



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1K90  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin and 3' deoxy-ATP  
Authors : Drum, C.L.; Yan, S.-Z.; Bard, J.; Shen, Y.-Q.; Lu, D.; Soelaiman, S.; Grabarek, Z.; Bohm, A.; Tang, W.-J.  
Deposited on : 2001-10-26  
Resolution : 2.75 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

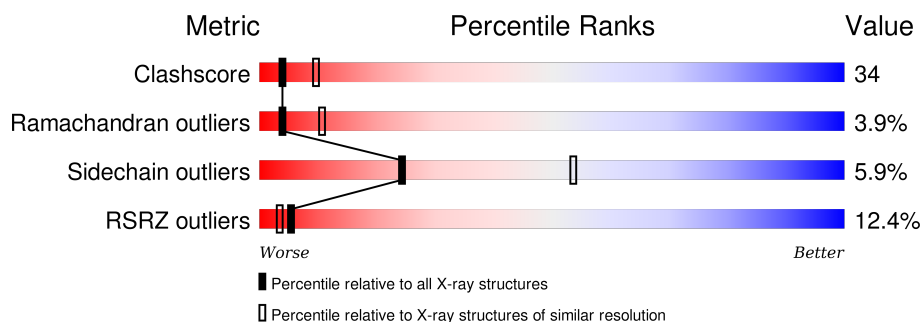
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 102246                      | 3829 (2.80-2.72)                                      |
| Ramachandran outliers | 100387                      | 3767 (2.80-2.72)                                      |
| Sidechain outliers    | 100360                      | 3770 (2.80-2.72)                                      |
| RSRZ outliers         | 91569                       | 3352 (2.80-2.72)                                      |

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     | 510    |                  |
| 1   | B     | 510    |                  |
| 1   | C     | 510    |                  |
| 2   | D     | 148    |                  |
| 2   | E     | 148    |                  |
| 2   | F     | 148    |                  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15357 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     | 485      | Total | C    | N   | O   | S | 65      | 0       | 0     |
|     |       |          | 3952  | 2528 | 673 | 748 | 3 |         |         |       |
| 1   | B     | 465      | Total | C    | N   | O   | S | 113     | 0       | 0     |
|     |       |          | 3794  | 2431 | 642 | 718 | 3 |         |         |       |
| 1   | C     | 503      | Total | C    | N   | O   | S | 166     | 0       | 0     |
|     |       |          | 4094  | 2616 | 696 | 779 | 3 |         |         |       |

- Molecule 2 is a protein called CALMODULIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | D     | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1125  | 690 | 181 | 245 | 9 |         |         |       |
| 2   | E     | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1125  | 690 | 181 | 245 | 9 |         |         |       |
| 2   | F     | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1125  | 690 | 181 | 245 | 9 |         |         |       |

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

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | D     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | F     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | E     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 4 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

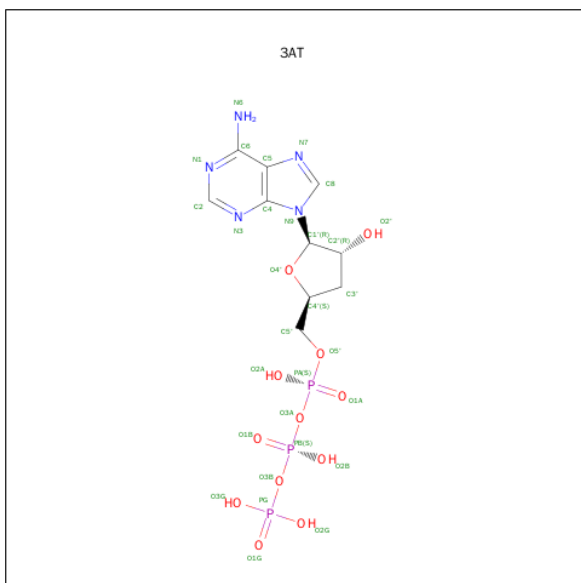
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | B     | 1        | Total | Yb | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | A     | 1        | Total Yb<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total Yb<br>1 1 | 0       | 0       |

- Molecule 5 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{12}\text{P}_3$ ).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 5   | A     | 1        | Total<br>30 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |