228:ASN:CB   | 2.70                     | 0.54              |
| 1:C:349:ASN:HD22 | 1:C:350:VAL:N    | 2.06                     | 0.54              |
| 1:E:654:ILE:C    | 1:E:655:ASN:HD22 | 2.10                     | 0.54              |
| 1:A:727:GLN:O    | 1:A:730:ASN:HB3  | 2.07                     | 0.54              |
| 1:A:654:ILE:C    | 1:A:655:ASN:HD22 | 2.11                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:688:PHE:C    | 1:E:688:PHE:CD2  | 2.79                     | 0.54              |
| 1:E:90:PRO:C     | 1:E:92:ASP:H     | 2.11                     | 0.54              |
| 1:F:97:TYR:HA    | 1:F:100:LEU:HD12 | 1.88                     | 0.54              |
| 2:P:109:MET:HG3  | 2:P:116:LEU:HD11 | 1.90                     | 0.54              |
| 1:D:414:LYS:NZ   | 1:D:419:ILE:O    | 2.36                     | 0.54              |
| 1:C:462:ILE:HD11 | 1:C:466:GLY:HA2  | 1.89                     | 0.54              |
| 1:D:431:LYS:C    | 1:D:432:TYR:HD2  | 2.09                     | 0.54              |
| 1:E:504:ILE:O    | 1:E:507:GLN:HB3  | 2.08                     | 0.54              |
| 1:A:165:GLN:C    | 1:A:167:LYS:H    | 2.11                     | 0.54              |
| 2:Q:95:ASP:OD2   | 2:Q:97:ASN:CG    | 2.46                     | 0.54              |
| 2:R:8:GLN:NE2    | 2:R:76:MET:SD    | 2.81                     | 0.54              |
| 1:C:659:THR:OG1  | 1:C:662:GLU:HB2  | 2.08                     | 0.54              |
| 1:F:525:LYS:HE3  | 2:T:114:GLU:HG2  | 1.90                     | 0.54              |
| 1:A:145:LYS:HD3  | 1:A:151:LYS:HD2  | 1.90                     | 0.54              |
| 1:A:530:THR:HG21 | 2:O:145:MET:CE   | 2.37                     | 0.54              |
| 1:D:510:GLN:O    | 1:D:514:ASP:HB2  | 2.07                     | 0.54              |
| 1:E:570:THR:O    | 1:E:570:THR:OG1  | 2.23                     | 0.54              |
| 1:E:307:LEU:HD12 | 1:E:307:LEU:H    | 1.73                     | 0.54              |
| 1:D:184:LYS:NZ   | 1:D:191:GLU:CB   | 2.66                     | 0.54              |
| 1:F:85:LEU:O     | 1:F:88:LYS:HE3   | 2.07                     | 0.54              |
| 1:E:412:GLU:C    | 1:E:414:LYS:N    | 2.60                     | 0.54              |
| 1:D:302:LEU:HB2  | 1:D:602:PHE:HD1  | 1.73                     | 0.54              |
| 1:B:579:THR:O    | 1:B:581:GLN:N    | 2.41                     | 0.54              |
| 1:F:462:ILE:HD11 | 1:F:466:GLY:HA2  | 1.88                     | 0.54              |
| 1:D:747:ASN:O    | 1:D:750:GLN:HB2  | 2.07                     | 0.54              |
| 1:C:435:LEU:H    | 1:C:445:ARG:HA   | 1.71                     | 0.54              |
| 1:C:360:VAL:O    | 1:C:363:TYR:HB2  | 2.07                     | 0.54              |
| 1:E:360:VAL:HG21 | 1:E:365:PRO:HB3  | 1.90                     | 0.54              |
| 1:F:247:TYR:HE2  | 1:F:256:VAL:HG11 | 1.73                     | 0.54              |
| 1:B:368:GLN:CB   | 1:B:380:VAL:HG13 | 2.38                     | 0.54              |
| 1:D:323:ASN:ND2  | 1:D:624:TYR:OH   | 2.31                     | 0.54              |
| 2:O:64:ASP:OD1   | 2:O:66:PRO:HD2   | 2.07                     | 0.54              |
| 2:S:64:ASP:OD1   | 2:S:66:PRO:HD2   | 2.07                     | 0.54              |
| 1:C:515:LYS:NZ   | 1:C:515:LYS:HB3  | 2.23                     | 0.54              |
| 1:D:535:LYS:HD2  | 1:D:536:TYR:CD2  | 2.42                     | 0.54              |
| 1:B:505:LYS:O    | 1:B:505:LYS:HD2  | 2.06                     | 0.54              |
| 1:A:90:PRO:HG2   | 1:A:93:VAL:HB    | 1.90                     | 0.54              |
| 1:B:657:ILE:HG21 | 1:B:704:TYR:CD1  | 2.43                     | 0.54              |
| 1:A:630:ARG:HG3  | 1:A:630:ARG:NH1  | 2.22                     | 0.54              |
| 1:D:629:ASN:ND2  | 1:D:631:SER:N    | 2.45                     | 0.54              |
| 1:D:792:VAL:HG12 | 1:D:796:ILE:HD11 | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:747:ASN:O    | 1:B:750:GLN:HB2  | 2.07                     | 0.54              |
| 1:E:435:LEU:H    | 1:E:445:ARG:HA   | 1.72                     | 0.54              |
| 1:E:360:VAL:O    | 1:E:363:TYR:HB2  | 2.08                     | 0.54              |
| 1:B:135:VAL:O    | 1:B:135:VAL:CG2  | 2.53                     | 0.54              |
| 1:D:443:GLU:HG2  | 1:D:458:LYS:HZ1  | 1.73                     | 0.54              |
| 1:E:123:GLU:CG   | 1:E:124:GLU:H    | 2.19                     | 0.54              |
| 1:B:735:VAL:O    | 1:B:738:SER:HB2  | 2.08                     | 0.54              |
| 2:S:8:GLN:NE2    | 2:S:76:MET:SD    | 2.80                     | 0.54              |
| 1:E:210:PHE:CD2  | 1:E:210:PHE:N    | 2.75                     | 0.54              |
| 1:E:510:GLN:O    | 1:E:514:ASP:HB2  | 2.07                     | 0.54              |
| 1:D:210:PHE:N    | 1:D:210:PHE:CD2  | 2.75                     | 0.54              |
| 1:E:92:ASP:C     | 1:E:94:LEU:N     | 2.57                     | 0.54              |
| 1:F:601:GLU:C    | 1:F:602:PHE:HD2  | 2.10                     | 0.54              |
| 1:A:302:LEU:HD22 | 1:A:602:PHE:HE1  | 1.71                     | 0.54              |
| 1:C:597:ASN:H    | 1:C:597:ASN:HD22 | 1.55                     | 0.54              |
| 1:B:217:LYS:CB   | 1:B:236:GLU:HG3  | 2.38                     | 0.54              |
| 1:A:735:VAL:HG12 | 1:A:741:ILE:HD11 | 1.88                     | 0.54              |
| 1:D:217:LYS:HB3  | 1:D:217:LYS:HZ3  | 1.72                     | 0.54              |
| 2:Q:76:MET:HG3   | 2:Q:76:MET:O     | 2.04                     | 0.54              |
| 1:C:515:LYS:O    | 1:C:515:LYS:HG2  | 2.08                     | 0.54              |
| 1:E:515:LYS:HB3  | 1:E:515:LYS:NZ   | 2.23                     | 0.54              |
| 1:B:525:LYS:HE3  | 2:P:114:GLU:HG2  | 1.89                     | 0.54              |
| 1:A:312:ALA:O    | 1:A:315:PHE:HB2  | 2.07                     | 0.54              |
| 1:C:312:ALA:O    | 1:C:315:PHE:HB2  | 2.08                     | 0.54              |
| 1:D:654:ILE:C    | 1:D:655:ASN:HD22 | 2.11                     | 0.54              |
| 1:D:618:ASN:O    | 1:D:622:LYS:HB3  | 2.07                     | 0.54              |
| 1:D:737:LYS:HA   | 1:D:737:LYS:HE2  | 1.89                     | 0.54              |
| 1:F:131:ARG:HH11 | 1:F:131:ARG:HG2  | 1.72                     | 0.54              |
| 1:E:191:GLU:C    | 1:E:193:LEU:N    | 2.61                     | 0.54              |
| 1:D:90:PRO:C     | 1:D:92:ASP:H     | 2.12                     | 0.54              |
| 1:C:97:TYR:HA    | 1:C:100:LEU:HD12 | 1.89                     | 0.54              |
| 1:B:170:TYR:C    | 1:B:172:GLU:N    | 2.61                     | 0.54              |
| 1:F:704:TYR:OH   | 1:F:759:GLN:NE2  | 2.40                     | 0.54              |
| 1:A:579:THR:O    | 1:A:581:GLN:N    | 2.41                     | 0.54              |
| 1:C:747:ASN:O    | 1:C:750:GLN:HB2  | 2.07                     | 0.54              |
| 2:S:32:LEU:HD21  | 2:S:71:MET:HE2   | 1.89                     | 0.54              |
| 1:B:435:LEU:CG   | 1:B:446:ILE:HG22 | 2.35                     | 0.54              |
| 1:C:431:LYS:C    | 1:C:432:TYR:HD2  | 2.10                     | 0.54              |
| 1:C:254:ARG:HG2  | 1:C:255:THR:N    | 2.22                     | 0.54              |
| 2:T:64:ASP:OD1   | 2:T:66:PRO:HD2   | 2.07                     | 0.54              |
| 1:E:515:LYS:O    | 1:E:515:LYS:HG2  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:73:ASN:HB3   | 1:B:74:GLU:OE1   | 2.08                     | 0.54              |
| 1:D:131:ARG:HH11 | 1:D:131:ARG:HG2  | 1.72                     | 0.54              |
| 1:E:184:LYS:HZ3  | 1:E:193:LEU:HD12 | 1.71                     | 0.54              |
| 1:D:175:LYS:O    | 1:D:178:SER:N    | 2.40                     | 0.54              |
| 1:B:295:VAL:HB   | 1:B:603:ILE:HG23 | 1.90                     | 0.54              |
| 2:S:109:MET:HG3  | 2:S:116:LEU:HD11 | 1.90                     | 0.54              |
| 2:S:121:VAL:C    | 2:S:123:GLN:N    | 2.60                     | 0.54              |
| 1:E:411:GLU:O    | 1:E:414:LYS:HB2  | 2.07                     | 0.54              |
| 1:C:325:TYR:CD1  | 1:C:598:PRO:HD3  | 2.43                     | 0.54              |
| 1:D:325:TYR:CD1  | 1:D:598:PRO:HD3  | 2.43                     | 0.54              |
| 1:F:107:THR:HG21 | 1:F:115:LYS:HD2  | 1.89                     | 0.54              |
| 1:E:297:LYS:HB3  | 1:E:297:LYS:HZ2  | 1.72                     | 0.54              |
| 1:F:630:ARG:HG3  | 1:F:630:ARG:HH11 | 1.73                     | 0.54              |
| 1:E:792:VAL:HG12 | 1:E:796:ILE:HD11 | 1.90                     | 0.54              |
| 1:D:115:LYS:HB3  | 1:D:115:LYS:HZ3  | 1.73                     | 0.54              |
| 1:B:360:VAL:HG21 | 1:B:365:PRO:HB3  | 1.89                     | 0.54              |
| 1:B:217:LYS:HZ2  | 1:B:236:GLU:HG3  | 1.73                     | 0.54              |
| 1:C:368:GLN:CB   | 1:C:380:VAL:HG13 | 2.37                     | 0.54              |
| 1:B:456:LYS:HB3  | 1:B:470:ASN:C    | 2.27                     | 0.54              |
| 1:B:312:ALA:O    | 1:B:315:PHE:HB2  | 2.07                     | 0.54              |
| 1:E:349:ASN:HD22 | 1:E:350:VAL:N    | 2.06                     | 0.54              |
| 1:A:109:ILE:HD13 | 1:A:157:LYS:HZ3  | 1.71                     | 0.54              |
| 1:A:534:ILE:HG22 | 1:A:535:LYS:N    | 2.23                     | 0.54              |
| 1:A:636:ALA:O    | 1:A:640:LYS:N    | 2.41                     | 0.54              |
| 1:F:510:GLN:O    | 1:F:514:ASP:HB2  | 2.07                     | 0.54              |
| 1:C:145:LYS:HD3  | 1:C:151:LYS:HD2  | 1.90                     | 0.54              |
| 1:D:727:GLN:O    | 1:D:730:ASN:HB3  | 2.06                     | 0.54              |
| 1:F:737:LYS:HA   | 1:F:737:LYS:HE2  | 1.89                     | 0.54              |
| 1:B:737:LYS:HE2  | 1:B:737:LYS:HA   | 1.90                     | 0.54              |
| 1:D:128:MET:HB2  | 1:D:239:HIS:NE2  | 2.22                     | 0.53              |
| 1:C:85:LEU:O     | 1:C:88:LYS:HE3   | 2.09                     | 0.53              |
| 1:C:412:GLU:C    | 1:C:414:LYS:N    | 2.60                     | 0.53              |
| 2:S:105:LEU:HD23 | 2:S:121:VAL:HG13 | 1.89                     | 0.53              |
| 1:A:412:GLU:C    | 1:A:414:LYS:N    | 2.61                     | 0.53              |
| 1:D:338:LEU:O    | 1:D:341:SER:HB3  | 2.08                     | 0.53              |
| 1:F:302:LEU:HB2  | 1:F:602:PHE:HD1  | 1.73                     | 0.53              |
| 1:F:302:LEU:HD22 | 1:F:602:PHE:HE1  | 1.72                     | 0.53              |
| 1:A:325:TYR:CD1  | 1:A:598:PRO:HD3  | 2.43                     | 0.53              |
| 1:B:597:ASN:ND2  | 1:B:601:GLU:N    | 2.51                     | 0.53              |
| 1:E:657:ILE:O    | 1:E:658:PRO:O    | 2.26                     | 0.53              |
| 1:B:360:VAL:O    | 1:B:363:TYR:HB2  | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:360:VAL:O    | 1:D:363:TYR:HB2  | 2.08                     | 0.53              |
| 2:P:44:THR:OG1   | 2:P:47:GLU:N     | 2.35                     | 0.53              |
| 1:E:659:THR:OG1  | 1:E:662:GLU:HB2  | 2.08                     | 0.53              |
| 2:Q:13:LYS:HZ3   | 2:Q:65:PHE:HB3   | 1.71                     | 0.53              |
| 1:C:73:ASN:HB3   | 1:C:74:GLU:OE1   | 2.07                     | 0.53              |
| 1:F:327:LEU:HD12 | 1:F:327:LEU:N    | 2.23                     | 0.53              |
| 1:B:145:LYS:HD3  | 1:B:151:LYS:HD2  | 1.90                     | 0.53              |
| 1:F:639:ASN:H    | 1:F:639:ASN:HD22 | 1.57                     | 0.53              |
| 1:F:90:PRO:C     | 1:F:92:ASP:H     | 2.12                     | 0.53              |
| 1:A:97:TYR:HA    | 1:A:100:LEU:HD12 | 1.89                     | 0.53              |
| 1:A:85:LEU:O     | 1:A:88:LYS:HE3   | 2.08                     | 0.53              |
| 2:S:106:ARG:CG   | 2:S:121:VAL:HG21 | 2.06                     | 0.53              |
| 1:A:411:GLU:O    | 1:A:414:LYS:HB2  | 2.08                     | 0.53              |
| 1:D:411:GLU:O    | 1:D:414:LYS:HB2  | 2.07                     | 0.53              |
| 1:C:657:ILE:HG21 | 1:C:704:TYR:CD1  | 2.44                     | 0.53              |
| 1:F:105:TYR:HB2  | 1:F:153:ILE:HG12 | 1.90                     | 0.53              |
| 1:C:279:ILE:CD1  | 1:C:279:ILE:H    | 2.21                     | 0.53              |
| 1:D:247:TYR:HE2  | 1:D:256:VAL:HG11 | 1.73                     | 0.53              |
| 1:F:504:ILE:O    | 1:F:507:GLN:HB3  | 2.08                     | 0.53              |
| 1:C:525:LYS:HE3  | 2:Q:114:GLU:HG2  | 1.89                     | 0.53              |
| 1:D:73:ASN:HB3   | 1:D:74:GLU:OE1   | 2.07                     | 0.53              |
| 1:E:327:LEU:HD12 | 1:E:327:LEU:N    | 2.23                     | 0.53              |
| 1:E:307:LEU:N    | 1:E:307:LEU:HD12 | 2.22                     | 0.53              |
| 1:B:636:ALA:O    | 1:B:640:LYS:N    | 2.42                     | 0.53              |
| 1:D:145:LYS:HD3  | 1:D:151:LYS:HD2  | 1.90                     | 0.53              |
| 1:D:90:PRO:HG2   | 1:D:93:VAL:HB    | 1.91                     | 0.53              |
| 1:C:88:LYS:HG2   | 1:C:88:LYS:O     | 2.07                     | 0.53              |
| 1:A:747:ASN:O    | 1:A:750:GLN:HB2  | 2.08                     | 0.53              |
| 1:C:792:VAL:HG12 | 1:C:796:ILE:HD11 | 1.90                     | 0.53              |
| 1:B:792:VAL:HG12 | 1:B:796:ILE:HD11 | 1.90                     | 0.53              |
| 1:E:368:GLN:CB   | 1:E:380:VAL:HG13 | 2.38                     | 0.53              |
| 1:E:324:THR:HG22 | 1:E:499:PRO:HA   | 1.90                     | 0.53              |
| 2:S:95:ASP:OD2   | 2:S:97:ASN:CG    | 2.46                     | 0.53              |
| 2:P:46:ALA:HA    | 2:P:49:GLN:NE2   | 2.20                     | 0.53              |
| 1:E:639:ASN:ND2  | 1:E:639:ASN:H    | 2.06                     | 0.53              |
| 1:F:210:PHE:CD2  | 1:F:210:PHE:N    | 2.75                     | 0.53              |
| 1:C:630:ARG:HG3  | 1:C:630:ARG:HH11 | 1.74                     | 0.53              |
| 1:B:630:ARG:HG3  | 1:B:630:ARG:HH11 | 1.74                     | 0.53              |
| 1:A:657:ILE:O    | 1:A:658:PRO:O    | 2.26                     | 0.53              |
| 1:C:105:TYR:HB2  | 1:C:153:ILE:HG12 | 1.90                     | 0.53              |
| 1:E:115:LYS:O    | 1:E:117:LEU:N    | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:446:ILE:HD11 | 1:B:451:ASN:CB   | 2.38                     | 0.53              |
| 1:D:165:GLN:C    | 1:D:167:LYS:H    | 2.11                     | 0.53              |
| 1:A:368:GLN:CB   | 1:A:380:VAL:HG13 | 2.39                     | 0.53              |
| 2:P:97:ASN:ND2   | 2:P:97:ASN:N     | 2.49                     | 0.53              |
| 1:A:659:THR:OG1  | 1:A:662:GLU:HB2  | 2.08                     | 0.53              |
| 1:B:659:THR:OG1  | 1:B:662:GLU:HB2  | 2.08                     | 0.53              |
| 1:B:515:LYS:O    | 1:B:515:LYS:HG2  | 2.08                     | 0.53              |
| 1:D:312:ALA:O    | 1:D:315:PHE:HB2  | 2.09                     | 0.53              |
| 1:C:530:THR:HG21 | 2:Q:145:MET:CE   | 2.39                     | 0.53              |
| 1:D:639:ASN:H    | 1:D:639:ASN:HD22 | 1.55                     | 0.53              |
| 1:D:639:ASN:ND2  | 1:D:639:ASN:H    | 2.07                     | 0.53              |
| 1:F:184:LYS:HZ1  | 1:F:193:LEU:HD12 | 1.74                     | 0.53              |
| 1:C:90:PRO:HG2   | 1:C:93:VAL:HB    | 1.91                     | 0.53              |
| 1:B:97:TYR:HA    | 1:B:100:LEU:HD12 | 1.89                     | 0.53              |
| 1:C:410:ILE:HG22 | 1:C:411:GLU:N    | 2.23                     | 0.53              |
| 2:T:109:MET:HG3  | 2:T:116:LEU:HD11 | 1.91                     | 0.53              |
| 1:E:105:TYR:HB2  | 1:E:153:ILE:HG12 | 1.90                     | 0.53              |
| 1:B:462:ILE:HD11 | 1:B:466:GLY:HA2  | 1.89                     | 0.53              |
| 1:D:435:LEU:H    | 1:D:445:ARG:HA   | 1.72                     | 0.53              |
| 1:C:247:TYR:HE2  | 1:C:256:VAL:HG11 | 1.73                     | 0.53              |
| 2:R:95:ASP:OD2   | 2:R:97:ASN:CG    | 2.46                     | 0.53              |
| 2:O:46:ALA:HA    | 2:O:49:GLN:NE2   | 2.20                     | 0.53              |
| 1:A:210:PHE:N    | 1:A:210:PHE:CD2  | 2.75                     | 0.53              |
| 1:E:145:LYS:HD3  | 1:E:151:LYS:HD2  | 1.90                     | 0.53              |
| 1:C:128:MET:HB2  | 1:C:239:HIS:NE2  | 2.22                     | 0.53              |
| 1:C:411:GLU:O    | 1:C:414:LYS:HB2  | 2.08                     | 0.53              |
| 1:E:410:ILE:HG22 | 1:E:411:GLU:N    | 2.24                     | 0.53              |
| 1:B:410:ILE:HG22 | 1:B:411:GLU:N    | 2.24                     | 0.53              |
| 1:E:325:TYR:CD1  | 1:E:598:PRO:HD3  | 2.43                     | 0.53              |
| 1:A:327:LEU:HD12 | 1:A:327:LEU:N    | 2.24                     | 0.53              |
| 1:F:635:ILE:CD1  | 1:F:635:ILE:H    | 2.01                     | 0.53              |
| 1:C:360:VAL:HG21 | 1:C:365:PRO:HB3  | 1.89                     | 0.53              |
| 1:B:165:GLN:C    | 1:B:167:LYS:H    | 2.12                     | 0.53              |
| 1:C:499:PRO:HD3  | 1:C:552:TRP:CH2  | 2.43                     | 0.53              |
| 1:D:515:LYS:NZ   | 1:D:515:LYS:HB3  | 2.24                     | 0.53              |
| 1:B:349:ASN:HD22 | 1:B:350:VAL:N    | 2.07                     | 0.53              |
| 1:E:90:PRO:HG2   | 1:E:93:VAL:HB    | 1.91                     | 0.53              |
| 1:D:180:ASP:CG   | 1:D:181:ILE:N    | 2.59                     | 0.53              |
| 1:C:170:TYR:C    | 1:C:172:GLU:N    | 2.62                     | 0.53              |
| 1:A:88:LYS:HG2   | 1:A:88:LYS:O     | 2.07                     | 0.53              |
| 1:A:410:ILE:HG22 | 1:A:411:GLU:N    | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:657:ILE:HG13 | 1:F:756:ILE:HD12 | 1.90                     | 0.53              |
| 1:F:792:VAL:HG12 | 1:F:796:ILE:HD11 | 1.91                     | 0.53              |
| 1:A:792:VAL:HG12 | 1:A:796:ILE:HD11 | 1.90                     | 0.53              |
| 1:E:499:PRO:HD3  | 1:E:552:TRP:CH2  | 2.44                     | 0.53              |
| 1:E:165:GLN:C    | 1:E:167:LYS:H    | 2.11                     | 0.53              |
| 1:E:247:TYR:HE2  | 1:E:256:VAL:HG11 | 1.74                     | 0.53              |
| 2:P:5:THR:HG23   | 2:P:8:GLN:HB2    | 1.91                     | 0.53              |
| 1:F:515:LYS:O    | 1:F:515:LYS:HG2  | 2.08                     | 0.53              |
| 1:D:525:LYS:HE3  | 2:R:114:GLU:HG2  | 1.90                     | 0.53              |
| 1:B:71:PHE:CD1   | 1:B:108:ASP:OD1  | 2.62                     | 0.53              |
| 1:F:534:ILE:HG22 | 1:F:535:LYS:N    | 2.24                     | 0.53              |
| 1:E:534:ILE:HG22 | 1:E:535:LYS:N    | 2.24                     | 0.53              |
| 1:B:639:ASN:HD22 | 1:B:639:ASN:H    | 1.56                     | 0.53              |
| 1:B:639:ASN:H    | 1:B:639:ASN:ND2  | 2.06                     | 0.53              |
| 1:E:209:LEU:HD23 | 1:E:260:TYR:CG   | 2.43                     | 0.53              |
| 1:C:639:ASN:H    | 1:C:639:ASN:ND2  | 2.06                     | 0.53              |
| 1:B:313:ASP:O    | 1:B:316:LYS:HB2  | 2.09                     | 0.53              |
| 1:E:737:LYS:HA   | 1:E:737:LYS:HE2  | 1.89                     | 0.53              |
| 1:C:131:ARG:HH11 | 1:C:131:ARG:HG2  | 1.73                     | 0.53              |
| 1:B:172:GLU:O    | 1:B:175:LYS:HB3  | 2.09                     | 0.53              |
| 1:A:92:ASP:C     | 1:A:94:LEU:N     | 2.58                     | 0.53              |
| 1:C:302:LEU:HB2  | 1:C:602:PHE:HD1  | 1.74                     | 0.53              |
| 1:F:410:ILE:HG22 | 1:F:411:GLU:N    | 2.24                     | 0.53              |
| 1:F:411:GLU:O    | 1:F:414:LYS:HB2  | 2.08                     | 0.53              |
| 1:E:302:LEU:HB2  | 1:E:602:PHE:HD1  | 1.74                     | 0.53              |
| 1:A:397:GLU:O    | 1:A:479:LYS:HA   | 2.09                     | 0.53              |
| 1:E:199:LEU:HD23 | 1:E:225:ILE:O    | 2.09                     | 0.53              |
| 1:D:546:LYS:CD   | 1:D:554:LYS:HE3  | 2.36                     | 0.53              |
| 1:B:247:TYR:HE2  | 1:B:256:VAL:HG11 | 1.74                     | 0.53              |
| 1:D:795:LYS:C    | 1:D:797:ILE:N    | 2.62                     | 0.53              |
| 1:A:515:LYS:O    | 1:A:515:LYS:HG2  | 2.09                     | 0.53              |
| 1:F:177:ILE:HA   | 1:F:180:ASP:CG   | 2.29                     | 0.53              |
| 1:B:199:LEU:HD21 | 1:B:226:ASP:OD2  | 2.09                     | 0.53              |
| 1:A:199:LEU:HD23 | 1:A:225:ILE:O    | 2.09                     | 0.53              |
| 2:P:121:VAL:C    | 2:P:123:GLN:N    | 2.61                     | 0.53              |
| 1:A:338:LEU:O    | 1:A:341:SER:HB3  | 2.09                     | 0.53              |
| 1:A:107:THR:HG21 | 1:A:115:LYS:HD2  | 1.91                     | 0.53              |
| 1:E:337:ASN:ND2  | 1:E:412:GLU:OE1  | 2.42                     | 0.53              |
| 1:B:338:LEU:O    | 1:B:341:SER:HB3  | 2.09                     | 0.53              |
| 1:D:199:LEU:HD23 | 1:D:225:ILE:O    | 2.09                     | 0.53              |
| 1:C:279:ILE:HD13 | 1:C:279:ILE:N    | 2.24                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:217:LYS:HB3  | 1:E:217:LYS:HZ3  | 1.73                     | 0.53              |
| 2:T:5:THR:HG23   | 2:T:8:GLN:HB2    | 1.91                     | 0.53              |
| 1:D:515:LYS:O    | 1:D:515:LYS:HG2  | 2.08                     | 0.53              |
| 1:C:639:ASN:HD22 | 1:C:639:ASN:H    | 1.55                     | 0.53              |
| 1:A:131:ARG:HH11 | 1:A:131:ARG:HG2  | 1.73                     | 0.53              |
| 1:B:210:PHE:CD2  | 1:B:210:PHE:N    | 2.75                     | 0.53              |
| 1:B:131:ARG:HH11 | 1:B:131:ARG:HG2  | 1.73                     | 0.53              |
| 1:E:184:LYS:CE   | 1:E:193:LEU:HB2  | 2.39                     | 0.53              |
| 1:C:90:PRO:C     | 1:C:92:ASP:H     | 2.12                     | 0.53              |
| 1:B:397:GLU:O    | 1:B:479:LYS:HA   | 2.09                     | 0.53              |
| 1:B:412:GLU:C    | 1:B:414:LYS:N    | 2.60                     | 0.53              |
| 1:E:355:SER:CB   | 1:E:371:SER:HA   | 2.39                     | 0.53              |
| 1:C:199:LEU:HD23 | 1:C:225:ILE:O    | 2.09                     | 0.53              |
| 1:D:405:LEU:N    | 1:D:405:LEU:HD12 | 2.24                     | 0.53              |
| 2:R:32:LEU:HD21  | 2:R:71:MET:HE2   | 1.90                     | 0.53              |
| 2:O:5:THR:CG2    | 2:O:8:GLN:HB2    | 2.39                     | 0.53              |
| 1:F:776:LEU:O    | 1:F:780:LEU:CD2  | 2.57                     | 0.53              |
| 1:F:349:ASN:HD22 | 1:F:350:VAL:N    | 2.07                     | 0.53              |
| 1:F:636:ALA:O    | 1:F:640:LYS:N    | 2.41                     | 0.53              |
| 1:E:664:ILE:HG21 | 2:S:15:ALA:HB2   | 1.92                     | 0.53              |
| 1:D:148:GLU:HG3  | 1:D:149:THR:N    | 2.23                     | 0.53              |
| 1:F:145:LYS:HD3  | 1:F:151:LYS:HD2  | 1.91                     | 0.53              |
| 1:E:148:GLU:HG3  | 1:E:149:THR:N    | 2.23                     | 0.53              |
| 1:B:248:TYR:O    | 1:B:248:TYR:CD2  | 2.62                     | 0.53              |
| 1:E:186:LYS:HZ1  | 1:E:234:LEU:CD1  | 2.23                     | 0.52              |
| 1:C:189:ASP:O    | 1:C:190:PRO:C    | 2.46                     | 0.52              |
| 1:A:170:TYR:C    | 1:A:172:GLU:N    | 2.61                     | 0.52              |
| 2:R:102:ALA:HB2  | 2:R:125:ILE:HG13 | 1.90                     | 0.52              |
| 1:B:327:LEU:HD12 | 1:B:327:LEU:N    | 2.24                     | 0.52              |
| 1:F:199:LEU:HD23 | 1:F:225:ILE:O    | 2.09                     | 0.52              |
| 1:F:134:LYS:HG2  | 1:F:136:PRO:CG   | 2.38                     | 0.52              |
| 1:F:318:ILE:N    | 1:F:318:ILE:HD12 | 2.22                     | 0.52              |
| 2:O:97:ASN:O     | 2:O:99:TYR:HD1   | 1.92                     | 0.52              |
| 1:C:731:GLU:O    | 1:C:735:VAL:HG23 | 2.09                     | 0.52              |
| 2:T:5:THR:CG2    | 2:T:8:GLN:HB2    | 2.39                     | 0.52              |
| 1:F:312:ALA:O    | 1:F:315:PHE:HB2  | 2.09                     | 0.52              |
| 1:C:654:ILE:C    | 1:C:655:ASN:HD22 | 2.13                     | 0.52              |
| 1:F:90:PRO:HG2   | 1:F:93:VAL:HB    | 1.91                     | 0.52              |
| 1:C:172:GLU:O    | 1:C:175:LYS:HB3  | 2.09                     | 0.52              |
| 1:B:90:PRO:HG2   | 1:B:93:VAL:HB    | 1.91                     | 0.52              |
| 1:D:597:ASN:ND2  | 1:D:601:GLU:N    | 2.53                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:630:ARG:HH11 | 1:D:630:ARG:HG3  | 1.74                     | 0.52              |
| 1:D:360:VAL:HG21 | 1:D:365:PRO:HB3  | 1.90                     | 0.52              |
| 1:F:135:VAL:O    | 1:F:135:VAL:CG2  | 2.52                     | 0.52              |
| 1:F:324:THR:HG22 | 1:F:499:PRO:HA   | 1.91                     | 0.52              |
| 1:A:499:PRO:HD3  | 1:A:552:TRP:CH2  | 2.45                     | 0.52              |
| 2:O:5:THR:HG23   | 2:O:8:GLN:HB2    | 1.91                     | 0.52              |
| 1:E:776:LEU:O    | 1:E:780:LEU:CD2  | 2.57                     | 0.52              |
| 1:B:776:LEU:O    | 1:B:780:LEU:CD2  | 2.57                     | 0.52              |
| 1:D:642:TYR:HE2  | 1:D:644:GLU:OE2  | 1.93                     | 0.52              |
| 1:F:209:LEU:HD23 | 1:F:260:TYR:CG   | 2.44                     | 0.52              |
| 1:F:642:TYR:HE2  | 1:F:644:GLU:OE2  | 1.92                     | 0.52              |
| 1:A:209:LEU:HD23 | 1:A:260:TYR:CG   | 2.45                     | 0.52              |
| 1:C:688:PHE:C    | 1:C:688:PHE:CD2  | 2.81                     | 0.52              |
| 2:Q:121:VAL:C    | 2:Q:123:GLN:N    | 2.60                     | 0.52              |
| 2:S:102:ALA:HB2  | 2:S:125:ILE:HG13 | 1.91                     | 0.52              |
| 1:A:718:ARG:NH1  | 1:A:767:GLN:NE2  | 2.53                     | 0.52              |
| 1:F:630:ARG:NH1  | 1:F:630:ARG:HG3  | 2.25                     | 0.52              |
| 1:D:435:LEU:CG   | 1:D:446:ILE:HG22 | 2.34                     | 0.52              |
| 1:D:318:ILE:N    | 1:D:318:ILE:HD12 | 2.22                     | 0.52              |
| 1:C:795:LYS:C    | 1:C:797:ILE:N    | 2.63                     | 0.52              |
| 1:F:735:VAL:O    | 1:F:738:SER:CB   | 2.58                     | 0.52              |
| 2:S:5:THR:CG2    | 2:S:8:GLN:HB2    | 2.39                     | 0.52              |
| 1:A:349:ASN:HD22 | 1:A:350:VAL:N    | 2.07                     | 0.52              |
| 1:F:535:LYS:HD2  | 1:F:536:TYR:CE2  | 2.44                     | 0.52              |
| 1:D:534:ILE:HG22 | 1:D:535:LYS:N    | 2.25                     | 0.52              |
| 1:D:664:ILE:HG21 | 2:R:15:ALA:HB2   | 1.91                     | 0.52              |
| 1:A:148:GLU:HG3  | 1:A:149:THR:N    | 2.23                     | 0.52              |
| 1:B:148:GLU:HG3  | 1:B:149:THR:N    | 2.23                     | 0.52              |
| 1:B:209:LEU:HD23 | 1:B:260:TYR:CG   | 2.44                     | 0.52              |
| 1:C:186:LYS:CA   | 1:C:190:PRO:HD3  | 2.18                     | 0.52              |
| 1:B:213:LYS:HB2  | 1:B:240:ALA:CB   | 2.40                     | 0.52              |
| 1:B:297:LYS:HZ2  | 1:B:297:LYS:HB3  | 1.74                     | 0.52              |
| 1:A:405:LEU:N    | 1:A:405:LEU:HD12 | 2.25                     | 0.52              |
| 1:F:360:VAL:O    | 1:F:363:TYR:HB2  | 2.09                     | 0.52              |
| 1:C:497:LEU:CD1  | 1:C:556:MET:HG2  | 2.36                     | 0.52              |
| 1:D:254:ARG:HG2  | 1:D:255:THR:N    | 2.23                     | 0.52              |
| 1:D:504:ILE:O    | 1:D:507:GLN:HB3  | 2.08                     | 0.52              |
| 1:B:499:PRO:HD3  | 1:B:552:TRP:CH2  | 2.44                     | 0.52              |
| 1:B:731:GLU:O    | 1:B:735:VAL:HG23 | 2.09                     | 0.52              |
| 2:R:76:MET:HG3   | 2:R:76:MET:O     | 2.04                     | 0.52              |
| 1:D:659:THR:OG1  | 1:D:662:GLU:HB2  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:535:LYS:HD2  | 1:A:536:TYR:CE2  | 2.45                     | 0.52              |
| 1:F:523:LEU:HD11 | 2:T:144:MET:HG2  | 1.91                     | 0.52              |
| 1:D:209:LEU:HD23 | 1:D:260:TYR:CG   | 2.44                     | 0.52              |
| 1:F:148:GLU:HG3  | 1:F:149:THR:N    | 2.23                     | 0.52              |
| 2:R:109:MET:HG3  | 2:R:116:LEU:HD11 | 1.91                     | 0.52              |
| 2:O:106:ARG:CG   | 2:O:121:VAL:HG21 | 2.08                     | 0.52              |
| 1:E:338:LEU:O    | 1:E:341:SER:HB3  | 2.08                     | 0.52              |
| 1:C:597:ASN:ND2  | 1:C:601:GLU:N    | 2.52                     | 0.52              |
| 1:B:302:LEU:HB2  | 1:B:602:PHE:HD1  | 1.73                     | 0.52              |
| 1:F:337:ASN:O    | 1:F:341:SER:N    | 2.28                     | 0.52              |
| 1:D:657:ILE:O    | 1:D:658:PRO:O    | 2.27                     | 0.52              |
| 1:B:105:TYR:HB2  | 1:B:153:ILE:HG12 | 1.91                     | 0.52              |
| 1:C:549:LEU:HD12 | 1:C:553:GLN:HB3  | 1.92                     | 0.52              |
| 1:F:546:LYS:CD   | 1:F:554:LYS:HE3  | 2.37                     | 0.52              |
| 1:B:246:SER:O    | 1:B:250:ALA:HB2  | 2.09                     | 0.52              |
| 1:B:255:THR:O    | 1:B:256:VAL:C    | 2.48                     | 0.52              |
| 1:F:499:PRO:HD3  | 1:F:552:TRP:CH2  | 2.44                     | 0.52              |
| 1:F:795:LYS:C    | 1:F:797:ILE:N    | 2.63                     | 0.52              |
| 2:T:95:ASP:OD2   | 2:T:97:ASN:CG    | 2.47                     | 0.52              |
| 2:O:76:MET:O     | 2:O:76:MET:HG3   | 2.04                     | 0.52              |
| 1:A:776:LEU:O    | 1:A:780:LEU:CD2  | 2.58                     | 0.52              |
| 2:Q:5:THR:CG2    | 2:Q:8:GLN:HB2    | 2.40                     | 0.52              |
| 1:A:73:ASN:ND2   | 1:A:74:GLU:OE2   | 2.42                     | 0.52              |
| 1:C:148:GLU:HG3  | 1:C:149:THR:N    | 2.23                     | 0.52              |
| 1:C:727:GLN:O    | 1:C:730:ASN:HB3  | 2.08                     | 0.52              |
| 1:F:313:ASP:O    | 1:F:316:LYS:HB2  | 2.09                     | 0.52              |
| 1:B:189:ASP:O    | 1:B:191:GLU:HG2  | 2.09                     | 0.52              |
| 2:Q:109:MET:HG3  | 2:Q:116:LEU:HD11 | 1.92                     | 0.52              |
| 1:A:302:LEU:HB2  | 1:A:602:PHE:HD1  | 1.73                     | 0.52              |
| 1:F:657:ILE:O    | 1:F:658:PRO:O    | 2.26                     | 0.52              |
| 1:A:667:LEU:HD13 | 1:A:678:VAL:HG21 | 1.90                     | 0.52              |
| 1:C:355:SER:CB   | 1:C:371:SER:HA   | 2.40                     | 0.52              |
| 1:E:405:LEU:HD12 | 1:E:405:LEU:N    | 2.25                     | 0.52              |
| 1:F:279:ILE:CD1  | 1:F:279:ILE:H    | 2.23                     | 0.52              |
| 1:A:217:LYS:CB   | 1:A:236:GLU:HG3  | 2.39                     | 0.52              |
| 1:F:165:GLN:C    | 1:F:167:LYS:H    | 2.12                     | 0.52              |
| 1:B:254:ARG:HG2  | 1:B:255:THR:N    | 2.23                     | 0.52              |
| 1:A:246:SER:O    | 1:A:250:ALA:HB2  | 2.10                     | 0.52              |
| 1:E:254:ARG:HG2  | 1:E:255:THR:N    | 2.23                     | 0.52              |
| 1:B:795:LYS:C    | 1:B:797:ILE:N    | 2.63                     | 0.52              |
| 1:F:731:GLU:O    | 1:F:735:VAL:HG23 | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:776:LEU:O    | 1:D:780:LEU:CD2  | 2.57                     | 0.52              |
| 2:S:5:THR:HG23   | 2:S:8:GLN:HB2    | 1.92                     | 0.52              |
| 1:B:73:ASN:ND2   | 1:B:74:GLU:OE2   | 2.42                     | 0.52              |
| 1:B:535:LYS:HD2  | 1:B:536:TYR:CE2  | 2.45                     | 0.52              |
| 1:C:639:ASN:HD22 | 1:C:639:ASN:N    | 2.07                     | 0.52              |
| 1:A:313:ASP:O    | 1:A:316:LYS:HB2  | 2.10                     | 0.52              |
| 1:E:98:SER:O     | 1:E:101:GLY:N    | 2.43                     | 0.52              |
| 1:F:654:ILE:C    | 1:F:655:ASN:HD22 | 2.13                     | 0.52              |
| 1:D:173:ILE:O    | 1:D:174:GLY:C    | 2.48                     | 0.52              |
| 1:C:630:ARG:HG3  | 1:C:630:ARG:NH1  | 2.25                     | 0.52              |
| 1:F:337:ASN:ND2  | 1:F:412:GLU:OE1  | 2.43                     | 0.52              |
| 1:A:105:TYR:HB2  | 1:A:153:ILE:HG12 | 1.90                     | 0.52              |
| 2:Q:32:LEU:HD21  | 2:Q:71:MET:HE1   | 1.90                     | 0.52              |
| 1:B:444:PHE:CD1  | 1:B:444:PHE:N    | 2.78                     | 0.52              |
| 1:B:275:GLY:O    | 1:B:278:LYS:HB2  | 2.10                     | 0.52              |
| 1:F:246:SER:O    | 1:F:250:ALA:HB2  | 2.09                     | 0.52              |
| 1:D:368:GLN:CB   | 1:D:380:VAL:HG13 | 2.39                     | 0.52              |
| 2:P:26:THR:HA    | 2:P:64:ASP:HA    | 1.92                     | 0.52              |
| 2:O:44:THR:OG1   | 2:O:47:GLU:N     | 2.34                     | 0.52              |
| 2:T:26:THR:HA    | 2:T:64:ASP:HA    | 1.92                     | 0.52              |
| 2:S:26:THR:HA    | 2:S:64:ASP:HA    | 1.92                     | 0.52              |
| 2:Q:26:THR:HA    | 2:Q:64:ASP:HA    | 1.92                     | 0.52              |
| 1:A:515:LYS:NZ   | 1:A:515:LYS:HB3  | 2.24                     | 0.52              |
| 1:E:73:ASN:ND2   | 1:E:74:GLU:OE2   | 2.42                     | 0.52              |
| 1:A:639:ASN:HD22 | 1:A:639:ASN:N    | 2.07                     | 0.52              |
| 1:E:636:ALA:O    | 1:E:640:LYS:N    | 2.42                     | 0.52              |
| 1:A:530:THR:HG21 | 2:O:145:MET:HE3  | 1.91                     | 0.52              |
| 1:E:530:THR:HG21 | 2:S:145:MET:HE3  | 1.92                     | 0.52              |
| 1:C:180:ASP:CG   | 1:C:181:ILE:N    | 2.57                     | 0.52              |
| 1:D:410:ILE:HG22 | 1:D:411:GLU:N    | 2.24                     | 0.52              |
| 1:F:764:LEU:C    | 1:F:766:HIS:H    | 2.13                     | 0.52              |
| 1:D:601:GLU:O    | 1:D:602:PHE:HD2  | 1.93                     | 0.52              |
| 1:B:480:ASN:C    | 1:B:480:ASN:HD22 | 2.08                     | 0.52              |
| 1:B:630:ARG:HG3  | 1:B:630:ARG:NH1  | 2.25                     | 0.52              |
| 1:F:397:GLU:O    | 1:F:479:LYS:HA   | 2.10                     | 0.52              |
| 1:C:246:SER:O    | 1:C:250:ALA:HB2  | 2.10                     | 0.52              |
| 1:B:318:ILE:N    | 1:B:318:ILE:HD12 | 2.23                     | 0.52              |
| 2:Q:44:THR:C     | 2:Q:46:ALA:N     | 2.63                     | 0.52              |
| 2:P:5:THR:CG2    | 2:P:8:GLN:HB2    | 2.39                     | 0.52              |
| 2:S:5:THR:HG23   | 2:S:8:GLN:H      | 1.75                     | 0.52              |
| 2:R:5:THR:HG23   | 2:R:8:GLN:HB2    | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:659:THR:OG1  | 1:F:662:GLU:HB2  | 2.10                     | 0.52              |
| 1:A:628:PHE:CE2  | 2:O:90:ARG:NH1   | 2.78                     | 0.52              |
| 1:A:636:ALA:HB3  | 1:A:639:ASN:HD21 | 1.75                     | 0.52              |
| 1:C:209:LEU:HD23 | 1:C:260:TYR:CG   | 2.45                     | 0.52              |
| 1:D:85:LEU:O     | 1:D:88:LYS:HE3   | 2.10                     | 0.52              |
| 1:C:179:LEU:O    | 1:C:183:SER:N    | 2.43                     | 0.52              |
| 1:A:90:PRO:C     | 1:A:92:ASP:H     | 2.12                     | 0.52              |
| 1:D:337:ASN:ND2  | 1:D:412:GLU:OE1  | 2.43                     | 0.52              |
| 1:C:327:LEU:HD12 | 1:C:327:LEU:N    | 2.24                     | 0.52              |
| 1:E:764:LEU:C    | 1:E:766:HIS:H    | 2.14                     | 0.52              |
| 1:F:355:SER:CB   | 1:F:371:SER:HA   | 2.40                     | 0.52              |
| 1:C:308:VAL:CB   | 1:C:311:HIS:ND1  | 2.71                     | 0.52              |
| 1:F:368:GLN:CB   | 1:F:380:VAL:HG13 | 2.39                     | 0.52              |
| 1:F:217:LYS:CB   | 1:F:236:GLU:HG3  | 2.40                     | 0.52              |
| 2:O:5:THR:HG23   | 2:O:8:GLN:H      | 1.75                     | 0.52              |
| 2:Q:5:THR:HG23   | 2:Q:8:GLN:HB2    | 1.92                     | 0.52              |
| 1:C:288:VAL:HG23 | 1:C:289:GLU:N    | 2.25                     | 0.52              |
| 1:C:534:ILE:HG22 | 1:C:535:LYS:N    | 2.23                     | 0.52              |
| 1:F:790:PHE:O    | 1:F:793:PHE:HB3  | 2.10                     | 0.52              |
| 1:E:180:ASP:O    | 1:E:183:SER:N    | 2.38                     | 0.52              |
| 1:D:180:ASP:O    | 1:D:183:SER:N    | 2.41                     | 0.52              |
| 2:O:105:LEU:HD23 | 2:O:121:VAL:HG13 | 1.92                     | 0.52              |
| 1:E:115:LYS:HB3  | 1:E:115:LYS:HZ3  | 1.75                     | 0.52              |
| 1:D:355:SER:CB   | 1:D:371:SER:HA   | 2.40                     | 0.52              |
| 1:A:435:LEU:CG   | 1:A:446:ILE:HG22 | 2.35                     | 0.52              |
| 1:E:275:GLY:O    | 1:E:278:LYS:HB2  | 2.10                     | 0.52              |
| 1:F:123:GLU:CG   | 1:F:124:GLU:H    | 2.19                     | 0.52              |
| 1:F:288:VAL:HG23 | 1:F:289:GLU:N    | 2.24                     | 0.52              |
| 1:B:515:LYS:NZ   | 1:B:515:LYS:HB3  | 2.25                     | 0.52              |
| 1:F:515:LYS:HB3  | 1:F:515:LYS:NZ   | 2.25                     | 0.52              |
| 1:C:636:ALA:HB3  | 1:C:639:ASN:HD21 | 1.74                     | 0.52              |
| 1:F:503:GLU:HA   | 1:F:506:LYS:HD3  | 1.92                     | 0.52              |
| 1:D:313:ASP:O    | 1:D:316:LYS:HB2  | 2.09                     | 0.52              |
| 1:D:170:TYR:C    | 1:D:172:GLU:N    | 2.61                     | 0.51              |
| 1:D:88:LYS:HG2   | 1:D:88:LYS:O     | 2.09                     | 0.51              |
| 1:A:337:ASN:ND2  | 1:A:412:GLU:OE1  | 2.43                     | 0.51              |
| 1:D:337:ASN:ND2  | 1:D:412:GLU:OE2  | 2.43                     | 0.51              |
| 1:B:764:LEU:C    | 1:B:766:HIS:H    | 2.13                     | 0.51              |
| 1:E:630:ARG:HH11 | 1:E:630:ARG:HG3  | 1.75                     | 0.51              |
| 1:B:405:LEU:HD12 | 1:B:405:LEU:N    | 2.25                     | 0.51              |
| 2:Q:97:ASN:O     | 2:Q:99:TYR:HD1   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:731:GLU:O    | 1:A:735:VAL:HG23 | 2.10                     | 0.51              |
| 2:R:5:THR:HG23   | 2:R:8:GLN:H      | 1.75                     | 0.51              |
| 1:F:530:THR:HG21 | 2:T:145:MET:CE   | 2.40                     | 0.51              |
| 1:D:535:LYS:HD2  | 1:D:536:TYR:CE2  | 2.45                     | 0.51              |
| 1:A:639:ASN:ND2  | 1:A:639:ASN:H    | 2.06                     | 0.51              |
| 1:A:230:ILE:HG13 | 1:A:237:PHE:CE2  | 2.45                     | 0.51              |
| 1:C:642:TYR:HE2  | 1:C:644:GLU:OE2  | 1.93                     | 0.51              |
| 1:C:313:ASP:O    | 1:C:316:LYS:HB2  | 2.09                     | 0.51              |
| 1:A:98:SER:O     | 1:A:101:GLY:N    | 2.43                     | 0.51              |
| 1:E:790:PHE:O    | 1:E:793:PHE:HB3  | 2.10                     | 0.51              |
| 1:E:85:LEU:O     | 1:E:88:LYS:HE3   | 2.10                     | 0.51              |
| 1:C:173:ILE:O    | 1:C:174:GLY:C    | 2.48                     | 0.51              |
| 1:A:172:GLU:O    | 1:A:175:LYS:HB3  | 2.09                     | 0.51              |
| 1:A:218:LEU:C    | 1:A:220:LEU:H    | 2.14                     | 0.51              |
| 1:B:725:GLY:O    | 1:B:728:ALA:HB3  | 2.11                     | 0.51              |
| 1:A:444:PHE:N    | 1:A:444:PHE:CD1  | 2.78                     | 0.51              |
| 1:B:122:GLU:OE1  | 1:B:147:ARG:CB   | 2.55                     | 0.51              |
| 1:A:499:PRO:HD2  | 1:A:625:LEU:O    | 2.10                     | 0.51              |
| 1:E:731:GLU:O    | 1:E:735:VAL:HG23 | 2.11                     | 0.51              |
| 2:R:5:THR:CG2    | 2:R:8:GLN:HB2    | 2.39                     | 0.51              |
| 2:Q:8:GLN:NE2    | 2:Q:76:MET:SD    | 2.82                     | 0.51              |
| 2:Q:13:LYS:HZ1   | 2:Q:65:PHE:CB    | 2.24                     | 0.51              |
| 1:B:628:PHE:CE2  | 2:P:90:ARG:NH1   | 2.78                     | 0.51              |
| 1:D:327:LEU:N    | 1:D:327:LEU:HD12 | 2.24                     | 0.51              |
| 1:C:98:SER:O     | 1:C:101:GLY:N    | 2.44                     | 0.51              |
| 1:F:180:ASP:CG   | 1:F:181:ILE:N    | 2.62                     | 0.51              |
| 1:A:186:LYS:HG2  | 1:A:186:LYS:O    | 2.09                     | 0.51              |
| 2:R:105:LEU:HD23 | 2:R:121:VAL:HG13 | 1.92                     | 0.51              |
| 2:R:121:VAL:C    | 2:R:123:GLN:N    | 2.62                     | 0.51              |
| 2:P:102:ALA:HB2  | 2:P:125:ILE:HG13 | 1.91                     | 0.51              |
| 2:O:102:ALA:HB2  | 2:O:125:ILE:HG13 | 1.92                     | 0.51              |
| 1:D:105:TYR:HB2  | 1:D:153:ILE:HG12 | 1.91                     | 0.51              |
| 1:C:105:TYR:HB2  | 1:C:153:ILE:CG1  | 2.41                     | 0.51              |
| 1:D:668:SER:CA   | 2:R:14:GLU:HG3   | 2.32                     | 0.51              |
| 1:B:165:GLN:C    | 1:B:167:LYS:N    | 2.64                     | 0.51              |
| 1:F:628:PHE:CE2  | 2:T:90:ARG:NH1   | 2.79                     | 0.51              |
| 1:F:73:ASN:ND2   | 1:F:74:GLU:OE2   | 2.42                     | 0.51              |
| 1:E:535:LYS:HD2  | 1:E:536:TYR:CE2  | 2.45                     | 0.51              |
| 1:C:636:ALA:O    | 1:C:640:LYS:N    | 2.42                     | 0.51              |
| 1:B:218:LEU:C    | 1:B:220:LEU:H    | 2.14                     | 0.51              |
| 1:F:295:VAL:HB   | 1:F:603:ILE:HG23 | 1.90                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:657:ILE:O    | 1:B:658:PRO:O    | 2.29                     | 0.51              |
| 1:D:581:GLN:HE21 | 1:D:629:ASN:H    | 1.58                     | 0.51              |
| 1:E:720:ILE:O    | 1:E:724:ARG:HG2  | 2.11                     | 0.51              |
| 1:F:308:VAL:CB   | 1:F:311:HIS:ND1  | 2.71                     | 0.51              |
| 1:F:275:GLY:O    | 1:F:278:LYS:HB2  | 2.11                     | 0.51              |
| 2:O:26:THR:HA    | 2:O:64:ASP:HA    | 1.92                     | 0.51              |
| 2:R:44:THR:C     | 2:R:46:ALA:N     | 2.64                     | 0.51              |
| 1:C:776:LEU:O    | 1:C:780:LEU:CD2  | 2.58                     | 0.51              |
| 1:D:731:GLU:O    | 1:D:735:VAL:HG23 | 2.10                     | 0.51              |
| 1:C:595:ILE:HG22 | 1:C:596:ILE:N    | 2.26                     | 0.51              |
| 1:E:636:ALA:HB3  | 1:E:639:ASN:HD21 | 1.74                     | 0.51              |
| 1:C:503:GLU:HA   | 1:C:506:LYS:HD3  | 1.93                     | 0.51              |
| 1:E:205:SER:C    | 1:E:207:ASP:H    | 2.14                     | 0.51              |
| 1:C:586:PHE:CD2  | 1:C:638:GLY:HA3  | 2.46                     | 0.51              |
| 1:D:168:GLU:C    | 1:D:170:TYR:N    | 2.64                     | 0.51              |
| 1:F:168:GLU:C    | 1:F:170:TYR:N    | 2.64                     | 0.51              |
| 2:O:121:VAL:C    | 2:O:123:GLN:N    | 2.61                     | 0.51              |
| 2:T:105:LEU:HD23 | 2:T:121:VAL:HG13 | 1.92                     | 0.51              |
| 1:D:275:GLY:O    | 1:D:278:LYS:HB2  | 2.11                     | 0.51              |
| 1:C:165:GLN:C    | 1:C:167:LYS:N    | 2.64                     | 0.51              |
| 1:A:255:THR:O    | 1:A:256:VAL:C    | 2.48                     | 0.51              |
| 1:E:795:LYS:C    | 1:E:797:ILE:N    | 2.63                     | 0.51              |
| 2:T:97:ASN:O     | 2:T:99:TYR:HD1   | 1.94                     | 0.51              |
| 2:R:26:THR:HA    | 2:R:64:ASP:HA    | 1.92                     | 0.51              |
| 2:T:5:THR:HG23   | 2:T:8:GLN:H      | 1.76                     | 0.51              |
| 1:E:694:VAL:HG23 | 2:S:18:LEU:HD11  | 1.93                     | 0.51              |
| 1:D:288:VAL:HG23 | 1:D:289:GLU:N    | 2.25                     | 0.51              |
| 1:D:530:THR:HG21 | 2:R:145:MET:CE   | 2.40                     | 0.51              |
| 1:B:534:ILE:HG22 | 1:B:535:LYS:N    | 2.24                     | 0.51              |
| 1:B:595:ILE:HG22 | 1:B:596:ILE:N    | 2.26                     | 0.51              |
| 1:E:595:ILE:HG22 | 1:E:596:ILE:N    | 2.25                     | 0.51              |
| 1:F:205:SER:C    | 1:F:207:ASP:H    | 2.14                     | 0.51              |
| 1:C:263:ASP:O    | 1:C:264:MET:C    | 2.49                     | 0.51              |
| 1:A:248:TYR:O    | 1:A:248:TYR:CD2  | 2.63                     | 0.51              |
| 1:D:172:GLU:O    | 1:D:175:LYS:HB3  | 2.10                     | 0.51              |
| 1:D:189:ASP:O    | 1:D:191:GLU:N    | 2.44                     | 0.51              |
| 2:P:105:LEU:HD23 | 2:P:121:VAL:HG13 | 1.92                     | 0.51              |
| 1:C:337:ASN:ND2  | 1:C:412:GLU:OE1  | 2.44                     | 0.51              |
| 1:A:355:SER:CB   | 1:A:371:SER:HA   | 2.40                     | 0.51              |
| 1:A:279:ILE:HD13 | 1:A:279:ILE:N    | 2.25                     | 0.51              |
| 1:E:546:LYS:CD   | 1:E:554:LYS:HE3  | 2.37                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:546:LYS:CD   | 1:C:554:LYS:HE3  | 2.38                     | 0.51              |
| 1:A:324:THR:HG22 | 1:A:499:PRO:HA   | 1.91                     | 0.51              |
| 1:D:694:VAL:HG23 | 2:R:18:LEU:HD21  | 1.92                     | 0.51              |
| 1:A:288:VAL:HG23 | 1:A:289:GLU:N    | 2.25                     | 0.51              |
| 1:C:535:LYS:HD2  | 1:C:536:TYR:CE2  | 2.45                     | 0.51              |
| 1:D:503:GLU:HA   | 1:D:506:LYS:HD3  | 1.93                     | 0.51              |
| 1:C:92:ASP:O     | 1:C:93:VAL:C     | 2.49                     | 0.51              |
| 1:B:173:ILE:O    | 1:B:174:GLY:C    | 2.49                     | 0.51              |
| 1:B:337:ASN:ND2  | 1:B:412:GLU:OE1  | 2.44                     | 0.51              |
| 1:D:397:GLU:O    | 1:D:479:LYS:HA   | 2.10                     | 0.51              |
| 1:B:722:ILE:HD13 | 1:B:764:LEU:HD23 | 1.92                     | 0.51              |
| 1:F:338:LEU:O    | 1:F:341:SER:HB3  | 2.11                     | 0.51              |
| 1:A:657:ILE:HG13 | 1:A:756:ILE:HD12 | 1.93                     | 0.51              |
| 1:E:279:ILE:HD13 | 1:E:279:ILE:N    | 2.26                     | 0.51              |
| 1:F:279:ILE:N    | 1:F:279:ILE:HD13 | 2.26                     | 0.51              |
| 1:B:497:LEU:CD1  | 1:B:556:MET:HG2  | 2.38                     | 0.51              |
| 1:A:165:GLN:C    | 1:A:167:LYS:N    | 2.64                     | 0.51              |
| 1:B:499:PRO:HD2  | 1:B:625:LEU:O    | 2.11                     | 0.51              |
| 1:D:795:LYS:C    | 1:D:797:ILE:H    | 2.14                     | 0.51              |
| 2:T:73:ALA:O     | 2:T:75:LYS:N     | 2.43                     | 0.51              |
| 1:B:288:VAL:HG23 | 1:B:289:GLU:N    | 2.25                     | 0.51              |
| 1:D:141:PHE:H    | 1:D:141:PHE:HD1  | 1.57                     | 0.51              |
| 1:F:636:ALA:HB3  | 1:F:639:ASN:HD21 | 1.75                     | 0.51              |
| 1:F:639:ASN:H    | 1:F:639:ASN:ND2  | 2.08                     | 0.51              |
| 1:D:636:ALA:O    | 1:D:640:LYS:N    | 2.43                     | 0.51              |
| 2:Q:36:MET:HE3   | 2:Q:43:PRO:HG3   | 1.93                     | 0.51              |
| 1:B:503:GLU:HA   | 1:B:506:LYS:HD3  | 1.92                     | 0.51              |
| 1:E:313:ASP:O    | 1:E:316:LYS:HB2  | 2.10                     | 0.51              |
| 1:B:115:LYS:O    | 1:B:117:LEU:N    | 2.43                     | 0.51              |
| 1:C:107:THR:HG21 | 1:C:115:LYS:CD   | 2.40                     | 0.51              |
| 1:C:405:LEU:HD12 | 1:C:405:LEU:N    | 2.26                     | 0.51              |
| 1:C:456:LYS:HB3  | 1:C:470:ASN:C    | 2.31                     | 0.51              |
| 1:C:324:THR:HG22 | 1:C:499:PRO:HA   | 1.91                     | 0.51              |
| 1:F:216:GLU:HG3  | 1:F:217:LYS:HG2  | 1.93                     | 0.51              |
| 2:Q:5:THR:HG23   | 2:Q:8:GLN:H      | 1.75                     | 0.51              |
| 1:C:649:ILE:HD13 | 2:Q:138:TYR:HB2  | 1.92                     | 0.51              |
| 1:D:98:SER:O     | 1:D:101:GLY:N    | 2.42                     | 0.51              |
| 1:B:618:ASN:O    | 1:B:622:LYS:HB3  | 2.11                     | 0.51              |
| 1:C:523:LEU:HD11 | 2:Q:144:MET:HG2  | 1.92                     | 0.51              |
| 1:E:170:TYR:C    | 1:E:172:GLU:N    | 2.62                     | 0.51              |
| 1:D:170:TYR:O    | 1:D:174:GLY:N    | 2.43                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:90:PRO:C     | 1:C:92:ASP:N     | 2.64                     | 0.51              |
| 1:A:115:LYS:O    | 1:A:117:LEU:N    | 2.44                     | 0.51              |
| 1:A:601:GLU:O    | 1:A:602:PHE:HD2  | 1.94                     | 0.51              |
| 1:E:105:TYR:HB2  | 1:E:153:ILE:CG1  | 2.41                     | 0.51              |
| 1:F:629:ASN:HD22 | 1:F:631:SER:N    | 1.97                     | 0.51              |
| 1:D:629:ASN:HD22 | 1:D:631:SER:N    | 1.97                     | 0.51              |
| 1:B:355:SER:CB   | 1:B:371:SER:HA   | 2.41                     | 0.51              |
| 2:Q:12:PHE:CD1   | 2:Q:72:MET:HG3   | 2.46                     | 0.51              |
| 1:D:432:TYR:CE1  | 1:D:445:ARG:CZ   | 2.94                     | 0.51              |
| 1:C:447:SER:OG   | 1:C:448:ASP:N    | 2.44                     | 0.51              |
| 1:A:451:ASN:OD1  | 1:A:451:ASN:N    | 2.29                     | 0.51              |
| 1:C:275:GLY:O    | 1:C:278:LYS:HB2  | 2.10                     | 0.51              |
| 1:B:216:GLU:HG3  | 1:B:217:LYS:HG2  | 1.93                     | 0.51              |
| 1:D:324:THR:HG22 | 1:D:499:PRO:HA   | 1.91                     | 0.51              |
| 2:P:44:THR:C     | 2:P:46:ALA:N     | 2.64                     | 0.51              |
| 1:F:263:ASP:O    | 1:F:264:MET:C    | 2.48                     | 0.51              |
| 1:A:525:LYS:HE3  | 2:O:114:GLU:HG2  | 1.93                     | 0.51              |
| 1:D:523:LEU:HD11 | 2:R:144:MET:HG2  | 1.93                     | 0.51              |
| 1:C:557:LEU:HD11 | 1:C:575:VAL:CG1  | 2.41                     | 0.51              |
| 1:D:248:TYR:O    | 1:D:248:TYR:CD2  | 2.64                     | 0.51              |
| 1:D:90:PRO:C     | 1:D:92:ASP:N     | 2.64                     | 0.51              |
| 1:F:177:ILE:HA   | 1:F:180:ASP:OD1  | 2.11                     | 0.51              |
| 1:C:92:ASP:O     | 1:C:94:LEU:N     | 2.44                     | 0.51              |
| 1:B:88:LYS:HG2   | 1:B:88:LYS:O     | 2.10                     | 0.51              |
| 1:C:480:ASN:ND2  | 1:C:480:ASN:C    | 2.64                     | 0.51              |
| 1:D:105:TYR:HB2  | 1:D:153:ILE:CG1  | 2.41                     | 0.51              |
| 1:B:657:ILE:HG13 | 1:B:756:ILE:HD12 | 1.93                     | 0.51              |
| 1:F:115:LYS:O    | 1:F:117:LEU:N    | 2.44                     | 0.51              |
| 1:F:337:ASN:ND2  | 1:F:412:GLU:OE2  | 2.44                     | 0.51              |
| 1:A:595:ILE:HG22 | 1:A:596:ILE:N    | 2.26                     | 0.51              |
| 1:A:581:GLN:HE21 | 1:A:629:ASN:H    | 1.58                     | 0.51              |
| 1:F:581:GLN:HE21 | 1:F:629:ASN:H    | 1.59                     | 0.51              |
| 1:F:105:TYR:HB2  | 1:F:153:ILE:CG1  | 2.41                     | 0.51              |
| 1:F:218:LEU:C    | 1:F:220:LEU:H    | 2.14                     | 0.51              |
| 1:B:447:SER:OG   | 1:B:448:ASP:N    | 2.44                     | 0.51              |
| 1:C:446:ILE:HD11 | 1:C:451:ASN:CB   | 2.41                     | 0.51              |
| 1:F:497:LEU:CD1  | 1:F:556:MET:HG2  | 2.38                     | 0.51              |
| 1:A:318:ILE:N    | 1:A:318:ILE:HD12 | 2.21                     | 0.51              |
| 1:D:499:PRO:HD3  | 1:D:552:TRP:CH2  | 2.45                     | 0.51              |
| 1:A:247:TYR:HE2  | 1:A:256:VAL:CG1  | 2.24                     | 0.51              |
| 1:B:324:THR:HG22 | 1:B:499:PRO:HA   | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:44:THR:C     | 2:T:46:ALA:N     | 2.64                     | 0.51              |
| 2:R:13:LYS:HZ3   | 2:R:65:PHE:CB    | 2.23                     | 0.51              |
| 2:P:8:GLN:NE2    | 2:P:76:MET:SD    | 2.84                     | 0.51              |
| 1:D:636:ALA:HB3  | 1:D:639:ASN:HD21 | 1.75                     | 0.51              |
| 1:D:557:LEU:HD11 | 1:D:575:VAL:CG1  | 2.41                     | 0.51              |
| 1:D:586:PHE:CD2  | 1:D:638:GLY:HA3  | 2.46                     | 0.51              |
| 1:A:205:SER:C    | 1:A:207:ASP:H    | 2.14                     | 0.51              |
| 1:F:170:TYR:C    | 1:F:172:GLU:N    | 2.61                     | 0.50              |
| 1:F:90:PRO:C     | 1:F:92:ASP:N     | 2.64                     | 0.50              |
| 1:F:92:ASP:O     | 1:F:94:LEU:N     | 2.44                     | 0.50              |
| 1:B:130:SER:HB2  | 1:B:170:TYR:CE2  | 2.46                     | 0.50              |
| 1:A:173:ILE:O    | 1:A:174:GLY:C    | 2.48                     | 0.50              |
| 1:C:397:GLU:O    | 1:C:479:LYS:HA   | 2.10                     | 0.50              |
| 1:D:716:LYS:O    | 1:D:717:LYS:C    | 2.49                     | 0.50              |
| 2:T:12:PHE:CD1   | 2:T:72:MET:HG3   | 2.46                     | 0.50              |
| 1:D:447:SER:OG   | 1:D:448:ASP:N    | 2.44                     | 0.50              |
| 1:C:432:TYR:CE1  | 1:C:445:ARG:CZ   | 2.94                     | 0.50              |
| 1:A:446:ILE:HD11 | 1:A:451:ASN:CB   | 2.40                     | 0.50              |
| 2:P:76:MET:O     | 2:P:76:MET:HG3   | 2.04                     | 0.50              |
| 2:P:5:THR:HG23   | 2:P:8:GLN:H      | 1.76                     | 0.50              |
| 1:E:639:ASN:HD22 | 1:E:639:ASN:N    | 2.08                     | 0.50              |
| 1:B:639:ASN:HD22 | 1:B:639:ASN:N    | 2.07                     | 0.50              |
| 1:A:503:GLU:HA   | 1:A:506:LYS:HD3  | 1.93                     | 0.50              |
| 1:D:790:PHE:O    | 1:D:793:PHE:HB3  | 2.11                     | 0.50              |
| 1:C:618:ASN:O    | 1:C:622:LYS:HB3  | 2.11                     | 0.50              |
| 1:B:654:ILE:C    | 1:B:655:ASN:HD22 | 2.14                     | 0.50              |
| 1:E:88:LYS:O     | 1:E:88:LYS:HG2   | 2.11                     | 0.50              |
| 1:C:94:LEU:C     | 1:C:96:ILE:H     | 2.15                     | 0.50              |
| 1:F:725:GLY:O    | 1:F:728:ALA:HB3  | 2.10                     | 0.50              |
| 2:S:124:MET:O    | 2:S:126:ARG:N    | 2.44                     | 0.50              |
| 1:E:337:ASN:ND2  | 1:E:412:GLU:OE2  | 2.44                     | 0.50              |
| 1:C:657:ILE:O    | 1:C:658:PRO:O    | 2.28                     | 0.50              |
| 1:D:397:GLU:HG3  | 1:D:480:ASN:HB3  | 1.94                     | 0.50              |
| 1:E:581:GLN:HE21 | 1:E:629:ASN:H    | 1.59                     | 0.50              |
| 1:B:581:GLN:HE21 | 1:B:629:ASN:H    | 1.58                     | 0.50              |
| 1:A:275:GLY:O    | 1:A:278:LYS:HB2  | 2.12                     | 0.50              |
| 1:E:279:ILE:C    | 1:E:281:GLU:H    | 2.15                     | 0.50              |
| 1:D:165:GLN:C    | 1:D:167:LYS:N    | 2.64                     | 0.50              |
| 1:D:499:PRO:HD2  | 1:D:625:LEU:O    | 2.11                     | 0.50              |
| 1:E:711:ILE:C    | 1:E:712:PHE:HD2  | 2.14                     | 0.50              |
| 1:A:795:LYS:C    | 1:A:797:ILE:N    | 2.63                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:36:MET:CE    | 2:P:43:PRO:HG3   | 2.41                     | 0.50              |
| 1:E:642:TYR:HE2  | 1:E:644:GLU:OE2  | 1.94                     | 0.50              |
| 1:A:664:ILE:HG21 | 2:O:15:ALA:HB2   | 1.93                     | 0.50              |
| 1:E:92:ASP:O     | 1:E:93:VAL:C     | 2.49                     | 0.50              |
| 1:E:92:ASP:O     | 1:E:94:LEU:N     | 2.44                     | 0.50              |
| 1:D:94:LEU:C     | 1:D:96:ILE:H     | 2.13                     | 0.50              |
| 1:B:92:ASP:O     | 1:B:94:LEU:N     | 2.45                     | 0.50              |
| 1:C:601:GLU:O    | 1:C:602:PHE:HD2  | 1.93                     | 0.50              |
| 1:B:337:ASN:ND2  | 1:B:412:GLU:OE2  | 2.43                     | 0.50              |
| 1:D:657:ILE:HG13 | 1:D:756:ILE:HD12 | 1.92                     | 0.50              |
| 1:A:279:ILE:C    | 1:A:281:GLU:H    | 2.15                     | 0.50              |
| 1:A:216:GLU:HG3  | 1:A:217:LYS:HG2  | 1.93                     | 0.50              |
| 1:F:254:ARG:HG2  | 1:F:255:THR:N    | 2.23                     | 0.50              |
| 1:F:255:THR:O    | 1:F:256:VAL:C    | 2.49                     | 0.50              |
| 1:D:255:THR:O    | 1:D:256:VAL:C    | 2.49                     | 0.50              |
| 1:C:735:VAL:O    | 1:C:738:SER:CB   | 2.59                     | 0.50              |
| 2:O:8:GLN:NE2    | 2:O:76:MET:SD    | 2.84                     | 0.50              |
| 1:E:288:VAL:HG23 | 1:E:289:GLU:N    | 2.25                     | 0.50              |
| 1:C:223:LYS:HZ3  | 1:C:228:ASN:HB3  | 1.75                     | 0.50              |
| 1:E:141:PHE:H    | 1:E:141:PHE:HD1  | 1.59                     | 0.50              |
| 1:F:595:ILE:HG22 | 1:F:596:ILE:N    | 2.25                     | 0.50              |
| 1:C:73:ASN:ND2   | 1:C:74:GLU:OE2   | 2.43                     | 0.50              |
| 1:F:639:ASN:HD22 | 1:F:639:ASN:N    | 2.08                     | 0.50              |
| 1:C:205:SER:C    | 1:C:207:ASP:H    | 2.14                     | 0.50              |
| 1:F:112:VAL:O    | 1:F:114:HIS:N    | 2.43                     | 0.50              |
| 1:E:246:SER:O    | 1:E:250:ALA:HB2  | 2.11                     | 0.50              |
| 1:E:90:PRO:C     | 1:E:92:ASP:N     | 2.64                     | 0.50              |
| 1:C:410:ILE:HD13 | 1:C:419:ILE:HD11 | 1.93                     | 0.50              |
| 2:T:102:ALA:HB2  | 2:T:125:ILE:HG13 | 1.93                     | 0.50              |
| 1:C:105:TYR:CB   | 1:C:153:ILE:HG12 | 2.42                     | 0.50              |
| 1:B:105:TYR:HB2  | 1:B:153:ILE:CG1  | 2.41                     | 0.50              |
| 1:C:446:ILE:HG13 | 1:C:452:GLU:O    | 2.11                     | 0.50              |
| 1:A:432:TYR:CE1  | 1:A:445:ARG:CZ   | 2.95                     | 0.50              |
| 1:C:279:ILE:C    | 1:C:281:GLU:H    | 2.15                     | 0.50              |
| 1:B:279:ILE:N    | 1:B:279:ILE:HD13 | 2.26                     | 0.50              |
| 1:C:122:GLU:HG3  | 1:C:147:ARG:H    | 1.75                     | 0.50              |
| 1:E:165:GLN:C    | 1:E:167:LYS:N    | 2.64                     | 0.50              |
| 1:A:795:LYS:C    | 1:A:797:ILE:H    | 2.15                     | 0.50              |
| 1:F:711:ILE:C    | 1:F:712:PHE:HD2  | 2.15                     | 0.50              |
| 1:F:716:LYS:O    | 1:F:717:LYS:C    | 2.50                     | 0.50              |
| 1:E:216:GLU:HG3  | 1:E:217:LYS:HG2  | 1.93                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:97:ASN:O     | 2:R:99:TYR:HD1   | 1.93                     | 0.50              |
| 1:C:664:ILE:HG21 | 2:Q:15:ALA:HB2   | 1.92                     | 0.50              |
| 1:A:642:TYR:HE2  | 1:A:644:GLU:OE2  | 1.93                     | 0.50              |
| 1:D:88:LYS:NZ    | 1:D:172:GLU:OE2  | 2.45                     | 0.50              |
| 1:F:88:LYS:HG2   | 1:F:88:LYS:O     | 2.10                     | 0.50              |
| 1:F:88:LYS:NZ    | 1:F:172:GLU:OE2  | 2.45                     | 0.50              |
| 1:B:199:LEU:HD23 | 1:B:225:ILE:O    | 2.11                     | 0.50              |
| 1:B:94:LEU:C     | 1:B:96:ILE:H     | 2.14                     | 0.50              |
| 1:A:90:PRO:C     | 1:A:92:ASP:N     | 2.64                     | 0.50              |
| 2:T:124:MET:O    | 2:T:126:ARG:N    | 2.45                     | 0.50              |
| 1:A:337:ASN:ND2  | 1:A:412:GLU:OE2  | 2.43                     | 0.50              |
| 1:F:297:LYS:HZ2  | 1:F:297:LYS:HB3  | 1.75                     | 0.50              |
| 1:B:549:LEU:HD12 | 1:B:553:GLN:HB3  | 1.93                     | 0.50              |
| 1:B:480:ASN:C    | 1:B:480:ASN:ND2  | 2.63                     | 0.50              |
| 1:F:444:PHE:CD1  | 1:F:444:PHE:N    | 2.79                     | 0.50              |
| 1:F:432:TYR:CE1  | 1:F:445:ARG:CZ   | 2.94                     | 0.50              |
| 1:C:720:ILE:O    | 1:C:724:ARG:HG2  | 2.12                     | 0.50              |
| 1:A:501:LEU:HD22 | 2:O:112:LEU:CD2  | 2.37                     | 0.50              |
| 1:A:546:LYS:CD   | 1:A:554:LYS:HE3  | 2.37                     | 0.50              |
| 1:C:255:THR:O    | 1:C:256:VAL:C    | 2.49                     | 0.50              |
| 1:A:66:LEU:HD12  | 1:A:104:ILE:H    | 1.77                     | 0.50              |
| 2:O:44:THR:C     | 2:O:46:ALA:N     | 2.64                     | 0.50              |
| 1:B:263:ASP:O    | 1:B:264:MET:C    | 2.50                     | 0.50              |
| 1:E:286:GLU:O    | 1:E:286:GLU:HG2  | 2.12                     | 0.50              |
| 1:A:649:ILE:HD13 | 2:O:138:TYR:HB2  | 1.93                     | 0.50              |
| 2:Q:138:TYR:CE1  | 2:Q:142:VAL:HG22 | 2.47                     | 0.50              |
| 2:S:138:TYR:CE1  | 2:S:142:VAL:HG22 | 2.46                     | 0.50              |
| 1:F:172:GLU:O    | 1:F:175:LYS:HB3  | 2.11                     | 0.50              |
| 1:C:184:LYS:HZ1  | 1:C:193:LEU:HD12 | 1.74                     | 0.50              |
| 1:B:90:PRO:C     | 1:B:92:ASP:N     | 2.63                     | 0.50              |
| 1:A:176:GLY:C    | 1:A:178:SER:N    | 2.65                     | 0.50              |
| 1:A:725:GLY:O    | 1:A:728:ALA:HB3  | 2.11                     | 0.50              |
| 2:P:124:MET:O    | 2:P:126:ARG:N    | 2.44                     | 0.50              |
| 1:C:480:ASN:HD22 | 1:C:480:ASN:C    | 2.09                     | 0.50              |
| 1:E:337:ASN:O    | 1:E:341:SER:N    | 2.29                     | 0.50              |
| 1:F:601:GLU:O    | 1:F:602:PHE:HD2  | 1.94                     | 0.50              |
| 1:B:409:ARG:CZ   | 1:B:413:LEU:HD21 | 2.42                     | 0.50              |
| 1:B:722:ILE:HD13 | 1:B:764:LEU:CD2  | 2.41                     | 0.50              |
| 1:E:105:TYR:CB   | 1:E:153:ILE:HG12 | 2.42                     | 0.50              |
| 1:C:629:ASN:C    | 1:C:629:ASN:ND2  | 2.58                     | 0.50              |
| 1:C:581:GLN:HE22 | 1:C:629:ASN:H    | 1.60                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:432:TYR:CE1  | 1:B:445:ARG:CZ   | 2.95                     | 0.50              |
| 2:R:12:PHE:CD1   | 2:R:72:MET:HG3   | 2.47                     | 0.50              |
| 1:E:122:GLU:HG3  | 1:E:147:ARG:H    | 1.77                     | 0.50              |
| 1:F:279:ILE:C    | 1:F:281:GLU:H    | 2.15                     | 0.50              |
| 1:F:165:GLN:C    | 1:F:167:LYS:N    | 2.64                     | 0.50              |
| 1:D:246:SER:O    | 1:D:250:ALA:HB2  | 2.12                     | 0.50              |
| 1:E:252:ASP:O    | 1:E:254:ARG:HD2  | 2.11                     | 0.50              |
| 1:C:216:GLU:HG3  | 1:C:217:LYS:HG2  | 1.93                     | 0.50              |
| 1:D:694:VAL:HG23 | 2:R:18:LEU:HD11  | 1.94                     | 0.50              |
| 1:D:286:GLU:HG2  | 1:D:286:GLU:O    | 2.12                     | 0.50              |
| 1:C:628:PHE:CE2  | 2:Q:90:ARG:NH1   | 2.80                     | 0.50              |
| 1:D:73:ASN:ND2   | 1:D:74:GLU:OE2   | 2.43                     | 0.50              |
| 1:B:636:ALA:HB3  | 1:B:639:ASN:HD21 | 1.76                     | 0.50              |
| 1:B:642:TYR:HE2  | 1:B:644:GLU:OE2  | 1.93                     | 0.50              |
| 1:E:170:TYR:O    | 1:E:174:GLY:N    | 2.45                     | 0.50              |
| 1:E:172:GLU:O    | 1:E:175:LYS:HB3  | 2.11                     | 0.50              |
| 1:B:88:LYS:NZ    | 1:B:172:GLU:OE2  | 2.44                     | 0.50              |
| 1:A:177:ILE:HA   | 1:A:180:ASP:CG   | 2.32                     | 0.50              |
| 1:C:725:GLY:O    | 1:C:728:ALA:HB3  | 2.12                     | 0.50              |
| 1:B:410:ILE:HD13 | 1:B:419:ILE:HD11 | 1.94                     | 0.50              |
| 1:E:397:GLU:O    | 1:E:479:LYS:HA   | 2.10                     | 0.50              |
| 1:A:482:GLU:HA   | 1:A:482:GLU:OE2  | 2.12                     | 0.50              |
| 1:A:105:TYR:HB2  | 1:A:153:ILE:CG1  | 2.42                     | 0.50              |
| 1:F:105:TYR:CB   | 1:F:153:ILE:HG12 | 2.42                     | 0.50              |
| 1:F:405:LEU:HD12 | 1:F:405:LEU:N    | 2.26                     | 0.50              |
| 1:C:444:PHE:N    | 1:C:444:PHE:CD1  | 2.78                     | 0.50              |
| 2:R:12:PHE:O     | 2:R:16:PHE:HB2   | 2.12                     | 0.50              |
| 1:E:444:PHE:CD1  | 1:E:444:PHE:N    | 2.78                     | 0.50              |
| 1:D:279:ILE:N    | 1:D:279:ILE:HD13 | 2.26                     | 0.50              |
| 1:C:252:ASP:O    | 1:C:254:ARG:HD2  | 2.11                     | 0.50              |
| 1:E:255:THR:O    | 1:E:256:VAL:C    | 2.48                     | 0.50              |
| 1:F:776:LEU:HD23 | 1:F:776:LEU:C    | 2.32                     | 0.50              |
| 1:A:263:ASP:O    | 1:A:264:MET:C    | 2.49                     | 0.50              |
| 1:C:141:PHE:H    | 1:C:141:PHE:HD1  | 1.57                     | 0.50              |
| 2:P:36:MET:HE2   | 2:P:43:PRO:HG3   | 1.93                     | 0.50              |
| 1:E:557:LEU:HD11 | 1:E:575:VAL:CG1  | 2.42                     | 0.50              |
| 2:T:36:MET:CE    | 2:T:43:PRO:HG3   | 2.42                     | 0.50              |
| 1:B:205:SER:C    | 1:B:207:ASP:H    | 2.14                     | 0.50              |
| 1:E:94:LEU:C     | 1:E:96:ILE:H     | 2.15                     | 0.50              |
| 1:D:183:SER:O    | 1:D:187:SER:HB2  | 2.07                     | 0.50              |
| 1:D:92:ASP:O     | 1:D:93:VAL:C     | 2.50                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:170:TYR:O    | 1:B:174:GLY:N    | 2.45                     | 0.50              |
| 1:C:657:ILE:HG13 | 1:C:756:ILE:HD12 | 1.91                     | 0.50              |
| 1:B:302:LEU:HD22 | 1:B:602:PHE:CE1  | 2.47                     | 0.50              |
| 1:C:501:LEU:HD22 | 2:Q:112:LEU:CD2  | 2.39                     | 0.50              |
| 1:F:664:ILE:HG21 | 2:T:15:ALA:HB2   | 1.94                     | 0.50              |
| 1:F:286:GLU:HG2  | 1:F:286:GLU:O    | 2.12                     | 0.50              |
| 2:Q:36:MET:CE    | 2:Q:43:PRO:HG3   | 2.42                     | 0.50              |
| 1:D:205:SER:C    | 1:D:207:ASP:H    | 2.14                     | 0.50              |
| 1:E:586:PHE:CD2  | 1:E:638:GLY:HA3  | 2.47                     | 0.50              |
| 1:A:753:LYS:O    | 1:A:754:GLU:C    | 2.50                     | 0.50              |
| 1:F:173:ILE:O    | 1:F:174:GLY:C    | 2.49                     | 0.50              |
| 1:A:183:SER:C    | 1:A:187:SER:CB   | 2.75                     | 0.50              |
| 1:A:94:LEU:C     | 1:A:96:ILE:H     | 2.14                     | 0.50              |
| 1:D:105:TYR:CB   | 1:D:153:ILE:HG12 | 2.42                     | 0.50              |
| 1:A:549:LEU:HD12 | 1:A:553:GLN:HB3  | 1.93                     | 0.50              |
| 1:B:581:GLN:HE22 | 1:B:629:ASN:H    | 1.60                     | 0.50              |
| 1:F:549:LEU:HD12 | 1:F:553:GLN:HB3  | 1.93                     | 0.50              |
| 2:S:12:PHE:CD1   | 2:S:72:MET:HG3   | 2.47                     | 0.50              |
| 2:Q:12:PHE:O     | 2:Q:16:PHE:HB2   | 2.12                     | 0.50              |
| 1:E:447:SER:OG   | 1:E:448:ASP:N    | 2.44                     | 0.50              |
| 1:F:499:PRO:HD2  | 1:F:625:LEU:O    | 2.12                     | 0.50              |
| 1:F:795:LYS:C    | 1:F:797:ILE:H    | 2.14                     | 0.50              |
| 1:C:776:LEU:HD23 | 1:C:776:LEU:C    | 2.32                     | 0.50              |
| 2:S:73:ALA:O     | 2:S:75:LYS:N     | 2.45                     | 0.50              |
| 1:E:776:LEU:HD23 | 1:E:776:LEU:C    | 2.32                     | 0.50              |
| 1:B:694:VAL:HG23 | 2:P:18:LEU:HD11  | 1.93                     | 0.50              |
| 1:A:286:GLU:O    | 1:A:286:GLU:HG2  | 2.11                     | 0.50              |
| 2:S:24:ASP:CG    | 2:S:25:GLY:H     | 2.15                     | 0.50              |
| 1:E:248:TYR:O    | 1:E:248:TYR:CD2  | 2.65                     | 0.50              |
| 1:C:170:TYR:O    | 1:C:174:GLY:N    | 2.44                     | 0.49              |
| 1:B:184:LYS:HZ1  | 1:B:193:LEU:HD12 | 1.74                     | 0.49              |
| 1:A:184:LYS:CE   | 1:A:193:LEU:HB2  | 2.42                     | 0.49              |
| 1:A:88:LYS:NZ    | 1:A:172:GLU:OE2  | 2.45                     | 0.49              |
| 1:A:409:ARG:CZ   | 1:A:413:LEU:HD21 | 2.42                     | 0.49              |
| 1:A:410:ILE:HD13 | 1:A:419:ILE:HD11 | 1.93                     | 0.49              |
| 1:D:66:LEU:HD12  | 1:D:104:ILE:H    | 1.77                     | 0.49              |
| 1:E:480:ASN:ND2  | 1:E:480:ASN:C    | 2.64                     | 0.49              |
| 1:B:107:THR:HG21 | 1:B:115:LYS:CD   | 2.42                     | 0.49              |
| 1:C:218:LEU:C    | 1:C:220:LEU:H    | 2.14                     | 0.49              |
| 1:A:446:ILE:HG13 | 1:A:452:GLU:O    | 2.11                     | 0.49              |
| 1:F:252:ASP:O    | 1:F:254:ARG:HD2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:499:PRO:HD2  | 1:E:625:LEU:O    | 2.12                     | 0.49              |
| 1:B:247:TYR:HE2  | 1:B:256:VAL:CG1  | 2.25                     | 0.49              |
| 2:P:13:LYS:HZ3   | 2:P:65:PHE:CB    | 2.23                     | 0.49              |
| 1:D:263:ASP:O    | 1:D:264:MET:C    | 2.50                     | 0.49              |
| 1:F:586:PHE:CD2  | 1:F:638:GLY:HA3  | 2.47                     | 0.49              |
| 1:B:482:GLU:OE2  | 1:B:482:GLU:HA   | 2.12                     | 0.49              |
| 1:E:186:LYS:NZ   | 1:E:234:LEU:HD12 | 2.27                     | 0.49              |
| 1:F:94:LEU:C     | 1:F:96:ILE:N     | 2.65                     | 0.49              |
| 1:C:184:LYS:CE   | 1:C:191:GLU:HB2  | 2.41                     | 0.49              |
| 1:A:295:VAL:HB   | 1:A:603:ILE:HG23 | 1.93                     | 0.49              |
| 1:D:410:ILE:HD13 | 1:D:419:ILE:HD11 | 1.93                     | 0.49              |
| 1:A:597:ASN:ND2  | 1:A:601:GLU:N    | 2.52                     | 0.49              |
| 1:D:630:ARG:HG3  | 1:D:630:ARG:NH1  | 2.26                     | 0.49              |
| 1:A:271:LEU:HA   | 1:A:275:GLY:HA3  | 1.93                     | 0.49              |
| 1:C:443:GLU:HG2  | 1:C:458:LYS:HZ1  | 1.71                     | 0.49              |
| 1:B:456:LYS:HB2  | 1:B:470:ASN:HA   | 1.93                     | 0.49              |
| 1:B:716:LYS:O    | 1:B:717:LYS:C    | 2.50                     | 0.49              |
| 1:D:123:GLU:CG   | 1:D:124:GLU:H    | 2.19                     | 0.49              |
| 1:A:711:ILE:C    | 1:A:712:PHE:HD2  | 2.15                     | 0.49              |
| 2:O:13:LYS:HZ3   | 2:O:65:PHE:HB3   | 1.77                     | 0.49              |
| 1:D:216:GLU:HG3  | 1:D:217:LYS:HG2  | 1.93                     | 0.49              |
| 1:F:288:VAL:C    | 1:F:290:LYS:H    | 2.16                     | 0.49              |
| 1:C:99:GLU:C     | 1:C:101:GLY:H    | 2.15                     | 0.49              |
| 1:D:595:ILE:HG22 | 1:D:596:ILE:N    | 2.28                     | 0.49              |
| 1:D:177:ILE:HA   | 1:D:180:ASP:CG   | 2.33                     | 0.49              |
| 1:D:94:LEU:C     | 1:D:96:ILE:N     | 2.65                     | 0.49              |
| 1:D:94:LEU:O     | 1:D:97:TYR:N     | 2.45                     | 0.49              |
| 1:C:94:LEU:C     | 1:C:96:ILE:N     | 2.66                     | 0.49              |
| 1:B:168:GLU:C    | 1:B:170:TYR:N    | 2.64                     | 0.49              |
| 1:A:180:ASP:CG   | 1:A:181:ILE:N    | 2.61                     | 0.49              |
| 1:C:711:ILE:C    | 1:C:712:PHE:HD2  | 2.15                     | 0.49              |
| 1:C:716:LYS:O    | 1:C:717:LYS:C    | 2.50                     | 0.49              |
| 1:E:597:ASN:ND2  | 1:E:601:GLU:N    | 2.52                     | 0.49              |
| 1:E:601:GLU:O    | 1:E:602:PHE:HD2  | 1.94                     | 0.49              |
| 1:E:549:LEU:HD12 | 1:E:553:GLN:HB3  | 1.95                     | 0.49              |
| 1:E:218:LEU:C    | 1:E:220:LEU:H    | 2.14                     | 0.49              |
| 1:D:444:PHE:N    | 1:D:444:PHE:CD1  | 2.79                     | 0.49              |
| 1:F:447:SER:OG   | 1:F:448:ASP:N    | 2.44                     | 0.49              |
| 1:D:271:LEU:HD13 | 1:D:276:PHE:CE2  | 2.47                     | 0.49              |
| 1:E:311:HIS:HD2  | 1:E:564:VAL:HB   | 1.77                     | 0.49              |
| 1:D:165:GLN:O    | 1:D:167:LYS:N    | 2.46                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:66:LEU:HD12  | 1:B:104:ILE:H    | 1.77                     | 0.49              |
| 2:P:97:ASN:O     | 2:P:99:TYR:HD1   | 1.95                     | 0.49              |
| 1:B:776:LEU:HD23 | 1:B:776:LEU:C    | 2.32                     | 0.49              |
| 2:P:138:TYR:CE1  | 2:P:142:VAL:HG22 | 2.46                     | 0.49              |
| 1:B:530:THR:HG21 | 2:P:145:MET:CE   | 2.41                     | 0.49              |
| 1:B:664:ILE:HG21 | 2:P:15:ALA:HB2   | 1.93                     | 0.49              |
| 1:C:88:LYS:NZ    | 1:C:172:GLU:OE2  | 2.46                     | 0.49              |
| 1:B:94:LEU:C     | 1:B:96:ILE:N     | 2.65                     | 0.49              |
| 2:Q:105:LEU:HD23 | 2:Q:121:VAL:HG13 | 1.93                     | 0.49              |
| 1:C:409:ARG:CZ   | 1:C:413:LEU:HD21 | 2.42                     | 0.49              |
| 1:F:410:ILE:HD13 | 1:F:419:ILE:HD11 | 1.93                     | 0.49              |
| 1:E:397:GLU:HG3  | 1:E:480:ASN:HB3  | 1.94                     | 0.49              |
| 1:E:432:TYR:CE1  | 1:E:445:ARG:CZ   | 2.94                     | 0.49              |
| 2:O:12:PHE:CD1   | 2:O:72:MET:HG3   | 2.47                     | 0.49              |
| 1:D:308:VAL:CB   | 1:D:311:HIS:ND1  | 2.71                     | 0.49              |
| 1:B:720:ILE:O    | 1:B:724:ARG:HG2  | 2.12                     | 0.49              |
| 1:D:122:GLU:HG3  | 1:D:147:ARG:H    | 1.77                     | 0.49              |
| 1:F:247:TYR:HE2  | 1:F:256:VAL:CG1  | 2.25                     | 0.49              |
| 1:C:217:LYS:CB   | 1:C:236:GLU:HG3  | 2.43                     | 0.49              |
| 1:A:716:LYS:O    | 1:A:717:LYS:C    | 2.50                     | 0.49              |
| 1:B:795:LYS:C    | 1:B:797:ILE:H    | 2.14                     | 0.49              |
| 1:C:66:LEU:HD12  | 1:C:104:ILE:H    | 1.78                     | 0.49              |
| 1:D:217:LYS:CB   | 1:D:236:GLU:HG3  | 2.42                     | 0.49              |
| 2:S:97:ASN:O     | 2:S:99:TYR:HD1   | 1.95                     | 0.49              |
| 1:D:127:SER:O    | 1:D:133:GLU:HG3  | 2.13                     | 0.49              |
| 2:S:36:MET:CE    | 2:S:43:PRO:HG3   | 2.43                     | 0.49              |
| 1:B:180:ASP:CG   | 1:B:181:ILE:N    | 2.62                     | 0.49              |
| 1:B:184:LYS:CE   | 1:B:191:GLU:HB2  | 2.41                     | 0.49              |
| 1:E:409:ARG:CZ   | 1:E:413:LEU:HD21 | 2.41                     | 0.49              |
| 1:F:397:GLU:HG3  | 1:F:480:ASN:HB3  | 1.93                     | 0.49              |
| 1:D:115:LYS:O    | 1:D:117:LEU:N    | 2.45                     | 0.49              |
| 1:B:426:ILE:HD13 | 1:B:431:LYS:HA   | 1.95                     | 0.49              |
| 1:E:285:LYS:C    | 1:E:287:GLY:H    | 2.16                     | 0.49              |
| 1:E:134:LYS:HG2  | 1:E:136:PRO:CG   | 2.42                     | 0.49              |
| 1:E:716:LYS:O    | 1:E:717:LYS:C    | 2.50                     | 0.49              |
| 1:B:711:ILE:C    | 1:B:712:PHE:HD2  | 2.15                     | 0.49              |
| 2:O:5:THR:O      | 2:O:8:GLN:HB3    | 2.12                     | 0.49              |
| 1:D:776:LEU:C    | 1:D:776:LEU:HD23 | 2.32                     | 0.49              |
| 1:D:628:PHE:CE2  | 2:R:90:ARG:NH1   | 2.80                     | 0.49              |
| 1:F:649:ILE:HD13 | 2:T:138:TYR:HB2  | 1.93                     | 0.49              |
| 1:E:99:GLU:C     | 1:E:101:GLY:H    | 2.15                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:557:LEU:HD11 | 1:F:575:VAL:CG1  | 2.43                     | 0.49              |
| 1:F:127:SER:O    | 1:F:133:GLU:HG3  | 2.13                     | 0.49              |
| 1:D:92:ASP:O     | 1:D:94:LEU:N     | 2.46                     | 0.49              |
| 1:F:92:ASP:O     | 1:F:93:VAL:C     | 2.49                     | 0.49              |
| 1:F:94:LEU:C     | 1:F:96:ILE:H     | 2.14                     | 0.49              |
| 1:D:725:GLY:O    | 1:D:728:ALA:HB3  | 2.13                     | 0.49              |
| 1:B:601:GLU:O    | 1:B:602:PHE:HD2  | 1.95                     | 0.49              |
| 1:C:581:GLN:HE21 | 1:C:629:ASN:H    | 1.59                     | 0.49              |
| 1:D:581:GLN:HE22 | 1:D:629:ASN:H    | 1.60                     | 0.49              |
| 1:D:218:LEU:C    | 1:D:220:LEU:H    | 2.14                     | 0.49              |
| 1:A:447:SER:OG   | 1:A:448:ASP:N    | 2.45                     | 0.49              |
| 1:F:720:ILE:O    | 1:F:724:ARG:HG2  | 2.12                     | 0.49              |
| 1:C:271:LEU:HA   | 1:C:275:GLY:HA3  | 1.95                     | 0.49              |
| 1:B:501:LEU:HD22 | 2:P:112:LEU:CD2  | 2.39                     | 0.49              |
| 1:D:497:LEU:CD1  | 1:D:556:MET:HG2  | 2.38                     | 0.49              |
| 1:F:694:VAL:HG23 | 2:T:18:LEU:HD11  | 1.95                     | 0.49              |
| 1:E:628:PHE:CE2  | 2:S:90:ARG:NH1   | 2.81                     | 0.49              |
| 1:C:127:SER:O    | 1:C:133:GLU:HG3  | 2.13                     | 0.49              |
| 2:O:36:MET:CE    | 2:O:43:PRO:HG3   | 2.42                     | 0.49              |
| 1:C:248:TYR:O    | 1:C:248:TYR:CD2  | 2.65                     | 0.49              |
| 1:E:168:GLU:C    | 1:E:170:TYR:N    | 2.64                     | 0.49              |
| 1:E:173:ILE:O    | 1:E:174:GLY:C    | 2.50                     | 0.49              |
| 1:E:177:ILE:HA   | 1:E:180:ASP:CG   | 2.33                     | 0.49              |
| 1:C:94:LEU:O     | 1:C:97:TYR:N     | 2.45                     | 0.49              |
| 1:B:92:ASP:O     | 1:B:93:VAL:C     | 2.50                     | 0.49              |
| 1:A:168:GLU:C    | 1:A:170:TYR:N    | 2.64                     | 0.49              |
| 1:E:725:GLY:O    | 1:E:728:ALA:HB3  | 2.13                     | 0.49              |
| 2:Q:124:MET:O    | 2:Q:126:ARG:N    | 2.46                     | 0.49              |
| 1:C:337:ASN:ND2  | 1:C:412:GLU:OE2  | 2.45                     | 0.49              |
| 1:E:410:ILE:HD13 | 1:E:419:ILE:HD11 | 1.93                     | 0.49              |
| 1:D:480:ASN:C    | 1:D:480:ASN:ND2  | 2.64                     | 0.49              |
| 1:A:105:TYR:CB   | 1:A:153:ILE:HG12 | 2.42                     | 0.49              |
| 2:S:12:PHE:O     | 2:S:16:PHE:HB2   | 2.13                     | 0.49              |
| 1:A:426:ILE:HD13 | 1:A:431:LYS:HA   | 1.95                     | 0.49              |
| 1:A:720:ILE:O    | 1:A:724:ARG:HG2  | 2.12                     | 0.49              |
| 1:D:720:ILE:O    | 1:D:724:ARG:HG2  | 2.12                     | 0.49              |
| 1:E:135:VAL:CG2  | 1:E:135:VAL:O    | 2.53                     | 0.49              |
| 1:E:694:VAL:HG23 | 2:S:18:LEU:HD21  | 1.94                     | 0.49              |
| 1:B:141:PHE:H    | 1:B:141:PHE:HD1  | 1.57                     | 0.49              |
| 2:T:138:TYR:CE1  | 2:T:142:VAL:HG22 | 2.47                     | 0.49              |
| 2:P:143:GLN:O    | 2:P:147:ALA:HB3  | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:263:ASP:O    | 1:E:264:MET:C    | 2.50                     | 0.49              |
| 1:E:753:LYS:O    | 1:E:754:GLU:C    | 2.51                     | 0.49              |
| 1:B:586:PHE:CD2  | 1:B:638:GLY:HA3  | 2.47                     | 0.49              |
| 1:E:94:LEU:C     | 1:E:96:ILE:N     | 2.66                     | 0.49              |
| 1:D:184:LYS:HE3  | 1:D:191:GLU:HB2  | 1.93                     | 0.49              |
| 1:F:184:LYS:NZ   | 1:F:191:GLU:CB   | 2.67                     | 0.49              |
| 1:F:94:LEU:O     | 1:F:97:TYR:N     | 2.45                     | 0.49              |
| 1:A:94:LEU:O     | 1:A:97:TYR:N     | 2.46                     | 0.49              |
| 2:Q:102:ALA:HB2  | 2:Q:125:ILE:HG13 | 1.93                     | 0.49              |
| 2:O:124:MET:O    | 2:O:126:ARG:N    | 2.46                     | 0.49              |
| 1:D:409:ARG:CZ   | 1:D:413:LEU:HD21 | 2.42                     | 0.49              |
| 1:D:764:LEU:O    | 1:D:766:HIS:N    | 2.46                     | 0.49              |
| 1:F:668:SER:CA   | 2:T:14:GLU:HG3   | 2.32                     | 0.49              |
| 2:P:12:PHE:CD1   | 2:P:72:MET:HG3   | 2.48                     | 0.49              |
| 1:A:285:LYS:C    | 1:A:287:GLY:H    | 2.16                     | 0.49              |
| 1:B:279:ILE:C    | 1:B:281:GLU:H    | 2.15                     | 0.49              |
| 1:D:134:LYS:HG2  | 1:D:136:PRO:CG   | 2.43                     | 0.49              |
| 1:A:252:ASP:O    | 1:A:254:ARG:HD2  | 2.11                     | 0.49              |
| 1:E:247:TYR:HE2  | 1:E:256:VAL:CG1  | 2.25                     | 0.49              |
| 1:E:795:LYS:C    | 1:E:797:ILE:H    | 2.15                     | 0.49              |
| 2:O:138:TYR:CE1  | 2:O:142:VAL:HG22 | 2.47                     | 0.49              |
| 1:A:71:PHE:CD1   | 1:A:108:ASP:OD1  | 2.66                     | 0.49              |
| 1:C:99:GLU:OE2   | 1:C:284:LYS:HD2  | 2.13                     | 0.49              |
| 1:E:277:GLU:HA   | 1:E:280:SER:OG   | 2.13                     | 0.49              |
| 2:R:36:MET:CE    | 2:R:43:PRO:HG3   | 2.43                     | 0.49              |
| 1:A:586:PHE:CD2  | 1:A:638:GLY:HA3  | 2.47                     | 0.49              |
| 1:C:176:GLY:C    | 1:C:178:SER:N    | 2.66                     | 0.49              |
| 1:B:201:ASP:HB3  | 1:B:202:ASP:OD2  | 2.12                     | 0.49              |
| 2:S:32:LEU:HD21  | 2:S:71:MET:HE1   | 1.95                     | 0.49              |
| 1:F:426:ILE:HD13 | 1:F:431:LYS:HA   | 1.95                     | 0.49              |
| 1:B:546:LYS:CD   | 1:B:554:LYS:HE3  | 2.39                     | 0.49              |
| 1:E:217:LYS:HB3  | 1:E:217:LYS:HZ2  | 1.75                     | 0.49              |
| 2:T:5:THR:O      | 2:T:8:GLN:HB3    | 2.12                     | 0.49              |
| 1:B:286:GLU:HG2  | 1:B:286:GLU:O    | 2.12                     | 0.49              |
| 1:A:628:PHE:HE2  | 2:O:90:ARG:CD    | 2.25                     | 0.49              |
| 2:O:36:MET:HE3   | 2:O:43:PRO:HG3   | 1.94                     | 0.49              |
| 1:E:127:SER:O    | 1:E:133:GLU:HG3  | 2.13                     | 0.49              |
| 2:R:111:ASN:C    | 2:R:113:GLY:H    | 2.17                     | 0.49              |
| 1:A:127:SER:O    | 1:A:133:GLU:HG3  | 2.13                     | 0.49              |
| 1:B:94:LEU:O     | 1:B:97:TYR:N     | 2.45                     | 0.49              |
| 1:A:213:LYS:HB2  | 1:A:240:ALA:CB   | 2.43                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:92:ASP:O     | 1:A:93:VAL:C     | 2.51                     | 0.49              |
| 1:E:302:LEU:HD22 | 1:E:602:PHE:CE1  | 2.48                     | 0.49              |
| 1:E:482:GLU:OE2  | 1:E:482:GLU:HA   | 2.12                     | 0.49              |
| 1:A:397:GLU:HG3  | 1:A:480:ASN:HB3  | 1.94                     | 0.49              |
| 1:C:115:LYS:O    | 1:C:117:LEU:N    | 2.45                     | 0.49              |
| 1:B:451:ASN:N    | 1:B:451:ASN:OD1  | 2.29                     | 0.49              |
| 1:E:501:LEU:HD22 | 2:S:112:LEU:CD2  | 2.35                     | 0.49              |
| 1:C:165:GLN:O    | 1:C:167:LYS:N    | 2.46                     | 0.49              |
| 1:F:66:LEU:HD12  | 1:F:104:ILE:H    | 1.78                     | 0.49              |
| 2:S:4:LEU:HA     | 2:S:8:GLN:OE1    | 2.13                     | 0.49              |
| 2:Q:4:LEU:HA     | 2:Q:8:GLN:OE1    | 2.13                     | 0.49              |
| 1:B:288:VAL:C    | 1:B:290:LYS:H    | 2.17                     | 0.49              |
| 1:A:99:GLU:C     | 1:A:101:GLY:H    | 2.15                     | 0.49              |
| 1:E:523:LEU:HD11 | 2:S:144:MET:HG2  | 1.94                     | 0.49              |
| 1:F:409:ARG:CZ   | 1:F:413:LEU:HD21 | 2.43                     | 0.48              |
| 1:D:549:LEU:HD12 | 1:D:553:GLN:HB3  | 1.94                     | 0.48              |
| 2:T:12:PHE:O     | 2:T:16:PHE:HB2   | 2.13                     | 0.48              |
| 2:O:48:LEU:HA    | 2:O:51:MET:CE    | 2.43                     | 0.48              |
| 1:D:271:LEU:HA   | 1:D:275:GLY:HA3  | 1.94                     | 0.48              |
| 1:D:311:HIS:HD2  | 1:D:564:VAL:HB   | 1.76                     | 0.48              |
| 1:A:165:GLN:O    | 1:A:167:LYS:N    | 2.46                     | 0.48              |
| 1:E:66:LEU:HD12  | 1:E:104:ILE:H    | 1.79                     | 0.48              |
| 2:S:5:THR:O      | 2:S:8:GLN:HB3    | 2.13                     | 0.48              |
| 1:B:753:LYS:O    | 1:B:754:GLU:C    | 2.52                     | 0.48              |
| 1:A:557:LEU:HD11 | 1:A:575:VAL:CG1  | 2.43                     | 0.48              |
| 1:F:248:TYR:O    | 1:F:248:TYR:CD2  | 2.66                     | 0.48              |
| 1:F:170:TYR:O    | 1:F:174:GLY:N    | 2.45                     | 0.48              |
| 1:C:177:ILE:HA   | 1:C:180:ASP:OD1  | 2.13                     | 0.48              |
| 1:A:175:LYS:HZ3  | 1:A:175:LYS:HB2  | 1.74                     | 0.48              |
| 1:D:597:ASN:ND2  | 1:D:601:GLU:HB2  | 2.28                     | 0.48              |
| 1:A:142:VAL:HG13 | 1:A:154:ILE:HD12 | 1.94                     | 0.48              |
| 2:R:32:LEU:HD21  | 2:R:71:MET:HE1   | 1.95                     | 0.48              |
| 2:P:12:PHE:O     | 2:P:16:PHE:HB2   | 2.13                     | 0.48              |
| 1:F:285:LYS:C    | 1:F:287:GLY:H    | 2.17                     | 0.48              |
| 1:B:252:ASP:O    | 1:B:254:ARG:HD2  | 2.12                     | 0.48              |
| 1:A:456:LYS:HB3  | 1:A:470:ASN:C    | 2.34                     | 0.48              |
| 2:P:4:LEU:HA     | 2:P:8:GLN:OE1    | 2.13                     | 0.48              |
| 1:E:530:THR:HG21 | 2:S:145:MET:CE   | 2.43                     | 0.48              |
| 1:B:230:ILE:HG13 | 1:B:237:PHE:CE2  | 2.47                     | 0.48              |
| 1:A:523:LEU:HD11 | 2:O:144:MET:HG2  | 1.94                     | 0.48              |
| 2:Q:143:GLN:O    | 2:Q:147:ALA:HB3  | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:T:131:ASP:N    | 2:T:131:ASP:OD1  | 2.46                     | 0.48              |
| 1:B:729:TYR:C    | 1:B:729:TYR:CD2  | 2.87                     | 0.48              |
| 1:E:175:LYS:HZ3  | 1:E:175:LYS:CB   | 2.26                     | 0.48              |
| 1:D:168:GLU:O    | 1:D:170:TYR:N    | 2.47                     | 0.48              |
| 1:D:186:LYS:NZ   | 1:D:234:LEU:HD12 | 2.28                     | 0.48              |
| 1:A:94:LEU:C     | 1:A:96:ILE:N     | 2.66                     | 0.48              |
| 2:T:116:LEU:HD13 | 2:T:121:VAL:HG22 | 1.95                     | 0.48              |
| 1:F:597:ASN:ND2  | 1:F:601:GLU:HB2  | 2.29                     | 0.48              |
| 1:C:597:ASN:ND2  | 1:C:601:GLU:HB2  | 2.28                     | 0.48              |
| 1:E:657:ILE:HG13 | 1:E:756:ILE:HD12 | 1.94                     | 0.48              |
| 1:C:152:LEU:CD2  | 1:C:154:ILE:HD11 | 2.40                     | 0.48              |
| 1:A:495:PHE:CD1  | 1:A:495:PHE:O    | 2.67                     | 0.48              |
| 1:D:711:ILE:C    | 1:D:712:PHE:HD2  | 2.15                     | 0.48              |
| 1:E:426:ILE:HD13 | 1:E:431:LYS:HA   | 1.95                     | 0.48              |
| 1:B:456:LYS:HB3  | 1:B:471:TRP:N    | 2.28                     | 0.48              |
| 1:C:795:LYS:C    | 1:C:797:ILE:H    | 2.15                     | 0.48              |
| 1:A:123:GLU:CG   | 1:A:124:GLU:H    | 2.20                     | 0.48              |
| 1:B:263:ASP:O    | 1:B:265:PHE:N    | 2.47                     | 0.48              |
| 1:B:515:LYS:NZ   | 1:B:516:VAL:HG23 | 2.29                     | 0.48              |
| 1:A:344:ALA:O    | 1:A:489:THR:HG22 | 2.13                     | 0.48              |
| 1:F:99:GLU:C     | 1:F:101:GLY:H    | 2.15                     | 0.48              |
| 1:B:184:LYS:HZ2  | 1:B:191:GLU:HB2  | 1.75                     | 0.48              |
| 2:R:124:MET:O    | 2:R:126:ARG:N    | 2.46                     | 0.48              |
| 2:P:116:LEU:HD13 | 2:P:121:VAL:HG22 | 1.95                     | 0.48              |
| 2:T:121:VAL:C    | 2:T:123:GLN:N    | 2.61                     | 0.48              |
| 1:C:482:GLU:HA   | 1:C:482:GLU:OE2  | 2.13                     | 0.48              |
| 1:C:302:LEU:HD22 | 1:C:602:PHE:CE1  | 2.48                     | 0.48              |
| 1:E:629:ASN:ND2  | 1:E:629:ASN:C    | 2.57                     | 0.48              |
| 1:C:629:ASN:ND2  | 1:C:631:SER:N    | 2.44                     | 0.48              |
| 1:E:107:THR:HG21 | 1:E:115:LYS:CD   | 2.43                     | 0.48              |
| 1:D:225:ILE:HG23 | 1:D:229:PHE:CE2  | 2.49                     | 0.48              |
| 1:D:279:ILE:C    | 1:D:281:GLU:H    | 2.15                     | 0.48              |
| 1:E:353:LYS:HB2  | 1:E:368:GLN:HE22 | 1.78                     | 0.48              |
| 1:C:247:TYR:HE2  | 1:C:256:VAL:CG1  | 2.26                     | 0.48              |
| 1:D:500:SER:O    | 1:D:504:ILE:HD13 | 2.13                     | 0.48              |
| 1:F:500:SER:O    | 1:F:504:ILE:HD13 | 2.14                     | 0.48              |
| 1:B:123:GLU:CG   | 1:B:124:GLU:H    | 2.20                     | 0.48              |
| 1:B:686:ASP:CB   | 1:B:739:LYS:HD2  | 2.42                     | 0.48              |
| 1:E:515:LYS:HZ3  | 1:E:516:VAL:HG23 | 1.78                     | 0.48              |
| 2:T:24:ASP:CG    | 2:T:25:GLY:H     | 2.16                     | 0.48              |
| 1:F:168:GLU:C    | 1:F:170:TYR:H    | 2.17                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:83:GLN:O     | 1:F:84:ASP:C     | 2.51                     | 0.48              |
| 1:C:168:GLU:C    | 1:C:170:TYR:H    | 2.17                     | 0.48              |
| 1:B:177:ILE:HA   | 1:B:180:ASP:CG   | 2.34                     | 0.48              |
| 1:B:597:ASN:ND2  | 1:B:601:GLU:HB2  | 2.29                     | 0.48              |
| 1:C:142:VAL:CG2  | 1:C:154:ILE:HG23 | 2.40                     | 0.48              |
| 1:F:482:GLU:HA   | 1:F:482:GLU:OE2  | 2.14                     | 0.48              |
| 1:D:764:LEU:C    | 1:D:766:HIS:N    | 2.65                     | 0.48              |
| 1:B:105:TYR:CB   | 1:B:153:ILE:HG12 | 2.42                     | 0.48              |
| 1:D:426:ILE:HD13 | 1:D:431:LYS:HA   | 1.95                     | 0.48              |
| 1:C:426:ILE:HD13 | 1:C:431:LYS:HA   | 1.95                     | 0.48              |
| 2:O:30:LYS:H     | 2:O:30:LYS:CD    | 2.20                     | 0.48              |
| 1:D:279:ILE:HG22 | 1:D:283:LEU:CD1  | 2.44                     | 0.48              |
| 1:F:279:ILE:HG22 | 1:F:283:LEU:CD1  | 2.44                     | 0.48              |
| 1:B:165:GLN:O    | 1:B:167:LYS:N    | 2.46                     | 0.48              |
| 1:E:165:GLN:O    | 1:E:167:LYS:N    | 2.46                     | 0.48              |
| 2:P:5:THR:O      | 2:P:8:GLN:HB3    | 2.13                     | 0.48              |
| 2:T:4:LEU:HA     | 2:T:8:GLN:OE1    | 2.14                     | 0.48              |
| 1:F:263:ASP:O    | 1:F:265:PHE:N    | 2.46                     | 0.48              |
| 1:C:210:PHE:HD2  | 1:C:210:PHE:N    | 2.11                     | 0.48              |
| 1:B:523:LEU:HD11 | 2:P:144:MET:HG2  | 1.94                     | 0.48              |
| 1:D:130:SER:C    | 1:D:132:GLY:H    | 2.17                     | 0.48              |
| 1:E:83:GLN:O     | 1:E:84:ASP:C     | 2.51                     | 0.48              |
| 1:F:176:GLY:C    | 1:F:178:SER:N    | 2.67                     | 0.48              |
| 1:F:234:LEU:HD23 | 1:F:235:THR:H    | 1.78                     | 0.48              |
| 1:F:97:TYR:CD2   | 1:F:102:GLY:HA3  | 2.48                     | 0.48              |
| 1:B:184:LYS:HZ1  | 1:B:191:GLU:HB2  | 1.75                     | 0.48              |
| 1:A:97:TYR:CE1   | 1:A:178:SER:HB2  | 2.48                     | 0.48              |
| 1:C:397:GLU:HG3  | 1:C:480:ASN:HB3  | 1.95                     | 0.48              |
| 1:F:302:LEU:HD22 | 1:F:602:PHE:CE1  | 2.49                     | 0.48              |
| 1:A:581:GLN:HE22 | 1:A:629:ASN:H    | 1.61                     | 0.48              |
| 1:F:311:HIS:HD2  | 1:F:564:VAL:HB   | 1.78                     | 0.48              |
| 1:F:165:GLN:O    | 1:F:167:LYS:N    | 2.47                     | 0.48              |
| 2:S:5:THR:HG23   | 2:S:8:GLN:CB     | 2.43                     | 0.48              |
| 1:A:776:LEU:C    | 1:A:776:LEU:HD23 | 2.33                     | 0.48              |
| 2:Q:5:THR:O      | 2:Q:8:GLN:HB3    | 2.13                     | 0.48              |
| 1:D:649:ILE:HD13 | 2:R:138:TYR:HB2  | 1.94                     | 0.48              |
| 1:C:263:ASP:O    | 1:C:265:PHE:N    | 2.46                     | 0.48              |
| 1:E:183:SER:C    | 1:E:187:SER:HB3  | 2.34                     | 0.48              |
| 1:C:180:ASP:O    | 1:C:183:SER:N    | 2.41                     | 0.48              |
| 1:C:184:LYS:CE   | 1:C:193:LEU:HB2  | 2.42                     | 0.48              |
| 1:B:181:ILE:HD12 | 1:B:238:GLN:OE1  | 2.14                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:337:ASN:O    | 1:A:341:SER:N    | 2.29                     | 0.48              |
| 1:F:480:ASN:ND2  | 1:F:480:ASN:C    | 2.64                     | 0.48              |
| 1:E:668:SER:CA   | 2:S:14:GLU:HG3   | 2.36                     | 0.48              |
| 1:B:308:VAL:CB   | 1:B:311:HIS:ND1  | 2.71                     | 0.48              |
| 2:R:91:VAL:HG12  | 2:R:92:PHE:N     | 2.29                     | 0.48              |
| 1:C:499:PRO:HD2  | 1:C:625:LEU:O    | 2.14                     | 0.48              |
| 2:R:5:THR:HG23   | 2:R:8:GLN:CB     | 2.44                     | 0.48              |
| 1:D:660:SER:O    | 1:D:663:PHE:HB3  | 2.13                     | 0.48              |
| 1:C:694:VAL:HG23 | 2:Q:18:LEU:HD21  | 1.95                     | 0.48              |
| 1:C:286:GLU:HG2  | 1:C:286:GLU:O    | 2.13                     | 0.48              |
| 1:B:98:SER:O     | 1:B:101:GLY:N    | 2.45                     | 0.48              |
| 1:D:482:GLU:OE2  | 1:D:482:GLU:HA   | 2.13                     | 0.48              |
| 1:C:729:TYR:CD2  | 1:C:729:TYR:C    | 2.87                     | 0.48              |
| 1:E:94:LEU:O     | 1:E:97:TYR:N     | 2.46                     | 0.48              |
| 1:F:184:LYS:CE   | 1:F:193:LEU:HB2  | 2.42                     | 0.48              |
| 1:C:177:ILE:HA   | 1:C:180:ASP:CG   | 2.33                     | 0.48              |
| 1:C:192:PHE:HA   | 1:C:195:LEU:HB3  | 1.95                     | 0.48              |
| 1:B:234:LEU:HD23 | 1:B:235:THR:H    | 1.79                     | 0.48              |
| 1:A:184:LYS:NZ   | 1:A:191:GLU:CB   | 2.73                     | 0.48              |
| 2:S:116:LEU:HD13 | 2:S:121:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:302:LEU:HD22 | 1:A:602:PHE:CE1  | 2.48                     | 0.48              |
| 1:F:656:THR:O    | 1:F:755:ARG:HD2  | 2.13                     | 0.48              |
| 1:B:635:ILE:CD1  | 1:B:635:ILE:H    | 1.99                     | 0.48              |
| 1:B:495:PHE:O    | 1:B:495:PHE:CD1  | 2.67                     | 0.48              |
| 1:F:435:LEU:CG   | 1:F:446:ILE:HG22 | 2.35                     | 0.48              |
| 1:B:443:GLU:CD   | 1:B:458:LYS:HG2  | 2.33                     | 0.48              |
| 1:A:288:VAL:C    | 1:A:290:LYS:H    | 2.17                     | 0.48              |
| 2:R:24:ASP:CG    | 2:R:25:GLY:H     | 2.17                     | 0.48              |
| 2:Q:24:ASP:CG    | 2:Q:25:GLY:H     | 2.17                     | 0.48              |
| 1:D:109:ILE:HD13 | 1:D:157:LYS:HZ3  | 1.77                     | 0.48              |
| 1:D:639:ASN:N    | 1:D:639:ASN:HD22 | 2.08                     | 0.48              |
| 1:D:99:GLU:C     | 1:D:101:GLY:H    | 2.16                     | 0.48              |
| 1:D:277:GLU:HA   | 1:D:280:SER:OG   | 2.14                     | 0.48              |
| 2:O:111:ASN:C    | 2:O:113:GLY:H    | 2.16                     | 0.48              |
| 1:F:277:GLU:HA   | 1:F:280:SER:OG   | 2.13                     | 0.48              |
| 2:S:111:ASN:C    | 2:S:113:GLY:H    | 2.17                     | 0.48              |
| 1:E:186:LYS:HG2  | 1:E:186:LYS:O    | 2.14                     | 0.48              |
| 1:F:168:GLU:O    | 1:F:170:TYR:N    | 2.47                     | 0.48              |
| 1:C:234:LEU:HD23 | 1:C:235:THR:H    | 1.79                     | 0.48              |
| 1:B:184:LYS:CE   | 1:B:193:LEU:HB2  | 2.42                     | 0.48              |
| 1:D:107:THR:HG21 | 1:D:115:LYS:CD   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:P:31:GLU:O     | 2:P:35:VAL:HG23  | 2.14                     | 0.48              |
| 1:E:308:VAL:CB   | 1:E:311:HIS:ND1  | 2.71                     | 0.48              |
| 1:D:135:VAL:N    | 1:D:136:PRO:HD3  | 2.27                     | 0.48              |
| 1:D:252:ASP:O    | 1:D:254:ARG:HD2  | 2.13                     | 0.48              |
| 1:C:318:ILE:HD12 | 1:C:318:ILE:N    | 2.24                     | 0.48              |
| 1:C:123:GLU:CG   | 1:C:124:GLU:H    | 2.19                     | 0.48              |
| 2:R:73:ALA:O     | 2:R:75:LYS:N     | 2.47                     | 0.48              |
| 1:E:660:SER:O    | 1:E:663:PHE:HB3  | 2.14                     | 0.48              |
| 1:C:660:SER:O    | 1:C:663:PHE:HB3  | 2.13                     | 0.48              |
| 1:F:609:GLU:O    | 1:F:610:MET:C    | 2.53                     | 0.48              |
| 2:P:24:ASP:CG    | 2:P:25:GLY:H     | 2.17                     | 0.48              |
| 1:E:210:PHE:HD2  | 1:E:210:PHE:N    | 2.12                     | 0.48              |
| 1:E:263:ASP:O    | 1:E:265:PHE:N    | 2.47                     | 0.48              |
| 1:B:99:GLU:C     | 1:B:101:GLY:H    | 2.16                     | 0.48              |
| 1:B:127:SER:O    | 1:B:133:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:790:PHE:O    | 1:A:793:PHE:HB3  | 2.14                     | 0.48              |
| 1:D:234:LEU:HD23 | 1:D:235:THR:H    | 1.79                     | 0.48              |
| 1:D:302:LEU:HD22 | 1:D:602:PHE:CE1  | 2.48                     | 0.48              |
| 1:B:713:SER:O    | 1:B:714:GLN:C    | 2.52                     | 0.48              |
| 1:E:597:ASN:ND2  | 1:E:601:GLU:HB2  | 2.29                     | 0.48              |
| 1:D:715:GLU:OE1  | 1:D:767:GLN:NE2  | 2.47                     | 0.48              |
| 1:F:629:ASN:C    | 1:F:629:ASN:ND2  | 2.57                     | 0.48              |
| 1:D:279:ILE:H    | 1:D:279:ILE:CD1  | 2.23                     | 0.48              |
| 1:C:311:HIS:HD2  | 1:C:564:VAL:HB   | 1.75                     | 0.48              |
| 1:B:285:LYS:C    | 1:B:287:GLY:H    | 2.16                     | 0.48              |
| 1:F:353:LYS:HB2  | 1:F:368:GLN:HE22 | 1.79                     | 0.48              |
| 1:D:353:LYS:HB2  | 1:D:368:GLN:HE22 | 1.79                     | 0.48              |
| 2:O:44:THR:O     | 2:O:46:ALA:N     | 2.47                     | 0.48              |
| 1:C:694:VAL:HG23 | 2:Q:18:LEU:HD11  | 1.96                     | 0.48              |
| 1:F:344:ALA:O    | 1:F:489:THR:HG22 | 2.13                     | 0.48              |
| 1:F:515:LYS:NZ   | 1:F:516:VAL:HG23 | 2.28                     | 0.48              |
| 2:R:138:TYR:CE1  | 2:R:142:VAL:HG22 | 2.49                     | 0.48              |
| 1:D:210:PHE:N    | 1:D:210:PHE:HD2  | 2.12                     | 0.48              |
| 1:A:210:PHE:N    | 1:A:210:PHE:HD2  | 2.12                     | 0.48              |
| 1:F:98:SER:O     | 1:F:101:GLY:N    | 2.44                     | 0.48              |
| 1:E:503:GLU:HA   | 1:E:506:LYS:HD3  | 1.95                     | 0.48              |
| 1:D:729:TYR:CD2  | 1:D:729:TYR:C    | 2.87                     | 0.48              |
| 1:E:88:LYS:NZ    | 1:E:172:GLU:OE2  | 2.47                     | 0.47              |
| 1:D:83:GLN:O     | 1:D:84:ASP:C     | 2.52                     | 0.47              |
| 1:A:234:LEU:HD23 | 1:A:235:THR:H    | 1.78                     | 0.47              |
| 2:Q:121:VAL:O    | 2:Q:122:ASP:C    | 2.52                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:715:GLU:HA   | 1:A:718:ARG:NH2  | 2.29                     | 0.47              |
| 1:F:581:GLN:HE22 | 1:F:629:ASN:H    | 1.61                     | 0.47              |
| 1:E:225:ILE:HG23 | 1:E:229:PHE:CE2  | 2.49                     | 0.47              |
| 1:F:446:ILE:HD11 | 1:F:451:ASN:CB   | 2.44                     | 0.47              |
| 1:E:279:ILE:HG22 | 1:E:283:LEU:CD1  | 2.44                     | 0.47              |
| 1:F:271:LEU:HA   | 1:F:275:GLY:HA3  | 1.95                     | 0.47              |
| 1:D:247:TYR:HE2  | 1:D:256:VAL:CG1  | 2.25                     | 0.47              |
| 1:B:353:LYS:HB2  | 1:B:368:GLN:HE22 | 1.79                     | 0.47              |
| 1:C:500:SER:O    | 1:C:504:ILE:HD13 | 2.13                     | 0.47              |
| 1:C:288:VAL:C    | 1:C:290:LYS:H    | 2.16                     | 0.47              |
| 1:A:686:ASP:CB   | 1:A:739:LYS:HD2  | 2.42                     | 0.47              |
| 2:O:24:ASP:CG    | 2:O:25:GLY:H     | 2.17                     | 0.47              |
| 2:T:143:GLN:O    | 2:T:147:ALA:HB3  | 2.15                     | 0.47              |
| 2:O:143:GLN:O    | 2:O:147:ALA:HB3  | 2.14                     | 0.47              |
| 1:C:753:LYS:O    | 1:C:754:GLU:C    | 2.52                     | 0.47              |
| 1:B:557:LEU:HD11 | 1:B:575:VAL:CG1  | 2.44                     | 0.47              |
| 1:E:168:GLU:O    | 1:E:170:TYR:N    | 2.47                     | 0.47              |
| 1:D:97:TYR:CD2   | 1:D:102:GLY:HA3  | 2.49                     | 0.47              |
| 1:C:168:GLU:C    | 1:C:170:TYR:N    | 2.64                     | 0.47              |
| 1:B:83:GLN:O     | 1:B:84:ASP:C     | 2.52                     | 0.47              |
| 2:O:116:LEU:HD13 | 2:O:121:VAL:HG22 | 1.95                     | 0.47              |
| 1:B:397:GLU:HG3  | 1:B:480:ASN:HB3  | 1.94                     | 0.47              |
| 1:F:153:ILE:C    | 1:F:154:ILE:HD13 | 2.34                     | 0.47              |
| 1:D:116:GLU:C    | 1:D:117:LEU:HD22 | 2.35                     | 0.47              |
| 2:O:12:PHE:O     | 2:O:16:PHE:HB2   | 2.13                     | 0.47              |
| 1:A:279:ILE:CD1  | 1:A:279:ILE:H    | 2.22                     | 0.47              |
| 1:C:500:SER:HA   | 1:C:624:TYR:CD2  | 2.49                     | 0.47              |
| 1:D:217:LYS:HB3  | 1:D:217:LYS:HZ2  | 1.77                     | 0.47              |
| 1:E:741:ILE:O    | 1:E:742:ALA:C    | 2.52                     | 0.47              |
| 2:P:5:THR:HG23   | 2:P:8:GLN:CB     | 2.44                     | 0.47              |
| 2:T:5:THR:HG23   | 2:T:8:GLN:CB     | 2.44                     | 0.47              |
| 2:P:44:THR:O     | 2:P:46:ALA:N     | 2.48                     | 0.47              |
| 2:S:44:THR:C     | 2:S:46:ALA:N     | 2.64                     | 0.47              |
| 1:C:515:LYS:NZ   | 1:C:516:VAL:HG23 | 2.30                     | 0.47              |
| 1:E:515:LYS:NZ   | 1:E:516:VAL:HG23 | 2.29                     | 0.47              |
| 1:D:609:GLU:O    | 1:D:610:MET:C    | 2.52                     | 0.47              |
| 1:F:515:LYS:HZ3  | 1:F:516:VAL:HG23 | 1.79                     | 0.47              |
| 1:D:515:LYS:NZ   | 1:D:516:VAL:HG23 | 2.29                     | 0.47              |
| 1:C:112:VAL:O    | 1:C:114:HIS:N    | 2.44                     | 0.47              |
| 1:C:277:GLU:HA   | 1:C:280:SER:OG   | 2.13                     | 0.47              |
| 1:D:176:GLY:C    | 1:D:178:SER:N    | 2.67                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:97:TYR:CD2   | 1:C:102:GLY:HA3  | 2.48                     | 0.47              |
| 1:A:92:ASP:O     | 1:A:94:LEU:N     | 2.47                     | 0.47              |
| 1:C:712:PHE:HD1  | 1:C:716:LYS:HG2  | 1.78                     | 0.47              |
| 1:B:142:VAL:HG13 | 1:B:154:ILE:HD12 | 1.94                     | 0.47              |
| 1:F:225:ILE:HG23 | 1:F:229:PHE:CE2  | 2.49                     | 0.47              |
| 1:E:279:ILE:H    | 1:E:279:ILE:CD1  | 2.23                     | 0.47              |
| 1:C:443:GLU:CD   | 1:C:458:LYS:HG2  | 2.35                     | 0.47              |
| 1:B:456:LYS:CB   | 1:B:470:ASN:C    | 2.83                     | 0.47              |
| 1:B:712:PHE:HD1  | 1:B:716:LYS:HG2  | 1.77                     | 0.47              |
| 2:R:4:LEU:HA     | 2:R:8:GLN:OE1    | 2.15                     | 0.47              |
| 1:A:263:ASP:O    | 1:A:265:PHE:N    | 2.47                     | 0.47              |
| 1:D:628:PHE:HE2  | 2:R:90:ARG:CD    | 2.26                     | 0.47              |
| 1:D:753:LYS:O    | 1:D:754:GLU:C    | 2.52                     | 0.47              |
| 2:R:101:SER:O    | 2:R:104:GLU:HG2  | 2.15                     | 0.47              |
| 1:B:277:GLU:HA   | 1:B:280:SER:OG   | 2.14                     | 0.47              |
| 1:A:729:TYR:C    | 1:A:729:TYR:CD2  | 2.87                     | 0.47              |
| 1:A:97:TYR:CD2   | 1:A:102:GLY:HA3  | 2.49                     | 0.47              |
| 1:A:83:GLN:O     | 1:A:84:ASP:C     | 2.52                     | 0.47              |
| 1:D:597:ASN:HD21 | 1:D:601:GLU:HB2  | 1.79                     | 0.47              |
| 1:B:629:ASN:ND2  | 1:B:631:SER:N    | 2.44                     | 0.47              |
| 1:E:713:SER:O    | 1:E:714:GLN:C    | 2.52                     | 0.47              |
| 1:D:446:ILE:HD11 | 1:D:451:ASN:CB   | 2.45                     | 0.47              |
| 2:P:48:LEU:HA    | 2:P:51:MET:CE    | 2.44                     | 0.47              |
| 1:A:311:HIS:HD2  | 1:A:564:VAL:HB   | 1.77                     | 0.47              |
| 1:E:271:LEU:HA   | 1:E:275:GLY:HA3  | 1.96                     | 0.47              |
| 1:A:254:ARG:HG2  | 1:A:255:THR:N    | 2.22                     | 0.47              |
| 1:B:323:ASN:O    | 1:B:324:THR:HG22 | 2.15                     | 0.47              |
| 2:Q:44:THR:O     | 2:Q:46:ALA:N     | 2.47                     | 0.47              |
| 2:T:13:LYS:HZ3   | 2:T:65:PHE:CB    | 2.25                     | 0.47              |
| 2:T:111:ASN:C    | 2:T:113:GLY:H    | 2.17                     | 0.47              |
| 1:F:753:LYS:O    | 1:F:754:GLU:C    | 2.52                     | 0.47              |
| 1:E:729:TYR:CD2  | 1:E:729:TYR:C    | 2.87                     | 0.47              |
| 1:E:94:LEU:O     | 1:E:96:ILE:N     | 2.48                     | 0.47              |
| 1:C:168:GLU:O    | 1:C:170:TYR:N    | 2.47                     | 0.47              |
| 1:A:94:LEU:O     | 1:A:96:ILE:N     | 2.48                     | 0.47              |
| 2:P:121:VAL:O    | 2:P:122:ASP:C    | 2.53                     | 0.47              |
| 2:S:121:VAL:O    | 2:S:122:ASP:C    | 2.53                     | 0.47              |
| 1:A:107:THR:HG21 | 1:A:115:LYS:CD   | 2.45                     | 0.47              |
| 1:E:715:GLU:OE1  | 1:E:767:GLN:NE2  | 2.47                     | 0.47              |
| 1:C:153:ILE:C    | 1:C:154:ILE:HD13 | 2.35                     | 0.47              |
| 2:T:48:LEU:HA    | 2:T:51:MET:CE    | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:446:ILE:HD11 | 1:B:451:ASN:HB2  | 1.97                     | 0.47              |
| 1:A:497:LEU:CD1  | 1:A:556:MET:HG2  | 2.38                     | 0.47              |
| 1:B:500:SER:HA   | 1:B:624:TYR:CD2  | 2.49                     | 0.47              |
| 1:E:712:PHE:HD1  | 1:E:716:LYS:HG2  | 1.78                     | 0.47              |
| 1:D:741:ILE:O    | 1:D:742:ALA:C    | 2.53                     | 0.47              |
| 2:S:44:THR:O     | 2:S:46:ALA:N     | 2.48                     | 0.47              |
| 1:E:649:ILE:HD13 | 2:S:138:TYR:HB2  | 1.96                     | 0.47              |
| 1:B:210:PHE:HD2  | 1:B:210:PHE:N    | 2.12                     | 0.47              |
| 1:D:263:ASP:O    | 1:D:265:PHE:N    | 2.48                     | 0.47              |
| 2:P:111:ASN:C    | 2:P:113:GLY:H    | 2.17                     | 0.47              |
| 1:F:94:LEU:O     | 1:F:96:ILE:N     | 2.48                     | 0.47              |
| 1:C:97:TYR:CE1   | 1:C:178:SER:HB2  | 2.49                     | 0.47              |
| 1:B:168:GLU:C    | 1:B:170:TYR:H    | 2.18                     | 0.47              |
| 1:B:225:ILE:HG23 | 1:B:229:PHE:CE2  | 2.49                     | 0.47              |
| 1:A:225:ILE:HG23 | 1:A:229:PHE:CE2  | 2.49                     | 0.47              |
| 2:R:116:LEU:HD13 | 2:R:121:VAL:HG22 | 1.96                     | 0.47              |
| 1:A:597:ASN:ND2  | 1:A:601:GLU:HB2  | 2.29                     | 0.47              |
| 1:F:715:GLU:HA   | 1:F:718:ARG:NH2  | 2.30                     | 0.47              |
| 1:C:713:SER:O    | 1:C:714:GLN:C    | 2.53                     | 0.47              |
| 1:B:343:VAL:HG12 | 1:B:344:ALA:O    | 2.15                     | 0.47              |
| 1:E:142:VAL:HG13 | 1:E:154:ILE:HD12 | 1.94                     | 0.47              |
| 1:A:656:THR:O    | 1:A:755:ARG:HD2  | 2.14                     | 0.47              |
| 1:A:152:LEU:CD2  | 1:A:154:ILE:HD11 | 2.39                     | 0.47              |
| 2:T:31:GLU:O     | 2:T:35:VAL:HG23  | 2.15                     | 0.47              |
| 1:C:279:ILE:HG22 | 1:C:283:LEU:CD1  | 2.45                     | 0.47              |
| 1:E:217:LYS:CB   | 1:E:236:GLU:HG3  | 2.45                     | 0.47              |
| 2:O:5:THR:HG23   | 2:O:8:GLN:CB     | 2.44                     | 0.47              |
| 2:T:44:THR:O     | 2:T:46:ALA:N     | 2.48                     | 0.47              |
| 1:B:660:SER:O    | 1:B:663:PHE:HB3  | 2.15                     | 0.47              |
| 2:Q:5:THR:HG23   | 2:Q:8:GLN:CB     | 2.44                     | 0.47              |
| 1:F:694:VAL:HG23 | 2:T:18:LEU:HD21  | 1.95                     | 0.47              |
| 1:A:516:VAL:O    | 1:A:519:THR:HG22 | 2.15                     | 0.47              |
| 1:D:489:THR:OG1  | 1:D:490:ALA:N    | 2.48                     | 0.47              |
| 1:E:628:PHE:HE2  | 2:S:90:ARG:CD    | 2.28                     | 0.47              |
| 1:B:649:ILE:HD13 | 2:P:138:TYR:HB2  | 1.96                     | 0.47              |
| 1:A:424:LYS:HG2  | 1:A:433:TYR:CD2  | 2.50                     | 0.47              |
| 2:Q:111:ASN:C    | 2:Q:113:GLY:H    | 2.16                     | 0.47              |
| 1:E:170:TYR:C    | 1:E:172:GLU:H    | 2.18                     | 0.47              |
| 1:E:97:TYR:CD2   | 1:E:102:GLY:HA3  | 2.50                     | 0.47              |
| 1:D:94:LEU:O     | 1:D:96:ILE:N     | 2.47                     | 0.47              |
| 1:B:176:GLY:C    | 1:B:178:SER:N    | 2.68                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:97:TYR:CD2   | 1:B:102:GLY:HA3  | 2.49                     | 0.47              |
| 1:A:168:GLU:O    | 1:A:170:TYR:N    | 2.47                     | 0.47              |
| 1:A:170:TYR:O    | 1:A:174:GLY:N    | 2.44                     | 0.47              |
| 2:P:102:ALA:HA   | 2:P:125:ILE:HG13 | 1.97                     | 0.47              |
| 1:A:116:GLU:C    | 1:A:117:LEU:HD22 | 2.35                     | 0.47              |
| 1:B:344:ALA:O    | 1:B:489:THR:HG22 | 2.15                     | 0.47              |
| 1:D:152:LEU:CD2  | 1:D:154:ILE:HD11 | 2.41                     | 0.47              |
| 1:A:764:LEU:C    | 1:A:766:HIS:H    | 2.18                     | 0.47              |
| 1:D:713:SER:O    | 1:D:714:GLN:C    | 2.53                     | 0.47              |
| 1:B:152:LEU:CD2  | 1:B:154:ILE:HD11 | 2.39                     | 0.47              |
| 1:F:142:VAL:HG13 | 1:F:154:ILE:HD12 | 1.94                     | 0.47              |
| 1:C:225:ILE:HG23 | 1:C:229:PHE:CE2  | 2.49                     | 0.47              |
| 1:C:136:PRO:O    | 1:C:139:SER:N    | 2.37                     | 0.47              |
| 2:P:30:LYS:CD    | 2:P:30:LYS:H     | 2.20                     | 0.47              |
| 1:C:285:LYS:C    | 1:C:287:GLY:H    | 2.17                     | 0.47              |
| 1:B:279:ILE:HG22 | 1:B:283:LEU:CD1  | 2.45                     | 0.47              |
| 1:B:271:LEU:HA   | 1:B:275:GLY:HA3  | 1.95                     | 0.47              |
| 1:E:318:ILE:CG2  | 1:E:322:LEU:HD12 | 2.45                     | 0.47              |
| 1:B:500:SER:O    | 1:B:504:ILE:HD13 | 2.14                     | 0.47              |
| 1:A:712:PHE:HB3  | 1:A:716:LYS:HG2  | 1.96                     | 0.47              |
| 1:F:712:PHE:HB3  | 1:F:716:LYS:HG2  | 1.97                     | 0.47              |
| 1:C:741:ILE:O    | 1:C:742:ALA:C    | 2.52                     | 0.47              |
| 1:F:741:ILE:O    | 1:F:742:ALA:C    | 2.52                     | 0.47              |
| 2:Q:73:ALA:O     | 2:Q:75:LYS:N     | 2.48                     | 0.47              |
| 1:F:660:SER:O    | 1:F:663:PHE:HB3  | 2.15                     | 0.47              |
| 1:E:288:VAL:C    | 1:E:290:LYS:H    | 2.16                     | 0.47              |
| 1:C:344:ALA:O    | 1:C:489:THR:HG22 | 2.15                     | 0.47              |
| 1:F:516:VAL:O    | 1:F:519:THR:HG22 | 2.15                     | 0.47              |
| 1:E:344:ALA:O    | 1:E:489:THR:HG22 | 2.14                     | 0.47              |
| 1:F:672:ARG:HD3  | 1:F:672:ARG:HA   | 1.68                     | 0.47              |
| 1:A:672:ARG:HD3  | 1:A:672:ARG:HA   | 1.68                     | 0.47              |
| 1:C:109:ILE:HD13 | 1:C:157:LYS:HZ3  | 1.80                     | 0.47              |
| 1:E:700:TYR:O    | 1:E:703:ASP:N    | 2.48                     | 0.47              |
| 1:C:616:GLU:HA   | 1:C:620:THR:HB   | 1.97                     | 0.47              |
| 1:F:424:LYS:HG2  | 1:F:433:TYR:CD2  | 2.50                     | 0.47              |
| 1:B:424:LYS:HG2  | 1:B:433:TYR:CD2  | 2.50                     | 0.47              |
| 1:F:764:LEU:C    | 1:F:766:HIS:N    | 2.68                     | 0.47              |
| 1:D:116:GLU:O    | 1:D:117:LEU:HD22 | 2.15                     | 0.47              |
| 1:D:285:LYS:C    | 1:D:287:GLY:H    | 2.17                     | 0.47              |
| 1:A:279:ILE:HG22 | 1:A:283:LEU:CD1  | 2.45                     | 0.47              |
| 1:C:353:LYS:H    | 1:C:368:GLN:HE22 | 1.63                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:44:THR:O     | 2:R:46:ALA:N     | 2.48                     | 0.47              |
| 2:R:5:THR:O      | 2:R:8:GLN:HB3    | 2.14                     | 0.47              |
| 2:S:13:LYS:HZ1   | 2:S:65:PHE:CB    | 2.27                     | 0.47              |
| 2:R:143:GLN:O    | 2:R:147:ALA:HB3  | 2.14                     | 0.47              |
| 1:A:277:GLU:HA   | 1:A:280:SER:OG   | 2.14                     | 0.47              |
| 1:D:616:GLU:HA   | 1:D:620:THR:HB   | 1.97                     | 0.47              |
| 1:D:186:LYS:HG2  | 1:D:186:LYS:O    | 2.15                     | 0.47              |
| 1:D:184:LYS:CE   | 1:D:193:LEU:HB2  | 2.42                     | 0.47              |
| 1:B:94:LEU:O     | 1:B:96:ILE:N     | 2.48                     | 0.47              |
| 2:T:102:ALA:HA   | 2:T:125:ILE:HG13 | 1.97                     | 0.47              |
| 1:C:656:THR:O    | 1:C:755:ARG:HD2  | 2.15                     | 0.47              |
| 1:B:656:THR:O    | 1:B:755:ARG:HD2  | 2.15                     | 0.47              |
| 1:F:116:GLU:C    | 1:F:117:LEU:HD22 | 2.35                     | 0.47              |
| 1:E:142:VAL:CG2  | 1:E:154:ILE:HG23 | 2.39                     | 0.47              |
| 1:C:107:THR:CG2  | 1:C:115:LYS:HD2  | 2.45                     | 0.47              |
| 1:E:116:GLU:C    | 1:E:117:LEU:HD22 | 2.36                     | 0.47              |
| 2:Q:32:LEU:HD21  | 2:Q:71:MET:HE2   | 1.94                     | 0.47              |
| 2:O:70:THR:O     | 2:O:71:MET:C     | 2.54                     | 0.47              |
| 2:R:31:GLU:O     | 2:R:35:VAL:HG23  | 2.14                     | 0.47              |
| 1:B:279:ILE:CD1  | 1:B:279:ILE:H    | 2.22                     | 0.47              |
| 1:F:134:LYS:C    | 1:F:136:PRO:CD   | 2.83                     | 0.47              |
| 1:C:456:LYS:HB2  | 1:C:470:ASN:HA   | 1.96                     | 0.47              |
| 1:B:540:ARG:HD3  | 1:B:627:TYR:OH   | 2.15                     | 0.47              |
| 2:O:4:LEU:HA     | 2:O:8:GLN:OE1    | 2.15                     | 0.47              |
| 1:C:790:PHE:O    | 1:C:793:PHE:HB3  | 2.15                     | 0.47              |
| 1:D:700:TYR:O    | 1:D:703:ASP:N    | 2.47                     | 0.47              |
| 1:E:234:LEU:HD23 | 1:E:235:THR:H    | 1.80                     | 0.47              |
| 1:C:184:LYS:HZ1  | 1:C:191:GLU:HB2  | 1.76                     | 0.47              |
| 1:F:597:ASN:HD21 | 1:F:601:GLU:HB2  | 1.80                     | 0.47              |
| 1:E:581:GLN:HE22 | 1:E:629:ASN:H    | 1.62                     | 0.47              |
| 1:B:115:LYS:HB2  | 1:B:118:GLN:HG2  | 1.97                     | 0.47              |
| 1:F:443:GLU:CD   | 1:F:458:LYS:HG2  | 2.35                     | 0.47              |
| 1:A:515:LYS:NZ   | 1:A:516:VAL:HG23 | 2.30                     | 0.47              |
| 1:E:628:PHE:CD1  | 1:E:645:TRP:CD1  | 3.03                     | 0.47              |
| 2:S:21:LYS:HD3   | 2:S:22:ASP:N     | 2.30                     | 0.47              |
| 1:A:270:LYS:HA   | 1:A:273:LYS:HB2  | 1.97                     | 0.47              |
| 1:E:178:SER:OG   | 1:E:179:LEU:CD2  | 2.63                     | 0.46              |
| 1:D:168:GLU:C    | 1:D:170:TYR:H    | 2.16                     | 0.46              |
| 1:B:168:GLU:O    | 1:B:170:TYR:N    | 2.48                     | 0.46              |
| 1:F:713:SER:O    | 1:F:714:GLN:C    | 2.53                     | 0.46              |
| 1:F:107:THR:HG21 | 1:F:115:LYS:CD   | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:153:ILE:C    | 1:E:154:ILE:HD13 | 2.35                     | 0.46              |
| 1:A:609:GLU:O    | 1:A:610:MET:C    | 2.53                     | 0.46              |
| 1:D:658:PRO:HG3  | 1:D:752:LEU:HD22 | 1.97                     | 0.46              |
| 1:B:153:ILE:C    | 1:B:154:ILE:HD13 | 2.35                     | 0.46              |
| 2:S:70:THR:O     | 2:S:71:MET:C     | 2.53                     | 0.46              |
| 1:C:435:LEU:CG   | 1:C:446:ILE:HG22 | 2.35                     | 0.46              |
| 2:T:30:LYS:H     | 2:T:30:LYS:CD    | 2.20                     | 0.46              |
| 1:F:318:ILE:CG2  | 1:F:322:LEU:HD12 | 2.44                     | 0.46              |
| 1:E:712:PHE:HB3  | 1:E:716:LYS:HG2  | 1.97                     | 0.46              |
| 1:D:443:GLU:CD   | 1:D:458:LYS:HG2  | 2.35                     | 0.46              |
| 1:A:500:SER:O    | 1:A:504:ILE:HD13 | 2.15                     | 0.46              |
| 2:T:65:PHE:CD1   | 2:T:66:PRO:HD3   | 2.50                     | 0.46              |
| 1:D:288:VAL:C    | 1:D:290:LYS:H    | 2.17                     | 0.46              |
| 1:F:343:VAL:HG12 | 1:F:344:ALA:O    | 2.15                     | 0.46              |
| 1:F:489:THR:OG1  | 1:F:490:ALA:N    | 2.49                     | 0.46              |
| 1:B:71:PHE:CB    | 1:B:108:ASP:HB2  | 2.45                     | 0.46              |
| 1:D:170:TYR:C    | 1:D:172:GLU:H    | 2.18                     | 0.46              |
| 1:D:188:LEU:HD22 | 1:D:188:LEU:N    | 2.26                     | 0.46              |
| 1:A:168:GLU:C    | 1:A:170:TYR:H    | 2.17                     | 0.46              |
| 1:A:170:TYR:C    | 1:A:172:GLU:H    | 2.18                     | 0.46              |
| 1:A:550:SER:N    | 1:A:553:GLN:NE2  | 2.45                     | 0.46              |
| 1:E:495:PHE:CD1  | 1:E:495:PHE:O    | 2.68                     | 0.46              |
| 1:E:630:ARG:NH1  | 1:E:630:ARG:HG3  | 2.27                     | 0.46              |
| 1:C:495:PHE:O    | 1:C:581:GLN:HG2  | 2.15                     | 0.46              |
| 1:A:713:SER:O    | 1:A:714:GLN:C    | 2.53                     | 0.46              |
| 1:D:712:PHE:HB3  | 1:D:716:LYS:HG2  | 1.97                     | 0.46              |
| 1:B:741:ILE:O    | 1:B:742:ALA:C    | 2.53                     | 0.46              |
| 2:R:13:LYS:HZ1   | 2:R:65:PHE:CB    | 2.28                     | 0.46              |
| 2:S:13:LYS:HZ3   | 2:S:65:PHE:CB    | 2.27                     | 0.46              |
| 1:A:694:VAL:HG23 | 2:O:18:LEU:HD11  | 1.97                     | 0.46              |
| 1:C:489:THR:OG1  | 1:C:490:ALA:N    | 2.48                     | 0.46              |
| 1:E:343:VAL:HG12 | 1:E:344:ALA:O    | 2.15                     | 0.46              |
| 1:F:616:GLU:HA   | 1:F:620:THR:HB   | 1.97                     | 0.46              |
| 1:C:508:ILE:CG2  | 1:C:509:PRO:HD2  | 2.45                     | 0.46              |
| 1:C:424:LYS:HG2  | 1:C:433:TYR:CD2  | 2.50                     | 0.46              |
| 1:F:729:TYR:CD2  | 1:F:729:TYR:C    | 2.87                     | 0.46              |
| 1:F:192:PHE:HB3  | 1:F:196:ILE:CD1  | 2.45                     | 0.46              |
| 1:C:213:LYS:HB2  | 1:C:240:ALA:CB   | 2.45                     | 0.46              |
| 1:E:697:ILE:C    | 1:E:699:GLY:N    | 2.69                     | 0.46              |
| 1:D:142:VAL:CG2  | 1:D:154:ILE:HG23 | 2.41                     | 0.46              |
| 1:E:658:PRO:HG3  | 1:E:752:LEU:HD22 | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:597:ASN:HD21 | 1:E:601:GLU:HB2  | 1.81                     | 0.46              |
| 1:A:153:ILE:C    | 1:A:154:ILE:HD13 | 2.35                     | 0.46              |
| 1:D:792:VAL:C    | 1:D:796:ILE:HG12 | 2.36                     | 0.46              |
| 1:E:446:ILE:HD11 | 1:E:451:ASN:CB   | 2.46                     | 0.46              |
| 1:C:271:LEU:HD13 | 1:C:276:PHE:CE2  | 2.50                     | 0.46              |
| 1:C:373:LYS:CD   | 1:C:376:GLN:NE2  | 2.75                     | 0.46              |
| 1:A:723:PHE:O    | 1:A:726:ILE:N    | 2.48                     | 0.46              |
| 1:F:712:PHE:HD1  | 1:F:716:LYS:HG2  | 1.78                     | 0.46              |
| 1:C:735:VAL:HG12 | 1:C:741:ILE:HD13 | 1.96                     | 0.46              |
| 1:B:609:GLU:O    | 1:B:610:MET:C    | 2.53                     | 0.46              |
| 1:F:210:PHE:N    | 1:F:210:PHE:HD2  | 2.12                     | 0.46              |
| 1:E:616:GLU:HA   | 1:E:620:THR:HB   | 1.97                     | 0.46              |
| 1:F:170:TYR:C    | 1:F:172:GLU:H    | 2.18                     | 0.46              |
| 2:Q:116:LEU:HD13 | 2:Q:121:VAL:HG22 | 1.96                     | 0.46              |
| 2:O:121:VAL:O    | 2:O:122:ASP:C    | 2.53                     | 0.46              |
| 1:C:116:GLU:C    | 1:C:117:LEU:HD22 | 2.35                     | 0.46              |
| 2:T:70:THR:O     | 2:T:71:MET:C     | 2.53                     | 0.46              |
| 1:C:134:LYS:CG   | 1:C:136:PRO:HD3  | 2.38                     | 0.46              |
| 1:C:724:ARG:NH1  | 1:C:724:ARG:CG   | 2.78                     | 0.46              |
| 1:F:271:LEU:HD13 | 1:F:276:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:353:LYS:H    | 1:A:368:GLN:HE22 | 1.63                     | 0.46              |
| 1:A:323:ASN:O    | 1:A:324:THR:HG22 | 2.16                     | 0.46              |
| 1:A:741:ILE:O    | 1:A:742:ALA:C    | 2.52                     | 0.46              |
| 2:S:143:GLN:O    | 2:S:147:ALA:HB3  | 2.15                     | 0.46              |
| 1:F:456:LYS:HB2  | 1:F:469:PHE:O    | 2.16                     | 0.46              |
| 1:E:130:SER:HB2  | 1:E:170:TYR:CE2  | 2.51                     | 0.46              |
| 1:E:97:TYR:CE1   | 1:E:178:SER:HB2  | 2.50                     | 0.46              |
| 1:E:189:ASP:O    | 1:E:191:GLU:HG2  | 2.16                     | 0.46              |
| 1:B:185:ASP:O    | 1:B:190:PRO:HG3  | 2.16                     | 0.46              |
| 1:C:630:ARG:CZ   | 2:Q:83:GLU:CG    | 2.94                     | 0.46              |
| 1:F:463:THR:HB   | 1:F:467:GLU:H    | 1.80                     | 0.46              |
| 1:A:359:PRO:O    | 1:A:361:ALA:N    | 2.48                     | 0.46              |
| 2:Q:70:THR:O     | 2:Q:71:MET:C     | 2.54                     | 0.46              |
| 2:R:48:LEU:HA    | 2:R:51:MET:CE    | 2.44                     | 0.46              |
| 1:F:628:PHE:HE2  | 2:T:90:ARG:CD    | 2.28                     | 0.46              |
| 1:C:315:PHE:CD2  | 1:C:560:LEU:HD22 | 2.51                     | 0.46              |
| 1:F:525:LYS:O    | 1:F:529:VAL:HG23 | 2.15                     | 0.46              |
| 2:P:143:GLN:O    | 2:P:147:ALA:CB   | 2.64                     | 0.46              |
| 1:F:508:ILE:CG2  | 1:F:509:PRO:HD2  | 2.46                     | 0.46              |
| 1:D:88:LYS:NZ    | 1:D:172:GLU:CD   | 2.69                     | 0.46              |
| 1:F:96:ILE:O     | 1:F:100:LEU:HG   | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:88:LYS:NZ    | 1:A:172:GLU:CD   | 2.68                     | 0.46              |
| 1:A:96:ILE:O     | 1:A:100:LEU:HG   | 2.15                     | 0.46              |
| 1:A:413:LEU:N    | 1:A:413:LEU:HD23 | 2.31                     | 0.46              |
| 1:C:723:PHE:O    | 1:C:726:ILE:N    | 2.49                     | 0.46              |
| 1:C:722:ILE:HD13 | 1:C:764:LEU:CD2  | 2.46                     | 0.46              |
| 1:E:152:LEU:CD2  | 1:E:154:ILE:HD11 | 2.39                     | 0.46              |
| 1:F:792:VAL:C    | 1:F:796:ILE:HG12 | 2.36                     | 0.46              |
| 1:D:359:PRO:HD2  | 1:D:444:PHE:CE2  | 2.51                     | 0.46              |
| 2:R:37:ARG:HH11  | 2:R:37:ARG:HG2   | 1.81                     | 0.46              |
| 2:Q:37:ARG:HH11  | 2:Q:37:ARG:HG2   | 1.80                     | 0.46              |
| 2:S:91:VAL:HG12  | 2:S:92:PHE:N     | 2.30                     | 0.46              |
| 1:D:540:ARG:HD3  | 1:D:627:TYR:OH   | 2.15                     | 0.46              |
| 1:F:323:ASN:O    | 1:F:324:THR:HG22 | 2.15                     | 0.46              |
| 1:C:123:GLU:O    | 1:C:146:LYS:NZ   | 2.49                     | 0.46              |
| 1:D:79:ILE:C     | 1:D:81:GLN:N     | 2.69                     | 0.46              |
| 1:E:609:GLU:O    | 1:E:610:MET:C    | 2.53                     | 0.46              |
| 1:D:424:LYS:HG2  | 1:D:433:TYR:CD2  | 2.50                     | 0.46              |
| 1:E:168:GLU:C    | 1:E:170:TYR:H    | 2.17                     | 0.46              |
| 1:A:480:ASN:C    | 1:A:480:ASN:ND2  | 2.64                     | 0.46              |
| 1:F:550:SER:N    | 1:F:553:GLN:NE2  | 2.45                     | 0.46              |
| 2:S:31:GLU:O     | 2:S:35:VAL:HG23  | 2.16                     | 0.46              |
| 1:F:359:PRO:HD2  | 1:F:444:PHE:CE2  | 2.51                     | 0.46              |
| 1:D:135:VAL:CG2  | 1:D:135:VAL:O    | 2.52                     | 0.46              |
| 1:E:443:GLU:CD   | 1:E:458:LYS:HG2  | 2.35                     | 0.46              |
| 1:A:353:LYS:HB2  | 1:A:368:GLN:HE22 | 1.81                     | 0.46              |
| 1:B:659:THR:O    | 1:B:660:SER:C    | 2.54                     | 0.46              |
| 1:A:75:THR:C     | 1:A:77:ASP:N     | 2.69                     | 0.46              |
| 1:A:515:LYS:HZ3  | 1:A:516:VAL:HG23 | 1.80                     | 0.46              |
| 1:A:525:LYS:O    | 1:A:529:VAL:HG23 | 2.15                     | 0.46              |
| 2:T:36:MET:HE3   | 2:T:43:PRO:HG3   | 1.98                     | 0.46              |
| 2:Q:143:GLN:O    | 2:Q:147:ALA:CB   | 2.64                     | 0.46              |
| 2:S:146:THR:O    | 2:S:147:ALA:C    | 2.54                     | 0.46              |
| 1:A:616:GLU:HA   | 1:A:620:THR:HB   | 1.97                     | 0.46              |
| 1:B:97:TYR:CE1   | 1:B:178:SER:HB2  | 2.50                     | 0.46              |
| 1:A:177:ILE:HA   | 1:A:180:ASP:OD1  | 2.16                     | 0.46              |
| 1:D:142:VAL:HG13 | 1:D:154:ILE:HD11 | 1.96                     | 0.46              |
| 1:E:495:PHE:O    | 1:E:581:GLN:HG2  | 2.15                     | 0.46              |
| 1:D:712:PHE:HD1  | 1:D:716:LYS:HG2  | 1.79                     | 0.46              |
| 2:S:16:PHE:CZ    | 2:S:27:ILE:HG23  | 2.51                     | 0.46              |
| 1:A:792:VAL:C    | 1:A:796:ILE:HG12 | 2.36                     | 0.46              |
| 1:D:353:LYS:H    | 1:D:368:GLN:HE22 | 1.63                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:540:ARG:HD2  | 1:B:582:ASP:OD2  | 2.16                     | 0.46              |
| 2:R:65:PHE:CD1   | 2:R:66:PRO:HD3   | 2.51                     | 0.46              |
| 1:D:525:LYS:O    | 1:D:529:VAL:HG23 | 2.16                     | 0.46              |
| 1:D:191:GLU:O    | 1:D:192:PHE:C    | 2.52                     | 0.46              |
| 1:C:170:TYR:C    | 1:C:172:GLU:H    | 2.18                     | 0.46              |
| 1:C:88:LYS:NZ    | 1:C:172:GLU:CD   | 2.70                     | 0.46              |
| 1:C:188:LEU:HD22 | 1:C:188:LEU:N    | 2.26                     | 0.46              |
| 2:R:121:VAL:O    | 2:R:122:ASP:C    | 2.54                     | 0.46              |
| 2:S:102:ALA:HA   | 2:S:125:ILE:HG13 | 1.97                     | 0.46              |
| 2:O:101:SER:O    | 2:O:104:GLU:HG2  | 2.16                     | 0.46              |
| 1:D:142:VAL:HG13 | 1:D:154:ILE:HD12 | 1.94                     | 0.46              |
| 1:F:115:LYS:HB2  | 1:F:118:GLN:HG2  | 1.98                     | 0.46              |
| 1:E:656:THR:O    | 1:E:755:ARG:HD2  | 2.15                     | 0.46              |
| 1:F:495:PHE:O    | 1:F:495:PHE:CD1  | 2.69                     | 0.46              |
| 1:E:792:VAL:C    | 1:E:796:ILE:HG12 | 2.36                     | 0.46              |
| 2:S:48:LEU:HA    | 2:S:51:MET:CE    | 2.44                     | 0.46              |
| 1:A:359:PRO:HD2  | 1:A:444:PHE:CE2  | 2.51                     | 0.46              |
| 1:B:353:LYS:H    | 1:B:368:GLN:HE22 | 1.64                     | 0.46              |
| 1:D:318:ILE:CG2  | 1:D:322:LEU:HD12 | 2.46                     | 0.46              |
| 2:O:65:PHE:CD1   | 2:O:66:PRO:HD3   | 2.51                     | 0.46              |
| 1:D:456:LYS:HB2  | 1:D:469:PHE:O    | 2.16                     | 0.46              |
| 1:D:687:GLU:O    | 1:D:690:LYS:N    | 2.49                     | 0.46              |
| 1:B:270:LYS:HA   | 1:B:273:LYS:HB2  | 1.98                     | 0.46              |
| 1:E:424:LYS:HG2  | 1:E:433:TYR:CD2  | 2.50                     | 0.46              |
| 1:D:559:ARG:HA   | 1:D:559:ARG:HD2  | 1.78                     | 0.46              |
| 1:B:140:ARG:HA   | 1:B:140:ARG:NE   | 2.31                     | 0.46              |
| 1:E:140:ARG:HA   | 1:E:140:ARG:NE   | 2.31                     | 0.46              |
| 1:C:186:LYS:HZ1  | 1:C:234:LEU:CD1  | 2.28                     | 0.46              |
| 1:B:170:TYR:C    | 1:B:172:GLU:H    | 2.18                     | 0.46              |
| 1:A:175:LYS:O    | 1:A:176:GLY:C    | 2.55                     | 0.46              |
| 1:B:715:GLU:HA   | 1:B:718:ARG:NH2  | 2.30                     | 0.46              |
| 1:E:479:LYS:HG2  | 1:E:488:LEU:CD2  | 2.30                     | 0.46              |
| 1:D:115:LYS:HZ2  | 1:D:116:GLU:HG2  | 1.78                     | 0.46              |
| 2:T:16:PHE:CZ    | 2:T:27:ILE:HG23  | 2.51                     | 0.46              |
| 1:E:462:ILE:HG12 | 1:E:463:THR:H    | 1.81                     | 0.46              |
| 2:Q:48:LEU:HA    | 2:Q:51:MET:CE    | 2.44                     | 0.46              |
| 1:A:446:ILE:HD11 | 1:A:451:ASN:HB2  | 1.98                     | 0.46              |
| 1:B:359:PRO:HD2  | 1:B:444:PHE:CE2  | 2.51                     | 0.46              |
| 1:B:359:PRO:O    | 1:B:361:ALA:N    | 2.49                     | 0.46              |
| 1:A:271:LEU:HD13 | 1:A:276:PHE:CE2  | 2.51                     | 0.46              |
| 1:B:311:HIS:HD2  | 1:B:564:VAL:HB   | 1.77                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:500:SER:O    | 1:E:504:ILE:HD13 | 2.16                     | 0.46              |
| 1:A:318:ILE:CG2  | 1:A:322:LEU:HD12 | 2.45                     | 0.46              |
| 1:D:500:SER:HA   | 1:D:624:TYR:CD2  | 2.51                     | 0.46              |
| 1:D:735:VAL:HG12 | 1:D:741:ILE:HD13 | 1.97                     | 0.46              |
| 1:A:777:TYR:CE1  | 1:A:782:PHE:CE1  | 3.04                     | 0.46              |
| 2:S:65:PHE:CD1   | 2:S:66:PRO:HD3   | 2.51                     | 0.46              |
| 1:E:79:ILE:C     | 1:E:81:GLN:N     | 2.69                     | 0.46              |
| 1:C:343:VAL:HG12 | 1:C:344:ALA:O    | 2.16                     | 0.46              |
| 1:A:343:VAL:HG12 | 1:A:344:ALA:O    | 2.16                     | 0.46              |
| 1:C:525:LYS:O    | 1:C:529:VAL:HG23 | 2.16                     | 0.46              |
| 1:E:109:ILE:HD13 | 1:E:157:LYS:HZ3  | 1.79                     | 0.46              |
| 1:B:671:ARG:NH1  | 1:B:677:GLY:HA3  | 2.31                     | 0.46              |
| 1:C:140:ARG:HA   | 1:C:140:ARG:NE   | 2.30                     | 0.46              |
| 1:D:96:ILE:O     | 1:D:100:LEU:HG   | 2.16                     | 0.45              |
| 1:D:153:ILE:C    | 1:D:154:ILE:HD13 | 2.36                     | 0.45              |
| 1:B:764:LEU:C    | 1:B:766:HIS:N    | 2.69                     | 0.45              |
| 1:B:764:LEU:O    | 1:B:766:HIS:N    | 2.49                     | 0.45              |
| 1:D:715:GLU:HA   | 1:D:718:ARG:NH2  | 2.30                     | 0.45              |
| 1:D:718:ARG:HH11 | 1:D:767:GLN:NE2  | 2.13                     | 0.45              |
| 1:F:495:PHE:O    | 1:F:581:GLN:HG2  | 2.16                     | 0.45              |
| 2:P:70:THR:O     | 2:P:71:MET:C     | 2.54                     | 0.45              |
| 1:E:271:LEU:HD13 | 1:E:276:PHE:CE2  | 2.50                     | 0.45              |
| 1:A:334:LEU:N    | 1:A:334:LEU:CD1  | 2.75                     | 0.45              |
| 1:E:497:LEU:CD1  | 1:E:556:MET:HG2  | 2.38                     | 0.45              |
| 1:B:443:GLU:OE2  | 1:B:458:LYS:HG2  | 2.15                     | 0.45              |
| 1:B:723:PHE:O    | 1:B:726:ILE:N    | 2.49                     | 0.45              |
| 1:F:777:TYR:CE1  | 1:F:782:PHE:CE1  | 3.04                     | 0.45              |
| 1:F:628:PHE:CD1  | 1:F:645:TRP:CD1  | 3.04                     | 0.45              |
| 1:B:525:LYS:O    | 1:B:529:VAL:HG23 | 2.15                     | 0.45              |
| 2:Q:21:LYS:HD3   | 2:Q:22:ASP:N     | 2.31                     | 0.45              |
| 2:P:21:LYS:HD3   | 2:P:22:ASP:N     | 2.31                     | 0.45              |
| 1:F:558:ASP:O    | 1:F:561:ASN:N    | 2.49                     | 0.45              |
| 1:D:97:TYR:CE1   | 1:D:178:SER:HB2  | 2.51                     | 0.45              |
| 1:F:175:LYS:O    | 1:F:176:GLY:C    | 2.55                     | 0.45              |
| 1:C:715:GLU:HA   | 1:C:718:ARG:NH2  | 2.30                     | 0.45              |
| 1:B:116:GLU:C    | 1:B:117:LEU:HD22 | 2.36                     | 0.45              |
| 2:T:12:PHE:HE1   | 2:T:72:MET:HB3   | 1.81                     | 0.45              |
| 1:C:792:VAL:C    | 1:C:796:ILE:HG12 | 2.36                     | 0.45              |
| 2:R:12:PHE:HE1   | 2:R:72:MET:HB3   | 1.81                     | 0.45              |
| 1:E:359:PRO:O    | 1:E:361:ALA:N    | 2.49                     | 0.45              |
| 2:O:37:ARG:HG2   | 2:O:37:ARG:HH11  | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:353:LYS:HB2  | 1:C:368:GLN:HE22 | 1.81                     | 0.45              |
| 1:D:540:ARG:HD2  | 1:D:582:ASP:OD2  | 2.16                     | 0.45              |
| 1:A:794:GLN:HB3  | 1:A:794:GLN:HE21 | 1.63                     | 0.45              |
| 1:E:75:THR:C     | 1:E:77:ASP:N     | 2.70                     | 0.45              |
| 1:B:75:THR:C     | 1:B:77:ASP:N     | 2.69                     | 0.45              |
| 1:D:515:LYS:HZ3  | 1:D:516:VAL:HG23 | 1.80                     | 0.45              |
| 1:B:482:GLU:O    | 1:B:484:VAL:HG22 | 2.17                     | 0.45              |
| 1:F:97:TYR:CE1   | 1:F:178:SER:HB2  | 2.51                     | 0.45              |
| 2:O:126:ARG:HG3  | 2:O:126:ARG:HH21 | 1.81                     | 0.45              |
| 1:C:712:PHE:HB3  | 1:C:716:LYS:HG2  | 1.97                     | 0.45              |
| 1:B:397:GLU:O    | 1:B:398:ILE:HD13 | 2.16                     | 0.45              |
| 1:B:489:THR:OG1  | 1:B:490:ALA:N    | 2.49                     | 0.45              |
| 1:F:413:LEU:HD23 | 1:F:413:LEU:N    | 2.31                     | 0.45              |
| 1:B:495:PHE:O    | 1:B:581:GLN:HG2  | 2.16                     | 0.45              |
| 1:A:397:GLU:O    | 1:A:398:ILE:HD13 | 2.16                     | 0.45              |
| 1:D:359:PRO:O    | 1:D:361:ALA:N    | 2.49                     | 0.45              |
| 1:E:359:PRO:HD2  | 1:E:444:PHE:CE2  | 2.51                     | 0.45              |
| 1:D:501:LEU:HD22 | 2:R:112:LEU:CD2  | 2.36                     | 0.45              |
| 1:B:724:ARG:NH1  | 1:B:724:ARG:CG   | 2.79                     | 0.45              |
| 1:C:456:LYS:HB3  | 1:C:471:TRP:N    | 2.31                     | 0.45              |
| 1:C:540:ARG:HD3  | 1:C:627:TYR:OH   | 2.16                     | 0.45              |
| 2:P:65:PHE:CD1   | 2:P:66:PRO:HD3   | 2.51                     | 0.45              |
| 1:A:777:TYR:HA   | 1:A:780:LEU:HD23 | 1.98                     | 0.45              |
| 1:B:777:TYR:HA   | 1:B:780:LEU:CD2  | 2.46                     | 0.45              |
| 1:B:516:VAL:O    | 1:B:519:THR:HG22 | 2.15                     | 0.45              |
| 1:C:628:PHE:HE2  | 2:Q:90:ARG:CD    | 2.27                     | 0.45              |
| 1:A:489:THR:OG1  | 1:A:490:ALA:N    | 2.49                     | 0.45              |
| 1:F:686:ASP:CB   | 1:F:739:LYS:HD2  | 2.46                     | 0.45              |
| 1:E:655:ASN:ND2  | 1:E:655:ASN:N    | 2.63                     | 0.45              |
| 1:E:456:LYS:HB2  | 1:E:469:PHE:O    | 2.17                     | 0.45              |
| 1:B:700:TYR:O    | 1:B:703:ASP:N    | 2.48                     | 0.45              |
| 1:E:508:ILE:CG2  | 1:E:509:PRO:HD2  | 2.45                     | 0.45              |
| 1:C:186:LYS:NZ   | 1:C:234:LEU:HD12 | 2.32                     | 0.45              |
| 1:D:697:ILE:C    | 1:D:699:GLY:N    | 2.70                     | 0.45              |
| 2:Q:102:ALA:HA   | 2:Q:125:ILE:HG13 | 1.98                     | 0.45              |
| 1:E:413:LEU:N    | 1:E:413:LEU:HD23 | 2.32                     | 0.45              |
| 1:A:722:ILE:HD13 | 1:A:764:LEU:HD23 | 1.99                     | 0.45              |
| 1:C:142:VAL:HG13 | 1:C:154:ILE:HD12 | 1.95                     | 0.45              |
| 1:E:397:GLU:O    | 1:E:398:ILE:HD13 | 2.17                     | 0.45              |
| 1:C:115:LYS:HB2  | 1:C:118:GLN:HG2  | 1.98                     | 0.45              |
| 1:D:107:THR:CG2  | 1:D:115:LYS:HD2  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:462:ILE:HG12 | 1:F:463:THR:H    | 1.82                     | 0.45              |
| 1:D:462:ILE:HG12 | 1:D:463:THR:H    | 1.81                     | 0.45              |
| 1:B:456:LYS:HB2  | 1:B:469:PHE:O    | 2.16                     | 0.45              |
| 1:D:516:VAL:O    | 1:D:519:THR:HG22 | 2.15                     | 0.45              |
| 1:D:655:ASN:ND2  | 1:D:655:ASN:N    | 2.64                     | 0.45              |
| 1:D:99:GLU:OE2   | 1:D:284:LYS:HD2  | 2.15                     | 0.45              |
| 1:B:508:ILE:CG2  | 1:B:509:PRO:HD2  | 2.46                     | 0.45              |
| 1:B:559:ARG:HD2  | 1:B:559:ARG:HA   | 1.79                     | 0.45              |
| 1:D:348:LEU:HA   | 1:D:348:LEU:HD23 | 1.82                     | 0.45              |
| 1:C:94:LEU:O     | 1:C:96:ILE:N     | 2.49                     | 0.45              |
| 1:B:196:ILE:HA   | 1:B:199:LEU:HG   | 1.99                     | 0.45              |
| 2:Q:126:ARG:HG3  | 2:Q:126:ARG:HH21 | 1.81                     | 0.45              |
| 2:T:126:ARG:HG3  | 2:T:126:ARG:HH21 | 1.81                     | 0.45              |
| 1:D:479:LYS:HG2  | 1:D:488:LEU:CD2  | 2.32                     | 0.45              |
| 1:B:767:GLN:HB3  | 1:B:768:LYS:H    | 1.53                     | 0.45              |
| 1:B:792:VAL:C    | 1:B:796:ILE:HG12 | 2.36                     | 0.45              |
| 1:A:540:ARG:HD3  | 1:A:627:TYR:OH   | 2.16                     | 0.45              |
| 1:F:540:ARG:HD3  | 1:F:627:TYR:OH   | 2.17                     | 0.45              |
| 1:D:777:TYR:HA   | 1:D:780:LEU:CD2  | 2.47                     | 0.45              |
| 1:B:777:TYR:CE1  | 1:B:782:PHE:CE1  | 3.05                     | 0.45              |
| 2:Q:65:PHE:CD1   | 2:Q:66:PRO:HD3   | 2.51                     | 0.45              |
| 1:C:516:VAL:O    | 1:C:519:THR:HG22 | 2.16                     | 0.45              |
| 2:T:21:LYS:HD3   | 2:T:22:ASP:N     | 2.32                     | 0.45              |
| 1:E:99:GLU:OE2   | 1:E:284:LYS:HD2  | 2.17                     | 0.45              |
| 2:O:102:ALA:HA   | 2:O:125:ILE:HG13 | 1.98                     | 0.45              |
| 1:A:495:PHE:O    | 1:A:581:GLN:HG2  | 2.17                     | 0.45              |
| 1:B:115:LYS:C    | 1:B:117:LEU:N    | 2.69                     | 0.45              |
| 1:D:719:LYS:O    | 1:D:721:SER:N    | 2.50                     | 0.45              |
| 1:C:463:THR:HB   | 1:C:467:GLU:H    | 1.81                     | 0.45              |
| 2:O:31:GLU:O     | 2:O:35:VAL:HG23  | 2.17                     | 0.45              |
| 1:C:359:PRO:O    | 1:C:361:ALA:N    | 2.49                     | 0.45              |
| 2:P:32:LEU:HD12  | 2:P:32:LEU:O     | 2.17                     | 0.45              |
| 1:F:135:VAL:N    | 1:F:136:PRO:HD3  | 2.32                     | 0.45              |
| 1:A:373:LYS:CD   | 1:A:376:GLN:NE2  | 2.76                     | 0.45              |
| 1:F:318:ILE:O    | 1:F:319:ALA:C    | 2.55                     | 0.45              |
| 1:F:324:THR:HB   | 1:F:499:PRO:CA   | 2.45                     | 0.45              |
| 1:A:691:LYS:O    | 1:A:693:SER:N    | 2.50                     | 0.45              |
| 1:A:660:SER:O    | 1:A:663:PHE:HB3  | 2.15                     | 0.45              |
| 2:T:13:LYS:HZ1   | 2:T:65:PHE:CB    | 2.28                     | 0.45              |
| 1:C:777:TYR:HA   | 1:C:780:LEU:CD2  | 2.46                     | 0.45              |
| 1:D:777:TYR:CE1  | 1:D:782:PHE:CE1  | 3.04                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:75:THR:C     | 1:D:77:ASP:N     | 2.70                     | 0.45              |
| 1:D:315:PHE:CD2  | 1:D:560:LEU:HD22 | 2.52                     | 0.45              |
| 1:E:687:GLU:O    | 1:E:690:LYS:N    | 2.50                     | 0.45              |
| 1:F:175:LYS:CB   | 1:F:175:LYS:HZ3  | 2.29                     | 0.45              |
| 1:C:413:LEU:HD23 | 1:C:413:LEU:N    | 2.32                     | 0.45              |
| 1:B:413:LEU:HD23 | 1:B:413:LEU:N    | 2.32                     | 0.45              |
| 1:D:495:PHE:O    | 1:D:581:GLN:HG2  | 2.16                     | 0.45              |
| 1:D:115:LYS:HB2  | 1:D:118:GLN:HG2  | 1.98                     | 0.45              |
| 2:O:32:LEU:O     | 2:O:32:LEU:HD12  | 2.17                     | 0.45              |
| 1:C:359:PRO:CB   | 1:C:405:LEU:HD21 | 2.47                     | 0.45              |
| 1:B:373:LYS:CD   | 1:B:376:GLN:NE2  | 2.75                     | 0.45              |
| 1:E:323:ASN:O    | 1:E:324:THR:HG22 | 2.16                     | 0.45              |
| 1:F:723:PHE:O    | 1:F:726:ILE:N    | 2.50                     | 0.45              |
| 1:D:777:TYR:HA   | 1:D:780:LEU:HD23 | 1.98                     | 0.45              |
| 1:C:79:ILE:C     | 1:C:81:GLN:N     | 2.70                     | 0.45              |
| 1:B:628:PHE:CD1  | 1:B:645:TRP:CD1  | 3.04                     | 0.45              |
| 1:F:141:PHE:H    | 1:F:141:PHE:HD1  | 1.59                     | 0.45              |
| 1:C:333:LYS:C    | 1:C:335:ALA:H    | 2.20                     | 0.45              |
| 1:F:140:ARG:HA   | 1:F:140:ARG:NE   | 2.31                     | 0.45              |
| 1:C:96:ILE:O     | 1:C:100:LEU:HG   | 2.16                     | 0.45              |
| 1:E:764:LEU:C    | 1:E:766:HIS:N    | 2.68                     | 0.45              |
| 1:D:721:SER:C    | 1:D:723:PHE:N    | 2.70                     | 0.45              |
| 1:B:271:LEU:HD13 | 1:B:276:PHE:CE2  | 2.51                     | 0.45              |
| 1:F:368:GLN:C    | 1:F:370:LEU:H    | 2.21                     | 0.45              |
| 1:A:318:ILE:O    | 1:A:319:ALA:C    | 2.55                     | 0.45              |
| 1:C:456:LYS:HB2  | 1:C:469:PHE:O    | 2.16                     | 0.45              |
| 1:B:318:ILE:CG2  | 1:B:322:LEU:HD12 | 2.45                     | 0.45              |
| 1:A:443:GLU:CD   | 1:A:458:LYS:HG2  | 2.35                     | 0.45              |
| 1:E:254:ARG:N    | 1:E:254:ARG:HD2  | 2.30                     | 0.45              |
| 1:F:794:GLN:HB3  | 1:F:794:GLN:HE21 | 1.63                     | 0.45              |
| 1:D:795:LYS:O    | 1:D:797:ILE:N    | 2.50                     | 0.45              |
| 1:F:719:LYS:O    | 1:F:721:SER:N    | 2.50                     | 0.45              |
| 1:F:735:VAL:HG12 | 1:F:741:ILE:HD13 | 1.97                     | 0.45              |
| 1:D:344:ALA:O    | 1:D:489:THR:HG22 | 2.16                     | 0.45              |
| 2:O:143:GLN:O    | 2:O:147:ALA:CB   | 2.64                     | 0.45              |
| 1:A:140:ARG:NE   | 1:A:140:ARG:HA   | 2.32                     | 0.45              |
| 1:E:175:LYS:O    | 1:E:176:GLY:C    | 2.56                     | 0.45              |
| 1:F:213:LYS:HB2  | 1:F:240:ALA:CB   | 2.47                     | 0.45              |
| 1:B:175:LYS:O    | 1:B:176:GLY:C    | 2.55                     | 0.45              |
| 1:A:175:LYS:HZ3  | 1:A:175:LYS:CB   | 2.29                     | 0.45              |
| 1:E:153:ILE:HG22 | 1:E:153:ILE:O    | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:142:VAL:HG13 | 1:C:154:ILE:HD11 | 1.97                     | 0.45              |
| 2:P:12:PHE:HE1   | 2:P:72:MET:HB3   | 1.82                     | 0.45              |
| 2:S:37:ARG:HH11  | 2:S:37:ARG:HG2   | 1.81                     | 0.45              |
| 1:D:254:ARG:N    | 1:D:254:ARG:HD2  | 2.31                     | 0.45              |
| 1:E:719:LYS:O    | 1:E:721:SER:N    | 2.50                     | 0.45              |
| 1:E:723:PHE:O    | 1:E:726:ILE:N    | 2.50                     | 0.45              |
| 1:E:123:GLU:O    | 1:E:146:LYS:NZ   | 2.50                     | 0.45              |
| 1:F:691:LYS:O    | 1:F:693:SER:N    | 2.50                     | 0.45              |
| 1:A:777:TYR:HA   | 1:A:780:LEU:CD2  | 2.47                     | 0.45              |
| 1:C:659:THR:O    | 1:C:660:SER:C    | 2.55                     | 0.45              |
| 1:B:79:ILE:C     | 1:B:81:GLN:N     | 2.70                     | 0.45              |
| 1:F:79:ILE:C     | 1:F:81:GLN:N     | 2.69                     | 0.45              |
| 1:C:609:GLU:O    | 1:C:610:MET:C    | 2.53                     | 0.45              |
| 2:P:146:THR:O    | 2:P:147:ALA:C    | 2.55                     | 0.45              |
| 1:B:333:LYS:C    | 1:B:335:ALA:H    | 2.21                     | 0.45              |
| 2:R:143:GLN:O    | 2:R:147:ALA:CB   | 2.65                     | 0.45              |
| 1:B:616:GLU:HA   | 1:B:620:THR:HB   | 1.97                     | 0.45              |
| 1:C:266:GLU:HA   | 1:C:269:ASN:HB3  | 1.99                     | 0.45              |
| 1:D:175:LYS:O    | 1:D:176:GLY:C    | 2.55                     | 0.45              |
| 1:C:173:ILE:HG13 | 1:C:242:SER:CB   | 2.36                     | 0.45              |
| 2:S:126:ARG:HH21 | 2:S:126:ARG:HG3  | 1.81                     | 0.45              |
| 1:D:413:LEU:HD23 | 1:D:413:LEU:N    | 2.32                     | 0.45              |
| 1:D:153:ILE:O    | 1:D:153:ILE:HG22 | 2.16                     | 0.45              |
| 1:F:116:GLU:O    | 1:F:117:LEU:HD22 | 2.17                     | 0.45              |
| 1:E:550:SER:N    | 1:E:553:GLN:NE2  | 2.46                     | 0.45              |
| 1:E:199:LEU:CD2  | 1:E:225:ILE:O    | 2.65                     | 0.45              |
| 2:S:32:LEU:O     | 2:S:32:LEU:HD12  | 2.17                     | 0.45              |
| 2:T:16:PHE:CE1   | 2:T:27:ILE:HD13  | 2.52                     | 0.45              |
| 2:Q:31:GLU:O     | 2:Q:35:VAL:HG23  | 2.16                     | 0.45              |
| 1:B:463:THR:HB   | 1:B:467:GLU:H    | 1.82                     | 0.45              |
| 2:R:16:PHE:CZ    | 2:R:27:ILE:HG23  | 2.52                     | 0.45              |
| 1:E:403:LEU:HD13 | 1:E:476:VAL:HG11 | 1.99                     | 0.45              |
| 1:A:324:THR:HB   | 1:A:499:PRO:CA   | 2.46                     | 0.45              |
| 1:A:712:PHE:HD1  | 1:A:716:LYS:HG2  | 1.79                     | 0.45              |
| 1:B:315:PHE:CD2  | 1:B:560:LEU:HD22 | 2.52                     | 0.45              |
| 1:A:333:LYS:C    | 1:A:335:ALA:H    | 2.21                     | 0.45              |
| 1:F:270:LYS:HA   | 1:F:273:LYS:HB2  | 1.99                     | 0.45              |
| 1:D:680:LYS:HG2  | 1:D:681:ASP:N    | 2.32                     | 0.45              |
| 1:F:687:GLU:O    | 1:F:690:LYS:N    | 2.50                     | 0.45              |
| 1:C:461:LYS:HD2  | 1:C:461:LYS:HA   | 1.82                     | 0.45              |
| 1:E:89:ILE:HG22  | 1:E:93:VAL:CG1   | 2.10                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:130:SER:C    | 1:B:132:GLY:H    | 2.20                     | 0.44              |
| 1:E:296:LEU:O    | 1:E:301:ALA:HB2  | 2.17                     | 0.44              |
| 2:P:101:SER:O    | 2:P:104:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:115:LYS:HB2  | 1:A:118:GLN:HG2  | 1.98                     | 0.44              |
| 1:C:597:ASN:HD21 | 1:C:601:GLU:HB2  | 1.79                     | 0.44              |
| 1:B:630:ARG:CZ   | 2:P:83:GLU:CG    | 2.94                     | 0.44              |
| 1:A:722:ILE:HD13 | 1:A:764:LEU:CD2  | 2.47                     | 0.44              |
| 1:F:478:ALA:HA   | 1:F:488:LEU:HG   | 1.98                     | 0.44              |
| 1:B:153:ILE:HG22 | 1:B:153:ILE:O    | 2.16                     | 0.44              |
| 1:C:116:GLU:O    | 1:C:117:LEU:HD22 | 2.17                     | 0.44              |
| 1:E:116:GLU:O    | 1:E:117:LEU:HD22 | 2.17                     | 0.44              |
| 1:F:199:LEU:CD2  | 1:F:225:ILE:O    | 2.65                     | 0.44              |
| 2:T:32:LEU:HD12  | 2:T:32:LEU:O     | 2.16                     | 0.44              |
| 1:F:359:PRO:O    | 1:F:361:ALA:N    | 2.50                     | 0.44              |
| 1:A:308:VAL:CB   | 1:A:311:HIS:ND1  | 2.71                     | 0.44              |
| 1:E:135:VAL:N    | 1:E:136:PRO:HD3  | 2.31                     | 0.44              |
| 1:F:353:LYS:H    | 1:F:368:GLN:HE22 | 1.65                     | 0.44              |
| 1:C:443:GLU:OE2  | 1:C:458:LYS:HG2  | 2.17                     | 0.44              |
| 1:A:456:LYS:HB2  | 1:A:470:ASN:HA   | 1.98                     | 0.44              |
| 1:B:712:PHE:HB3  | 1:B:716:LYS:HG2  | 1.98                     | 0.44              |
| 1:D:123:GLU:O    | 1:D:146:LYS:NZ   | 2.50                     | 0.44              |
| 1:B:795:LYS:O    | 1:B:797:ILE:N    | 2.51                     | 0.44              |
| 2:S:5:THR:O      | 2:S:8:GLN:N      | 2.50                     | 0.44              |
| 1:E:777:TYR:HA   | 1:E:780:LEU:CD2  | 2.47                     | 0.44              |
| 1:B:777:TYR:HA   | 1:B:780:LEU:HD23 | 1.98                     | 0.44              |
| 1:A:694:VAL:HG23 | 2:O:18:LEU:HD21  | 1.97                     | 0.44              |
| 1:E:516:VAL:O    | 1:E:519:THR:HG22 | 2.16                     | 0.44              |
| 2:R:21:LYS:HD3   | 2:R:22:ASP:N     | 2.32                     | 0.44              |
| 1:E:209:LEU:HD23 | 1:E:260:TYR:CD2  | 2.52                     | 0.44              |
| 1:F:700:TYR:O    | 1:F:703:ASP:N    | 2.51                     | 0.44              |
| 2:R:131:ASP:N    | 2:R:131:ASP:OD1  | 2.46                     | 0.44              |
| 1:C:482:GLU:O    | 1:C:484:VAL:HG22 | 2.17                     | 0.44              |
| 1:D:478:ALA:HA   | 1:D:488:LEU:HG   | 2.00                     | 0.44              |
| 1:C:495:PHE:O    | 1:C:495:PHE:CD1  | 2.70                     | 0.44              |
| 1:B:142:VAL:CG2  | 1:B:154:ILE:HG23 | 2.41                     | 0.44              |
| 1:E:115:LYS:HB2  | 1:E:118:GLN:HG2  | 1.99                     | 0.44              |
| 1:D:789:ASN:O    | 1:D:792:VAL:HB   | 2.18                     | 0.44              |
| 1:A:462:ILE:HG12 | 1:A:463:THR:H    | 1.81                     | 0.44              |
| 1:A:359:PRO:CB   | 1:A:405:LEU:HD21 | 2.47                     | 0.44              |
| 1:B:134:LYS:CG   | 1:B:136:PRO:HD3  | 2.37                     | 0.44              |
| 1:D:403:LEU:HD13 | 1:D:476:VAL:HG11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:745:TYR:O    | 1:E:746:LYS:C    | 2.56                     | 0.44              |
| 1:E:720:ILE:HA   | 1:E:720:ILE:HD12 | 1.87                     | 0.44              |
| 1:F:441:VAL:O    | 1:F:442:TYR:CD2  | 2.70                     | 0.44              |
| 1:C:540:ARG:HD2  | 1:C:582:ASP:OD2  | 2.17                     | 0.44              |
| 1:A:441:VAL:O    | 1:A:442:TYR:CD2  | 2.70                     | 0.44              |
| 1:F:123:GLU:O    | 1:F:146:LYS:NZ   | 2.50                     | 0.44              |
| 1:E:735:VAL:HG12 | 1:E:741:ILE:HD13 | 1.97                     | 0.44              |
| 1:C:777:TYR:HA   | 1:C:780:LEU:HD23 | 1.98                     | 0.44              |
| 1:B:709:ASN:OD1  | 2:P:130:ILE:O    | 2.35                     | 0.44              |
| 1:E:489:THR:OG1  | 1:E:490:ALA:N    | 2.49                     | 0.44              |
| 1:F:315:PHE:CD2  | 1:F:560:LEU:HD22 | 2.52                     | 0.44              |
| 1:A:71:PHE:CB    | 1:A:108:ASP:HB2  | 2.46                     | 0.44              |
| 1:A:655:ASN:ND2  | 1:A:655:ASN:N    | 2.64                     | 0.44              |
| 2:S:146:THR:O    | 2:S:148:LYS:N    | 2.51                     | 0.44              |
| 1:A:508:ILE:CG2  | 1:A:509:PRO:HD2  | 2.46                     | 0.44              |
| 1:D:508:ILE:CG2  | 1:D:509:PRO:HD2  | 2.46                     | 0.44              |
| 1:A:583:ASN:ND2  | 1:A:587:PRO:HA   | 2.32                     | 0.44              |
| 1:E:96:ILE:O     | 1:E:100:LEU:HG   | 2.17                     | 0.44              |
| 1:C:83:GLN:O     | 1:C:84:ASP:C     | 2.52                     | 0.44              |
| 1:A:191:GLU:C    | 1:A:193:LEU:N    | 2.70                     | 0.44              |
| 1:E:732:ILE:HG23 | 1:E:749:PHE:HD1  | 1.82                     | 0.44              |
| 2:T:121:VAL:O    | 2:T:122:ASP:C    | 2.55                     | 0.44              |
| 1:A:116:GLU:O    | 1:A:117:LEU:HD22 | 2.17                     | 0.44              |
| 1:C:716:LYS:O    | 1:C:719:LYS:N    | 2.50                     | 0.44              |
| 1:C:579:THR:C    | 1:C:581:GLN:H    | 2.21                     | 0.44              |
| 1:E:789:ASN:O    | 1:E:792:VAL:HB   | 2.18                     | 0.44              |
| 1:E:115:LYS:C    | 1:E:117:LEU:N    | 2.69                     | 0.44              |
| 2:S:16:PHE:CE1   | 2:S:27:ILE:HD13  | 2.53                     | 0.44              |
| 2:S:12:PHE:HE1   | 2:S:72:MET:HB3   | 1.81                     | 0.44              |
| 1:D:463:THR:HB   | 1:D:467:GLU:H    | 1.81                     | 0.44              |
| 2:Q:16:PHE:CE1   | 2:Q:27:ILE:HD13  | 2.53                     | 0.44              |
| 1:D:359:PRO:CB   | 1:D:405:LEU:HD21 | 2.47                     | 0.44              |
| 1:F:122:GLU:HG3  | 1:F:147:ARG:H    | 1.82                     | 0.44              |
| 2:R:94:LYS:NZ    | 2:R:94:LYS:CB    | 2.76                     | 0.44              |
| 1:E:353:LYS:H    | 1:E:368:GLN:HE22 | 1.64                     | 0.44              |
| 1:E:324:THR:HB   | 1:E:499:PRO:CA   | 2.46                     | 0.44              |
| 1:E:500:SER:HA   | 1:E:624:TYR:CD2  | 2.53                     | 0.44              |
| 1:E:323:ASN:ND2  | 1:E:624:TYR:OH   | 2.32                     | 0.44              |
| 1:E:540:ARG:HD3  | 1:E:627:TYR:OH   | 2.18                     | 0.44              |
| 1:E:716:LYS:O    | 1:E:719:LYS:N    | 2.51                     | 0.44              |
| 1:A:795:LYS:O    | 1:A:797:ILE:N    | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:716:LYS:O    | 1:F:719:LYS:N    | 2.51                     | 0.44              |
| 1:E:693:SER:OG   | 1:E:731:GLU:OE1  | 2.34                     | 0.44              |
| 2:Q:5:THR:O      | 2:Q:8:GLN:N      | 2.50                     | 0.44              |
| 1:A:79:ILE:C     | 1:A:81:GLN:N     | 2.69                     | 0.44              |
| 1:E:315:PHE:CD2  | 1:E:560:LEU:HD22 | 2.52                     | 0.44              |
| 1:E:525:LYS:O    | 1:E:529:VAL:HG23 | 2.17                     | 0.44              |
| 2:O:21:LYS:HD3   | 2:O:22:ASP:N     | 2.32                     | 0.44              |
| 1:E:611:THR:O    | 1:E:615:ILE:HG13 | 2.18                     | 0.44              |
| 2:R:146:THR:O    | 2:R:147:ALA:C    | 2.55                     | 0.44              |
| 1:C:508:ILE:HG22 | 1:C:509:PRO:HD2  | 1.99                     | 0.44              |
| 1:B:687:GLU:O    | 1:B:690:LYS:N    | 2.51                     | 0.44              |
| 1:E:270:LYS:HA   | 1:E:273:LYS:HB2  | 1.98                     | 0.44              |
| 1:C:178:SER:OG   | 1:C:179:LEU:CD2  | 2.65                     | 0.44              |
| 1:B:96:ILE:O     | 1:B:100:LEU:HG   | 2.17                     | 0.44              |
| 1:B:97:TYR:CE2   | 1:B:102:GLY:HA3  | 2.53                     | 0.44              |
| 1:B:88:LYS:NZ    | 1:B:172:GLU:CD   | 2.70                     | 0.44              |
| 1:A:173:ILE:HG13 | 1:A:242:SER:CB   | 2.37                     | 0.44              |
| 1:F:764:LEU:O    | 1:F:766:HIS:N    | 2.50                     | 0.44              |
| 1:E:715:GLU:HA   | 1:E:718:ARG:NH2  | 2.32                     | 0.44              |
| 1:D:656:THR:O    | 1:D:755:ARG:HD2  | 2.16                     | 0.44              |
| 1:D:495:PHE:O    | 1:D:495:PHE:CD1  | 2.70                     | 0.44              |
| 2:T:12:PHE:CE1   | 2:T:72:MET:HG3   | 2.52                     | 0.44              |
| 2:Q:16:PHE:CZ    | 2:Q:27:ILE:HG23  | 2.52                     | 0.44              |
| 2:R:70:THR:O     | 2:R:71:MET:C     | 2.53                     | 0.44              |
| 1:F:432:TYR:HE1  | 1:F:445:ARG:CZ   | 2.31                     | 0.44              |
| 2:Q:9:ILE:HD12   | 2:Q:69:LEU:HD21  | 2.00                     | 0.44              |
| 1:C:323:ASN:ND2  | 1:C:624:TYR:OH   | 2.35                     | 0.44              |
| 1:C:318:ILE:CG2  | 1:C:322:LEU:HD12 | 2.45                     | 0.44              |
| 1:C:777:TYR:CE1  | 1:C:782:PHE:CE1  | 3.05                     | 0.44              |
| 2:P:73:ALA:O     | 2:P:75:LYS:N     | 2.50                     | 0.44              |
| 2:S:5:THR:O      | 2:S:6:GLU:C      | 2.56                     | 0.44              |
| 1:C:75:THR:C     | 1:C:77:ASP:N     | 2.70                     | 0.44              |
| 1:F:333:LYS:C    | 1:F:335:ALA:H    | 2.21                     | 0.44              |
| 1:C:298:GLY:C    | 1:C:300:LYS:H    | 2.21                     | 0.44              |
| 1:D:112:VAL:O    | 1:D:114:HIS:N    | 2.49                     | 0.44              |
| 1:E:112:VAL:O    | 1:E:114:HIS:N    | 2.49                     | 0.44              |
| 1:C:270:LYS:HA   | 1:C:273:LYS:HB2  | 1.99                     | 0.44              |
| 1:C:191:GLU:O    | 1:C:192:PHE:C    | 2.56                     | 0.44              |
| 1:A:238:GLN:C    | 1:A:240:ALA:N    | 2.71                     | 0.44              |
| 1:A:697:ILE:C    | 1:A:699:GLY:N    | 2.70                     | 0.44              |
| 1:F:732:ILE:HG23 | 1:F:749:PHE:HD1  | 1.83                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:101:SER:O    | 2:S:104:GLU:HG2  | 2.17                     | 0.44              |
| 1:F:715:GLU:OE1  | 1:F:767:GLN:NE2  | 2.50                     | 0.44              |
| 1:C:658:PRO:HG3  | 1:C:752:LEU:HD22 | 1.99                     | 0.44              |
| 1:F:115:LYS:C    | 1:F:117:LEU:N    | 2.70                     | 0.44              |
| 1:C:199:LEU:CD2  | 1:C:225:ILE:O    | 2.65                     | 0.44              |
| 2:S:70:THR:C     | 2:S:72:MET:N     | 2.71                     | 0.44              |
| 1:A:432:TYR:HE1  | 1:A:445:ARG:CZ   | 2.31                     | 0.44              |
| 2:O:12:PHE:HE1   | 2:O:72:MET:HB3   | 1.82                     | 0.44              |
| 1:C:359:PRO:HD2  | 1:C:444:PHE:CE2  | 2.52                     | 0.44              |
| 2:P:32:LEU:HD21  | 2:P:71:MET:HE2   | 1.99                     | 0.44              |
| 1:C:441:VAL:O    | 1:C:442:TYR:CD2  | 2.70                     | 0.44              |
| 1:C:456:LYS:CB   | 1:C:470:ASN:C    | 2.86                     | 0.44              |
| 1:A:716:LYS:O    | 1:A:719:LYS:N    | 2.50                     | 0.44              |
| 1:A:735:VAL:O    | 1:A:738:SER:CB   | 2.65                     | 0.44              |
| 1:F:777:TYR:HA   | 1:F:780:LEU:CD2  | 2.47                     | 0.44              |
| 1:A:628:PHE:CD1  | 1:A:645:TRP:CD1  | 3.04                     | 0.44              |
| 1:F:75:THR:C     | 1:F:77:ASP:N     | 2.70                     | 0.44              |
| 1:C:345:THR:HB   | 1:C:491:ASP:CB   | 2.47                     | 0.44              |
| 1:C:628:PHE:CD1  | 1:C:645:TRP:CD1  | 3.05                     | 0.44              |
| 1:A:315:PHE:CD2  | 1:A:560:LEU:HD22 | 2.53                     | 0.44              |
| 2:O:146:THR:O    | 2:O:147:ALA:C    | 2.55                     | 0.44              |
| 1:D:557:LEU:HD11 | 1:D:575:VAL:HG11 | 2.00                     | 0.44              |
| 1:F:99:GLU:OE2   | 1:F:284:LYS:HD2  | 2.18                     | 0.44              |
| 1:E:508:ILE:HG22 | 1:E:509:PRO:HD2  | 1.99                     | 0.44              |
| 1:D:266:GLU:HA   | 1:D:269:ASN:HB3  | 2.00                     | 0.44              |
| 1:F:186:LYS:O    | 1:F:186:LYS:HG2  | 2.16                     | 0.44              |
| 1:F:88:LYS:NZ    | 1:F:172:GLU:CD   | 2.70                     | 0.44              |
| 1:B:697:ILE:C    | 1:B:699:GLY:N    | 2.69                     | 0.44              |
| 1:D:296:LEU:O    | 1:D:301:ALA:HB2  | 2.18                     | 0.44              |
| 2:T:101:SER:O    | 2:T:104:GLU:HG2  | 2.17                     | 0.44              |
| 1:C:719:LYS:O    | 1:C:721:SER:N    | 2.51                     | 0.44              |
| 1:B:597:ASN:HD21 | 1:B:601:GLU:HB2  | 1.80                     | 0.44              |
| 1:A:764:LEU:O    | 1:A:766:HIS:N    | 2.50                     | 0.44              |
| 1:C:153:ILE:HG22 | 1:C:153:ILE:O    | 2.16                     | 0.44              |
| 1:F:397:GLU:O    | 1:F:398:ILE:HD13 | 2.18                     | 0.44              |
| 1:D:630:ARG:CZ   | 2:R:83:GLU:CG    | 2.96                     | 0.44              |
| 1:A:134:LYS:CG   | 1:A:136:PRO:HD3  | 2.37                     | 0.44              |
| 1:C:403:LEU:HD13 | 1:C:476:VAL:HG11 | 2.00                     | 0.44              |
| 2:P:16:PHE:CZ    | 2:P:27:ILE:HG23  | 2.52                     | 0.44              |
| 2:T:37:ARG:HH11  | 2:T:37:ARG:HG2   | 1.82                     | 0.44              |
| 1:C:311:HIS:O    | 1:C:314:ALA:HB3  | 2.16                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:540:ARG:HD2  | 1:E:582:ASP:OD2  | 2.18                     | 0.44              |
| 1:D:318:ILE:O    | 1:D:319:ALA:C    | 2.55                     | 0.44              |
| 1:C:323:ASN:O    | 1:C:324:THR:HG22 | 2.18                     | 0.44              |
| 1:B:716:LYS:O    | 1:B:719:LYS:N    | 2.51                     | 0.44              |
| 1:B:794:GLN:HB3  | 1:B:794:GLN:HE21 | 1.62                     | 0.44              |
| 1:A:735:VAL:HG12 | 1:A:741:ILE:HD13 | 1.97                     | 0.44              |
| 1:D:693:SER:OG   | 1:D:731:GLU:OE1  | 2.36                     | 0.44              |
| 1:E:777:TYR:HA   | 1:E:780:LEU:HD23 | 1.99                     | 0.44              |
| 1:E:777:TYR:CE1  | 1:E:782:PHE:CE1  | 3.05                     | 0.44              |
| 2:R:5:THR:O      | 2:R:6:GLU:C      | 2.56                     | 0.44              |
| 2:R:5:THR:O      | 2:R:8:GLN:N      | 2.50                     | 0.44              |
| 1:B:515:LYS:HZ3  | 1:B:516:VAL:HG23 | 1.83                     | 0.44              |
| 1:C:686:ASP:CB   | 1:C:739:LYS:HD2  | 2.46                     | 0.44              |
| 1:B:109:ILE:HD13 | 1:B:157:LYS:HZ2  | 1.82                     | 0.44              |
| 1:E:333:LYS:C    | 1:E:335:ALA:H    | 2.21                     | 0.44              |
| 1:C:210:PHE:HD2  | 1:C:210:PHE:H    | 1.66                     | 0.44              |
| 1:C:773:PHE:O    | 1:C:775:LEU:N    | 2.50                     | 0.44              |
| 1:B:266:GLU:HA   | 1:B:269:ASN:HB3  | 1.99                     | 0.44              |
| 1:A:180:ASP:O    | 1:A:183:SER:N    | 2.46                     | 0.44              |
| 1:A:199:LEU:CD2  | 1:A:225:ILE:O    | 2.65                     | 0.44              |
| 1:E:697:ILE:C    | 1:E:699:GLY:H    | 2.21                     | 0.44              |
| 1:F:697:ILE:C    | 1:F:699:GLY:N    | 2.71                     | 0.44              |
| 1:F:658:PRO:HG3  | 1:F:752:LEU:HD22 | 2.00                     | 0.44              |
| 1:B:718:ARG:HH11 | 1:B:767:GLN:NE2  | 2.15                     | 0.44              |
| 1:B:495:PHE:CD1  | 1:B:495:PHE:C    | 2.91                     | 0.44              |
| 1:E:478:ALA:HA   | 1:E:488:LEU:HG   | 2.00                     | 0.44              |
| 1:B:107:THR:CG2  | 1:B:115:LYS:HD2  | 2.48                     | 0.44              |
| 1:D:579:THR:C    | 1:D:581:GLN:H    | 2.21                     | 0.44              |
| 1:E:405:LEU:CD1  | 1:E:405:LEU:N    | 2.81                     | 0.44              |
| 1:D:134:LYS:C    | 1:D:136:PRO:CD   | 2.83                     | 0.44              |
| 2:O:92:PHE:C     | 2:O:94:LYS:N     | 2.71                     | 0.44              |
| 1:B:441:VAL:O    | 1:B:442:TYR:CD2  | 2.71                     | 0.44              |
| 1:A:456:LYS:HB2  | 1:A:469:PHE:O    | 2.18                     | 0.44              |
| 1:F:693:SER:OG   | 1:F:731:GLU:OE1  | 2.36                     | 0.44              |
| 1:F:659:THR:O    | 1:F:660:SER:C    | 2.55                     | 0.44              |
| 1:B:694:VAL:HG23 | 2:P:18:LEU:HD21  | 1.98                     | 0.44              |
| 1:C:709:ASN:OD1  | 2:Q:130:ILE:O    | 2.36                     | 0.44              |
| 1:B:672:ARG:HA   | 1:B:672:ARG:HD3  | 1.69                     | 0.44              |
| 1:A:298:GLY:C    | 1:A:300:LYS:H    | 2.21                     | 0.44              |
| 1:F:97:TYR:CE2   | 1:F:102:GLY:HA3  | 2.52                     | 0.44              |
| 1:F:175:LYS:HB2  | 1:F:175:LYS:HZ3  | 1.74                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:192:PHE:HB3  | 1:A:196:ILE:CD1  | 2.48                     | 0.44              |
| 1:C:295:VAL:HB   | 1:C:603:ILE:CG2  | 2.48                     | 0.44              |
| 1:D:732:ILE:HG23 | 1:D:749:PHE:HD1  | 1.83                     | 0.44              |
| 1:C:697:ILE:C    | 1:C:699:GLY:N    | 2.70                     | 0.44              |
| 2:R:102:ALA:HA   | 2:R:125:ILE:HG13 | 1.99                     | 0.44              |
| 2:R:126:ARG:HH21 | 2:R:126:ARG:HG3  | 1.82                     | 0.44              |
| 1:D:397:GLU:O    | 1:D:398:ILE:HD13 | 2.18                     | 0.44              |
| 1:B:629:ASN:ND2  | 1:B:629:ASN:C    | 2.59                     | 0.44              |
| 1:D:752:LEU:O    | 1:D:756:ILE:HG12 | 2.18                     | 0.44              |
| 1:F:142:VAL:CG2  | 1:F:154:ILE:HG23 | 2.40                     | 0.44              |
| 1:A:463:THR:HB   | 1:A:467:GLU:H    | 1.82                     | 0.44              |
| 1:D:199:LEU:CD2  | 1:D:225:ILE:O    | 2.65                     | 0.44              |
| 1:F:745:TYR:O    | 1:F:746:LYS:C    | 2.56                     | 0.44              |
| 1:B:134:LYS:C    | 1:B:136:PRO:CD   | 2.85                     | 0.44              |
| 2:Q:12:PHE:HE1   | 2:Q:72:MET:HB3   | 1.82                     | 0.44              |
| 2:P:37:ARG:HG2   | 2:P:37:ARG:HH11  | 1.82                     | 0.44              |
| 1:F:501:LEU:HD22 | 2:T:112:LEU:CD2  | 2.41                     | 0.44              |
| 1:D:441:VAL:O    | 1:D:442:TYR:CD2  | 2.71                     | 0.44              |
| 1:B:305:SER:OG   | 1:B:306:GLY:N    | 2.50                     | 0.44              |
| 1:C:795:LYS:O    | 1:C:797:ILE:N    | 2.51                     | 0.44              |
| 1:E:795:LYS:O    | 1:E:797:ILE:N    | 2.51                     | 0.44              |
| 1:B:123:GLU:O    | 1:B:146:LYS:NZ   | 2.50                     | 0.44              |
| 1:B:223:LYS:HZ3  | 1:B:228:ASN:HB3  | 1.82                     | 0.44              |
| 1:F:532:LEU:HD23 | 1:F:532:LEU:HA   | 1.84                     | 0.44              |
| 1:C:71:PHE:CG    | 1:C:73:ASN:HB2   | 2.53                     | 0.44              |
| 1:E:639:ASN:ND2  | 1:E:639:ASN:N    | 2.66                     | 0.44              |
| 2:R:36:MET:HE3   | 2:R:43:PRO:HG3   | 2.00                     | 0.44              |
| 2:S:131:ASP:N    | 2:S:131:ASP:OD1  | 2.45                     | 0.44              |
| 1:D:173:ILE:HG13 | 1:D:242:SER:CB   | 2.36                     | 0.44              |
| 1:F:238:GLN:C    | 1:F:240:ALA:N    | 2.71                     | 0.44              |
| 2:P:124:MET:O    | 2:P:125:ILE:C    | 2.56                     | 0.44              |
| 1:A:658:PRO:HG3  | 1:A:752:LEU:HD22 | 1.98                     | 0.44              |
| 1:A:630:ARG:CZ   | 2:O:83:GLU:CG    | 2.94                     | 0.44              |
| 1:E:115:LYS:HB2  | 1:E:118:GLN:CG   | 2.48                     | 0.44              |
| 1:A:405:LEU:N    | 1:A:405:LEU:CD1  | 2.81                     | 0.44              |
| 1:D:405:LEU:N    | 1:D:405:LEU:CD1  | 2.80                     | 0.44              |
| 1:D:720:ILE:HD12 | 1:D:720:ILE:HA   | 1.87                     | 0.44              |
| 2:P:92:PHE:C     | 2:P:94:LYS:N     | 2.71                     | 0.44              |
| 1:E:443:GLU:HG2  | 1:E:458:LYS:HZ1  | 1.78                     | 0.44              |
| 1:B:368:GLN:C    | 1:B:370:LEU:H    | 2.21                     | 0.44              |
| 1:A:66:LEU:CD1   | 1:A:103:GLU:HA   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:693:SER:OG   | 1:A:731:GLU:OE1  | 2.36                     | 0.44              |
| 2:P:13:LYS:HZ1   | 2:P:65:PHE:CB    | 2.30                     | 0.44              |
| 1:A:659:THR:O    | 1:A:660:SER:C    | 2.56                     | 0.44              |
| 1:E:691:LYS:O    | 1:E:693:SER:N    | 2.51                     | 0.44              |
| 2:P:5:THR:O      | 2:P:8:GLN:N      | 2.51                     | 0.44              |
| 1:E:345:THR:HB   | 1:E:491:ASP:CB   | 2.47                     | 0.44              |
| 1:B:209:LEU:HD23 | 1:B:260:TYR:CD2  | 2.53                     | 0.44              |
| 1:F:298:GLY:C    | 1:F:300:LYS:H    | 2.21                     | 0.44              |
| 1:D:140:ARG:NE   | 1:D:140:ARG:HA   | 2.31                     | 0.44              |
| 1:D:186:LYS:HZ1  | 1:D:234:LEU:CD1  | 2.31                     | 0.43              |
| 1:A:732:ILE:HG23 | 1:A:749:PHE:HD1  | 1.82                     | 0.43              |
| 1:A:115:LYS:C    | 1:A:117:LEU:N    | 2.71                     | 0.43              |
| 1:C:722:ILE:HD13 | 1:C:764:LEU:HD23 | 1.99                     | 0.43              |
| 1:E:764:LEU:O    | 1:E:766:HIS:N    | 2.51                     | 0.43              |
| 1:F:482:GLU:O    | 1:F:484:VAL:HG22 | 2.18                     | 0.43              |
| 1:A:478:ALA:HA   | 1:A:488:LEU:HG   | 2.00                     | 0.43              |
| 1:A:405:LEU:HD13 | 1:A:453:VAL:CG2  | 2.38                     | 0.43              |
| 1:A:136:PRO:HG2  | 1:A:139:SER:HG   | 1.83                     | 0.43              |
| 2:Q:12:PHE:CE1   | 2:Q:72:MET:HG3   | 2.53                     | 0.43              |
| 1:F:446:ILE:HG13 | 1:F:452:GLU:O    | 2.17                     | 0.43              |
| 2:S:30:LYS:H     | 2:S:30:LYS:CD    | 2.20                     | 0.43              |
| 1:E:443:GLU:OE2  | 1:E:458:LYS:HG2  | 2.17                     | 0.43              |
| 1:A:368:GLN:C    | 1:A:370:LEU:H    | 2.21                     | 0.43              |
| 1:D:443:GLU:OE2  | 1:D:458:LYS:HG2  | 2.18                     | 0.43              |
| 1:B:721:SER:C    | 1:B:723:PHE:N    | 2.71                     | 0.43              |
| 2:R:97:ASN:O     | 2:R:99:TYR:CD1   | 2.71                     | 0.43              |
| 1:F:777:TYR:HA   | 1:F:780:LEU:HD23 | 1.98                     | 0.43              |
| 1:A:532:LEU:HA   | 1:A:532:LEU:HD23 | 1.86                     | 0.43              |
| 1:C:610:MET:O    | 1:C:614:PHE:N    | 2.38                     | 0.43              |
| 1:E:71:PHE:CG    | 1:E:73:ASN:HB2   | 2.53                     | 0.43              |
| 1:B:109:ILE:HG13 | 1:B:109:ILE:H    | 1.64                     | 0.43              |
| 1:B:109:ILE:HD13 | 1:B:157:LYS:HZ3  | 1.83                     | 0.43              |
| 1:B:403:LEU:HD13 | 1:B:476:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:687:GLU:O    | 1:C:690:LYS:N    | 2.50                     | 0.43              |
| 1:C:700:TYR:O    | 1:C:703:ASP:N    | 2.51                     | 0.43              |
| 1:F:771:ILE:HG12 | 1:F:771:ILE:H    | 1.57                     | 0.43              |
| 1:E:176:GLY:C    | 1:E:178:SER:N    | 2.67                     | 0.43              |
| 1:F:234:LEU:HG   | 1:F:235:THR:N    | 2.33                     | 0.43              |
| 1:A:234:LEU:HG   | 1:A:235:THR:N    | 2.33                     | 0.43              |
| 1:E:142:VAL:HG13 | 1:E:154:ILE:HD11 | 1.96                     | 0.43              |
| 1:A:153:ILE:O    | 1:A:153:ILE:HG22 | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:403:LEU:HD13 | 1:A:476:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:462:ILE:HG12 | 1:C:463:THR:H    | 1.82                     | 0.43              |
| 1:D:667:LEU:O    | 1:D:668:SER:C    | 2.56                     | 0.43              |
| 1:F:403:LEU:HD13 | 1:F:476:VAL:HG11 | 2.00                     | 0.43              |
| 1:C:432:TYR:HE1  | 1:C:445:ARG:CZ   | 2.31                     | 0.43              |
| 1:C:446:ILE:HD11 | 1:C:451:ASN:HB2  | 1.99                     | 0.43              |
| 1:E:432:TYR:HE1  | 1:E:445:ARG:CZ   | 2.31                     | 0.43              |
| 2:O:16:PHE:CE1   | 2:O:27:ILE:HD13  | 2.52                     | 0.43              |
| 2:R:9:ILE:HD12   | 2:R:69:LEU:HD21  | 2.00                     | 0.43              |
| 1:A:540:ARG:HD2  | 1:A:582:ASP:OD2  | 2.18                     | 0.43              |
| 1:A:456:LYS:HB3  | 1:A:471:TRP:N    | 2.33                     | 0.43              |
| 1:F:66:LEU:CD1   | 1:F:103:GLU:HA   | 2.48                     | 0.43              |
| 1:D:694:VAL:HG22 | 2:R:18:LEU:HD21  | 2.00                     | 0.43              |
| 2:Q:5:THR:O      | 2:Q:6:GLU:C      | 2.56                     | 0.43              |
| 1:E:210:PHE:H    | 1:E:210:PHE:HD2  | 1.66                     | 0.43              |
| 1:D:639:ASN:ND2  | 1:D:639:ASN:N    | 2.66                     | 0.43              |
| 1:D:438:ASN:HA   | 1:D:438:ASN:HD22 | 1.53                     | 0.43              |
| 1:F:88:LYS:HZ2   | 1:F:172:GLU:CD   | 2.21                     | 0.43              |
| 1:C:175:LYS:O    | 1:C:176:GLY:C    | 2.55                     | 0.43              |
| 1:C:83:GLN:C     | 1:C:85:LEU:N     | 2.72                     | 0.43              |
| 1:D:697:ILE:C    | 1:D:699:GLY:H    | 2.22                     | 0.43              |
| 2:T:105:LEU:HB2  | 2:T:125:ILE:HD11 | 2.01                     | 0.43              |
| 1:B:478:ALA:HA   | 1:B:488:LEU:HG   | 2.00                     | 0.43              |
| 1:D:657:ILE:HG21 | 1:D:704:TYR:CE1  | 2.54                     | 0.43              |
| 1:C:115:LYS:C    | 1:C:117:LEU:N    | 2.71                     | 0.43              |
| 1:F:152:LEU:CD2  | 1:F:154:ILE:HD11 | 2.40                     | 0.43              |
| 1:D:432:TYR:HE1  | 1:D:445:ARG:CZ   | 2.31                     | 0.43              |
| 1:B:432:TYR:HE1  | 1:B:445:ARG:CZ   | 2.31                     | 0.43              |
| 1:B:359:PRO:CB   | 1:B:405:LEU:HD21 | 2.49                     | 0.43              |
| 1:C:359:PRO:HB2  | 1:C:405:LEU:HD21 | 2.00                     | 0.43              |
| 2:R:70:THR:C     | 2:R:72:MET:N     | 2.71                     | 0.43              |
| 2:Q:91:VAL:HG12  | 2:Q:92:PHE:N     | 2.33                     | 0.43              |
| 2:Q:94:LYS:CB    | 2:Q:94:LYS:NZ    | 2.76                     | 0.43              |
| 1:D:323:ASN:O    | 1:D:324:THR:HG22 | 2.18                     | 0.43              |
| 1:E:255:THR:O    | 1:E:257:LEU:N    | 2.52                     | 0.43              |
| 1:F:795:LYS:O    | 1:F:797:ILE:N    | 2.50                     | 0.43              |
| 1:A:719:LYS:O    | 1:A:721:SER:N    | 2.50                     | 0.43              |
| 1:B:735:VAL:O    | 1:B:738:SER:CB   | 2.66                     | 0.43              |
| 2:O:5:THR:O      | 2:O:8:GLN:N      | 2.50                     | 0.43              |
| 1:F:595:ILE:HD12 | 1:F:614:PHE:CE2  | 2.54                     | 0.43              |
| 1:D:71:PHE:CG    | 1:D:73:ASN:HB2   | 2.53                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:109:ILE:HG13 | 1:F:109:ILE:H    | 1.64                     | 0.43              |
| 2:T:143:GLN:O    | 2:T:147:ALA:CB   | 2.66                     | 0.43              |
| 1:F:639:ASN:ND2  | 1:F:639:ASN:N    | 2.66                     | 0.43              |
| 2:Q:146:THR:O    | 2:Q:147:ALA:C    | 2.56                     | 0.43              |
| 1:B:298:GLY:C    | 1:B:300:LYS:H    | 2.22                     | 0.43              |
| 1:C:558:ASP:O    | 1:C:561:ASN:N    | 2.52                     | 0.43              |
| 1:A:700:TYR:O    | 1:A:703:ASP:N    | 2.51                     | 0.43              |
| 1:D:298:GLY:C    | 1:D:300:LYS:H    | 2.21                     | 0.43              |
| 1:A:266:GLU:HA   | 1:A:269:ASN:HB3  | 1.99                     | 0.43              |
| 1:A:558:ASP:O    | 1:A:561:ASN:N    | 2.52                     | 0.43              |
| 1:E:559:ARG:HA   | 1:E:559:ARG:HD2  | 1.79                     | 0.43              |
| 1:D:270:LYS:HA   | 1:D:273:LYS:HB2  | 1.99                     | 0.43              |
| 1:F:186:LYS:NZ   | 1:F:234:LEU:HD12 | 2.33                     | 0.43              |
| 1:C:97:TYR:CE2   | 1:C:102:GLY:HA3  | 2.53                     | 0.43              |
| 1:C:130:SER:C    | 1:C:132:GLY:H    | 2.22                     | 0.43              |
| 2:Q:101:SER:O    | 2:Q:104:GLU:HG2  | 2.17                     | 0.43              |
| 2:T:101:SER:OG   | 2:T:104:GLU:HG2  | 2.18                     | 0.43              |
| 1:C:397:GLU:O    | 1:C:398:ILE:HD13 | 2.18                     | 0.43              |
| 1:C:715:GLU:OE1  | 1:C:767:GLN:NE2  | 2.49                     | 0.43              |
| 1:A:482:GLU:O    | 1:A:484:VAL:HG22 | 2.19                     | 0.43              |
| 1:D:723:PHE:O    | 1:D:726:ILE:N    | 2.50                     | 0.43              |
| 1:D:581:GLN:NE2  | 1:D:629:ASN:N    | 2.60                     | 0.43              |
| 1:B:142:VAL:HG13 | 1:B:154:ILE:HD11 | 1.97                     | 0.43              |
| 1:A:745:TYR:O    | 1:A:746:LYS:C    | 2.55                     | 0.43              |
| 1:E:463:THR:HB   | 1:E:467:GLU:H    | 1.83                     | 0.43              |
| 1:A:134:LYS:C    | 1:A:136:PRO:CD   | 2.85                     | 0.43              |
| 2:Q:32:LEU:HD12  | 2:Q:32:LEU:O     | 2.17                     | 0.43              |
| 1:F:405:LEU:CD1  | 1:F:405:LEU:N    | 2.82                     | 0.43              |
| 2:S:92:PHE:C     | 2:S:94:LYS:N     | 2.71                     | 0.43              |
| 1:C:443:GLU:O    | 1:C:455:TYR:HA   | 2.17                     | 0.43              |
| 1:F:540:ARG:HD2  | 1:F:582:ASP:OD2  | 2.19                     | 0.43              |
| 1:D:123:GLU:CG   | 1:D:124:GLU:N    | 2.71                     | 0.43              |
| 1:B:691:LYS:O    | 1:B:693:SER:N    | 2.51                     | 0.43              |
| 1:C:197:LYS:NZ   | 1:C:267:TYR:CD2  | 2.87                     | 0.43              |
| 1:B:71:PHE:CG    | 1:B:73:ASN:HB2   | 2.53                     | 0.43              |
| 1:F:210:PHE:H    | 1:F:210:PHE:HD2  | 1.66                     | 0.43              |
| 1:A:671:ARG:NH1  | 1:A:677:GLY:HA3  | 2.33                     | 0.43              |
| 1:E:234:LEU:HG   | 1:E:235:THR:N    | 2.34                     | 0.43              |
| 1:E:238:GLN:C    | 1:E:240:ALA:N    | 2.71                     | 0.43              |
| 1:C:173:ILE:HG23 | 1:C:174:GLY:H    | 1.83                     | 0.43              |
| 1:C:581:GLN:NE2  | 1:C:629:ASN:N    | 2.61                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:716:LYS:O    | 1:D:719:LYS:N    | 2.50                     | 0.43              |
| 1:D:115:LYS:HB2  | 1:D:118:GLN:CG   | 2.48                     | 0.43              |
| 1:B:405:LEU:N    | 1:B:405:LEU:CD1  | 2.81                     | 0.43              |
| 1:B:405:LEU:HD13 | 1:B:453:VAL:CG2  | 2.39                     | 0.43              |
| 2:O:16:PHE:CZ    | 2:O:27:ILE:HG23  | 2.53                     | 0.43              |
| 2:R:32:LEU:HD12  | 2:R:32:LEU:O     | 2.18                     | 0.43              |
| 1:D:311:HIS:O    | 1:D:314:ALA:HB3  | 2.17                     | 0.43              |
| 1:E:311:HIS:O    | 1:E:314:ALA:HB3  | 2.19                     | 0.43              |
| 1:E:318:ILE:O    | 1:E:319:ALA:C    | 2.57                     | 0.43              |
| 1:F:443:GLU:O    | 1:F:455:TYR:HA   | 2.19                     | 0.43              |
| 1:B:255:THR:O    | 1:B:257:LEU:N    | 2.52                     | 0.43              |
| 1:B:318:ILE:O    | 1:B:319:ALA:C    | 2.56                     | 0.43              |
| 1:D:443:GLU:O    | 1:D:455:TYR:HA   | 2.18                     | 0.43              |
| 1:A:209:LEU:HD23 | 1:A:260:TYR:CD2  | 2.54                     | 0.43              |
| 1:E:595:ILE:HD12 | 1:E:614:PHE:CE2  | 2.53                     | 0.43              |
| 1:D:482:GLU:O    | 1:D:484:VAL:HG22 | 2.19                     | 0.43              |
| 2:S:143:GLN:O    | 2:S:147:ALA:CB   | 2.66                     | 0.43              |
| 1:A:687:GLU:O    | 1:A:690:LYS:N    | 2.52                     | 0.43              |
| 1:B:773:PHE:O    | 1:B:775:LEU:N    | 2.52                     | 0.43              |
| 1:B:790:PHE:O    | 1:B:793:PHE:HB3  | 2.18                     | 0.43              |
| 1:D:773:PHE:O    | 1:D:775:LEU:N    | 2.51                     | 0.43              |
| 2:T:55:VAL:HB    | 2:T:67:GLU:OE1   | 2.18                     | 0.43              |
| 1:F:180:ASP:O    | 1:F:183:SER:N    | 2.45                     | 0.43              |
| 2:P:126:ARG:HH21 | 2:P:126:ARG:HG3  | 1.84                     | 0.43              |
| 1:A:142:VAL:CG2  | 1:A:154:ILE:HG23 | 2.41                     | 0.43              |
| 2:P:70:THR:C     | 2:P:72:MET:N     | 2.72                     | 0.43              |
| 2:P:91:VAL:HG12  | 2:P:92:PHE:N     | 2.33                     | 0.43              |
| 1:E:443:GLU:O    | 1:E:455:TYR:HA   | 2.18                     | 0.43              |
| 1:A:443:GLU:O    | 1:A:455:TYR:HA   | 2.18                     | 0.43              |
| 1:F:721:SER:C    | 1:F:723:PHE:N    | 2.70                     | 0.43              |
| 1:B:693:SER:OG   | 1:B:731:GLU:OE1  | 2.36                     | 0.43              |
| 1:D:628:PHE:CD1  | 1:D:645:TRP:CD1  | 3.07                     | 0.43              |
| 1:D:709:ASN:OD1  | 2:R:130:ILE:O    | 2.37                     | 0.43              |
| 1:A:141:PHE:H    | 1:A:141:PHE:HD1  | 1.59                     | 0.43              |
| 1:B:611:THR:O    | 1:B:615:ILE:HG13 | 2.18                     | 0.43              |
| 1:C:557:LEU:HD11 | 1:C:575:VAL:HG11 | 2.01                     | 0.43              |
| 1:B:655:ASN:N    | 1:B:655:ASN:ND2  | 2.66                     | 0.43              |
| 2:R:146:THR:O    | 2:R:148:LYS:N    | 2.52                     | 0.43              |
| 1:D:773:PHE:O    | 1:D:774:LYS:C    | 2.57                     | 0.43              |
| 1:E:266:GLU:HA   | 1:E:269:ASN:HB3  | 2.00                     | 0.43              |
| 1:D:234:LEU:HG   | 1:D:235:THR:N    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:234:LEU:HG   | 1:C:235:THR:N    | 2.33                     | 0.43              |
| 1:C:97:TYR:CE1   | 1:C:178:SER:CB   | 3.02                     | 0.43              |
| 1:A:130:SER:HB2  | 1:A:170:TYR:CZ   | 2.53                     | 0.43              |
| 1:A:97:TYR:CE2   | 1:A:102:GLY:HA3  | 2.53                     | 0.43              |
| 1:B:714:GLN:O    | 1:B:715:GLU:C    | 2.57                     | 0.43              |
| 1:B:520:PRO:HG2  | 1:B:521:ASN:N    | 2.33                     | 0.43              |
| 1:C:115:LYS:HB2  | 1:C:118:GLN:CG   | 2.49                     | 0.43              |
| 2:P:16:PHE:CE1   | 2:P:27:ILE:HD13  | 2.54                     | 0.43              |
| 2:Q:92:PHE:C     | 2:Q:94:LYS:N     | 2.71                     | 0.43              |
| 1:E:255:THR:C    | 1:E:257:LEU:N    | 2.72                     | 0.43              |
| 1:B:735:VAL:HG12 | 1:B:741:ILE:HD13 | 1.96                     | 0.43              |
| 2:P:145:MET:HB3  | 2:P:146:THR:H    | 1.63                     | 0.43              |
| 1:D:333:LYS:C    | 1:D:335:ALA:H    | 2.21                     | 0.43              |
| 1:D:209:LEU:HD23 | 1:D:260:TYR:CD2  | 2.54                     | 0.43              |
| 1:C:209:LEU:HD23 | 1:C:260:TYR:CD2  | 2.54                     | 0.43              |
| 1:F:508:ILE:HG22 | 1:F:509:PRO:HD2  | 2.00                     | 0.43              |
| 1:D:665:LYS:HG3  | 2:R:11:GLU:CD    | 2.39                     | 0.43              |
| 1:F:680:LYS:HG2  | 1:F:681:ASP:N    | 2.34                     | 0.43              |
| 1:E:771:ILE:HG12 | 1:E:771:ILE:H    | 1.57                     | 0.43              |
| 1:B:461:LYS:HA   | 1:B:461:LYS:HD2  | 1.82                     | 0.43              |
| 1:E:170:TYR:O    | 1:E:172:GLU:N    | 2.52                     | 0.43              |
| 1:E:88:LYS:NZ    | 1:E:172:GLU:CD   | 2.72                     | 0.43              |
| 1:D:238:GLN:C    | 1:D:240:ALA:N    | 2.71                     | 0.43              |
| 1:B:170:TYR:O    | 1:B:172:GLU:N    | 2.52                     | 0.43              |
| 1:B:83:GLN:C     | 1:B:85:LEU:N     | 2.72                     | 0.43              |
| 1:A:170:TYR:O    | 1:A:172:GLU:N    | 2.52                     | 0.43              |
| 1:A:196:ILE:HA   | 1:A:199:LEU:HG   | 1.99                     | 0.43              |
| 2:P:101:SER:OG   | 2:P:104:GLU:HG2  | 2.19                     | 0.43              |
| 1:C:478:ALA:HA   | 1:C:488:LEU:HG   | 2.00                     | 0.43              |
| 1:B:550:SER:N    | 1:B:553:GLN:NE2  | 2.44                     | 0.43              |
| 1:F:789:ASN:O    | 1:F:792:VAL:HB   | 2.19                     | 0.43              |
| 2:Q:70:THR:C     | 2:Q:72:MET:N     | 2.72                     | 0.43              |
| 2:O:9:ILE:HD12   | 2:O:69:LEU:HD21  | 2.01                     | 0.43              |
| 1:E:368:GLN:C    | 1:E:370:LEU:H    | 2.21                     | 0.43              |
| 1:D:373:LYS:CD   | 1:D:376:GLN:NE2  | 2.76                     | 0.43              |
| 1:D:255:THR:O    | 1:D:257:LEU:N    | 2.51                     | 0.43              |
| 1:B:443:GLU:HG3  | 1:B:458:LYS:CG   | 2.48                     | 0.43              |
| 1:B:443:GLU:O    | 1:B:455:TYR:HA   | 2.18                     | 0.43              |
| 1:D:305:SER:OG   | 1:D:306:GLY:N    | 2.49                     | 0.43              |
| 1:C:305:SER:OG   | 1:C:306:GLY:N    | 2.50                     | 0.43              |
| 2:R:44:THR:OG1   | 2:R:47:GLU:HB2   | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:532:LEU:HA   | 1:E:532:LEU:HD23 | 1.85                     | 0.43              |
| 1:D:210:PHE:H    | 1:D:210:PHE:HD2  | 1.67                     | 0.43              |
| 1:B:508:ILE:HG22 | 1:B:509:PRO:HD2  | 2.00                     | 0.43              |
| 1:B:773:PHE:O    | 1:B:774:LYS:C    | 2.57                     | 0.43              |
| 1:E:773:PHE:O    | 1:E:774:LYS:C    | 2.57                     | 0.43              |
| 1:A:680:LYS:HG2  | 1:A:681:ASP:N    | 2.34                     | 0.43              |
| 1:F:773:PHE:O    | 1:F:775:LEU:N    | 2.51                     | 0.43              |
| 1:F:701:LEU:HD23 | 1:F:701:LEU:HA   | 1.80                     | 0.43              |
| 1:D:97:TYR:CE2   | 1:D:102:GLY:HA3  | 2.53                     | 0.43              |
| 2:S:105:LEU:HB2  | 2:S:125:ILE:HD11 | 2.01                     | 0.43              |
| 1:C:755:ARG:O    | 1:C:756:ILE:C    | 2.57                     | 0.43              |
| 1:A:657:ILE:HA   | 1:A:658:PRO:HD2  | 1.87                     | 0.43              |
| 1:A:610:MET:O    | 1:A:614:PHE:N    | 2.37                     | 0.43              |
| 1:D:550:SER:N    | 1:D:553:GLN:NE2  | 2.44                     | 0.43              |
| 2:S:12:PHE:CE1   | 2:S:72:MET:HG3   | 2.53                     | 0.43              |
| 2:T:32:LEU:HD21  | 2:T:71:MET:HE1   | 2.00                     | 0.43              |
| 2:T:70:THR:C     | 2:T:72:MET:N     | 2.72                     | 0.43              |
| 1:F:359:PRO:CB   | 1:F:405:LEU:HD21 | 2.48                     | 0.43              |
| 2:O:12:PHE:CE1   | 2:O:72:MET:HG3   | 2.54                     | 0.43              |
| 1:C:720:ILE:HA   | 1:C:720:ILE:HD12 | 1.87                     | 0.43              |
| 2:T:5:THR:O      | 2:T:8:GLN:N      | 2.51                     | 0.43              |
| 1:E:659:THR:O    | 1:E:660:SER:C    | 2.57                     | 0.43              |
| 1:A:75:THR:O     | 1:A:77:ASP:N     | 2.51                     | 0.43              |
| 1:D:343:VAL:HG12 | 1:D:344:ALA:O    | 2.17                     | 0.43              |
| 1:F:628:PHE:CD2  | 1:F:628:PHE:N    | 2.87                     | 0.43              |
| 1:C:350:VAL:HG12 | 1:C:352:GLY:H    | 1.84                     | 0.43              |
| 2:T:146:THR:O    | 2:T:148:LYS:N    | 2.52                     | 0.43              |
| 2:O:146:THR:O    | 2:O:148:LYS:N    | 2.51                     | 0.43              |
| 1:F:655:ASN:ND2  | 1:F:655:ASN:N    | 2.65                     | 0.43              |
| 1:D:508:ILE:HG22 | 1:D:509:PRO:HD2  | 2.01                     | 0.43              |
| 1:D:170:TYR:O    | 1:D:172:GLU:N    | 2.52                     | 0.43              |
| 1:B:238:GLN:C    | 1:B:240:ALA:N    | 2.72                     | 0.43              |
| 1:A:182:ILE:O    | 1:A:187:SER:OG   | 2.36                     | 0.43              |
| 1:D:295:VAL:HB   | 1:D:603:ILE:CG2  | 2.46                     | 0.43              |
| 1:F:755:ARG:O    | 1:F:756:ILE:C    | 2.57                     | 0.43              |
| 1:C:752:LEU:O    | 1:C:756:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:764:LEU:C    | 1:A:766:HIS:N    | 2.72                     | 0.43              |
| 1:A:581:GLN:HE21 | 1:A:629:ASN:N    | 2.17                     | 0.43              |
| 1:E:107:THR:CG2  | 1:E:115:LYS:HD2  | 2.47                     | 0.43              |
| 1:D:745:TYR:O    | 1:D:746:LYS:C    | 2.56                     | 0.43              |
| 1:C:405:LEU:CD1  | 1:C:405:LEU:N    | 2.82                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:279:ILE:HG22 | 1:E:283:LEU:HD11 | 2.01                     | 0.43              |
| 1:C:493:ASP:OD2  | 1:C:577:HIS:NE2  | 2.51                     | 0.43              |
| 2:T:92:PHE:C     | 2:T:94:LYS:N     | 2.71                     | 0.43              |
| 1:D:625:LEU:C    | 1:D:625:LEU:CD1  | 2.84                     | 0.43              |
| 1:A:500:SER:HA   | 1:A:624:TYR:CD2  | 2.54                     | 0.43              |
| 2:O:5:THR:O      | 2:O:6:GLU:C      | 2.57                     | 0.43              |
| 1:E:731:GLU:HA   | 1:E:734:ASN:HB2  | 2.01                     | 0.43              |
| 1:E:558:ASP:O    | 1:E:561:ASN:N    | 2.52                     | 0.43              |
| 1:F:223:LYS:HZ1  | 1:F:228:ASN:HB3  | 1.81                     | 0.43              |
| 1:A:71:PHE:CG    | 1:A:73:ASN:HB2   | 2.53                     | 0.43              |
| 2:P:146:THR:O    | 2:P:148:LYS:N    | 2.52                     | 0.43              |
| 1:F:209:LEU:HD23 | 1:F:260:TYR:CD2  | 2.54                     | 0.43              |
| 1:B:558:ASP:O    | 1:B:561:ASN:N    | 2.52                     | 0.43              |
| 1:A:773:PHE:O    | 1:A:774:LYS:C    | 2.57                     | 0.43              |
| 1:A:348:LEU:HD23 | 1:A:348:LEU:HA   | 1.82                     | 0.43              |
| 1:E:685:LYS:HA   | 1:E:685:LYS:HD3  | 1.86                     | 0.43              |
| 1:D:184:LYS:HZ1  | 1:D:191:GLU:CB   | 2.29                     | 0.42              |
| 1:F:184:LYS:HZ2  | 1:F:191:GLU:CB   | 2.27                     | 0.42              |
| 1:B:234:LEU:HG   | 1:B:235:THR:N    | 2.34                     | 0.42              |
| 1:A:173:ILE:HG23 | 1:A:174:GLY:H    | 1.84                     | 0.42              |
| 2:P:105:LEU:HB2  | 2:P:125:ILE:HD11 | 2.01                     | 0.42              |
| 2:S:124:MET:O    | 2:S:125:ILE:C    | 2.57                     | 0.42              |
| 1:C:495:PHE:C    | 1:C:495:PHE:CD1  | 2.93                     | 0.42              |
| 1:F:153:ILE:HG22 | 1:F:153:ILE:O    | 2.18                     | 0.42              |
| 1:D:115:LYS:C    | 1:D:117:LEU:N    | 2.71                     | 0.42              |
| 1:E:667:LEU:O    | 1:E:668:SER:C    | 2.56                     | 0.42              |
| 1:C:380:VAL:C    | 1:C:382:LYS:H    | 2.22                     | 0.42              |
| 1:B:719:LYS:O    | 1:B:721:SER:N    | 2.52                     | 0.42              |
| 1:C:318:ILE:O    | 1:C:319:ALA:C    | 2.56                     | 0.42              |
| 1:E:66:LEU:CD1   | 1:E:103:GLU:HA   | 2.48                     | 0.42              |
| 2:P:5:THR:O      | 2:P:6:GLU:C      | 2.57                     | 0.42              |
| 2:S:65:PHE:CD1   | 2:S:65:PHE:N     | 2.85                     | 0.42              |
| 1:C:515:LYS:HZ3  | 1:C:516:VAL:HG23 | 1.84                     | 0.42              |
| 1:D:558:ASP:O    | 1:D:561:ASN:N    | 2.52                     | 0.42              |
| 2:P:89:PHE:CD1   | 2:P:141:PHE:CD2  | 3.05                     | 0.42              |
| 2:O:145:MET:HB3  | 2:O:146:THR:H    | 1.63                     | 0.42              |
| 1:B:210:PHE:HD2  | 1:B:210:PHE:H    | 1.67                     | 0.42              |
| 1:A:508:ILE:HG22 | 1:A:509:PRO:HD2  | 2.00                     | 0.42              |
| 1:C:155:ASN:C    | 1:C:156:ILE:HG13 | 2.39                     | 0.42              |
| 1:E:680:LYS:HG2  | 1:E:681:ASP:N    | 2.34                     | 0.42              |
| 1:E:781:ASN:ND2  | 1:E:783:THR:OG1  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:701:LEU:HD23 | 1:E:701:LEU:HA   | 1.80                     | 0.42              |
| 1:D:771:ILE:HG12 | 1:D:771:ILE:H    | 1.57                     | 0.42              |
| 1:F:170:TYR:O    | 1:F:172:GLU:N    | 2.52                     | 0.42              |
| 1:F:191:GLU:C    | 1:F:193:LEU:N    | 2.71                     | 0.42              |
| 2:O:109:MET:HG3  | 2:O:116:LEU:CD1  | 2.49                     | 0.42              |
| 2:O:124:MET:O    | 2:O:125:ILE:C    | 2.57                     | 0.42              |
| 2:T:117:THR:HG23 | 2:T:120:GLU:CB   | 2.39                     | 0.42              |
| 1:A:597:ASN:HD21 | 1:A:601:GLU:HB2  | 1.80                     | 0.42              |
| 1:B:579:THR:C    | 1:B:581:GLN:H    | 2.22                     | 0.42              |
| 1:B:581:GLN:HE21 | 1:B:629:ASN:N    | 2.16                     | 0.42              |
| 1:E:718:ARG:HH11 | 1:E:767:GLN:NE2  | 2.16                     | 0.42              |
| 1:F:630:ARG:CZ   | 2:T:83:GLU:CG    | 2.96                     | 0.42              |
| 1:F:463:THR:HB   | 1:F:467:GLU:N    | 2.34                     | 0.42              |
| 1:B:136:PRO:HG2  | 1:B:139:SER:HG   | 1.84                     | 0.42              |
| 2:O:70:THR:C     | 2:O:72:MET:N     | 2.72                     | 0.42              |
| 1:F:373:LYS:CD   | 1:F:376:GLN:NE2  | 2.75                     | 0.42              |
| 2:S:94:LYS:CB    | 2:S:94:LYS:NZ    | 2.76                     | 0.42              |
| 2:Q:97:ASN:O     | 2:Q:99:TYR:CD1   | 2.72                     | 0.42              |
| 1:E:794:GLN:HE21 | 1:E:794:GLN:HB3  | 1.62                     | 0.42              |
| 2:O:73:ALA:O     | 2:O:75:LYS:N     | 2.51                     | 0.42              |
| 1:B:197:LYS:CD   | 1:B:197:LYS:O    | 2.66                     | 0.42              |
| 1:B:79:ILE:O     | 1:B:81:GLN:N     | 2.52                     | 0.42              |
| 1:A:75:THR:HB    | 1:A:76:LEU:H     | 1.65                     | 0.42              |
| 2:S:137:ASN:OD1  | 2:S:139:GLU:N    | 2.52                     | 0.42              |
| 1:A:628:PHE:N    | 1:A:628:PHE:CD2  | 2.87                     | 0.42              |
| 1:D:345:THR:HB   | 1:D:491:ASP:CB   | 2.47                     | 0.42              |
| 1:D:595:ILE:HD12 | 1:D:614:PHE:CE2  | 2.54                     | 0.42              |
| 1:E:773:PHE:O    | 1:E:775:LEU:N    | 2.52                     | 0.42              |
| 1:E:541:LYS:HB3  | 1:E:542:PRO:HD2  | 2.01                     | 0.42              |
| 1:F:438:ASN:HA   | 1:F:438:ASN:HD22 | 1.53                     | 0.42              |
| 1:E:177:ILE:HA   | 1:E:180:ASP:OD1  | 2.19                     | 0.42              |
| 1:F:130:SER:C    | 1:F:132:GLY:H    | 2.23                     | 0.42              |
| 2:O:105:LEU:HB2  | 2:O:125:ILE:HD11 | 2.01                     | 0.42              |
| 1:D:520:PRO:HG2  | 1:D:521:ASN:N    | 2.33                     | 0.42              |
| 1:C:763:LEU:HA   | 1:C:763:LEU:HD23 | 1.89                     | 0.42              |
| 1:C:767:GLN:O    | 1:C:767:GLN:HG2  | 2.19                     | 0.42              |
| 1:B:327:LEU:O    | 1:B:495:PHE:N    | 2.49                     | 0.42              |
| 1:A:495:PHE:CD1  | 1:A:495:PHE:C    | 2.92                     | 0.42              |
| 1:F:142:VAL:HG13 | 1:F:154:ILE:HD11 | 1.96                     | 0.42              |
| 1:F:665:LYS:O    | 1:F:668:SER:HB3  | 2.20                     | 0.42              |
| 1:A:359:PRO:HB2  | 1:A:405:LEU:HD21 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:359:PRO:HG2  | 1:F:360:VAL:N    | 2.32                     | 0.42              |
| 1:E:665:LYS:O    | 1:E:668:SER:HB3  | 2.19                     | 0.42              |
| 1:C:405:LEU:HD13 | 1:C:453:VAL:CG2  | 2.38                     | 0.42              |
| 2:R:92:PHE:C     | 2:R:94:LYS:N     | 2.71                     | 0.42              |
| 2:O:97:ASN:O     | 2:O:99:TYR:CD1   | 2.71                     | 0.42              |
| 1:E:305:SER:OG   | 1:E:306:GLY:N    | 2.51                     | 0.42              |
| 1:E:694:VAL:HG22 | 2:S:18:LEU:HD21  | 1.99                     | 0.42              |
| 1:B:197:LYS:NZ   | 1:B:264:MET:SD   | 2.88                     | 0.42              |
| 1:A:709:ASN:OD1  | 2:O:130:ILE:O    | 2.37                     | 0.42              |
| 1:A:611:THR:O    | 1:A:615:ILE:HG13 | 2.18                     | 0.42              |
| 1:C:773:PHE:O    | 1:C:774:LYS:C    | 2.57                     | 0.42              |
| 1:F:266:GLU:HA   | 1:F:269:ASN:HB3  | 2.00                     | 0.42              |
| 1:C:680:LYS:HG2  | 1:C:681:ASP:N    | 2.33                     | 0.42              |
| 1:F:473:ASN:OD1  | 1:F:473:ASN:N    | 2.53                     | 0.42              |
| 1:E:186:LYS:O    | 1:E:188:LEU:O    | 2.38                     | 0.42              |
| 1:E:97:TYR:CE2   | 1:E:102:GLY:HA3  | 2.54                     | 0.42              |
| 1:B:191:GLU:C    | 1:B:193:LEU:N    | 2.72                     | 0.42              |
| 1:C:697:ILE:C    | 1:C:699:GLY:H    | 2.22                     | 0.42              |
| 1:C:732:ILE:HG23 | 1:C:749:PHE:HD1  | 1.84                     | 0.42              |
| 1:D:413:LEU:HB2  | 1:D:419:ILE:HG12 | 2.01                     | 0.42              |
| 1:A:714:GLN:O    | 1:A:715:GLU:C    | 2.58                     | 0.42              |
| 1:A:755:ARG:O    | 1:A:756:ILE:C    | 2.57                     | 0.42              |
| 1:E:482:GLU:O    | 1:E:484:VAL:HG22 | 2.20                     | 0.42              |
| 1:D:714:GLN:O    | 1:D:715:GLU:C    | 2.58                     | 0.42              |
| 1:C:745:TYR:O    | 1:C:746:LYS:C    | 2.56                     | 0.42              |
| 1:C:462:ILE:CG1  | 1:C:463:THR:N    | 2.80                     | 0.42              |
| 2:R:16:PHE:CE1   | 2:R:27:ILE:HD13  | 2.54                     | 0.42              |
| 1:E:359:PRO:CB   | 1:E:405:LEU:HD21 | 2.49                     | 0.42              |
| 1:B:311:HIS:O    | 1:B:314:ALA:HB3  | 2.18                     | 0.42              |
| 1:A:311:HIS:O    | 1:A:314:ALA:HB3  | 2.19                     | 0.42              |
| 1:F:311:HIS:O    | 1:F:314:ALA:HB3  | 2.19                     | 0.42              |
| 1:D:493:ASP:OD2  | 1:D:577:HIS:NE2  | 2.52                     | 0.42              |
| 2:T:9:ILE:HD12   | 2:T:69:LEU:HD21  | 2.01                     | 0.42              |
| 1:C:455:TYR:O    | 1:C:471:TRP:HA   | 2.19                     | 0.42              |
| 1:A:255:THR:O    | 1:A:257:LEU:N    | 2.52                     | 0.42              |
| 1:A:380:VAL:C    | 1:A:382:LYS:H    | 2.23                     | 0.42              |
| 1:B:66:LEU:CD1   | 1:B:103:GLU:HA   | 2.49                     | 0.42              |
| 2:Q:44:THR:OG1   | 2:Q:47:GLU:HB2   | 2.19                     | 0.42              |
| 1:C:776:LEU:CD2  | 1:C:776:LEU:C    | 2.88                     | 0.42              |
| 1:D:691:LYS:O    | 1:D:693:SER:N    | 2.52                     | 0.42              |
| 1:E:686:ASP:CB   | 1:E:739:LYS:HD2  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:S:36:MET:HE2   | 2:S:43:PRO:HG3   | 2.01                     | 0.42              |
| 1:B:384:ASN:O    | 1:B:385:LEU:C    | 2.58                     | 0.42              |
| 1:C:192:PHE:HB3  | 1:C:196:ILE:CD1  | 2.49                     | 0.42              |
| 1:B:658:PRO:HG3  | 1:B:752:LEU:HD22 | 2.00                     | 0.42              |
| 1:B:715:GLU:OE1  | 1:B:767:GLN:NE2  | 2.52                     | 0.42              |
| 1:E:579:THR:C    | 1:E:581:GLN:H    | 2.22                     | 0.42              |
| 1:A:579:THR:C    | 1:A:581:GLN:H    | 2.22                     | 0.42              |
| 1:A:595:ILE:HD12 | 1:A:614:PHE:CE2  | 2.54                     | 0.42              |
| 1:C:136:PRO:HG2  | 1:C:139:SER:HG   | 1.85                     | 0.42              |
| 2:P:12:PHE:CE1   | 2:P:72:MET:HG3   | 2.55                     | 0.42              |
| 1:B:332:ASN:ND2  | 1:B:334:LEU:HD13 | 2.34                     | 0.42              |
| 1:C:794:GLN:O    | 1:C:797:ILE:CG1  | 2.64                     | 0.42              |
| 1:D:731:GLU:HA   | 1:D:734:ASN:HB2  | 2.02                     | 0.42              |
| 2:Q:13:LYS:N     | 2:Q:13:LYS:HD2   | 2.35                     | 0.42              |
| 1:F:75:THR:O     | 1:F:77:ASP:N     | 2.52                     | 0.42              |
| 2:T:137:ASN:OD1  | 2:T:139:GLU:N    | 2.53                     | 0.42              |
| 1:E:628:PHE:N    | 1:E:628:PHE:CD2  | 2.87                     | 0.42              |
| 1:B:350:VAL:HG12 | 1:B:352:GLY:H    | 1.85                     | 0.42              |
| 2:T:146:THR:O    | 2:T:147:ALA:C    | 2.56                     | 0.42              |
| 1:E:557:LEU:HD11 | 1:E:575:VAL:HG11 | 2.02                     | 0.42              |
| 1:D:456:LYS:HB3  | 1:D:470:ASN:C    | 2.39                     | 0.42              |
| 1:F:671:ARG:NH1  | 1:F:677:GLY:HA3  | 2.34                     | 0.42              |
| 1:F:685:LYS:HD3  | 1:F:685:LYS:HA   | 1.86                     | 0.42              |
| 1:D:83:GLN:C     | 1:D:85:LEU:N     | 2.72                     | 0.42              |
| 1:B:697:ILE:C    | 1:B:699:GLY:H    | 2.22                     | 0.42              |
| 1:F:296:LEU:O    | 1:F:301:ALA:HB2  | 2.19                     | 0.42              |
| 2:Q:105:LEU:HB2  | 2:Q:125:ILE:HD11 | 2.01                     | 0.42              |
| 1:F:767:GLN:HB3  | 1:F:768:LYS:H    | 1.61                     | 0.42              |
| 1:C:721:SER:C    | 1:C:723:PHE:N    | 2.70                     | 0.42              |
| 1:B:581:GLN:NE2  | 1:B:629:ASN:N    | 2.60                     | 0.42              |
| 1:E:752:LEU:O    | 1:E:756:ILE:HG12 | 2.20                     | 0.42              |
| 1:B:115:LYS:HB2  | 1:B:118:GLN:CG   | 2.49                     | 0.42              |
| 1:A:746:LYS:NZ   | 1:A:747:ASN:HD21 | 2.17                     | 0.42              |
| 1:C:665:LYS:O    | 1:C:668:SER:HB3  | 2.19                     | 0.42              |
| 1:B:745:TYR:O    | 1:B:746:LYS:C    | 2.57                     | 0.42              |
| 1:D:359:PRO:HB2  | 1:D:405:LEU:HD21 | 2.00                     | 0.42              |
| 1:A:281:GLU:O    | 1:A:285:LYS:HG2  | 2.20                     | 0.42              |
| 1:F:255:THR:C    | 1:F:257:LEU:N    | 2.72                     | 0.42              |
| 1:F:500:SER:HA   | 1:F:624:TYR:CD2  | 2.54                     | 0.42              |
| 1:A:731:GLU:HA   | 1:A:734:ASN:HB2  | 2.02                     | 0.42              |
| 1:D:776:LEU:C    | 1:D:776:LEU:CD2  | 2.88                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:776:LEU:C    | 1:F:776:LEU:CD2  | 2.88                     | 0.42              |
| 2:P:52:ILE:HG23  | 2:P:53:ASN:N     | 2.35                     | 0.42              |
| 2:S:65:PHE:HB2   | 2:S:66:PRO:CD    | 2.49                     | 0.42              |
| 1:A:79:ILE:O     | 1:A:81:GLN:N     | 2.53                     | 0.42              |
| 1:F:709:ASN:OD1  | 2:T:130:ILE:O    | 2.37                     | 0.42              |
| 1:A:223:LYS:HZ1  | 1:A:228:ASN:HB3  | 1.82                     | 0.42              |
| 1:C:595:ILE:HD12 | 1:C:614:PHE:CE2  | 2.55                     | 0.42              |
| 1:D:525:LYS:NZ   | 2:R:114:GLU:OE1  | 2.51                     | 0.42              |
| 1:C:307:LEU:H    | 1:C:307:LEU:CD1  | 2.33                     | 0.42              |
| 2:Q:146:THR:O    | 2:Q:148:LYS:N    | 2.52                     | 0.42              |
| 1:B:99:GLU:OE2   | 1:B:284:LYS:HD2  | 2.18                     | 0.42              |
| 1:B:620:THR:HG22 | 1:B:621:GLY:N    | 2.34                     | 0.42              |
| 1:B:680:LYS:HG2  | 1:B:681:ASP:N    | 2.34                     | 0.42              |
| 1:A:384:ASN:O    | 1:A:385:LEU:C    | 2.58                     | 0.42              |
| 1:D:181:ILE:O    | 1:D:186:LYS:HB3  | 2.20                     | 0.42              |
| 1:C:238:GLN:C    | 1:C:240:ALA:N    | 2.71                     | 0.42              |
| 1:A:83:GLN:C     | 1:A:85:LEU:N     | 2.72                     | 0.42              |
| 2:Q:121:VAL:O    | 2:Q:123:GLN:N    | 2.53                     | 0.42              |
| 2:S:101:SER:OG   | 2:S:104:GLU:HG2  | 2.19                     | 0.42              |
| 1:A:657:ILE:HG21 | 1:A:704:TYR:CE1  | 2.54                     | 0.42              |
| 1:E:714:GLN:O    | 1:E:715:GLU:C    | 2.58                     | 0.42              |
| 1:B:116:GLU:O    | 1:B:117:LEU:HD22 | 2.20                     | 0.42              |
| 1:E:788:ASP:C    | 1:E:792:VAL:HG23 | 2.37                     | 0.42              |
| 1:B:462:ILE:HG12 | 1:B:463:THR:H    | 1.81                     | 0.42              |
| 2:R:12:PHE:CE1   | 2:R:72:MET:HG3   | 2.54                     | 0.42              |
| 1:F:443:GLU:OE2  | 1:F:458:LYS:HG2  | 2.18                     | 0.42              |
| 1:D:324:THR:HB   | 1:D:499:PRO:CA   | 2.47                     | 0.42              |
| 1:C:693:SER:OG   | 1:C:731:GLU:OE1  | 2.36                     | 0.42              |
| 1:B:731:GLU:HA   | 1:B:734:ASN:HB2  | 2.01                     | 0.42              |
| 1:E:776:LEU:CD2  | 1:E:776:LEU:C    | 2.88                     | 0.42              |
| 1:B:776:LEU:CD2  | 1:B:776:LEU:C    | 2.88                     | 0.42              |
| 1:D:75:THR:O     | 1:D:77:ASP:N     | 2.53                     | 0.42              |
| 1:B:628:PHE:HE2  | 2:P:90:ARG:CD    | 2.28                     | 0.42              |
| 1:B:532:LEU:HD23 | 1:B:532:LEU:HA   | 1.86                     | 0.42              |
| 1:D:350:VAL:HG12 | 1:D:352:GLY:H    | 1.85                     | 0.42              |
| 1:A:307:LEU:CD1  | 1:A:307:LEU:H    | 2.33                     | 0.42              |
| 1:A:636:ALA:O    | 1:A:637:PRO:C    | 2.58                     | 0.42              |
| 2:P:42:ASN:HA    | 2:P:43:PRO:HD2   | 1.87                     | 0.42              |
| 1:F:773:PHE:O    | 1:F:774:LYS:C    | 2.57                     | 0.42              |
| 1:A:773:PHE:O    | 1:A:775:LEU:N    | 2.52                     | 0.42              |
| 2:Q:131:ASP:N    | 2:Q:131:ASP:OD1  | 2.46                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:88:LYS:HZ2   | 1:D:172:GLU:CD   | 2.23                     | 0.42              |
| 1:A:179:LEU:O    | 1:A:183:SER:N    | 2.53                     | 0.42              |
| 1:B:732:ILE:HG23 | 1:B:749:PHE:HD1  | 1.83                     | 0.42              |
| 2:R:124:MET:O    | 2:R:125:ILE:C    | 2.57                     | 0.42              |
| 2:P:104:GLU:O    | 2:P:105:LEU:C    | 2.58                     | 0.42              |
| 2:S:109:MET:HG3  | 2:S:116:LEU:CD1  | 2.49                     | 0.42              |
| 2:S:121:VAL:O    | 2:S:123:GLN:N    | 2.53                     | 0.42              |
| 2:O:104:GLU:O    | 2:O:105:LEU:C    | 2.58                     | 0.42              |
| 1:C:714:GLN:O    | 1:C:715:GLU:C    | 2.57                     | 0.42              |
| 1:E:520:PRO:HG2  | 1:E:521:ASN:N    | 2.33                     | 0.42              |
| 1:D:447:SER:CB   | 1:D:450:ASN:O    | 2.66                     | 0.42              |
| 1:E:405:LEU:HD13 | 1:E:453:VAL:CG2  | 2.40                     | 0.42              |
| 1:D:332:ASN:ND2  | 1:D:334:LEU:HD13 | 2.33                     | 0.42              |
| 1:E:441:VAL:O    | 1:E:442:TYR:CD2  | 2.72                     | 0.42              |
| 1:A:443:GLU:OE2  | 1:A:458:LYS:HG2  | 2.19                     | 0.42              |
| 1:F:305:SER:OG   | 1:F:306:GLY:N    | 2.50                     | 0.42              |
| 2:S:97:ASN:O     | 2:S:99:TYR:CD1   | 2.73                     | 0.42              |
| 2:T:65:PHE:HB2   | 2:T:66:PRO:CD    | 2.49                     | 0.42              |
| 1:A:197:LYS:NZ   | 1:A:264:MET:SD   | 2.92                     | 0.42              |
| 1:E:709:ASN:OD1  | 2:S:130:ILE:O    | 2.38                     | 0.42              |
| 1:A:210:PHE:H    | 1:A:210:PHE:HD2  | 1.67                     | 0.42              |
| 1:C:636:ALA:O    | 1:C:637:PRO:C    | 2.58                     | 0.42              |
| 1:F:456:LYS:HB3  | 1:F:470:ASN:C    | 2.40                     | 0.42              |
| 1:D:671:ARG:NH1  | 1:D:677:GLY:HA3  | 2.34                     | 0.42              |
| 1:D:173:ILE:HG23 | 1:D:174:GLY:H    | 1.84                     | 0.42              |
| 1:C:192:PHE:O    | 1:C:193:LEU:C    | 2.58                     | 0.42              |
| 1:B:177:ILE:HA   | 1:B:180:ASP:OD2  | 2.20                     | 0.42              |
| 1:B:192:PHE:HB3  | 1:B:196:ILE:CD1  | 2.50                     | 0.42              |
| 1:A:184:LYS:HZ1  | 1:A:191:GLU:CB   | 2.32                     | 0.42              |
| 1:E:295:VAL:HB   | 1:E:603:ILE:CG2  | 2.49                     | 0.42              |
| 2:Q:124:MET:O    | 2:Q:125:ILE:C    | 2.57                     | 0.42              |
| 1:A:413:LEU:HB2  | 1:A:419:ILE:HG12 | 2.02                     | 0.42              |
| 1:E:495:PHE:CD1  | 1:E:495:PHE:C    | 2.92                     | 0.42              |
| 1:E:581:GLN:NE2  | 1:E:629:ASN:N    | 2.62                     | 0.42              |
| 1:F:579:THR:C    | 1:F:581:GLN:H    | 2.22                     | 0.42              |
| 1:D:495:PHE:C    | 1:D:495:PHE:CD1  | 2.93                     | 0.42              |
| 1:C:667:LEU:O    | 1:C:668:SER:C    | 2.58                     | 0.42              |
| 1:D:446:ILE:HG13 | 1:D:452:GLU:O    | 2.19                     | 0.42              |
| 1:E:447:SER:CB   | 1:E:450:ASN:O    | 2.67                     | 0.42              |
| 1:D:279:ILE:HG22 | 1:D:283:LEU:HD11 | 2.02                     | 0.42              |
| 1:C:278:LYS:O    | 1:C:279:ILE:C    | 2.58                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:279:ILE:HG22 | 1:C:283:LEU:HD11 | 2.01                     | 0.42              |
| 1:B:217:LYS:HB2  | 1:B:236:GLU:HG3  | 2.02                     | 0.42              |
| 2:S:9:ILE:HD12   | 2:S:69:LEU:HD21  | 2.02                     | 0.42              |
| 2:P:9:ILE:HD12   | 2:P:69:LEU:HD21  | 2.02                     | 0.42              |
| 1:D:255:THR:C    | 1:D:257:LEU:N    | 2.72                     | 0.42              |
| 1:B:380:VAL:C    | 1:B:382:LYS:H    | 2.23                     | 0.42              |
| 1:A:250:ALA:O    | 1:A:252:ASP:N    | 2.53                     | 0.42              |
| 1:C:731:GLU:HA   | 1:C:734:ASN:HB2  | 2.02                     | 0.42              |
| 2:R:52:ILE:HG23  | 2:R:53:ASN:N     | 2.35                     | 0.42              |
| 1:E:691:LYS:O    | 1:E:692:GLU:C    | 2.58                     | 0.42              |
| 1:A:776:LEU:C    | 1:A:776:LEU:CD2  | 2.88                     | 0.42              |
| 1:B:197:LYS:NZ   | 1:B:267:TYR:CD2  | 2.88                     | 0.42              |
| 1:B:628:PHE:CD2  | 1:B:628:PHE:N    | 2.86                     | 0.42              |
| 1:C:71:PHE:CD1   | 1:C:108:ASP:OD1  | 2.73                     | 0.42              |
| 1:B:583:ASN:ND2  | 1:B:587:PRO:HA   | 2.35                     | 0.42              |
| 1:F:384:ASN:O    | 1:F:385:LEU:C    | 2.58                     | 0.42              |
| 1:E:583:ASN:ND2  | 1:E:587:PRO:HA   | 2.35                     | 0.42              |
| 1:C:701:LEU:HD23 | 1:C:701:LEU:HA   | 1.81                     | 0.42              |
| 1:E:83:GLN:C     | 1:E:85:LEU:N     | 2.71                     | 0.42              |
| 1:C:188:LEU:H    | 1:C:188:LEU:HD22 | 1.65                     | 0.42              |
| 1:B:755:ARG:O    | 1:B:756:ILE:C    | 2.57                     | 0.42              |
| 1:D:581:GLN:HE21 | 1:D:629:ASN:N    | 2.16                     | 0.42              |
| 1:A:142:VAL:HG13 | 1:A:154:ILE:HD11 | 1.97                     | 0.42              |
| 1:E:113:GLU:HA   | 1:E:118:GLN:HB3  | 2.02                     | 0.42              |
| 1:B:359:PRO:HB2  | 1:B:405:LEU:HD21 | 2.02                     | 0.42              |
| 1:B:281:GLU:O    | 1:B:285:LYS:HG2  | 2.20                     | 0.42              |
| 1:D:136:PRO:O    | 1:D:138:ALA:N    | 2.53                     | 0.42              |
| 1:E:380:VAL:C    | 1:E:382:LYS:H    | 2.23                     | 0.42              |
| 1:E:443:GLU:CG   | 1:E:458:LYS:CG   | 2.95                     | 0.42              |
| 1:C:255:THR:O    | 1:C:257:LEU:N    | 2.52                     | 0.42              |
| 1:D:504:ILE:HD12 | 1:D:504:ILE:N    | 2.35                     | 0.42              |
| 1:A:443:GLU:HG3  | 1:A:458:LYS:CG   | 2.49                     | 0.42              |
| 2:T:97:ASN:O     | 2:T:99:TYR:CD1   | 2.72                     | 0.42              |
| 1:B:691:LYS:O    | 1:B:692:GLU:C    | 2.58                     | 0.42              |
| 1:D:197:LYS:NZ   | 1:D:267:TYR:CD2  | 2.88                     | 0.42              |
| 1:F:197:LYS:NZ   | 1:F:267:TYR:CD2  | 2.88                     | 0.42              |
| 1:E:79:ILE:O     | 1:E:81:GLN:N     | 2.53                     | 0.42              |
| 2:R:137:ASN:OD1  | 2:R:139:GLU:N    | 2.53                     | 0.42              |
| 1:F:71:PHE:CG    | 1:F:73:ASN:HB2   | 2.54                     | 0.42              |
| 1:B:307:LEU:CD1  | 1:B:307:LEU:H    | 2.32                     | 0.42              |
| 1:C:655:ASN:N    | 1:C:655:ASN:ND2  | 2.66                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:784:GLU:HG3  | 1:B:785:ASN:N    | 2.35                     | 0.42              |
| 1:E:298:GLY:C    | 1:E:300:LYS:H    | 2.22                     | 0.42              |
| 1:D:583:ASN:ND2  | 1:D:587:PRO:HA   | 2.35                     | 0.42              |
| 1:E:192:PHE:O    | 1:E:193:LEU:C    | 2.57                     | 0.41              |
| 1:D:192:PHE:O    | 1:D:193:LEU:C    | 2.59                     | 0.41              |
| 1:D:192:PHE:HB3  | 1:D:196:ILE:CD1  | 2.50                     | 0.41              |
| 1:B:186:LYS:O    | 1:B:188:LEU:O    | 2.38                     | 0.41              |
| 2:R:109:MET:HG3  | 2:R:116:LEU:CD1  | 2.50                     | 0.41              |
| 1:C:718:ARG:O    | 1:C:722:ILE:CG1  | 2.66                     | 0.41              |
| 1:B:752:LEU:O    | 1:B:756:ILE:HG12 | 2.20                     | 0.41              |
| 1:E:630:ARG:CZ   | 2:S:83:GLU:CG    | 2.98                     | 0.41              |
| 1:C:327:LEU:O    | 1:C:495:PHE:N    | 2.48                     | 0.41              |
| 1:A:715:GLU:OE1  | 1:A:767:GLN:NE2  | 2.53                     | 0.41              |
| 1:E:657:ILE:HG21 | 1:E:704:TYR:CE1  | 2.55                     | 0.41              |
| 1:E:281:GLU:O    | 1:E:285:LYS:HG2  | 2.19                     | 0.41              |
| 1:A:254:ARG:HD2  | 1:A:254:ARG:N    | 2.31                     | 0.41              |
| 1:C:691:LYS:O    | 1:C:693:SER:N    | 2.53                     | 0.41              |
| 1:E:233:ASN:HB3  | 1:E:236:GLU:HB2  | 2.02                     | 0.41              |
| 2:O:65:PHE:HB2   | 2:O:66:PRO:CD    | 2.50                     | 0.41              |
| 2:S:44:THR:OG1   | 2:S:47:GLU:HB2   | 2.21                     | 0.41              |
| 1:F:79:ILE:O     | 1:F:81:GLN:N     | 2.52                     | 0.41              |
| 1:E:512:GLU:O    | 1:E:516:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:672:ARG:HA   | 1:C:672:ARG:HD3  | 1.69                     | 0.41              |
| 2:S:89:PHE:CD1   | 2:S:141:PHE:CD2  | 3.06                     | 0.41              |
| 1:A:109:ILE:HG13 | 1:A:109:ILE:H    | 1.64                     | 0.41              |
| 1:A:781:ASN:O    | 1:A:789:ASN:ND2  | 2.53                     | 0.41              |
| 1:F:583:ASN:ND2  | 1:F:587:PRO:HA   | 2.34                     | 0.41              |
| 1:E:186:LYS:HZ1  | 1:E:234:LEU:HD13 | 1.84                     | 0.41              |
| 1:D:186:LYS:O    | 1:D:188:LEU:O    | 2.38                     | 0.41              |
| 1:F:178:SER:OG   | 1:F:179:LEU:CD2  | 2.68                     | 0.41              |
| 1:F:186:LYS:HA   | 1:F:190:PRO:CD   | 2.26                     | 0.41              |
| 1:F:189:ASP:O    | 1:F:191:GLU:N    | 2.52                     | 0.41              |
| 1:F:83:GLN:C     | 1:F:85:LEU:N     | 2.72                     | 0.41              |
| 2:P:109:MET:HG3  | 2:P:116:LEU:CD1  | 2.49                     | 0.41              |
| 1:C:410:ILE:C    | 1:C:412:GLU:H    | 2.24                     | 0.41              |
| 1:B:413:LEU:HB2  | 1:B:419:ILE:HG12 | 2.02                     | 0.41              |
| 1:E:581:GLN:HE21 | 1:E:629:ASN:N    | 2.18                     | 0.41              |
| 1:F:581:GLN:HE21 | 1:F:629:ASN:N    | 2.18                     | 0.41              |
| 1:A:665:LYS:O    | 1:A:668:SER:HB3  | 2.21                     | 0.41              |
| 1:B:665:LYS:HG3  | 2:P:11:GLU:CD    | 2.41                     | 0.41              |
| 1:F:746:LYS:NZ   | 1:F:747:ASN:HD21 | 2.17                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:27:ILE:HA    | 2:Q:31:GLU:OE2   | 2.20                     | 0.41              |
| 1:F:444:PHE:N    | 1:F:444:PHE:HD1  | 2.18                     | 0.41              |
| 1:E:450:ASN:ND2  | 1:E:452:GLU:CD   | 2.74                     | 0.41              |
| 2:R:27:ILE:HA    | 2:R:31:GLU:OE2   | 2.20                     | 0.41              |
| 1:F:450:ASN:ND2  | 1:F:452:GLU:CD   | 2.74                     | 0.41              |
| 1:E:359:PRO:HG2  | 1:E:360:VAL:N    | 2.32                     | 0.41              |
| 1:F:279:ILE:HG22 | 1:F:283:LEU:HD11 | 2.01                     | 0.41              |
| 1:F:136:PRO:HG2  | 1:F:139:SER:HG   | 1.86                     | 0.41              |
| 2:S:69:LEU:HD12  | 2:S:69:LEU:HA    | 1.84                     | 0.41              |
| 1:A:721:SER:C    | 1:A:723:PHE:N    | 2.70                     | 0.41              |
| 1:F:731:GLU:HA   | 1:F:734:ASN:HB2  | 2.02                     | 0.41              |
| 1:E:197:LYS:NZ   | 1:E:267:TYR:CD2  | 2.89                     | 0.41              |
| 1:C:109:ILE:HD13 | 1:C:157:LYS:HZ2  | 1.85                     | 0.41              |
| 2:R:101:SER:OG   | 2:R:104:GLU:HG2  | 2.20                     | 0.41              |
| 1:B:155:ASN:C    | 1:B:156:ILE:HG13 | 2.40                     | 0.41              |
| 2:R:55:VAL:HB    | 2:R:67:GLU:OE1   | 2.20                     | 0.41              |
| 1:E:438:ASN:HA   | 1:E:438:ASN:HD22 | 1.53                     | 0.41              |
| 1:D:473:ASN:N    | 1:D:473:ASN:OD1  | 2.53                     | 0.41              |
| 1:A:701:LEU:HD23 | 1:A:701:LEU:HA   | 1.79                     | 0.41              |
| 2:R:105:LEU:HB2  | 2:R:125:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:107:THR:CG2  | 1:A:115:LYS:HD2  | 2.50                     | 0.41              |
| 1:F:657:ILE:HA   | 1:F:658:PRO:HD2  | 1.87                     | 0.41              |
| 1:F:495:PHE:C    | 1:F:495:PHE:CD1  | 2.93                     | 0.41              |
| 1:B:746:LYS:NZ   | 1:B:747:ASN:HD21 | 2.17                     | 0.41              |
| 1:D:463:THR:HB   | 1:D:467:GLU:N    | 2.35                     | 0.41              |
| 1:B:450:ASN:ND2  | 1:B:452:GLU:CD   | 2.74                     | 0.41              |
| 1:E:665:LYS:HG3  | 2:S:11:GLU:CD    | 2.40                     | 0.41              |
| 1:B:278:LYS:O    | 1:B:279:ILE:C    | 2.59                     | 0.41              |
| 1:F:255:THR:O    | 1:F:257:LEU:N    | 2.52                     | 0.41              |
| 1:E:134:LYS:C    | 1:E:136:PRO:CD   | 2.85                     | 0.41              |
| 1:F:380:VAL:C    | 1:F:382:LYS:H    | 2.23                     | 0.41              |
| 1:C:794:GLN:HE21 | 1:C:794:GLN:HB3  | 1.62                     | 0.41              |
| 2:R:49:GLN:CA    | 2:R:52:ILE:HG22  | 2.48                     | 0.41              |
| 2:P:44:THR:OG1   | 2:P:47:GLU:HB2   | 2.21                     | 0.41              |
| 1:F:197:LYS:NZ   | 1:F:264:MET:SD   | 2.90                     | 0.41              |
| 1:E:75:THR:O     | 1:E:77:ASP:N     | 2.52                     | 0.41              |
| 1:B:75:THR:O     | 1:B:77:ASP:N     | 2.52                     | 0.41              |
| 2:Q:137:ASN:OD1  | 2:Q:139:GLU:N    | 2.53                     | 0.41              |
| 1:D:628:PHE:CD2  | 1:D:628:PHE:N    | 2.86                     | 0.41              |
| 1:A:684:ASP:C    | 1:A:686:ASP:H    | 2.24                     | 0.41              |
| 1:B:375:GLY:O    | 1:B:377:GLN:N    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:610:MET:O    | 1:F:614:PHE:N    | 2.38                     | 0.41              |
| 1:E:672:ARG:HA   | 1:E:672:ARG:HD3  | 1.68                     | 0.41              |
| 1:B:108:ASP:O    | 1:B:110:ASP:OD1  | 2.39                     | 0.41              |
| 1:C:684:ASP:C    | 1:C:686:ASP:H    | 2.23                     | 0.41              |
| 1:A:300:LYS:HE2  | 1:A:300:LYS:HB3  | 1.94                     | 0.41              |
| 1:C:384:ASN:O    | 1:C:385:LEU:C    | 2.58                     | 0.41              |
| 1:C:541:LYS:HB3  | 1:C:542:PRO:HD2  | 2.02                     | 0.41              |
| 1:D:177:ILE:HA   | 1:D:180:ASP:OD1  | 2.20                     | 0.41              |
| 1:D:213:LYS:HB2  | 1:D:240:ALA:CB   | 2.49                     | 0.41              |
| 1:C:213:LYS:CD   | 1:C:240:ALA:HB1  | 2.48                     | 0.41              |
| 1:A:97:TYR:CE1   | 1:A:178:SER:CB   | 3.03                     | 0.41              |
| 2:T:104:GLU:O    | 2:T:105:LEU:C    | 2.58                     | 0.41              |
| 1:F:718:ARG:HH11 | 1:F:767:GLN:NE2  | 2.17                     | 0.41              |
| 1:D:105:TYR:HB2  | 1:D:153:ILE:HA   | 2.02                     | 0.41              |
| 1:F:520:PRO:HG2  | 1:F:521:ASN:N    | 2.33                     | 0.41              |
| 1:F:113:GLU:HA   | 1:F:118:GLN:HB3  | 2.03                     | 0.41              |
| 1:D:755:ARG:O    | 1:D:756:ILE:C    | 2.58                     | 0.41              |
| 1:F:201:ASP:HB3  | 1:F:202:ASP:OD2  | 2.21                     | 0.41              |
| 1:E:201:ASP:HB3  | 1:E:202:ASP:OD2  | 2.21                     | 0.41              |
| 1:A:444:PHE:HD1  | 1:A:444:PHE:N    | 2.18                     | 0.41              |
| 1:D:446:ILE:HD11 | 1:D:451:ASN:HB2  | 2.01                     | 0.41              |
| 1:D:403:LEU:HG   | 1:D:405:LEU:CD1  | 2.51                     | 0.41              |
| 1:B:279:ILE:C    | 1:B:281:GLU:N    | 2.74                     | 0.41              |
| 2:P:94:LYS:CB    | 2:P:94:LYS:NZ    | 2.76                     | 0.41              |
| 1:B:318:ILE:H    | 1:B:318:ILE:CD1  | 2.28                     | 0.41              |
| 1:A:456:LYS:CB   | 1:A:470:ASN:C    | 2.89                     | 0.41              |
| 1:C:233:ASN:HB3  | 1:C:236:GLU:HB2  | 2.02                     | 0.41              |
| 1:D:233:ASN:HB3  | 1:D:236:GLU:HB2  | 2.02                     | 0.41              |
| 1:E:223:LYS:HZ1  | 1:E:228:ASN:HB3  | 1.83                     | 0.41              |
| 1:F:684:ASP:C    | 1:F:686:ASP:H    | 2.24                     | 0.41              |
| 1:D:109:ILE:H    | 1:D:109:ILE:HG13 | 1.64                     | 0.41              |
| 1:D:611:THR:O    | 1:D:615:ILE:HG13 | 2.21                     | 0.41              |
| 1:C:611:THR:HG22 | 1:C:615:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:155:ASN:C    | 1:A:156:ILE:HG13 | 2.41                     | 0.41              |
| 1:B:173:ILE:C    | 1:B:175:LYS:H    | 2.23                     | 0.41              |
| 1:C:413:LEU:HB2  | 1:C:419:ILE:HG12 | 2.01                     | 0.41              |
| 1:B:154:ILE:HG13 | 1:B:171:TYR:CD1  | 2.55                     | 0.41              |
| 1:D:746:LYS:NZ   | 1:D:747:ASN:HD21 | 2.17                     | 0.41              |
| 2:O:16:PHE:HA    | 2:O:35:VAL:HG11  | 2.02                     | 0.41              |
| 2:P:28:THR:N     | 2:P:31:GLU:OE2   | 2.49                     | 0.41              |
| 1:A:318:ILE:H    | 1:A:318:ILE:CD1  | 2.26                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:380:VAL:C    | 1:D:382:LYS:H    | 2.23                     | 0.41              |
| 2:P:13:LYS:N     | 2:P:13:LYS:HD2   | 2.36                     | 0.41              |
| 2:O:44:THR:OG1   | 2:O:47:GLU:HB2   | 2.20                     | 0.41              |
| 2:S:6:GLU:CG     | 2:S:7:GLU:N      | 2.80                     | 0.41              |
| 1:F:350:VAL:HG12 | 1:F:352:GLY:H    | 1.84                     | 0.41              |
| 1:A:350:VAL:HG12 | 1:A:352:GLY:H    | 1.85                     | 0.41              |
| 1:A:108:ASP:O    | 1:A:110:ASP:OD1  | 2.39                     | 0.41              |
| 1:E:350:VAL:HG12 | 1:E:352:GLY:H    | 1.85                     | 0.41              |
| 1:B:473:ASN:N    | 1:B:473:ASN:OD1  | 2.53                     | 0.41              |
| 1:E:130:SER:C    | 1:E:132:GLY:H    | 2.24                     | 0.41              |
| 1:D:173:ILE:HG23 | 1:D:174:GLY:N    | 2.35                     | 0.41              |
| 1:C:173:ILE:C    | 1:C:175:LYS:H    | 2.23                     | 0.41              |
| 1:B:173:ILE:HG23 | 1:B:174:GLY:H    | 1.85                     | 0.41              |
| 1:B:295:VAL:HB   | 1:B:603:ILE:CG2  | 2.51                     | 0.41              |
| 1:A:115:LYS:HB2  | 1:A:118:GLN:CG   | 2.50                     | 0.41              |
| 1:A:113:GLU:HA   | 1:A:118:GLN:HB3  | 2.02                     | 0.41              |
| 1:F:657:ILE:HG21 | 1:F:704:TYR:CE1  | 2.56                     | 0.41              |
| 1:F:752:LEU:O    | 1:F:756:ILE:HG12 | 2.21                     | 0.41              |
| 1:D:721:SER:O    | 1:D:722:ILE:C    | 2.59                     | 0.41              |
| 1:A:667:LEU:O    | 1:A:668:SER:C    | 2.58                     | 0.41              |
| 1:D:113:GLU:HA   | 1:D:118:GLN:HB3  | 2.02                     | 0.41              |
| 1:C:450:ASN:ND2  | 1:C:452:GLU:CD   | 2.74                     | 0.41              |
| 1:E:746:LYS:NZ   | 1:E:747:ASN:HD21 | 2.17                     | 0.41              |
| 1:E:359:PRO:HB2  | 1:E:405:LEU:HD21 | 2.02                     | 0.41              |
| 1:B:493:ASP:OD2  | 1:B:577:HIS:NE2  | 2.51                     | 0.41              |
| 2:P:97:ASN:O     | 2:P:99:TYR:CD1   | 2.73                     | 0.41              |
| 2:T:5:THR:O      | 2:T:6:GLU:C      | 2.57                     | 0.41              |
| 2:T:6:GLU:CG     | 2:T:7:GLU:N      | 2.80                     | 0.41              |
| 1:D:659:THR:O    | 1:D:660:SER:C    | 2.57                     | 0.41              |
| 1:C:611:THR:O    | 1:C:615:ILE:HG13 | 2.20                     | 0.41              |
| 1:F:307:LEU:CD1  | 1:F:307:LEU:H    | 2.33                     | 0.41              |
| 1:E:424:LYS:HE3  | 1:E:424:LYS:HB3  | 1.94                     | 0.41              |
| 1:D:384:ASN:O    | 1:D:385:LEU:C    | 2.58                     | 0.41              |
| 1:E:97:TYR:CE1   | 1:E:178:SER:CB   | 3.03                     | 0.41              |
| 1:F:97:TYR:CE1   | 1:F:178:SER:CB   | 3.03                     | 0.41              |
| 1:C:173:ILE:HG23 | 1:C:174:GLY:N    | 2.35                     | 0.41              |
| 1:B:97:TYR:CE1   | 1:B:178:SER:CB   | 3.03                     | 0.41              |
| 2:R:117:THR:HG23 | 2:R:120:GLU:CB   | 2.39                     | 0.41              |
| 1:C:520:PRO:HG2  | 1:C:521:ASN:N    | 2.33                     | 0.41              |
| 1:E:413:LEU:HB2  | 1:E:419:ILE:HG12 | 2.02                     | 0.41              |
| 1:B:657:ILE:HA   | 1:B:658:PRO:HD2  | 1.88                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:107:THR:CG2  | 1:F:115:LYS:HD2  | 2.50                     | 0.41              |
| 1:F:115:LYS:HB2  | 1:F:118:GLN:CG   | 2.49                     | 0.41              |
| 1:A:327:LEU:HG   | 1:A:595:ILE:HG23 | 2.03                     | 0.41              |
| 1:A:450:ASN:ND2  | 1:A:452:GLU:CD   | 2.74                     | 0.41              |
| 1:A:279:ILE:HG22 | 1:A:283:LEU:HD11 | 2.02                     | 0.41              |
| 1:F:493:ASP:OD2  | 1:F:577:HIS:NE2  | 2.51                     | 0.41              |
| 1:C:501:LEU:HA   | 1:C:501:LEU:HD23 | 1.89                     | 0.41              |
| 1:C:255:THR:C    | 1:C:257:LEU:N    | 2.72                     | 0.41              |
| 1:A:455:TYR:O    | 1:A:471:TRP:HA   | 2.21                     | 0.41              |
| 1:A:691:LYS:O    | 1:A:692:GLU:C    | 2.58                     | 0.41              |
| 2:Q:52:ILE:HG23  | 2:Q:53:ASN:N     | 2.35                     | 0.41              |
| 2:S:52:ILE:HG23  | 2:S:53:ASN:N     | 2.35                     | 0.41              |
| 1:A:197:LYS:NZ   | 1:A:267:TYR:CD2  | 2.88                     | 0.41              |
| 1:D:636:ALA:O    | 1:D:637:PRO:C    | 2.59                     | 0.41              |
| 1:B:595:ILE:HD12 | 1:B:614:PHE:CE2  | 2.56                     | 0.41              |
| 1:A:784:GLU:HG3  | 1:A:785:ASN:N    | 2.36                     | 0.41              |
| 1:E:384:ASN:O    | 1:E:385:LEU:C    | 2.59                     | 0.41              |
| 1:E:461:LYS:HA   | 1:E:461:LYS:HD2  | 1.82                     | 0.41              |
| 1:D:90:PRO:HD2   | 1:D:93:VAL:HG11  | 2.03                     | 0.41              |
| 1:A:186:LYS:HZ1  | 1:A:234:LEU:CD1  | 2.34                     | 0.41              |
| 2:Q:109:MET:HG3  | 2:Q:116:LEU:CD1  | 2.51                     | 0.41              |
| 2:T:124:MET:O    | 2:T:125:ILE:C    | 2.57                     | 0.41              |
| 1:D:410:ILE:C    | 1:D:412:GLU:H    | 2.24                     | 0.41              |
| 1:B:667:LEU:O    | 1:B:668:SER:C    | 2.58                     | 0.41              |
| 1:E:446:ILE:HD11 | 1:E:451:ASN:HB2  | 2.02                     | 0.41              |
| 1:C:403:LEU:HG   | 1:C:405:LEU:CD1  | 2.51                     | 0.41              |
| 1:E:444:PHE:N    | 1:E:444:PHE:HD1  | 2.18                     | 0.41              |
| 1:C:368:GLN:C    | 1:C:370:LEU:H    | 2.22                     | 0.41              |
| 1:A:305:SER:OG   | 1:A:306:GLY:N    | 2.52                     | 0.41              |
| 2:T:44:THR:OG1   | 2:T:47:GLU:HB2   | 2.20                     | 0.41              |
| 1:B:512:GLU:O    | 1:B:516:VAL:HG23 | 2.20                     | 0.41              |
| 1:D:561:ASN:C    | 1:D:563:ALA:N    | 2.73                     | 0.41              |
| 1:E:109:ILE:HG13 | 1:E:109:ILE:H    | 1.64                     | 0.41              |
| 1:E:611:THR:HG22 | 1:E:615:ILE:CD1  | 2.50                     | 0.41              |
| 1:D:620:THR:HG22 | 1:D:621:GLY:N    | 2.36                     | 0.41              |
| 1:E:620:THR:HG22 | 1:E:621:GLY:N    | 2.36                     | 0.41              |
| 1:E:671:ARG:NH1  | 1:E:677:GLY:HA3  | 2.35                     | 0.41              |
| 1:F:108:ASP:O    | 1:F:110:ASP:OD1  | 2.39                     | 0.41              |
| 1:A:685:LYS:HA   | 1:A:685:LYS:HD3  | 1.85                     | 0.41              |
| 1:E:473:ASN:OD1  | 1:E:473:ASN:N    | 2.54                     | 0.41              |
| 1:E:173:ILE:HG13 | 1:E:242:SER:CB   | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:184:LYS:HZ1  | 1:E:193:LEU:HD12 | 1.79                     | 0.41              |
| 1:C:170:TYR:O    | 1:C:172:GLU:N    | 2.53                     | 0.41              |
| 1:C:186:LYS:HZ1  | 1:C:234:LEU:HD13 | 1.86                     | 0.41              |
| 1:B:199:LEU:CD2  | 1:B:225:ILE:O    | 2.68                     | 0.41              |
| 1:B:192:PHE:O    | 1:B:193:LEU:C    | 2.59                     | 0.41              |
| 1:A:292:ARG:NE   | 1:A:617:LYS:HE3  | 2.36                     | 0.41              |
| 2:Q:101:SER:OG   | 2:Q:104:GLU:HG2  | 2.20                     | 0.41              |
| 2:S:104:GLU:O    | 2:S:105:LEU:C    | 2.58                     | 0.41              |
| 1:C:481:VAL:O    | 1:C:484:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:768:LYS:HA   | 1:B:768:LYS:HD3  | 1.86                     | 0.41              |
| 1:F:410:ILE:C    | 1:F:412:GLU:H    | 2.24                     | 0.41              |
| 1:E:755:ARG:O    | 1:E:756:ILE:C    | 2.59                     | 0.41              |
| 1:E:657:ILE:HA   | 1:E:658:PRO:HD2  | 1.88                     | 0.41              |
| 1:E:481:VAL:O    | 1:E:484:VAL:HG23 | 2.21                     | 0.41              |
| 1:F:481:VAL:O    | 1:F:484:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:229:PHE:CD1  | 1:C:229:PHE:O    | 2.74                     | 0.41              |
| 1:B:665:LYS:O    | 1:B:668:SER:HB3  | 2.21                     | 0.41              |
| 1:E:463:THR:HB   | 1:E:467:GLU:N    | 2.36                     | 0.41              |
| 1:D:450:ASN:ND2  | 1:D:452:GLU:CD   | 2.74                     | 0.41              |
| 1:A:724:ARG:CG   | 1:A:724:ARG:NH1  | 2.78                     | 0.41              |
| 1:D:279:ILE:C    | 1:D:281:GLU:N    | 2.74                     | 0.41              |
| 1:E:724:ARG:CG   | 1:E:724:ARG:NH1  | 2.78                     | 0.41              |
| 1:F:370:LEU:HA   | 1:F:370:LEU:HD23 | 1.92                     | 0.41              |
| 1:D:250:ALA:C    | 1:D:252:ASP:H    | 2.24                     | 0.41              |
| 1:F:323:ASN:ND2  | 1:F:624:TYR:OH   | 2.37                     | 0.41              |
| 1:A:443:GLU:CG   | 1:A:458:LYS:CG   | 2.95                     | 0.41              |
| 1:D:368:GLN:C    | 1:D:370:LEU:H    | 2.22                     | 0.41              |
| 1:D:794:GLN:O    | 1:D:797:ILE:CG1  | 2.64                     | 0.41              |
| 1:D:794:GLN:HB3  | 1:D:794:GLN:HE21 | 1.62                     | 0.41              |
| 1:C:66:LEU:CD1   | 1:C:103:GLU:HA   | 2.49                     | 0.41              |
| 2:T:52:ILE:HG23  | 2:T:53:ASN:N     | 2.35                     | 0.41              |
| 1:D:691:LYS:O    | 1:D:692:GLU:C    | 2.59                     | 0.41              |
| 1:B:694:VAL:HG22 | 2:P:18:LEU:HD21  | 2.02                     | 0.41              |
| 1:F:288:VAL:C    | 1:F:290:LYS:N    | 2.74                     | 0.41              |
| 1:C:79:ILE:O     | 1:C:81:GLN:N     | 2.54                     | 0.41              |
| 1:B:684:ASP:C    | 1:B:686:ASP:H    | 2.23                     | 0.41              |
| 2:O:137:ASN:OD1  | 2:O:139:GLU:N    | 2.54                     | 0.41              |
| 1:A:345:THR:HB   | 1:A:491:ASP:CB   | 2.46                     | 0.41              |
| 1:F:375:GLY:O    | 1:F:377:GLN:N    | 2.54                     | 0.41              |
| 1:E:561:ASN:O    | 1:E:562:GLU:C    | 2.59                     | 0.41              |
| 1:B:71:PHE:HD1   | 1:B:108:ASP:OD1  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:89:PHE:HB2   | 2:Q:141:PHE:CD2  | 2.56                     | 0.41              |
| 1:C:108:ASP:O    | 1:C:110:ASP:OD1  | 2.39                     | 0.41              |
| 2:T:89:PHE:HB2   | 2:T:141:PHE:CD2  | 2.56                     | 0.41              |
| 1:D:611:THR:HG22 | 1:D:615:ILE:CD1  | 2.51                     | 0.41              |
| 1:E:593:ILE:C    | 1:E:604:LEU:HD12 | 2.41                     | 0.41              |
| 1:F:636:ALA:O    | 1:F:637:PRO:C    | 2.59                     | 0.41              |
| 1:C:313:ASP:O    | 1:C:316:LYS:CB   | 2.69                     | 0.41              |
| 1:D:612:GLY:O    | 1:D:616:GLU:HG3  | 2.20                     | 0.41              |
| 1:C:561:ASN:O    | 1:C:562:GLU:C    | 2.59                     | 0.41              |
| 1:C:661:ALA:HB2  | 2:Q:38:SER:O     | 2.21                     | 0.41              |
| 1:B:541:LYS:HB3  | 1:B:542:PRO:HD2  | 2.02                     | 0.41              |
| 1:C:473:ASN:OD1  | 1:C:473:ASN:N    | 2.53                     | 0.41              |
| 1:D:461:LYS:HA   | 1:D:461:LYS:HD2  | 1.82                     | 0.41              |
| 1:D:770:ASN:HA   | 1:D:770:ASN:HD22 | 1.70                     | 0.41              |
| 1:C:438:ASN:HD22 | 1:C:438:ASN:HA   | 1.53                     | 0.41              |
| 1:D:97:TYR:CE1   | 1:D:178:SER:CB   | 3.04                     | 0.41              |
| 1:B:173:ILE:HG13 | 1:B:242:SER:CB   | 2.37                     | 0.41              |
| 1:A:189:ASP:O    | 1:A:191:GLU:HG2  | 2.21                     | 0.41              |
| 1:B:292:ARG:NE   | 1:B:617:LYS:HE3  | 2.36                     | 0.41              |
| 2:T:3:GLN:N      | 2:T:77:LYS:CE    | 2.63                     | 0.41              |
| 1:A:520:PRO:HG2  | 1:A:521:ASN:N    | 2.33                     | 0.41              |
| 1:A:752:LEU:O    | 1:A:756:ILE:HG12 | 2.20                     | 0.41              |
| 1:C:746:LYS:NZ   | 1:C:747:ASN:HD21 | 2.18                     | 0.41              |
| 1:F:667:LEU:O    | 1:F:668:SER:C    | 2.58                     | 0.41              |
| 1:A:403:LEU:HG   | 1:A:405:LEU:CD1  | 2.51                     | 0.41              |
| 1:A:136:PRO:O    | 1:A:138:ALA:N    | 2.54                     | 0.41              |
| 1:C:463:THR:HB   | 1:C:467:GLU:N    | 2.35                     | 0.41              |
| 1:F:359:PRO:HB2  | 1:F:405:LEU:HD21 | 2.02                     | 0.41              |
| 1:C:447:SER:CB   | 1:C:450:ASN:O    | 2.69                     | 0.41              |
| 1:D:359:PRO:HG2  | 1:D:360:VAL:N    | 2.30                     | 0.41              |
| 1:D:444:PHE:N    | 1:D:444:PHE:HD1  | 2.19                     | 0.41              |
| 1:F:724:ARG:CG   | 1:F:724:ARG:NH1  | 2.78                     | 0.41              |
| 1:A:279:ILE:C    | 1:A:281:GLU:N    | 2.74                     | 0.41              |
| 1:C:281:GLU:O    | 1:C:285:LYS:HG2  | 2.21                     | 0.41              |
| 1:F:278:LYS:O    | 1:F:279:ILE:C    | 2.59                     | 0.41              |
| 1:D:250:ALA:O    | 1:D:252:ASP:N    | 2.53                     | 0.41              |
| 1:B:254:ARG:HD2  | 1:B:254:ARG:N    | 2.31                     | 0.41              |
| 1:A:66:LEU:HD12  | 1:A:104:ILE:N    | 2.36                     | 0.41              |
| 1:A:255:THR:C    | 1:A:257:LEU:N    | 2.72                     | 0.41              |
| 1:E:721:SER:C    | 1:E:723:PHE:N    | 2.71                     | 0.41              |
| 1:C:324:THR:HB   | 1:C:499:PRO:CA   | 2.45                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:66:LEU:HD12  | 1:C:104:ILE:N    | 2.36                     | 0.41              |
| 2:Q:6:GLU:CG     | 2:Q:7:GLU:N      | 2.81                     | 0.41              |
| 2:S:13:LYS:HD2   | 2:S:13:LYS:N     | 2.36                     | 0.41              |
| 1:A:512:GLU:O    | 1:A:516:VAL:HG23 | 2.21                     | 0.41              |
| 1:E:375:GLY:O    | 1:E:377:GLN:N    | 2.54                     | 0.41              |
| 1:D:684:ASP:C    | 1:D:686:ASP:H    | 2.23                     | 0.41              |
| 1:E:684:ASP:C    | 1:E:686:ASP:H    | 2.24                     | 0.41              |
| 2:S:36:MET:O     | 2:S:39:LEU:N     | 2.53                     | 0.41              |
| 1:C:671:ARG:NH1  | 1:C:677:GLY:HA3  | 2.36                     | 0.41              |
| 1:C:231:LYS:O    | 1:C:232:GLU:C    | 2.57                     | 0.41              |
| 1:F:119:ASP:HB3  | 1:F:120:LEU:H    | 1.75                     | 0.41              |
| 1:F:173:ILE:HG23 | 1:F:174:GLY:H    | 1.85                     | 0.40              |
| 1:C:89:ILE:HG22  | 1:C:93:VAL:CG1   | 2.10                     | 0.40              |
| 1:A:238:GLN:C    | 1:A:240:ALA:H    | 2.24                     | 0.40              |
| 1:A:697:ILE:C    | 1:A:699:GLY:H    | 2.23                     | 0.40              |
| 1:F:697:ILE:C    | 1:F:699:GLY:H    | 2.23                     | 0.40              |
| 2:O:101:SER:OG   | 2:O:104:GLU:HG2  | 2.21                     | 0.40              |
| 1:E:105:TYR:HB2  | 1:E:153:ILE:HA   | 2.02                     | 0.40              |
| 1:C:581:GLN:HE21 | 1:C:629:ASN:N    | 2.17                     | 0.40              |
| 1:D:718:ARG:O    | 1:D:722:ILE:CG1  | 2.67                     | 0.40              |
| 1:A:462:ILE:CG1  | 1:A:463:THR:N    | 2.80                     | 0.40              |
| 2:T:16:PHE:HA    | 2:T:35:VAL:HG11  | 2.03                     | 0.40              |
| 1:D:201:ASP:HB3  | 1:D:202:ASP:OD2  | 2.21                     | 0.40              |
| 1:F:403:LEU:HG   | 1:F:405:LEU:CD1  | 2.51                     | 0.40              |
| 1:C:444:PHE:HD1  | 1:C:444:PHE:N    | 2.18                     | 0.40              |
| 1:F:446:ILE:HD11 | 1:F:451:ASN:HB2  | 2.01                     | 0.40              |
| 1:E:403:LEU:HG   | 1:E:405:LEU:CD1  | 2.51                     | 0.40              |
| 2:R:30:LYS:CD    | 2:R:30:LYS:H     | 2.19                     | 0.40              |
| 1:B:279:ILE:HG22 | 1:B:283:LEU:HD11 | 2.03                     | 0.40              |
| 1:E:279:ILE:C    | 1:E:281:GLU:N    | 2.74                     | 0.40              |
| 1:A:233:ASN:HB3  | 1:A:236:GLU:HB2  | 2.02                     | 0.40              |
| 1:E:504:ILE:HD12 | 1:E:504:ILE:N    | 2.36                     | 0.40              |
| 1:F:233:ASN:HB3  | 1:F:236:GLU:HB2  | 2.02                     | 0.40              |
| 2:T:13:LYS:C     | 2:T:15:ALA:N     | 2.74                     | 0.40              |
| 1:C:75:THR:O     | 1:C:77:ASP:N     | 2.53                     | 0.40              |
| 1:D:79:ILE:O     | 1:D:81:GLN:N     | 2.53                     | 0.40              |
| 1:E:427:ASP:O    | 1:E:428:ASN:CB   | 2.68                     | 0.40              |
| 1:C:628:PHE:N    | 1:C:628:PHE:CD2  | 2.88                     | 0.40              |
| 1:A:375:GLY:O    | 1:A:377:GLN:N    | 2.54                     | 0.40              |
| 1:A:611:THR:HG22 | 1:A:615:ILE:CD1  | 2.52                     | 0.40              |
| 1:F:611:THR:O    | 1:F:615:ILE:HG13 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:307:LEU:CD1  | 1:D:307:LEU:H    | 2.33                     | 0.40              |
| 2:Q:42:ASN:HA    | 2:Q:43:PRO:HD2   | 1.87                     | 0.40              |
| 1:F:456:LYS:HB2  | 1:F:470:ASN:HA   | 2.03                     | 0.40              |
| 1:D:356:ASP:O    | 1:D:357:TRP:HB3  | 2.21                     | 0.40              |
| 1:D:159:TYR:O    | 1:D:160:ALA:HB2  | 2.21                     | 0.40              |
| 1:A:661:ALA:HB2  | 2:O:38:SER:O     | 2.21                     | 0.40              |
| 1:F:182:ILE:O    | 1:F:187:SER:OG   | 2.39                     | 0.40              |
| 1:A:100:LEU:HD22 | 1:A:182:ILE:HG21 | 2.04                     | 0.40              |
| 1:A:201:ASP:HB3  | 1:A:202:ASP:OD2  | 2.21                     | 0.40              |
| 1:C:292:ARG:NE   | 1:C:617:LYS:HE3  | 2.36                     | 0.40              |
| 2:Q:104:GLU:O    | 2:Q:105:LEU:C    | 2.59                     | 0.40              |
| 1:C:579:THR:C    | 1:C:581:GLN:N    | 2.75                     | 0.40              |
| 1:A:481:VAL:O    | 1:A:484:VAL:HG23 | 2.22                     | 0.40              |
| 1:A:136:PRO:O    | 1:A:139:SER:N    | 2.37                     | 0.40              |
| 2:O:27:ILE:HA    | 2:O:31:GLU:OE2   | 2.21                     | 0.40              |
| 2:P:16:PHE:HA    | 2:P:35:VAL:HG11  | 2.01                     | 0.40              |
| 1:D:281:GLU:O    | 1:D:285:LYS:HG2  | 2.20                     | 0.40              |
| 1:A:278:LYS:O    | 1:A:279:ILE:C    | 2.58                     | 0.40              |
| 1:F:281:GLU:O    | 1:F:285:LYS:HG2  | 2.21                     | 0.40              |
| 1:F:254:ARG:CD   | 1:F:254:ARG:H    | 2.30                     | 0.40              |
| 1:B:443:GLU:CG   | 1:B:458:LYS:CG   | 2.94                     | 0.40              |
| 1:D:197:LYS:CD   | 1:D:197:LYS:O    | 2.66                     | 0.40              |
| 1:E:75:THR:HB    | 1:E:76:LEU:H     | 1.66                     | 0.40              |
| 1:C:288:VAL:C    | 1:C:290:LYS:N    | 2.75                     | 0.40              |
| 2:P:140:GLU:O    | 2:P:143:GLN:HB2  | 2.21                     | 0.40              |
| 1:E:307:LEU:H    | 1:E:307:LEU:CD1  | 2.34                     | 0.40              |
| 1:F:313:ASP:O    | 1:F:316:LYS:CB   | 2.70                     | 0.40              |
| 1:B:561:ASN:O    | 1:B:562:GLU:C    | 2.60                     | 0.40              |
| 1:B:159:TYR:N    | 1:B:159:TYR:CD1  | 2.89                     | 0.40              |
| 1:D:238:GLN:C    | 1:D:240:ALA:H    | 2.25                     | 0.40              |
| 1:C:175:LYS:HB2  | 1:C:175:LYS:HZ3  | 1.79                     | 0.40              |
| 1:B:184:LYS:HE3  | 1:B:191:GLU:HB2  | 2.02                     | 0.40              |
| 1:B:229:PHE:CD1  | 1:B:229:PHE:O    | 2.74                     | 0.40              |
| 1:A:173:ILE:C    | 1:A:175:LYS:H    | 2.25                     | 0.40              |
| 1:A:184:LYS:HZ2  | 1:A:191:GLU:HB2  | 1.82                     | 0.40              |
| 1:C:297:LYS:NZ   | 1:C:601:GLU:HB3  | 2.24                     | 0.40              |
| 1:C:721:SER:O    | 1:C:722:ILE:C    | 2.60                     | 0.40              |
| 1:D:104:ILE:HG23 | 1:D:152:LEU:HB3  | 2.04                     | 0.40              |
| 1:E:657:ILE:O    | 1:E:658:PRO:C    | 2.59                     | 0.40              |
| 1:A:105:TYR:HB2  | 1:A:153:ILE:HA   | 2.03                     | 0.40              |
| 1:B:105:TYR:HB2  | 1:B:153:ILE:HA   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:789:ASN:O    | 1:C:792:VAL:HB   | 2.21                     | 0.40              |
| 2:R:16:PHE:HA    | 2:R:35:VAL:HG11  | 2.04                     | 0.40              |
| 1:C:279:ILE:C    | 1:C:281:GLU:N    | 2.74                     | 0.40              |
| 1:E:332:ASN:ND2  | 1:E:334:LEU:HD13 | 2.34                     | 0.40              |
| 1:C:443:GLU:CG   | 1:C:458:LYS:CG   | 2.95                     | 0.40              |
| 1:C:250:ALA:C    | 1:C:252:ASP:H    | 2.25                     | 0.40              |
| 1:F:66:LEU:HD12  | 1:F:104:ILE:N    | 2.37                     | 0.40              |
| 1:B:304:ALA:O    | 1:B:305:SER:C    | 2.60                     | 0.40              |
| 2:R:13:LYS:HD2   | 2:R:13:LYS:N     | 2.36                     | 0.40              |
| 2:Q:13:LYS:HZ3   | 2:Q:65:PHE:CB    | 2.33                     | 0.40              |
| 1:C:375:GLY:O    | 1:C:377:GLN:N    | 2.55                     | 0.40              |
| 1:D:375:GLY:O    | 1:D:377:GLN:N    | 2.54                     | 0.40              |
| 1:E:210:PHE:CD1  | 1:E:214:PHE:HD1  | 2.39                     | 0.40              |
| 1:C:557:LEU:HD11 | 1:C:575:VAL:HG12 | 2.03                     | 0.40              |
| 1:D:241:PHE:HA   | 1:D:264:MET:HE1  | 2.03                     | 0.40              |
| 1:E:612:GLY:O    | 1:E:616:GLU:HG3  | 2.21                     | 0.40              |
| 1:B:781:ASN:O    | 1:B:789:ASN:ND2  | 2.54                     | 0.40              |
| 1:F:541:LYS:HB3  | 1:F:542:PRO:HD2  | 2.03                     | 0.40              |
| 1:E:238:GLN:C    | 1:E:240:ALA:H    | 2.24                     | 0.40              |
| 1:F:173:ILE:C    | 1:F:175:LYS:H    | 2.24                     | 0.40              |
| 1:D:292:ARG:NE   | 1:D:617:LYS:HE3  | 2.37                     | 0.40              |
| 2:T:109:MET:HG3  | 2:T:116:LEU:CD1  | 2.50                     | 0.40              |
| 1:A:410:ILE:C    | 1:A:412:GLU:H    | 2.24                     | 0.40              |
| 1:F:714:GLN:O    | 1:F:715:GLU:C    | 2.58                     | 0.40              |
| 1:C:718:ARG:HH11 | 1:C:767:GLN:NE2  | 2.19                     | 0.40              |
| 1:C:113:GLU:HA   | 1:C:118:GLN:HB3  | 2.03                     | 0.40              |
| 1:D:229:PHE:O    | 1:D:229:PHE:CD1  | 2.74                     | 0.40              |
| 1:A:135:VAL:N    | 1:A:136:PRO:HD3  | 2.36                     | 0.40              |
| 2:O:71:MET:HG2   | 2:O:71:MET:O     | 2.22                     | 0.40              |
| 1:F:250:ALA:C    | 1:F:252:ASP:H    | 2.24                     | 0.40              |
| 1:E:373:LYS:CD   | 1:E:376:GLN:NE2  | 2.76                     | 0.40              |
| 1:F:318:ILE:CD1  | 1:F:318:ILE:H    | 2.28                     | 0.40              |
| 1:E:66:LEU:HD12  | 1:E:104:ILE:N    | 2.37                     | 0.40              |
| 1:E:561:ASN:C    | 1:E:563:ALA:N    | 2.73                     | 0.40              |
| 1:D:611:THR:HG22 | 1:D:615:ILE:HD12 | 2.04                     | 0.40              |
| 2:T:145:MET:HB3  | 2:T:146:THR:H    | 1.63                     | 0.40              |
| 1:B:611:THR:HG22 | 1:B:615:ILE:CD1  | 2.52                     | 0.40              |
| 1:A:639:ASN:HD22 | 1:A:639:ASN:C    | 2.25                     | 0.40              |
| 1:A:593:ILE:C    | 1:A:604:LEU:HD12 | 2.41                     | 0.40              |
| 1:B:313:ASP:O    | 1:B:316:LYS:CB   | 2.68                     | 0.40              |
| 1:D:313:ASP:O    | 1:D:316:LYS:CB   | 2.69                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:620:THR:HG22 | 1:A:621:GLY:N    | 2.36                     | 0.40              |
| 1:C:583:ASN:ND2  | 1:C:587:PRO:HA   | 2.37                     | 0.40              |
| 1:D:108:ASP:O    | 1:D:110:ASP:OD1  | 2.39                     | 0.40              |
| 2:S:55:VAL:HB    | 2:S:67:GLU:OE1   | 2.21                     | 0.40              |
| 1:A:770:ASN:HA   | 1:A:770:ASN:HD22 | 1.70                     | 0.40              |
| 1:A:159:TYR:CD1  | 1:A:159:TYR:N    | 2.89                     | 0.40              |
| 1:C:348:LEU:HA   | 1:C:348:LEU:HD23 | 1.82                     | 0.40              |
| 1:A:473:ASN:OD1  | 1:A:473:ASN:N    | 2.54                     | 0.40              |
| 1:F:192:PHE:O    | 1:F:193:LEU:C    | 2.59                     | 0.40              |
| 1:B:183:SER:O    | 1:B:187:SER:HB2  | 2.20                     | 0.40              |
| 1:E:410:ILE:C    | 1:E:412:GLU:H    | 2.24                     | 0.40              |
| 1:B:345:THR:C    | 1:B:488:LEU:HD22 | 2.42                     | 0.40              |
| 1:F:413:LEU:HB2  | 1:F:419:ILE:HG12 | 2.02                     | 0.40              |
| 1:E:767:GLN:HB3  | 1:E:768:LYS:H    | 1.53                     | 0.40              |
| 1:A:327:LEU:O    | 1:A:495:PHE:N    | 2.49                     | 0.40              |
| 1:D:722:ILE:HD13 | 1:D:764:LEU:CD2  | 2.52                     | 0.40              |
| 1:D:579:THR:C    | 1:D:581:GLN:N    | 2.75                     | 0.40              |
| 1:A:154:ILE:HG13 | 1:A:171:TYR:CD1  | 2.56                     | 0.40              |
| 2:S:27:ILE:HA    | 2:S:31:GLU:OE2   | 2.21                     | 0.40              |
| 1:A:359:PRO:HG2  | 1:A:360:VAL:N    | 2.33                     | 0.40              |
| 1:B:136:PRO:O    | 1:B:138:ALA:N    | 2.55                     | 0.40              |
| 1:E:446:ILE:HG13 | 1:E:452:GLU:O    | 2.21                     | 0.40              |
| 1:C:134:LYS:C    | 1:C:136:PRO:CD   | 2.85                     | 0.40              |
| 1:F:447:SER:CB   | 1:F:450:ASN:O    | 2.68                     | 0.40              |
| 1:D:278:LYS:O    | 1:D:279:ILE:C    | 2.58                     | 0.40              |
| 2:S:9:ILE:HD12   | 2:S:69:LEU:CD1   | 2.44                     | 0.40              |
| 2:T:91:VAL:HG12  | 2:T:92:PHE:N     | 2.34                     | 0.40              |
| 1:B:455:TYR:O    | 1:B:471:TRP:HA   | 2.19                     | 0.40              |
| 1:B:250:ALA:O    | 1:B:252:ASP:N    | 2.54                     | 0.40              |
| 1:F:512:GLU:O    | 1:F:516:VAL:HG23 | 2.22                     | 0.40              |
| 1:D:73:ASN:O     | 1:D:74:GLU:O     | 2.40                     | 0.40              |
| 1:E:611:THR:HG22 | 1:E:615:ILE:HD12 | 2.04                     | 0.40              |
| 1:B:688:PHE:C    | 1:B:688:PHE:HD2  | 2.25                     | 0.40              |
| 1:B:639:ASN:HD22 | 1:B:639:ASN:C    | 2.24                     | 0.40              |
| 1:A:210:PHE:CD1  | 1:A:214:PHE:HD1  | 2.40                     | 0.40              |
| 1:C:131:ARG:HG2  | 1:C:131:ARG:NH1  | 2.37                     | 0.40              |
| 1:A:99:GLU:OE2   | 1:A:284:LYS:HD2  | 2.22                     | 0.40              |

All (8) 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) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:D:685:LYS:NZ | 1:D:685:LYS:NZ[2_657] | 2.03                     | 0.17              |
| 1:A:75:THR:CG2 | 1:E:786:GLU:O[4_556]  | 2.09                     | 0.11              |
| 1:B:786:GLU:O  | 1:D:75:THR:CG2[4_656] | 2.12                     | 0.08              |
| 1:F:75:THR:CG2 | 1:F:786:GLU:O[2_557]  | 2.13                     | 0.07              |
| 1:B:75:THR:CG2 | 1:D:786:GLU:O[4_656]  | 2.14                     | 0.06              |
| 1:A:786:GLU:O  | 1:E:75:THR:CG2[4_556] | 2.15                     | 0.05              |
| 1:C:75:THR:CG2 | 1:C:786:GLU:O[2_756]  | 2.15                     | 0.05              |
| 1:C:685:LYS:NZ | 1:E:685:LYS:NZ[2_657] | 2.16                     | 0.04              |

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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     | 733/777 (94%)   | 497 (68%)  | 179 (24%)  | 57 (8%)  | 1           | 9  |
| 1   | B     | 733/777 (94%)   | 494 (67%)  | 183 (25%)  | 56 (8%)  | 1           | 10 |
| 1   | C     | 733/777 (94%)   | 491 (67%)  | 187 (26%)  | 55 (8%)  | 1           | 11 |
| 1   | D     | 733/777 (94%)   | 492 (67%)  | 187 (26%)  | 54 (7%)  | 1           | 11 |
| 1   | E     | 733/777 (94%)   | 490 (67%)  | 186 (25%)  | 57 (8%)  | 1           | 9  |
| 1   | F     | 733/777 (94%)   | 492 (67%)  | 186 (25%)  | 55 (8%)  | 1           | 11 |
| 2   | O     | 144/149 (97%)   | 103 (72%)  | 30 (21%)   | 11 (8%)  | 1           | 10 |
| 2   | P     | 144/149 (97%)   | 103 (72%)  | 30 (21%)   | 11 (8%)  | 1           | 10 |
| 2   | Q     | 144/149 (97%)   | 103 (72%)  | 30 (21%)   | 11 (8%)  | 1           | 10 |
| 2   | R     | 144/149 (97%)   | 103 (72%)  | 29 (20%)   | 12 (8%)  | 1           | 8  |
| 2   | S     | 144/149 (97%)   | 103 (72%)  | 30 (21%)   | 11 (8%)  | 1           | 10 |
| 2   | T     | 144/149 (97%)   | 103 (72%)  | 30 (21%)   | 11 (8%)  | 1           | 10 |
| All | All   | 5262/5556 (95%) | 3574 (68%) | 1287 (24%) | 401 (8%) | 1           | 10 |

All (401) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 176 | GLY  |
| 1   | A     | 183 | SER  |
| 1   | A     | 302 | LEU  |
| 1   | A     | 787 | THR  |
| 1   | B     | 137 | PHE  |
| 1   | B     | 176 | GLY  |
| 1   | B     | 183 | SER  |
| 1   | B     | 302 | LEU  |
| 1   | B     | 787 | THR  |
| 1   | C     | 113 | GLU  |
| 1   | C     | 176 | GLY  |
| 1   | C     | 183 | SER  |
| 1   | C     | 302 | LEU  |
| 1   | C     | 787 | THR  |
| 1   | D     | 113 | GLU  |
| 1   | D     | 136 | PRO  |
| 1   | D     | 137 | PHE  |
| 1   | D     | 176 | GLY  |
| 1   | D     | 183 | SER  |
| 1   | D     | 302 | LEU  |
| 1   | D     | 787 | THR  |
| 1   | E     | 113 | GLU  |
| 1   | E     | 136 | PRO  |
| 1   | E     | 176 | GLY  |
| 1   | E     | 183 | SER  |
| 1   | E     | 302 | LEU  |
| 1   | E     | 787 | THR  |
| 1   | F     | 113 | GLU  |
| 1   | F     | 137 | PHE  |
| 1   | F     | 176 | GLY  |
| 1   | F     | 183 | SER  |
| 1   | F     | 302 | LEU  |
| 1   | F     | 787 | THR  |
| 2   | O     | 23  | GLY  |
| 2   | O     | 71  | MET  |
| 2   | O     | 145 | MET  |
| 2   | P     | 23  | GLY  |
| 2   | P     | 71  | MET  |
| 2   | P     | 145 | MET  |
| 2   | Q     | 23  | GLY  |
| 2   | R     | 23  | GLY  |
| 2   | R     | 71  | MET  |
| 2   | R     | 145 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S     | 23  | GLY  |
| 2   | S     | 71  | MET  |
| 2   | S     | 145 | MET  |
| 2   | T     | 23  | GLY  |
| 2   | T     | 71  | MET  |
| 2   | T     | 145 | MET  |
| 1   | A     | 73  | ASN  |
| 1   | A     | 74  | GLU  |
| 1   | A     | 84  | ASP  |
| 1   | A     | 91  | LYS  |
| 1   | A     | 113 | GLU  |
| 1   | A     | 116 | GLU  |
| 1   | A     | 136 | PRO  |
| 1   | A     | 137 | PHE  |
| 1   | A     | 174 | GLY  |
| 1   | A     | 192 | PHE  |
| 1   | A     | 200 | SER  |
| 1   | A     | 278 | LYS  |
| 1   | A     | 334 | LEU  |
| 1   | A     | 376 | GLN  |
| 1   | A     | 434 | LEU  |
| 1   | A     | 449 | GLU  |
| 1   | A     | 510 | GLN  |
| 1   | A     | 580 | GLU  |
| 1   | A     | 620 | THR  |
| 1   | A     | 658 | PRO  |
| 1   | A     | 730 | ASN  |
| 1   | B     | 73  | ASN  |
| 1   | B     | 74  | GLU  |
| 1   | B     | 84  | ASP  |
| 1   | B     | 91  | LYS  |
| 1   | B     | 113 | GLU  |
| 1   | B     | 116 | GLU  |
| 1   | B     | 136 | PRO  |
| 1   | B     | 174 | GLY  |
| 1   | B     | 278 | LYS  |
| 1   | B     | 334 | LEU  |
| 1   | B     | 376 | GLN  |
| 1   | B     | 434 | LEU  |
| 1   | B     | 510 | GLN  |
| 1   | B     | 580 | GLU  |
| 1   | B     | 620 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 658 | PRO  |
| 1   | B     | 730 | ASN  |
| 1   | C     | 73  | ASN  |
| 1   | C     | 74  | GLU  |
| 1   | C     | 84  | ASP  |
| 1   | C     | 91  | LYS  |
| 1   | C     | 116 | GLU  |
| 1   | C     | 136 | PRO  |
| 1   | C     | 137 | PHE  |
| 1   | C     | 174 | GLY  |
| 1   | C     | 200 | SER  |
| 1   | C     | 278 | LYS  |
| 1   | C     | 334 | LEU  |
| 1   | C     | 372 | LYS  |
| 1   | C     | 376 | GLN  |
| 1   | C     | 434 | LEU  |
| 1   | C     | 580 | GLU  |
| 1   | C     | 620 | THR  |
| 1   | C     | 658 | PRO  |
| 1   | C     | 730 | ASN  |
| 1   | D     | 73  | ASN  |
| 1   | D     | 74  | GLU  |
| 1   | D     | 84  | ASP  |
| 1   | D     | 91  | LYS  |
| 1   | D     | 116 | GLU  |
| 1   | D     | 174 | GLY  |
| 1   | D     | 200 | SER  |
| 1   | D     | 278 | LYS  |
| 1   | D     | 334 | LEU  |
| 1   | D     | 372 | LYS  |
| 1   | D     | 376 | GLN  |
| 1   | D     | 434 | LEU  |
| 1   | D     | 449 | GLU  |
| 1   | D     | 580 | GLU  |
| 1   | D     | 620 | THR  |
| 1   | D     | 658 | PRO  |
| 1   | D     | 730 | ASN  |
| 1   | E     | 73  | ASN  |
| 1   | E     | 74  | GLU  |
| 1   | E     | 84  | ASP  |
| 1   | E     | 91  | LYS  |
| 1   | E     | 116 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 137 | PHE  |
| 1   | E     | 174 | GLY  |
| 1   | E     | 192 | PHE  |
| 1   | E     | 200 | SER  |
| 1   | E     | 278 | LYS  |
| 1   | E     | 334 | LEU  |
| 1   | E     | 372 | LYS  |
| 1   | E     | 376 | GLN  |
| 1   | E     | 434 | LEU  |
| 1   | E     | 449 | GLU  |
| 1   | E     | 510 | GLN  |
| 1   | E     | 580 | GLU  |
| 1   | E     | 620 | THR  |
| 1   | E     | 658 | PRO  |
| 1   | E     | 730 | ASN  |
| 1   | F     | 73  | ASN  |
| 1   | F     | 74  | GLU  |
| 1   | F     | 84  | ASP  |
| 1   | F     | 91  | LYS  |
| 1   | F     | 116 | GLU  |
| 1   | F     | 136 | PRO  |
| 1   | F     | 174 | GLY  |
| 1   | F     | 200 | SER  |
| 1   | F     | 278 | LYS  |
| 1   | F     | 334 | LEU  |
| 1   | F     | 372 | LYS  |
| 1   | F     | 376 | GLN  |
| 1   | F     | 434 | LEU  |
| 1   | F     | 449 | GLU  |
| 1   | F     | 510 | GLN  |
| 1   | F     | 580 | GLU  |
| 1   | F     | 620 | THR  |
| 1   | F     | 658 | PRO  |
| 1   | F     | 730 | ASN  |
| 2   | O     | 45  | GLU  |
| 2   | O     | 93  | ASP  |
| 2   | O     | 118 | ASP  |
| 2   | O     | 125 | ILE  |
| 2   | P     | 45  | GLU  |
| 2   | P     | 93  | ASP  |
| 2   | P     | 118 | ASP  |
| 2   | P     | 125 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Q     | 45  | GLU  |
| 2   | Q     | 71  | MET  |
| 2   | Q     | 93  | ASP  |
| 2   | Q     | 118 | ASP  |
| 2   | Q     | 125 | ILE  |
| 2   | Q     | 145 | MET  |
| 2   | R     | 45  | GLU  |
| 2   | R     | 74  | ARG  |
| 2   | R     | 93  | ASP  |
| 2   | R     | 118 | ASP  |
| 2   | R     | 125 | ILE  |
| 2   | S     | 45  | GLU  |
| 2   | S     | 74  | ARG  |
| 2   | S     | 93  | ASP  |
| 2   | S     | 118 | ASP  |
| 2   | S     | 125 | ILE  |
| 2   | T     | 45  | GLU  |
| 2   | T     | 74  | ARG  |
| 2   | T     | 93  | ASP  |
| 2   | T     | 118 | ASP  |
| 2   | T     | 125 | ILE  |
| 1   | A     | 76  | LEU  |
| 1   | A     | 251 | PRO  |
| 1   | A     | 260 | TYR  |
| 1   | A     | 299 | GLU  |
| 1   | A     | 372 | LYS  |
| 1   | A     | 406 | ASP  |
| 1   | A     | 734 | ASN  |
| 1   | A     | 765 | THR  |
| 1   | A     | 774 | LYS  |
| 1   | B     | 76  | LEU  |
| 1   | B     | 180 | ASP  |
| 1   | B     | 200 | SER  |
| 1   | B     | 251 | PRO  |
| 1   | B     | 260 | TYR  |
| 1   | B     | 299 | GLU  |
| 1   | B     | 372 | LYS  |
| 1   | B     | 406 | ASP  |
| 1   | B     | 449 | GLU  |
| 1   | B     | 734 | ASN  |
| 1   | B     | 765 | THR  |
| 1   | B     | 774 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 76  | LEU  |
| 1   | C     | 251 | PRO  |
| 1   | C     | 260 | TYR  |
| 1   | C     | 299 | GLU  |
| 1   | C     | 406 | ASP  |
| 1   | C     | 449 | GLU  |
| 1   | C     | 510 | GLN  |
| 1   | C     | 734 | ASN  |
| 1   | C     | 774 | LYS  |
| 1   | D     | 76  | LEU  |
| 1   | D     | 251 | PRO  |
| 1   | D     | 260 | TYR  |
| 1   | D     | 299 | GLU  |
| 1   | D     | 406 | ASP  |
| 1   | D     | 510 | GLN  |
| 1   | D     | 720 | ILE  |
| 1   | D     | 734 | ASN  |
| 1   | D     | 765 | THR  |
| 1   | D     | 774 | LYS  |
| 1   | E     | 76  | LEU  |
| 1   | E     | 251 | PRO  |
| 1   | E     | 260 | TYR  |
| 1   | E     | 299 | GLU  |
| 1   | E     | 406 | ASP  |
| 1   | E     | 734 | ASN  |
| 1   | E     | 774 | LYS  |
| 1   | F     | 76  | LEU  |
| 1   | F     | 192 | PHE  |
| 1   | F     | 251 | PRO  |
| 1   | F     | 260 | TYR  |
| 1   | F     | 299 | GLU  |
| 1   | F     | 406 | ASP  |
| 1   | F     | 734 | ASN  |
| 1   | F     | 774 | LYS  |
| 2   | O     | 25  | GLY  |
| 2   | O     | 74  | ARG  |
| 2   | P     | 25  | GLY  |
| 2   | P     | 74  | ARG  |
| 2   | Q     | 74  | ARG  |
| 2   | R     | 25  | GLY  |
| 2   | S     | 25  | GLY  |
| 2   | T     | 25  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 95  | GLU  |
| 1   | A     | 121 | SER  |
| 1   | A     | 166 | SER  |
| 1   | A     | 360 | VAL  |
| 1   | A     | 393 | GLU  |
| 1   | A     | 459 | GLU  |
| 1   | A     | 691 | LYS  |
| 1   | A     | 720 | ILE  |
| 1   | B     | 95  | GLU  |
| 1   | B     | 121 | SER  |
| 1   | B     | 166 | SER  |
| 1   | B     | 192 | PHE  |
| 1   | B     | 393 | GLU  |
| 1   | B     | 691 | LYS  |
| 1   | B     | 720 | ILE  |
| 1   | C     | 121 | SER  |
| 1   | C     | 166 | SER  |
| 1   | C     | 393 | GLU  |
| 1   | C     | 691 | LYS  |
| 1   | C     | 720 | ILE  |
| 1   | D     | 95  | GLU  |
| 1   | D     | 121 | SER  |
| 1   | D     | 166 | SER  |
| 1   | D     | 393 | GLU  |
| 1   | D     | 691 | LYS  |
| 1   | E     | 95  | GLU  |
| 1   | E     | 121 | SER  |
| 1   | E     | 166 | SER  |
| 1   | E     | 180 | ASP  |
| 1   | E     | 393 | GLU  |
| 1   | E     | 691 | LYS  |
| 1   | E     | 720 | ILE  |
| 1   | F     | 95  | GLU  |
| 1   | F     | 121 | SER  |
| 1   | F     | 166 | SER  |
| 1   | F     | 393 | GLU  |
| 1   | F     | 459 | GLU  |
| 1   | F     | 691 | LYS  |
| 1   | F     | 720 | ILE  |
| 1   | F     | 765 | THR  |
| 2   | Q     | 25  | GLY  |
| 1   | A     | 80  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 123 | GLU  |
| 1   | A     | 159 | TYR  |
| 1   | A     | 323 | ASN  |
| 1   | A     | 423 | LYS  |
| 1   | A     | 546 | LYS  |
| 1   | A     | 637 | PRO  |
| 1   | B     | 80  | GLN  |
| 1   | B     | 123 | GLU  |
| 1   | B     | 159 | TYR  |
| 1   | B     | 264 | MET  |
| 1   | B     | 323 | ASN  |
| 1   | B     | 360 | VAL  |
| 1   | B     | 423 | LYS  |
| 1   | B     | 459 | GLU  |
| 1   | B     | 546 | LYS  |
| 1   | B     | 637 | PRO  |
| 1   | C     | 80  | GLN  |
| 1   | C     | 95  | GLU  |
| 1   | C     | 123 | GLU  |
| 1   | C     | 159 | TYR  |
| 1   | C     | 190 | PRO  |
| 1   | C     | 323 | ASN  |
| 1   | C     | 360 | VAL  |
| 1   | C     | 423 | LYS  |
| 1   | C     | 459 | GLU  |
| 1   | C     | 546 | LYS  |
| 1   | C     | 637 | PRO  |
| 1   | D     | 80  | GLN  |
| 1   | D     | 123 | GLU  |
| 1   | D     | 323 | ASN  |
| 1   | D     | 360 | VAL  |
| 1   | D     | 423 | LYS  |
| 1   | D     | 459 | GLU  |
| 1   | D     | 546 | LYS  |
| 1   | D     | 605 | THR  |
| 1   | D     | 637 | PRO  |
| 1   | E     | 80  | GLN  |
| 1   | E     | 123 | GLU  |
| 1   | E     | 323 | ASN  |
| 1   | E     | 360 | VAL  |
| 1   | E     | 423 | LYS  |
| 1   | E     | 459 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 637 | PRO  |
| 1   | E     | 757 | THR  |
| 1   | E     | 765 | THR  |
| 1   | F     | 80  | GLN  |
| 1   | F     | 123 | GLU  |
| 1   | F     | 159 | TYR  |
| 1   | F     | 323 | ASN  |
| 1   | F     | 360 | VAL  |
| 1   | F     | 423 | LYS  |
| 1   | F     | 546 | LYS  |
| 1   | F     | 637 | PRO  |
| 2   | O     | 147 | ALA  |
| 2   | P     | 147 | ALA  |
| 2   | Q     | 147 | ALA  |
| 2   | R     | 147 | ALA  |
| 2   | S     | 147 | ALA  |
| 2   | T     | 147 | ALA  |
| 1   | A     | 264 | MET  |
| 1   | A     | 460 | GLY  |
| 1   | A     | 605 | THR  |
| 1   | A     | 692 | GLU  |
| 1   | A     | 757 | THR  |
| 1   | B     | 460 | GLY  |
| 1   | B     | 605 | THR  |
| 1   | B     | 692 | GLU  |
| 1   | C     | 206 | SER  |
| 1   | C     | 264 | MET  |
| 1   | C     | 605 | THR  |
| 1   | D     | 206 | SER  |
| 1   | D     | 264 | MET  |
| 1   | D     | 460 | GLY  |
| 1   | D     | 757 | THR  |
| 1   | E     | 206 | SER  |
| 1   | E     | 264 | MET  |
| 1   | E     | 460 | GLY  |
| 1   | E     | 546 | LYS  |
| 1   | E     | 605 | THR  |
| 1   | E     | 692 | GLU  |
| 1   | F     | 264 | MET  |
| 1   | F     | 460 | GLY  |
| 1   | F     | 692 | GLU  |
| 1   | F     | 757 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 133 | ASP  |
| 1   | C     | 460 | GLY  |
| 1   | A     | 177 | ILE  |
| 1   | A     | 537 | GLY  |
| 1   | C     | 537 | GLY  |
| 1   | D     | 537 | GLY  |
| 2   | O     | 59  | GLY  |
| 2   | P     | 59  | GLY  |
| 2   | Q     | 59  | GLY  |
| 2   | T     | 59  | GLY  |
| 1   | B     | 537 | GLY  |
| 1   | D     | 177 | ILE  |
| 1   | E     | 537 | GLY  |
| 1   | F     | 537 | GLY  |
| 2   | R     | 59  | GLY  |
| 2   | S     | 59  | GLY  |
| 1   | B     | 177 | ILE  |
| 1   | C     | 177 | ILE  |
| 1   | F     | 177 | ILE  |
| 1   | A     | 279 | ILE  |
| 1   | C     | 279 | ILE  |
| 1   | E     | 177 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 664/705 (94%) | 562 (85%) | 102 (15%) | 3           | 16 |
| 1   | B     | 664/705 (94%) | 558 (84%) | 106 (16%) | 3           | 14 |
| 1   | C     | 664/705 (94%) | 560 (84%) | 104 (16%) | 3           | 15 |
| 1   | D     | 664/705 (94%) | 558 (84%) | 106 (16%) | 3           | 14 |
| 1   | E     | 664/705 (94%) | 558 (84%) | 106 (16%) | 3           | 14 |
| 1   | F     | 664/705 (94%) | 558 (84%) | 106 (16%) | 3           | 14 |
| 2   | O     | 123/127 (97%) | 103 (84%) | 20 (16%)  | 3           | 14 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 2   | P     | 123/127 (97%)   | 105 (85%)  | 18 (15%)  | 4           | 18 |
| 2   | Q     | 123/127 (97%)   | 104 (85%)  | 19 (15%)  | 3           | 16 |
| 2   | R     | 123/127 (97%)   | 103 (84%)  | 20 (16%)  | 3           | 14 |
| 2   | S     | 123/127 (97%)   | 105 (85%)  | 18 (15%)  | 4           | 18 |
| 2   | T     | 123/127 (97%)   | 104 (85%)  | 19 (15%)  | 3           | 16 |
| All | All   | 4722/4992 (95%) | 3978 (84%) | 744 (16%) | 3           | 15 |

All (744) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 70  | GLU  |
| 1   | A     | 71  | PHE  |
| 1   | A     | 72  | THR  |
| 1   | A     | 77  | ASP  |
| 1   | A     | 80  | GLN  |
| 1   | A     | 87  | LYS  |
| 1   | A     | 88  | LYS  |
| 1   | A     | 97  | TYR  |
| 1   | A     | 99  | GLU  |
| 1   | A     | 110 | ASP  |
| 1   | A     | 113 | GLU  |
| 1   | A     | 115 | LYS  |
| 1   | A     | 120 | LEU  |
| 1   | A     | 122 | GLU  |
| 1   | A     | 128 | MET  |
| 1   | A     | 129 | ASN  |
| 1   | A     | 133 | GLU  |
| 1   | A     | 135 | VAL  |
| 1   | A     | 140 | ARG  |
| 1   | A     | 141 | PHE  |
| 1   | A     | 148 | GLU  |
| 1   | A     | 149 | THR  |
| 1   | A     | 152 | LEU  |
| 1   | A     | 153 | ILE  |
| 1   | A     | 156 | ILE  |
| 1   | A     | 158 | ASP  |
| 1   | A     | 170 | TYR  |
| 1   | A     | 172 | GLU  |
| 1   | A     | 173 | ILE  |
| 1   | A     | 179 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 182 | ILE  |
| 1   | A     | 188 | LEU  |
| 1   | A     | 197 | LYS  |
| 1   | A     | 201 | ASP  |
| 1   | A     | 202 | ASP  |
| 1   | A     | 210 | PHE  |
| 1   | A     | 212 | GLN  |
| 1   | A     | 217 | LYS  |
| 1   | A     | 218 | LEU  |
| 1   | A     | 221 | ASN  |
| 1   | A     | 223 | LYS  |
| 1   | A     | 253 | HIS  |
| 1   | A     | 254 | ARG  |
| 1   | A     | 279 | ILE  |
| 1   | A     | 284 | LYS  |
| 1   | A     | 292 | ARG  |
| 1   | A     | 293 | ILE  |
| 1   | A     | 296 | LEU  |
| 1   | A     | 299 | GLU  |
| 1   | A     | 305 | SER  |
| 1   | A     | 323 | ASN  |
| 1   | A     | 334 | LEU  |
| 1   | A     | 336 | THR  |
| 1   | A     | 349 | ASN  |
| 1   | A     | 377 | GLN  |
| 1   | A     | 395 | GLU  |
| 1   | A     | 397 | GLU  |
| 1   | A     | 400 | LYS  |
| 1   | A     | 401 | ILE  |
| 1   | A     | 414 | LYS  |
| 1   | A     | 415 | GLU  |
| 1   | A     | 416 | ASN  |
| 1   | A     | 434 | LEU  |
| 1   | A     | 438 | ASN  |
| 1   | A     | 444 | PHE  |
| 1   | A     | 451 | ASN  |
| 1   | A     | 455 | TYR  |
| 1   | A     | 472 | ARG  |
| 1   | A     | 479 | LYS  |
| 1   | A     | 480 | ASN  |
| 1   | A     | 481 | VAL  |
| 1   | A     | 484 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 500 | SER  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 515 | LYS  |
| 1   | A     | 521 | ASN  |
| 1   | A     | 524 | GLU  |
| 1   | A     | 533 | LEU  |
| 1   | A     | 562 | GLU  |
| 1   | A     | 570 | THR  |
| 1   | A     | 582 | ASP  |
| 1   | A     | 597 | ASN  |
| 1   | A     | 623 | ASP  |
| 1   | A     | 629 | ASN  |
| 1   | A     | 635 | ILE  |
| 1   | A     | 639 | ASN  |
| 1   | A     | 659 | THR  |
| 1   | A     | 665 | LYS  |
| 1   | A     | 672 | ARG  |
| 1   | A     | 678 | VAL  |
| 1   | A     | 688 | PHE  |
| 1   | A     | 709 | ASN  |
| 1   | A     | 714 | GLN  |
| 1   | A     | 726 | ILE  |
| 1   | A     | 729 | TYR  |
| 1   | A     | 734 | ASN  |
| 1   | A     | 744 | GLU  |
| 1   | A     | 755 | ARG  |
| 1   | A     | 770 | ASN  |
| 1   | A     | 781 | ASN  |
| 1   | A     | 786 | GLU  |
| 1   | A     | 794 | GLN  |
| 1   | B     | 70  | GLU  |
| 1   | B     | 71  | PHE  |
| 1   | B     | 72  | THR  |
| 1   | B     | 77  | ASP  |
| 1   | B     | 80  | GLN  |
| 1   | B     | 87  | LYS  |
| 1   | B     | 88  | LYS  |
| 1   | B     | 97  | TYR  |
| 1   | B     | 99  | GLU  |
| 1   | B     | 110 | ASP  |
| 1   | B     | 113 | GLU  |
| 1   | B     | 115 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 120 | LEU  |
| 1   | B     | 122 | GLU  |
| 1   | B     | 128 | MET  |
| 1   | B     | 129 | ASN  |
| 1   | B     | 133 | GLU  |
| 1   | B     | 135 | VAL  |
| 1   | B     | 140 | ARG  |
| 1   | B     | 141 | PHE  |
| 1   | B     | 148 | GLU  |
| 1   | B     | 149 | THR  |
| 1   | B     | 152 | LEU  |
| 1   | B     | 153 | ILE  |
| 1   | B     | 156 | ILE  |
| 1   | B     | 158 | ASP  |
| 1   | B     | 170 | TYR  |
| 1   | B     | 172 | GLU  |
| 1   | B     | 173 | ILE  |
| 1   | B     | 179 | LEU  |
| 1   | B     | 180 | ASP  |
| 1   | B     | 182 | ILE  |
| 1   | B     | 188 | LEU  |
| 1   | B     | 197 | LYS  |
| 1   | B     | 201 | ASP  |
| 1   | B     | 202 | ASP  |
| 1   | B     | 210 | PHE  |
| 1   | B     | 212 | GLN  |
| 1   | B     | 217 | LYS  |
| 1   | B     | 218 | LEU  |
| 1   | B     | 221 | ASN  |
| 1   | B     | 223 | LYS  |
| 1   | B     | 253 | HIS  |
| 1   | B     | 254 | ARG  |
| 1   | B     | 279 | ILE  |
| 1   | B     | 284 | LYS  |
| 1   | B     | 292 | ARG  |
| 1   | B     | 293 | ILE  |
| 1   | B     | 296 | LEU  |
| 1   | B     | 299 | GLU  |
| 1   | B     | 305 | SER  |
| 1   | B     | 309 | PRO  |
| 1   | B     | 323 | ASN  |
| 1   | B     | 334 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 336 | THR  |
| 1   | B     | 349 | ASN  |
| 1   | B     | 377 | GLN  |
| 1   | B     | 395 | GLU  |
| 1   | B     | 397 | GLU  |
| 1   | B     | 400 | LYS  |
| 1   | B     | 401 | ILE  |
| 1   | B     | 414 | LYS  |
| 1   | B     | 415 | GLU  |
| 1   | B     | 416 | ASN  |
| 1   | B     | 434 | LEU  |
| 1   | B     | 438 | ASN  |
| 1   | B     | 444 | PHE  |
| 1   | B     | 451 | ASN  |
| 1   | B     | 455 | TYR  |
| 1   | B     | 472 | ARG  |
| 1   | B     | 479 | LYS  |
| 1   | B     | 480 | ASN  |
| 1   | B     | 481 | VAL  |
| 1   | B     | 484 | VAL  |
| 1   | B     | 499 | PRO  |
| 1   | B     | 500 | SER  |
| 1   | B     | 507 | GLN  |
| 1   | B     | 515 | LYS  |
| 1   | B     | 521 | ASN  |
| 1   | B     | 524 | GLU  |
| 1   | B     | 533 | LEU  |
| 1   | B     | 562 | GLU  |
| 1   | B     | 570 | THR  |
| 1   | B     | 582 | ASP  |
| 1   | B     | 597 | ASN  |
| 1   | B     | 623 | ASP  |
| 1   | B     | 629 | ASN  |
| 1   | B     | 635 | ILE  |
| 1   | B     | 639 | ASN  |
| 1   | B     | 659 | THR  |
| 1   | B     | 665 | LYS  |
| 1   | B     | 672 | ARG  |
| 1   | B     | 678 | VAL  |
| 1   | B     | 688 | PHE  |
| 1   | B     | 709 | ASN  |
| 1   | B     | 714 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 726 | ILE  |
| 1   | B     | 729 | TYR  |
| 1   | B     | 734 | ASN  |
| 1   | B     | 744 | GLU  |
| 1   | B     | 755 | ARG  |
| 1   | B     | 766 | HIS  |
| 1   | B     | 770 | ASN  |
| 1   | B     | 781 | ASN  |
| 1   | B     | 786 | GLU  |
| 1   | B     | 794 | GLN  |
| 1   | C     | 70  | GLU  |
| 1   | C     | 71  | PHE  |
| 1   | C     | 72  | THR  |
| 1   | C     | 77  | ASP  |
| 1   | C     | 80  | GLN  |
| 1   | C     | 88  | LYS  |
| 1   | C     | 97  | TYR  |
| 1   | C     | 99  | GLU  |
| 1   | C     | 110 | ASP  |
| 1   | C     | 113 | GLU  |
| 1   | C     | 115 | LYS  |
| 1   | C     | 120 | LEU  |
| 1   | C     | 122 | GLU  |
| 1   | C     | 128 | MET  |
| 1   | C     | 129 | ASN  |
| 1   | C     | 133 | GLU  |
| 1   | C     | 135 | VAL  |
| 1   | C     | 140 | ARG  |
| 1   | C     | 141 | PHE  |
| 1   | C     | 148 | GLU  |
| 1   | C     | 149 | THR  |
| 1   | C     | 152 | LEU  |
| 1   | C     | 153 | ILE  |
| 1   | C     | 156 | ILE  |
| 1   | C     | 158 | ASP  |
| 1   | C     | 170 | TYR  |
| 1   | C     | 172 | GLU  |
| 1   | C     | 173 | ILE  |
| 1   | C     | 179 | LEU  |
| 1   | C     | 182 | ILE  |
| 1   | C     | 188 | LEU  |
| 1   | C     | 197 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 201 | ASP  |
| 1   | C     | 202 | ASP  |
| 1   | C     | 210 | PHE  |
| 1   | C     | 212 | GLN  |
| 1   | C     | 217 | LYS  |
| 1   | C     | 218 | LEU  |
| 1   | C     | 221 | ASN  |
| 1   | C     | 223 | LYS  |
| 1   | C     | 253 | HIS  |
| 1   | C     | 254 | ARG  |
| 1   | C     | 279 | ILE  |
| 1   | C     | 284 | LYS  |
| 1   | C     | 292 | ARG  |
| 1   | C     | 293 | ILE  |
| 1   | C     | 296 | LEU  |
| 1   | C     | 299 | GLU  |
| 1   | C     | 305 | SER  |
| 1   | C     | 323 | ASN  |
| 1   | C     | 334 | LEU  |
| 1   | C     | 336 | THR  |
| 1   | C     | 349 | ASN  |
| 1   | C     | 377 | GLN  |
| 1   | C     | 395 | GLU  |
| 1   | C     | 397 | GLU  |
| 1   | C     | 400 | LYS  |
| 1   | C     | 401 | ILE  |
| 1   | C     | 414 | LYS  |
| 1   | C     | 415 | GLU  |
| 1   | C     | 416 | ASN  |
| 1   | C     | 434 | LEU  |
| 1   | C     | 438 | ASN  |
| 1   | C     | 444 | PHE  |
| 1   | C     | 451 | ASN  |
| 1   | C     | 455 | TYR  |
| 1   | C     | 472 | ARG  |
| 1   | C     | 479 | LYS  |
| 1   | C     | 480 | ASN  |
| 1   | C     | 481 | VAL  |
| 1   | C     | 484 | VAL  |
| 1   | C     | 499 | PRO  |
| 1   | C     | 500 | SER  |
| 1   | C     | 507 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 515 | LYS  |
| 1   | C     | 521 | ASN  |
| 1   | C     | 524 | GLU  |
| 1   | C     | 533 | LEU  |
| 1   | C     | 562 | GLU  |
| 1   | C     | 570 | THR  |
| 1   | C     | 582 | ASP  |
| 1   | C     | 597 | ASN  |
| 1   | C     | 623 | ASP  |
| 1   | C     | 629 | ASN  |
| 1   | C     | 635 | ILE  |
| 1   | C     | 639 | ASN  |
| 1   | C     | 659 | THR  |
| 1   | C     | 665 | LYS  |
| 1   | C     | 672 | ARG  |
| 1   | C     | 678 | VAL  |
| 1   | C     | 688 | PHE  |
| 1   | C     | 709 | ASN  |
| 1   | C     | 714 | GLN  |
| 1   | C     | 726 | ILE  |
| 1   | C     | 729 | TYR  |
| 1   | C     | 734 | ASN  |
| 1   | C     | 744 | GLU  |
| 1   | C     | 755 | ARG  |
| 1   | C     | 767 | GLN  |
| 1   | C     | 769 | SER  |
| 1   | C     | 770 | ASN  |
| 1   | C     | 781 | ASN  |
| 1   | C     | 786 | GLU  |
| 1   | C     | 794 | GLN  |
| 1   | D     | 70  | GLU  |
| 1   | D     | 71  | PHE  |
| 1   | D     | 72  | THR  |
| 1   | D     | 77  | ASP  |
| 1   | D     | 80  | GLN  |
| 1   | D     | 87  | LYS  |
| 1   | D     | 88  | LYS  |
| 1   | D     | 97  | TYR  |
| 1   | D     | 99  | GLU  |
| 1   | D     | 110 | ASP  |
| 1   | D     | 113 | GLU  |
| 1   | D     | 115 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 120 | LEU  |
| 1   | D     | 122 | GLU  |
| 1   | D     | 128 | MET  |
| 1   | D     | 129 | ASN  |
| 1   | D     | 133 | GLU  |
| 1   | D     | 135 | VAL  |
| 1   | D     | 140 | ARG  |
| 1   | D     | 141 | PHE  |
| 1   | D     | 148 | GLU  |
| 1   | D     | 149 | THR  |
| 1   | D     | 152 | LEU  |
| 1   | D     | 153 | ILE  |
| 1   | D     | 156 | ILE  |
| 1   | D     | 158 | ASP  |
| 1   | D     | 161 | ILE  |
| 1   | D     | 170 | TYR  |
| 1   | D     | 172 | GLU  |
| 1   | D     | 173 | ILE  |
| 1   | D     | 179 | LEU  |
| 1   | D     | 182 | ILE  |
| 1   | D     | 188 | LEU  |
| 1   | D     | 197 | LYS  |
| 1   | D     | 201 | ASP  |
| 1   | D     | 202 | ASP  |
| 1   | D     | 210 | PHE  |
| 1   | D     | 212 | GLN  |
| 1   | D     | 217 | LYS  |
| 1   | D     | 218 | LEU  |
| 1   | D     | 221 | ASN  |
| 1   | D     | 223 | LYS  |
| 1   | D     | 253 | HIS  |
| 1   | D     | 254 | ARG  |
| 1   | D     | 279 | ILE  |
| 1   | D     | 284 | LYS  |
| 1   | D     | 292 | ARG  |
| 1   | D     | 293 | ILE  |
| 1   | D     | 296 | LEU  |
| 1   | D     | 299 | GLU  |
| 1   | D     | 305 | SER  |
| 1   | D     | 323 | ASN  |
| 1   | D     | 334 | LEU  |
| 1   | D     | 336 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 349 | ASN  |
| 1   | D     | 377 | GLN  |
| 1   | D     | 395 | GLU  |
| 1   | D     | 397 | GLU  |
| 1   | D     | 400 | LYS  |
| 1   | D     | 401 | ILE  |
| 1   | D     | 414 | LYS  |
| 1   | D     | 415 | GLU  |
| 1   | D     | 416 | ASN  |
| 1   | D     | 434 | LEU  |
| 1   | D     | 438 | ASN  |
| 1   | D     | 444 | PHE  |
| 1   | D     | 451 | ASN  |
| 1   | D     | 455 | TYR  |
| 1   | D     | 472 | ARG  |
| 1   | D     | 479 | LYS  |
| 1   | D     | 480 | ASN  |
| 1   | D     | 481 | VAL  |
| 1   | D     | 484 | VAL  |
| 1   | D     | 499 | PRO  |
| 1   | D     | 500 | SER  |
| 1   | D     | 507 | GLN  |
| 1   | D     | 515 | LYS  |
| 1   | D     | 521 | ASN  |
| 1   | D     | 524 | GLU  |
| 1   | D     | 533 | LEU  |
| 1   | D     | 562 | GLU  |
| 1   | D     | 570 | THR  |
| 1   | D     | 582 | ASP  |
| 1   | D     | 597 | ASN  |
| 1   | D     | 623 | ASP  |
| 1   | D     | 629 | ASN  |
| 1   | D     | 635 | ILE  |
| 1   | D     | 639 | ASN  |
| 1   | D     | 659 | THR  |
| 1   | D     | 665 | LYS  |
| 1   | D     | 672 | ARG  |
| 1   | D     | 678 | VAL  |
| 1   | D     | 688 | PHE  |
| 1   | D     | 709 | ASN  |
| 1   | D     | 714 | GLN  |
| 1   | D     | 726 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 729 | TYR  |
| 1   | D     | 734 | ASN  |
| 1   | D     | 744 | GLU  |
| 1   | D     | 755 | ARG  |
| 1   | D     | 766 | HIS  |
| 1   | D     | 769 | SER  |
| 1   | D     | 770 | ASN  |
| 1   | D     | 781 | ASN  |
| 1   | D     | 786 | GLU  |
| 1   | D     | 794 | GLN  |
| 1   | E     | 70  | GLU  |
| 1   | E     | 71  | PHE  |
| 1   | E     | 72  | THR  |
| 1   | E     | 77  | ASP  |
| 1   | E     | 80  | GLN  |
| 1   | E     | 88  | LYS  |
| 1   | E     | 97  | TYR  |
| 1   | E     | 99  | GLU  |
| 1   | E     | 110 | ASP  |
| 1   | E     | 113 | GLU  |
| 1   | E     | 115 | LYS  |
| 1   | E     | 120 | LEU  |
| 1   | E     | 122 | GLU  |
| 1   | E     | 128 | MET  |
| 1   | E     | 129 | ASN  |
| 1   | E     | 133 | GLU  |
| 1   | E     | 135 | VAL  |
| 1   | E     | 140 | ARG  |
| 1   | E     | 141 | PHE  |
| 1   | E     | 148 | GLU  |
| 1   | E     | 149 | THR  |
| 1   | E     | 152 | LEU  |
| 1   | E     | 153 | ILE  |
| 1   | E     | 156 | ILE  |
| 1   | E     | 158 | ASP  |
| 1   | E     | 161 | ILE  |
| 1   | E     | 170 | TYR  |
| 1   | E     | 172 | GLU  |
| 1   | E     | 173 | ILE  |
| 1   | E     | 179 | LEU  |
| 1   | E     | 182 | ILE  |
| 1   | E     | 188 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 197 | LYS  |
| 1   | E     | 201 | ASP  |
| 1   | E     | 202 | ASP  |
| 1   | E     | 210 | PHE  |
| 1   | E     | 212 | GLN  |
| 1   | E     | 217 | LYS  |
| 1   | E     | 218 | LEU  |
| 1   | E     | 221 | ASN  |
| 1   | E     | 223 | LYS  |
| 1   | E     | 253 | HIS  |
| 1   | E     | 254 | ARG  |
| 1   | E     | 279 | ILE  |
| 1   | E     | 284 | LYS  |
| 1   | E     | 292 | ARG  |
| 1   | E     | 293 | ILE  |
| 1   | E     | 296 | LEU  |
| 1   | E     | 299 | GLU  |
| 1   | E     | 305 | SER  |
| 1   | E     | 323 | ASN  |
| 1   | E     | 334 | LEU  |
| 1   | E     | 336 | THR  |
| 1   | E     | 349 | ASN  |
| 1   | E     | 377 | GLN  |
| 1   | E     | 395 | GLU  |
| 1   | E     | 397 | GLU  |
| 1   | E     | 400 | LYS  |
| 1   | E     | 401 | ILE  |
| 1   | E     | 414 | LYS  |
| 1   | E     | 415 | GLU  |
| 1   | E     | 416 | ASN  |
| 1   | E     | 434 | LEU  |
| 1   | E     | 438 | ASN  |
| 1   | E     | 444 | PHE  |
| 1   | E     | 451 | ASN  |
| 1   | E     | 455 | TYR  |
| 1   | E     | 472 | ARG  |
| 1   | E     | 479 | LYS  |
| 1   | E     | 480 | ASN  |
| 1   | E     | 481 | VAL  |
| 1   | E     | 484 | VAL  |
| 1   | E     | 499 | PRO  |
| 1   | E     | 500 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 507 | GLN  |
| 1   | E     | 515 | LYS  |
| 1   | E     | 521 | ASN  |
| 1   | E     | 524 | GLU  |
| 1   | E     | 533 | LEU  |
| 1   | E     | 562 | GLU  |
| 1   | E     | 570 | THR  |
| 1   | E     | 582 | ASP  |
| 1   | E     | 597 | ASN  |
| 1   | E     | 623 | ASP  |
| 1   | E     | 629 | ASN  |
| 1   | E     | 635 | ILE  |
| 1   | E     | 639 | ASN  |
| 1   | E     | 648 | PRO  |
| 1   | E     | 659 | THR  |
| 1   | E     | 665 | LYS  |
| 1   | E     | 672 | ARG  |
| 1   | E     | 678 | VAL  |
| 1   | E     | 688 | PHE  |
| 1   | E     | 709 | ASN  |
| 1   | E     | 714 | GLN  |
| 1   | E     | 726 | ILE  |
| 1   | E     | 729 | TYR  |
| 1   | E     | 734 | ASN  |
| 1   | E     | 744 | GLU  |
| 1   | E     | 755 | ARG  |
| 1   | E     | 766 | HIS  |
| 1   | E     | 769 | SER  |
| 1   | E     | 770 | ASN  |
| 1   | E     | 781 | ASN  |
| 1   | E     | 786 | GLU  |
| 1   | E     | 794 | GLN  |
| 1   | F     | 65  | ASN  |
| 1   | F     | 70  | GLU  |
| 1   | F     | 71  | PHE  |
| 1   | F     | 72  | THR  |
| 1   | F     | 77  | ASP  |
| 1   | F     | 80  | GLN  |
| 1   | F     | 87  | LYS  |
| 1   | F     | 88  | LYS  |
| 1   | F     | 97  | TYR  |
| 1   | F     | 99  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 110 | ASP  |
| 1   | F     | 113 | GLU  |
| 1   | F     | 115 | LYS  |
| 1   | F     | 120 | LEU  |
| 1   | F     | 122 | GLU  |
| 1   | F     | 128 | MET  |
| 1   | F     | 129 | ASN  |
| 1   | F     | 133 | GLU  |
| 1   | F     | 135 | VAL  |
| 1   | F     | 140 | ARG  |
| 1   | F     | 141 | PHE  |
| 1   | F     | 148 | GLU  |
| 1   | F     | 149 | THR  |
| 1   | F     | 152 | LEU  |
| 1   | F     | 153 | ILE  |
| 1   | F     | 156 | ILE  |
| 1   | F     | 158 | ASP  |
| 1   | F     | 170 | TYR  |
| 1   | F     | 172 | GLU  |
| 1   | F     | 173 | ILE  |
| 1   | F     | 179 | LEU  |
| 1   | F     | 182 | ILE  |
| 1   | F     | 188 | LEU  |
| 1   | F     | 197 | LYS  |
| 1   | F     | 201 | ASP  |
| 1   | F     | 202 | ASP  |
| 1   | F     | 210 | PHE  |
| 1   | F     | 212 | GLN  |
| 1   | F     | 217 | LYS  |
| 1   | F     | 218 | LEU  |
| 1   | F     | 221 | ASN  |
| 1   | F     | 223 | LYS  |
| 1   | F     | 253 | HIS  |
| 1   | F     | 254 | ARG  |
| 1   | F     | 279 | ILE  |
| 1   | F     | 284 | LYS  |
| 1   | F     | 292 | ARG  |
| 1   | F     | 293 | ILE  |
| 1   | F     | 296 | LEU  |
| 1   | F     | 299 | GLU  |
| 1   | F     | 305 | SER  |
| 1   | F     | 323 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 334 | LEU  |
| 1   | F     | 336 | THR  |
| 1   | F     | 349 | ASN  |
| 1   | F     | 377 | GLN  |
| 1   | F     | 395 | GLU  |
| 1   | F     | 397 | GLU  |
| 1   | F     | 400 | LYS  |
| 1   | F     | 401 | ILE  |
| 1   | F     | 414 | LYS  |
| 1   | F     | 415 | GLU  |
| 1   | F     | 416 | ASN  |
| 1   | F     | 434 | LEU  |
| 1   | F     | 438 | ASN  |
| 1   | F     | 444 | PHE  |
| 1   | F     | 451 | ASN  |
| 1   | F     | 455 | TYR  |
| 1   | F     | 472 | ARG  |
| 1   | F     | 479 | LYS  |
| 1   | F     | 480 | ASN  |
| 1   | F     | 481 | VAL  |
| 1   | F     | 484 | VAL  |
| 1   | F     | 499 | PRO  |
| 1   | F     | 500 | SER  |
| 1   | F     | 507 | GLN  |
| 1   | F     | 515 | LYS  |
| 1   | F     | 521 | ASN  |
| 1   | F     | 524 | GLU  |
| 1   | F     | 533 | LEU  |
| 1   | F     | 562 | GLU  |
| 1   | F     | 570 | THR  |
| 1   | F     | 582 | ASP  |
| 1   | F     | 597 | ASN  |
| 1   | F     | 623 | ASP  |
| 1   | F     | 629 | ASN  |
| 1   | F     | 635 | ILE  |
| 1   | F     | 639 | ASN  |
| 1   | F     | 659 | THR  |
| 1   | F     | 665 | LYS  |
| 1   | F     | 672 | ARG  |
| 1   | F     | 678 | VAL  |
| 1   | F     | 688 | PHE  |
| 1   | F     | 709 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 714 | GLN  |
| 1   | F     | 726 | ILE  |
| 1   | F     | 729 | TYR  |
| 1   | F     | 734 | ASN  |
| 1   | F     | 744 | GLU  |
| 1   | F     | 755 | ARG  |
| 1   | F     | 766 | HIS  |
| 1   | F     | 769 | SER  |
| 1   | F     | 770 | ASN  |
| 1   | F     | 781 | ASN  |
| 1   | F     | 786 | GLU  |
| 1   | F     | 794 | GLN  |
| 2   | O     | 13  | LYS  |
| 2   | O     | 14  | GLU  |
| 2   | O     | 18  | LEU  |
| 2   | O     | 30  | LYS  |
| 2   | O     | 34  | THR  |
| 2   | O     | 36  | MET  |
| 2   | O     | 39  | LEU  |
| 2   | O     | 49  | GLN  |
| 2   | O     | 50  | ASP  |
| 2   | O     | 54  | GLU  |
| 2   | O     | 55  | VAL  |
| 2   | O     | 56  | ASP  |
| 2   | O     | 62  | THR  |
| 2   | O     | 65  | PHE  |
| 2   | O     | 74  | ARG  |
| 2   | O     | 76  | MET  |
| 2   | O     | 97  | ASN  |
| 2   | O     | 106 | ARG  |
| 2   | O     | 117 | THR  |
| 2   | O     | 123 | GLN  |
| 2   | P     | 13  | LYS  |
| 2   | P     | 14  | GLU  |
| 2   | P     | 18  | LEU  |
| 2   | P     | 36  | MET  |
| 2   | P     | 39  | LEU  |
| 2   | P     | 49  | GLN  |
| 2   | P     | 50  | ASP  |
| 2   | P     | 54  | GLU  |
| 2   | P     | 55  | VAL  |
| 2   | P     | 56  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 62  | THR  |
| 2   | P     | 65  | PHE  |
| 2   | P     | 74  | ARG  |
| 2   | P     | 76  | MET  |
| 2   | P     | 97  | ASN  |
| 2   | P     | 106 | ARG  |
| 2   | P     | 117 | THR  |
| 2   | P     | 123 | GLN  |
| 2   | Q     | 13  | LYS  |
| 2   | Q     | 14  | GLU  |
| 2   | Q     | 18  | LEU  |
| 2   | Q     | 30  | LYS  |
| 2   | Q     | 36  | MET  |
| 2   | Q     | 39  | LEU  |
| 2   | Q     | 49  | GLN  |
| 2   | Q     | 50  | ASP  |
| 2   | Q     | 54  | GLU  |
| 2   | Q     | 55  | VAL  |
| 2   | Q     | 56  | ASP  |
| 2   | Q     | 62  | THR  |
| 2   | Q     | 65  | PHE  |
| 2   | Q     | 74  | ARG  |
| 2   | Q     | 76  | MET  |
| 2   | Q     | 97  | ASN  |
| 2   | Q     | 106 | ARG  |
| 2   | Q     | 117 | THR  |
| 2   | Q     | 123 | GLN  |
| 2   | R     | 13  | LYS  |
| 2   | R     | 14  | GLU  |
| 2   | R     | 18  | LEU  |
| 2   | R     | 30  | LYS  |
| 2   | R     | 34  | THR  |
| 2   | R     | 36  | MET  |
| 2   | R     | 39  | LEU  |
| 2   | R     | 49  | GLN  |
| 2   | R     | 50  | ASP  |
| 2   | R     | 54  | GLU  |
| 2   | R     | 55  | VAL  |
| 2   | R     | 56  | ASP  |
| 2   | R     | 62  | THR  |
| 2   | R     | 65  | PHE  |
| 2   | R     | 74  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 76  | MET  |
| 2   | R     | 97  | ASN  |
| 2   | R     | 106 | ARG  |
| 2   | R     | 117 | THR  |
| 2   | R     | 123 | GLN  |
| 2   | S     | 13  | LYS  |
| 2   | S     | 14  | GLU  |
| 2   | S     | 18  | LEU  |
| 2   | S     | 34  | THR  |
| 2   | S     | 39  | LEU  |
| 2   | S     | 49  | GLN  |
| 2   | S     | 50  | ASP  |
| 2   | S     | 54  | GLU  |
| 2   | S     | 55  | VAL  |
| 2   | S     | 56  | ASP  |
| 2   | S     | 62  | THR  |
| 2   | S     | 65  | PHE  |
| 2   | S     | 74  | ARG  |
| 2   | S     | 76  | MET  |
| 2   | S     | 97  | ASN  |
| 2   | S     | 106 | ARG  |
| 2   | S     | 117 | THR  |
| 2   | S     | 123 | GLN  |
| 2   | T     | 13  | LYS  |
| 2   | T     | 14  | GLU  |
| 2   | T     | 18  | LEU  |
| 2   | T     | 36  | MET  |
| 2   | T     | 39  | LEU  |
| 2   | T     | 49  | GLN  |
| 2   | T     | 50  | ASP  |
| 2   | T     | 54  | GLU  |
| 2   | T     | 55  | VAL  |
| 2   | T     | 56  | ASP  |
| 2   | T     | 62  | THR  |
| 2   | T     | 65  | PHE  |
| 2   | T     | 74  | ARG  |
| 2   | T     | 76  | MET  |
| 2   | T     | 97  | ASN  |
| 2   | T     | 106 | ARG  |
| 2   | T     | 117 | THR  |
| 2   | T     | 123 | GLN  |
| 2   | T     | 133 | ASP  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (225) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 64  | ASN  |
| 1   | A     | 73  | ASN  |
| 1   | A     | 81  | GLN  |
| 1   | A     | 83  | GLN  |
| 1   | A     | 129 | ASN  |
| 1   | A     | 212 | GLN  |
| 1   | A     | 323 | ASN  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 349 | ASN  |
| 1   | A     | 368 | GLN  |
| 1   | A     | 376 | GLN  |
| 1   | A     | 387 | ASN  |
| 1   | A     | 438 | ASN  |
| 1   | A     | 480 | ASN  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 510 | GLN  |
| 1   | A     | 518 | ASN  |
| 1   | A     | 551 | ASN  |
| 1   | A     | 553 | GLN  |
| 1   | A     | 576 | ASN  |
| 1   | A     | 577 | HIS  |
| 1   | A     | 581 | GLN  |
| 1   | A     | 597 | ASN  |
| 1   | A     | 629 | ASN  |
| 1   | A     | 639 | ASN  |
| 1   | A     | 655 | ASN  |
| 1   | A     | 709 | ASN  |
| 1   | A     | 747 | ASN  |
| 1   | A     | 750 | GLN  |
| 1   | A     | 759 | GLN  |
| 1   | A     | 767 | GLN  |
| 1   | A     | 770 | ASN  |
| 1   | A     | 781 | ASN  |
| 1   | A     | 794 | GLN  |
| 1   | B     | 64  | ASN  |
| 1   | B     | 73  | ASN  |
| 1   | B     | 81  | GLN  |
| 1   | B     | 83  | GLN  |
| 1   | B     | 129 | ASN  |
| 1   | B     | 212 | GLN  |
| 1   | B     | 323 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 337 | ASN  |
| 1   | B     | 349 | ASN  |
| 1   | B     | 368 | GLN  |
| 1   | B     | 376 | GLN  |
| 1   | B     | 387 | ASN  |
| 1   | B     | 438 | ASN  |
| 1   | B     | 480 | ASN  |
| 1   | B     | 507 | GLN  |
| 1   | B     | 510 | GLN  |
| 1   | B     | 518 | ASN  |
| 1   | B     | 551 | ASN  |
| 1   | B     | 553 | GLN  |
| 1   | B     | 576 | ASN  |
| 1   | B     | 577 | HIS  |
| 1   | B     | 581 | GLN  |
| 1   | B     | 597 | ASN  |
| 1   | B     | 629 | ASN  |
| 1   | B     | 639 | ASN  |
| 1   | B     | 655 | ASN  |
| 1   | B     | 709 | ASN  |
| 1   | B     | 727 | GLN  |
| 1   | B     | 747 | ASN  |
| 1   | B     | 750 | GLN  |
| 1   | B     | 759 | GLN  |
| 1   | B     | 767 | GLN  |
| 1   | B     | 770 | ASN  |
| 1   | B     | 781 | ASN  |
| 1   | B     | 794 | GLN  |
| 1   | C     | 73  | ASN  |
| 1   | C     | 81  | GLN  |
| 1   | C     | 83  | GLN  |
| 1   | C     | 129 | ASN  |
| 1   | C     | 212 | GLN  |
| 1   | C     | 323 | ASN  |
| 1   | C     | 337 | ASN  |
| 1   | C     | 349 | ASN  |
| 1   | C     | 368 | GLN  |
| 1   | C     | 376 | GLN  |
| 1   | C     | 387 | ASN  |
| 1   | C     | 438 | ASN  |
| 1   | C     | 480 | ASN  |
| 1   | C     | 507 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 510 | GLN  |
| 1   | C     | 518 | ASN  |
| 1   | C     | 551 | ASN  |
| 1   | C     | 553 | GLN  |
| 1   | C     | 576 | ASN  |
| 1   | C     | 577 | HIS  |
| 1   | C     | 581 | GLN  |
| 1   | C     | 597 | ASN  |
| 1   | C     | 629 | ASN  |
| 1   | C     | 639 | ASN  |
| 1   | C     | 655 | ASN  |
| 1   | C     | 709 | ASN  |
| 1   | C     | 727 | GLN  |
| 1   | C     | 740 | GLN  |
| 1   | C     | 747 | ASN  |
| 1   | C     | 750 | GLN  |
| 1   | C     | 759 | GLN  |
| 1   | C     | 767 | GLN  |
| 1   | C     | 770 | ASN  |
| 1   | C     | 781 | ASN  |
| 1   | C     | 794 | GLN  |
| 1   | D     | 64  | ASN  |
| 1   | D     | 73  | ASN  |
| 1   | D     | 81  | GLN  |
| 1   | D     | 83  | GLN  |
| 1   | D     | 129 | ASN  |
| 1   | D     | 212 | GLN  |
| 1   | D     | 323 | ASN  |
| 1   | D     | 337 | ASN  |
| 1   | D     | 349 | ASN  |
| 1   | D     | 368 | GLN  |
| 1   | D     | 376 | GLN  |
| 1   | D     | 387 | ASN  |
| 1   | D     | 438 | ASN  |
| 1   | D     | 480 | ASN  |
| 1   | D     | 507 | GLN  |
| 1   | D     | 510 | GLN  |
| 1   | D     | 518 | ASN  |
| 1   | D     | 551 | ASN  |
| 1   | D     | 553 | GLN  |
| 1   | D     | 576 | ASN  |
| 1   | D     | 577 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 581 | GLN  |
| 1   | D     | 597 | ASN  |
| 1   | D     | 629 | ASN  |
| 1   | D     | 639 | ASN  |
| 1   | D     | 655 | ASN  |
| 1   | D     | 709 | ASN  |
| 1   | D     | 727 | GLN  |
| 1   | D     | 747 | ASN  |
| 1   | D     | 750 | GLN  |
| 1   | D     | 759 | GLN  |
| 1   | D     | 767 | GLN  |
| 1   | D     | 770 | ASN  |
| 1   | D     | 781 | ASN  |
| 1   | D     | 794 | GLN  |
| 1   | E     | 73  | ASN  |
| 1   | E     | 81  | GLN  |
| 1   | E     | 83  | GLN  |
| 1   | E     | 129 | ASN  |
| 1   | E     | 212 | GLN  |
| 1   | E     | 323 | ASN  |
| 1   | E     | 337 | ASN  |
| 1   | E     | 349 | ASN  |
| 1   | E     | 368 | GLN  |
| 1   | E     | 376 | GLN  |
| 1   | E     | 387 | ASN  |
| 1   | E     | 438 | ASN  |
| 1   | E     | 480 | ASN  |
| 1   | E     | 507 | GLN  |
| 1   | E     | 510 | GLN  |
| 1   | E     | 518 | ASN  |
| 1   | E     | 551 | ASN  |
| 1   | E     | 553 | GLN  |
| 1   | E     | 576 | ASN  |
| 1   | E     | 577 | HIS  |
| 1   | E     | 581 | GLN  |
| 1   | E     | 597 | ASN  |
| 1   | E     | 629 | ASN  |
| 1   | E     | 639 | ASN  |
| 1   | E     | 655 | ASN  |
| 1   | E     | 709 | ASN  |
| 1   | E     | 727 | GLN  |
| 1   | E     | 747 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 750 | GLN  |
| 1   | E     | 759 | GLN  |
| 1   | E     | 767 | GLN  |
| 1   | E     | 770 | ASN  |
| 1   | E     | 781 | ASN  |
| 1   | E     | 794 | GLN  |
| 1   | F     | 65  | ASN  |
| 1   | F     | 73  | ASN  |
| 1   | F     | 81  | GLN  |
| 1   | F     | 83  | GLN  |
| 1   | F     | 129 | ASN  |
| 1   | F     | 212 | GLN  |
| 1   | F     | 323 | ASN  |
| 1   | F     | 337 | ASN  |
| 1   | F     | 349 | ASN  |
| 1   | F     | 368 | GLN  |
| 1   | F     | 376 | GLN  |
| 1   | F     | 387 | ASN  |
| 1   | F     | 438 | ASN  |
| 1   | F     | 480 | ASN  |
| 1   | F     | 507 | GLN  |
| 1   | F     | 510 | GLN  |
| 1   | F     | 518 | ASN  |
| 1   | F     | 551 | ASN  |
| 1   | F     | 553 | GLN  |
| 1   | F     | 576 | ASN  |
| 1   | F     | 577 | HIS  |
| 1   | F     | 581 | GLN  |
| 1   | F     | 597 | ASN  |
| 1   | F     | 629 | ASN  |
| 1   | F     | 639 | ASN  |
| 1   | F     | 655 | ASN  |
| 1   | F     | 709 | ASN  |
| 1   | F     | 747 | ASN  |
| 1   | F     | 750 | GLN  |
| 1   | F     | 759 | GLN  |
| 1   | F     | 767 | GLN  |
| 1   | F     | 770 | ASN  |
| 1   | F     | 781 | ASN  |
| 1   | F     | 794 | GLN  |
| 2   | O     | 49  | GLN  |
| 2   | O     | 111 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 143 | GLN  |
| 2   | P     | 49  | GLN  |
| 2   | P     | 111 | ASN  |
| 2   | P     | 143 | GLN  |
| 2   | Q     | 49  | GLN  |
| 2   | Q     | 111 | ASN  |
| 2   | Q     | 143 | GLN  |
| 2   | R     | 49  | GLN  |
| 2   | R     | 111 | ASN  |
| 2   | R     | 143 | GLN  |
| 2   | S     | 49  | GLN  |
| 2   | S     | 111 | ASN  |
| 2   | S     | 143 | GLN  |
| 2   | T     | 49  | GLN  |
| 2   | T     | 111 | ASN  |
| 2   | T     | 143 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 30 are monoatomic - leaving 6 for Mogul analysis.

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 |
| 5   | 3AT  | A     | 903 | 4    | 24,32,32     | 1.41 | 4 (16%)  | 26,50,50    | 1.37 | 4 (15%)  |
| 5   | 3AT  | B     | 904 | 4    | 24,32,32     | 1.40 | 4 (16%)  | 26,50,50    | 1.35 | 4 (15%)  |
| 5   | 3AT  | C     | 905 | 4    | 24,32,32     | 1.45 | 4 (16%)  | 26,50,50    | 1.37 | 4 (15%)  |
| 5   | 3AT  | D     | 906 | 4    | 24,32,32     | 1.42 | 4 (16%)  | 26,50,50    | 1.34 | 4 (15%)  |
| 5   | 3AT  | E     | 907 | 4    | 24,32,32     | 1.37 | 4 (16%)  | 26,50,50    | 1.31 | 4 (15%)  |
| 5   | 3AT  | F     | 908 | 4    | 24,32,32     | 1.36 | 4 (16%)  | 26,50,50    | 1.33 | 4 (15%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | 3AT  | A     | 903 | 4    | -       | 0/18/34/34 | 0/3/3/3 |
| 5   | 3AT  | B     | 904 | 4    | -       | 0/18/34/34 | 0/3/3/3 |
| 5   | 3AT  | C     | 905 | 4    | -       | 0/18/34/34 | 0/3/3/3 |
| 5   | 3AT  | D     | 906 | 4    | -       | 0/18/34/34 | 0/3/3/3 |
| 5   | 3AT  | E     | 907 | 4    | -       | 0/18/34/34 | 0/3/3/3 |
| 5   | 3AT  | F     | 908 | 4    | -       | 0/18/34/34 | 0/3/3/3 |

All (24) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | C     | 905 | 3AT  | PG-O2G | -3.16 | 1.43        | 1.54     |
| 5   | E     | 907 | 3AT  | PG-O2G | -3.14 | 1.43        | 1.54     |
| 5   | A     | 903 | 3AT  | PG-O2G | -3.04 | 1.43        | 1.54     |
| 5   | B     | 904 | 3AT  | PG-O2G | -3.01 | 1.43        | 1.54     |
| 5   | D     | 906 | 3AT  | PG-O2G | -2.89 | 1.44        | 1.54     |
| 5   | F     | 908 | 3AT  | PG-O2G | -2.86 | 1.44        | 1.54     |
| 5   | B     | 904 | 3AT  | C8-N7  | -2.72 | 1.29        | 1.34     |
| 5   | E     | 907 | 3AT  | C8-N7  | -2.63 | 1.29        | 1.34     |
| 5   | D     | 906 | 3AT  | C8-N7  | -2.61 | 1.29        | 1.34     |
| 5   | F     | 908 | 3AT  | C8-N7  | -2.60 | 1.29        | 1.34     |
| 5   | C     | 905 | 3AT  | C8-N7  | -2.59 | 1.29        | 1.34     |
| 5   | A     | 903 | 3AT  | C8-N7  | -2.50 | 1.29        | 1.34     |
| 5   | E     | 907 | 3AT  | C2-N3  | 2.24  | 1.36        | 1.32     |
| 5   | B     | 904 | 3AT  | C2-N3  | 2.35  | 1.36        | 1.32     |
| 5   | F     | 908 | 3AT  | C2-N3  | 2.36  | 1.36        | 1.32     |
| 5   | D     | 906 | 3AT  | C2-N3  | 2.38  | 1.36        | 1.32     |
| 5   | A     | 903 | 3AT  | C2-N3  | 2.39  | 1.36        | 1.32     |
| 5   | C     | 905 | 3AT  | C2-N3  | 2.39  | 1.36        | 1.32     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 5   | E     | 907 | 3AT  | C4-N3 | 2.55 | 1.39        | 1.35     |
| 5   | F     | 908 | 3AT  | C4-N3 | 2.72 | 1.39        | 1.35     |
| 5   | B     | 904 | 3AT  | C4-N3 | 2.90 | 1.39        | 1.35     |
| 5   | C     | 905 | 3AT  | C4-N3 | 3.14 | 1.40        | 1.35     |
| 5   | A     | 903 | 3AT  | C4-N3 | 3.21 | 1.40        | 1.35     |
| 5   | D     | 906 | 3AT  | C4-N3 | 3.39 | 1.40        | 1.35     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | C     | 905 | 3AT  | N3-C2-N1   | -3.23 | 126.42      | 128.89   |
| 5   | A     | 903 | 3AT  | N3-C2-N1   | -3.09 | 126.53      | 128.89   |
| 5   | B     | 904 | 3AT  | N3-C2-N1   | -3.02 | 126.58      | 128.89   |
| 5   | F     | 908 | 3AT  | N3-C2-N1   | -2.98 | 126.61      | 128.89   |
| 5   | D     | 906 | 3AT  | N3-C2-N1   | -2.94 | 126.64      | 128.89   |
| 5   | E     | 907 | 3AT  | N3-C2-N1   | -2.65 | 126.87      | 128.89   |
| 5   | B     | 904 | 3AT  | O2A-PA-O3A | 2.76  | 117.63      | 105.09   |
| 5   | E     | 907 | 3AT  | O2A-PA-O3A | 2.79  | 117.73      | 105.09   |
| 5   | F     | 908 | 3AT  | O2A-PA-O3A | 2.80  | 117.79      | 105.09   |
| 5   | D     | 906 | 3AT  | O2A-PA-O3A | 2.84  | 117.97      | 105.09   |
| 5   | A     | 903 | 3AT  | O2A-PA-O3A | 2.84  | 117.97      | 105.09   |
| 5   | C     | 905 | 3AT  | O2A-PA-O3A | 2.84  | 117.99      | 105.09   |
| 5   | D     | 906 | 3AT  | C4-C5-N7   | 2.85  | 112.11      | 109.48   |
| 5   | E     | 907 | 3AT  | C4-C5-N7   | 2.88  | 112.12      | 109.48   |
| 5   | C     | 905 | 3AT  | C4-C5-N7   | 2.90  | 112.14      | 109.48   |
| 5   | F     | 908 | 3AT  | C4-C5-N7   | 2.93  | 112.18      | 109.48   |
| 5   | B     | 904 | 3AT  | C4-C5-N7   | 2.96  | 112.20      | 109.48   |
| 5   | A     | 903 | 3AT  | C4-C5-N7   | 3.09  | 112.32      | 109.48   |
| 5   | D     | 906 | 3AT  | PB-O3B-PG  | 3.32  | 143.78      | 132.67   |
| 5   | E     | 907 | 3AT  | PB-O3B-PG  | 3.35  | 143.91      | 132.67   |
| 5   | F     | 908 | 3AT  | PB-O3B-PG  | 3.37  | 143.97      | 132.67   |
| 5   | A     | 903 | 3AT  | PB-O3B-PG  | 3.38  | 144.01      | 132.67   |
| 5   | C     | 905 | 3AT  | PB-O3B-PG  | 3.40  | 144.06      | 132.67   |
| 5   | B     | 904 | 3AT  | PB-O3B-PG  | 3.46  | 144.25      | 132.67   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 903 | 3AT  | 1       | 0            |
| 5   | B     | 904 | 3AT  | 1       | 0            |
| 5   | C     | 905 | 3AT  | 1       | 0            |
| 5   | D     | 906 | 3AT  | 1       | 0            |
| 5   | E     | 907 | 3AT  | 1       | 0            |
| 5   | F     | 908 | 3AT  | 1       | 0            |

## 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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 735/777 (94%)   | 0.37   | 39 (5%) 30 30  | 26, 80, 136, 148      | 0     |
| 1   | B     | 735/777 (94%)   | 0.30   | 32 (4%) 38 37  | 27, 80, 136, 148      | 0     |
| 1   | C     | 735/777 (94%)   | 0.31   | 26 (3%) 48 47  | 27, 80, 136, 148      | 0     |
| 1   | D     | 735/777 (94%)   | 0.32   | 29 (3%) 43 42  | 27, 80, 136, 150      | 0     |
| 1   | E     | 735/777 (94%)   | 0.34   | 36 (4%) 33 32  | 26, 80, 136, 148      | 0     |
| 1   | F     | 735/777 (94%)   | 0.36   | 41 (5%) 28 27  | 27, 80, 136, 148      | 0     |
| 2   | O     | 146/149 (97%)   | 0.13   | 2 (1%) 78 79   | 33, 63, 124, 131      | 0     |
| 2   | P     | 146/149 (97%)   | 0.13   | 2 (1%) 78 79   | 33, 63, 124, 131      | 0     |
| 2   | Q     | 146/149 (97%)   | 0.12   | 2 (1%) 78 79   | 33, 62, 124, 131      | 0     |
| 2   | R     | 146/149 (97%)   | 0.16   | 2 (1%) 78 79   | 33, 63, 124, 131      | 0     |
| 2   | S     | 146/149 (97%)   | 0.15   | 4 (2%) 58 58   | 32, 62, 124, 131      | 0     |
| 2   | T     | 146/149 (97%)   | 0.12   | 3 (2%) 67 67   | 33, 62, 124, 131      | 0     |
| All | All   | 5286/5556 (95%) | 0.30   | 218 (4%) 41 40 | 26, 76, 134, 150      | 0     |

All (218) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 126 | ASN  | 8.7  |
| 1   | D     | 162 | ASN  | 7.9  |
| 1   | A     | 222 | ASN  | 7.8  |
| 1   | D     | 171 | TYR  | 7.5  |
| 1   | B     | 126 | ASN  | 7.3  |
| 1   | B     | 171 | TYR  | 7.0  |
| 1   | F     | 162 | ASN  | 7.0  |
| 1   | E     | 171 | TYR  | 6.7  |
| 1   | D     | 225 | ILE  | 6.6  |
| 1   | C     | 171 | TYR  | 6.6  |
| 1   | A     | 171 | TYR  | 6.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 225 | ILE  | 6.5  |
| 1   | C     | 225 | ILE  | 6.2  |
| 1   | C     | 162 | ASN  | 6.0  |
| 1   | B     | 218 | LEU  | 5.9  |
| 1   | A     | 786 | GLU  | 5.8  |
| 1   | F     | 163 | SER  | 5.7  |
| 1   | E     | 125 | LYS  | 5.6  |
| 1   | C     | 126 | ASN  | 5.6  |
| 1   | F     | 225 | ILE  | 5.6  |
| 1   | B     | 212 | GLN  | 5.6  |
| 1   | F     | 171 | TYR  | 5.5  |
| 1   | E     | 225 | ILE  | 5.4  |
| 1   | A     | 162 | ASN  | 5.4  |
| 1   | A     | 221 | ASN  | 5.3  |
| 1   | B     | 162 | ASN  | 5.3  |
| 1   | E     | 111 | LEU  | 5.2  |
| 1   | F     | 212 | GLN  | 5.2  |
| 1   | C     | 222 | ASN  | 5.2  |
| 1   | B     | 786 | GLU  | 5.2  |
| 1   | E     | 127 | SER  | 5.2  |
| 1   | C     | 163 | SER  | 5.1  |
| 1   | A     | 111 | LEU  | 5.1  |
| 1   | D     | 163 | SER  | 5.0  |
| 1   | F     | 126 | ASN  | 4.9  |
| 1   | E     | 218 | LEU  | 4.9  |
| 1   | F     | 204 | ASP  | 4.8  |
| 1   | D     | 126 | ASN  | 4.7  |
| 1   | D     | 125 | LYS  | 4.7  |
| 1   | F     | 260 | TYR  | 4.7  |
| 1   | A     | 214 | PHE  | 4.7  |
| 1   | B     | 237 | PHE  | 4.6  |
| 1   | F     | 222 | ASN  | 4.6  |
| 1   | D     | 206 | SER  | 4.6  |
| 1   | F     | 237 | PHE  | 4.6  |
| 1   | A     | 212 | GLN  | 4.4  |
| 1   | A     | 160 | ALA  | 4.4  |
| 1   | C     | 226 | ASP  | 4.4  |
| 1   | E     | 162 | ASN  | 4.3  |
| 1   | B     | 125 | LYS  | 4.2  |
| 1   | A     | 126 | ASN  | 4.2  |
| 1   | A     | 163 | SER  | 4.2  |
| 1   | C     | 260 | TYR  | 4.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 786 | GLU  | 4.1  |
| 1   | A     | 260 | TYR  | 3.9  |
| 1   | A     | 218 | LEU  | 3.9  |
| 1   | D     | 76  | LEU  | 3.9  |
| 1   | C     | 214 | PHE  | 3.9  |
| 1   | E     | 212 | GLN  | 3.8  |
| 1   | D     | 229 | PHE  | 3.8  |
| 1   | F     | 230 | ILE  | 3.7  |
| 1   | A     | 129 | ASN  | 3.7  |
| 1   | F     | 221 | ASN  | 3.7  |
| 1   | A     | 127 | SER  | 3.6  |
| 1   | D     | 111 | LEU  | 3.6  |
| 1   | A     | 230 | ILE  | 3.6  |
| 1   | D     | 230 | ILE  | 3.5  |
| 1   | F     | 192 | PHE  | 3.5  |
| 2   | S     | 78  | ASP  | 3.5  |
| 1   | C     | 156 | ILE  | 3.4  |
| 1   | E     | 214 | PHE  | 3.4  |
| 2   | R     | 63  | ILE  | 3.4  |
| 1   | A     | 225 | ILE  | 3.4  |
| 1   | B     | 191 | GLU  | 3.4  |
| 2   | Q     | 63  | ILE  | 3.3  |
| 1   | C     | 157 | LYS  | 3.3  |
| 1   | D     | 110 | ASP  | 3.3  |
| 1   | F     | 226 | ASP  | 3.3  |
| 1   | E     | 230 | ILE  | 3.3  |
| 1   | B     | 204 | ASP  | 3.2  |
| 1   | F     | 185 | ASP  | 3.2  |
| 1   | B     | 127 | SER  | 3.2  |
| 1   | A     | 161 | ILE  | 3.2  |
| 1   | D     | 318 | ILE  | 3.2  |
| 1   | F     | 434 | LEU  | 3.2  |
| 1   | E     | 770 | ASN  | 3.1  |
| 1   | F     | 201 | ASP  | 3.1  |
| 1   | A     | 206 | SER  | 3.1  |
| 1   | C     | 218 | LEU  | 3.1  |
| 1   | B     | 214 | PHE  | 3.0  |
| 1   | F     | 111 | LEU  | 3.0  |
| 1   | F     | 156 | ILE  | 3.0  |
| 1   | B     | 160 | ALA  | 3.0  |
| 1   | D     | 237 | PHE  | 3.0  |
| 1   | B     | 156 | ILE  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 237 | PHE  | 2.9  |
| 1   | C     | 259 | LEU  | 2.9  |
| 1   | D     | 161 | ILE  | 2.9  |
| 1   | E     | 135 | VAL  | 2.9  |
| 1   | F     | 184 | LYS  | 2.9  |
| 1   | D     | 421 | LYS  | 2.9  |
| 1   | F     | 441 | VAL  | 2.9  |
| 2   | S     | 52  | ILE  | 2.9  |
| 1   | E     | 444 | PHE  | 2.9  |
| 1   | F     | 205 | SER  | 2.9  |
| 1   | E     | 357 | TRP  | 2.8  |
| 1   | B     | 114 | HIS  | 2.8  |
| 1   | B     | 222 | ASN  | 2.8  |
| 1   | E     | 206 | SER  | 2.8  |
| 1   | E     | 370 | LEU  | 2.8  |
| 1   | B     | 70  | GLU  | 2.8  |
| 1   | C     | 127 | SER  | 2.8  |
| 1   | F     | 420 | LEU  | 2.8  |
| 1   | B     | 118 | GLN  | 2.7  |
| 1   | F     | 218 | LEU  | 2.7  |
| 1   | B     | 787 | THR  | 2.7  |
| 1   | F     | 398 | ILE  | 2.7  |
| 1   | E     | 187 | SER  | 2.7  |
| 1   | C     | 76  | LEU  | 2.7  |
| 1   | F     | 160 | ALA  | 2.7  |
| 1   | E     | 786 | GLU  | 2.7  |
| 1   | D     | 433 | TYR  | 2.6  |
| 1   | B     | 206 | SER  | 2.6  |
| 1   | C     | 191 | GLU  | 2.6  |
| 1   | A     | 203 | SER  | 2.6  |
| 1   | E     | 217 | LYS  | 2.6  |
| 1   | A     | 359 | PRO  | 2.6  |
| 1   | E     | 339 | ILE  | 2.6  |
| 1   | E     | 434 | LEU  | 2.6  |
| 2   | S     | 63  | ILE  | 2.6  |
| 1   | D     | 398 | ILE  | 2.6  |
| 1   | F     | 203 | SER  | 2.6  |
| 1   | A     | 357 | TRP  | 2.6  |
| 1   | A     | 234 | LEU  | 2.6  |
| 1   | C     | 407 | HIS  | 2.5  |
| 2   | P     | 52  | ILE  | 2.5  |
| 1   | E     | 118 | GLN  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 203 | SER  | 2.5  |
| 1   | F     | 114 | HIS  | 2.5  |
| 1   | C     | 230 | ILE  | 2.5  |
| 1   | D     | 245 | PHE  | 2.5  |
| 1   | A     | 208 | LEU  | 2.5  |
| 1   | D     | 212 | GLN  | 2.4  |
| 1   | C     | 213 | LYS  | 2.4  |
| 1   | B     | 357 | TRP  | 2.4  |
| 1   | D     | 213 | LYS  | 2.4  |
| 1   | E     | 419 | ILE  | 2.4  |
| 2   | O     | 77  | LYS  | 2.4  |
| 1   | E     | 435 | LEU  | 2.4  |
| 1   | F     | 229 | PHE  | 2.4  |
| 1   | A     | 158 | ASP  | 2.4  |
| 1   | C     | 111 | LEU  | 2.4  |
| 1   | F     | 214 | PHE  | 2.4  |
| 1   | F     | 405 | LEU  | 2.4  |
| 1   | F     | 191 | GLU  | 2.4  |
| 1   | A     | 370 | LEU  | 2.4  |
| 1   | F     | 435 | LEU  | 2.4  |
| 1   | A     | 66  | LEU  | 2.3  |
| 1   | A     | 213 | LYS  | 2.3  |
| 1   | A     | 76  | LEU  | 2.3  |
| 1   | C     | 185 | ASP  | 2.3  |
| 1   | F     | 158 | ASP  | 2.3  |
| 1   | D     | 87  | LYS  | 2.3  |
| 1   | C     | 192 | PHE  | 2.3  |
| 1   | E     | 769 | SER  | 2.3  |
| 1   | C     | 110 | ASP  | 2.3  |
| 1   | A     | 192 | PHE  | 2.3  |
| 1   | B     | 192 | PHE  | 2.3  |
| 1   | D     | 192 | PHE  | 2.3  |
| 2   | O     | 63  | ILE  | 2.3  |
| 1   | E     | 283 | LEU  | 2.2  |
| 1   | B     | 76  | LEU  | 2.2  |
| 1   | E     | 237 | PHE  | 2.2  |
| 1   | B     | 185 | ASP  | 2.2  |
| 2   | R     | 78  | ASP  | 2.2  |
| 1   | E     | 184 | LYS  | 2.2  |
| 1   | B     | 72  | THR  | 2.2  |
| 1   | A     | 155 | ASN  | 2.2  |
| 1   | C     | 435 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | Q     | 116 | LEU  | 2.2  |
| 1   | A     | 227 | ILE  | 2.2  |
| 2   | T     | 52  | ILE  | 2.2  |
| 1   | A     | 282 | SER  | 2.2  |
| 2   | T     | 74  | ARG  | 2.2  |
| 1   | E     | 222 | ASN  | 2.2  |
| 1   | E     | 110 | ASP  | 2.2  |
| 1   | A     | 421 | LYS  | 2.2  |
| 2   | S     | 79  | THR  | 2.2  |
| 1   | D     | 773 | PHE  | 2.2  |
| 2   | P     | 63  | ILE  | 2.1  |
| 1   | A     | 125 | LYS  | 2.1  |
| 1   | F     | 446 | ILE  | 2.1  |
| 1   | D     | 239 | HIS  | 2.1  |
| 1   | B     | 155 | ASN  | 2.1  |
| 1   | E     | 70  | GLU  | 2.1  |
| 1   | C     | 398 | ILE  | 2.1  |
| 1   | A     | 446 | ILE  | 2.1  |
| 1   | F     | 259 | LEU  | 2.1  |
| 1   | B     | 777 | TYR  | 2.1  |
| 1   | F     | 159 | TYR  | 2.1  |
| 1   | B     | 205 | SER  | 2.1  |
| 1   | B     | 208 | LEU  | 2.1  |
| 1   | F     | 76  | LEU  | 2.1  |
| 1   | C     | 140 | ARG  | 2.1  |
| 1   | E     | 131 | ARG  | 2.1  |
| 1   | F     | 476 | VAL  | 2.1  |
| 1   | A     | 177 | ILE  | 2.0  |
| 2   | T     | 116 | LEU  | 2.0  |
| 1   | F     | 125 | LYS  | 2.0  |
| 1   | A     | 131 | ARG  | 2.0  |
| 1   | D     | 156 | ILE  | 2.0  |
| 1   | B     | 444 | PHE  | 2.0  |
| 1   | D     | 259 | LEU  | 2.0  |
| 1   | B     | 282 | SER  | 2.0  |
| 1   | E     | 105 | TYR  | 2.0  |
| 1   | D     | 214 | PHE  | 2.0  |
| 1   | E     | 201 | ASP  | 2.0  |
| 1   | F     | 130 | SER  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 5   | 3AT  | A     | 903 | 30/30 | 0.92 | 0.24 | -0.25 | 60,74,93,94                | 0     |
| 5   | 3AT  | C     | 905 | 30/30 | 0.92 | 0.22 | -0.32 | 62,73,94,95                | 0     |
| 5   | 3AT  | B     | 904 | 30/30 | 0.92 | 0.23 | -0.39 | 58,73,93,94                | 0     |
| 3   | CA   | T     | 812 | 1/1   | 0.98 | 0.16 | -0.56 | 49,49,49,49                | 0     |
| 3   | CA   | Q     | 806 | 1/1   | 0.97 | 0.16 | -0.62 | 57,57,57,57                | 0     |
| 3   | CA   | P     | 703 | 1/1   | 0.97 | 0.15 | -0.66 | 62,62,62,62                | 0     |
| 5   | 3AT  | E     | 907 | 30/30 | 0.93 | 0.22 | -0.69 | 60,74,96,97                | 0     |
| 5   | 3AT  | F     | 908 | 30/30 | 0.92 | 0.21 | -0.71 | 61,75,94,95                | 0     |
| 3   | CA   | O     | 802 | 1/1   | 0.98 | 0.14 | -0.84 | 52,52,52,52                | 0     |
| 5   | 3AT  | D     | 906 | 30/30 | 0.92 | 0.21 | -0.85 | 58,74,94,95                | 0     |
| 3   | CA   | T     | 811 | 1/1   | 0.95 | 0.17 | -1.04 | 33,33,33,33                | 0     |
| 3   | CA   | S     | 809 | 1/1   | 0.95 | 0.16 | -1.04 | 26,26,26,26                | 0     |
| 3   | CA   | S     | 709 | 1/1   | 0.96 | 0.11 | -1.08 | 57,57,57,57                | 0     |
| 3   | CA   | O     | 801 | 1/1   | 0.98 | 0.16 | -1.08 | 30,30,30,30                | 0     |
| 3   | CA   | R     | 807 | 1/1   | 0.97 | 0.14 | -1.15 | 33,33,33,33                | 0     |
| 3   | CA   | R     | 808 | 1/1   | 0.98 | 0.11 | -1.19 | 54,54,54,54                | 0     |
| 3   | CA   | Q     | 705 | 1/1   | 0.93 | 0.10 | -1.20 | 55,55,55,55                | 0     |
| 3   | CA   | P     | 804 | 1/1   | 0.98 | 0.10 | -1.29 | 52,52,52,52                | 0     |
| 3   | CA   | S     | 810 | 1/1   | 0.99 | 0.12 | -1.44 | 56,56,56,56                | 0     |
| 3   | CA   | T     | 711 | 1/1   | 0.96 | 0.10 | -1.44 | 55,55,55,55                | 0     |
| 3   | CA   | R     | 707 | 1/1   | 0.96 | 0.10 | -1.64 | 62,62,62,62                | 0     |
| 3   | CA   | P     | 803 | 1/1   | 0.98 | 0.14 | -1.71 | 31,31,31,31                | 0     |
| 3   | CA   | Q     | 805 | 1/1   | 0.95 | 0.17 | -2.04 | 27,27,27,27                | 0     |
| 3   | CA   | O     | 701 | 1/1   | 0.93 | 0.06 | -3.16 | 51,51,51,51                | 0     |
| 4   | MG   | C     | 903 | 1/1   | 0.93 | 0.15 | -     | 9,9,9,9                    | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|-----------------------------|-------|
| 4   | MG   | F     | 907 | 1/1   | 0.98 | 0.11 | -    | 34,34,34,34                 | 0     |
| 4   | MG   | E     | 906 | 1/1   | 0.97 | 0.14 | -    | 26,26,26,26                 | 0     |
| 4   | MG   | A     | 902 | 1/1   | 0.97 | 0.16 | -    | 28,28,28,28                 | 0     |
| 4   | MG   | F     | 906 | 1/1   | 0.97 | 0.15 | -    | 11,11,11,11                 | 0     |
| 4   | MG   | E     | 905 | 1/1   | 0.98 | 0.13 | -    | 20,20,20,20                 | 0     |
| 4   | MG   | D     | 905 | 1/1   | 0.97 | 0.10 | -    | 43,43,43,43                 | 0     |
| 4   | MG   | A     | 901 | 1/1   | 0.96 | 0.20 | -    | 5,5,5,5                     | 0     |
| 4   | MG   | B     | 902 | 1/1   | 0.94 | 0.21 | -    | 17,17,17,17                 | 0     |
| 4   | MG   | C     | 904 | 1/1   | 0.98 | 0.15 | -    | 26,26,26,26                 | 0     |
| 4   | MG   | D     | 904 | 1/1   | 0.95 | 0.17 | -    | 8,8,8,8                     | 0     |
| 4   | MG   | B     | 903 | 1/1   | 0.98 | 0.13 | -    | 25,25,25,25                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.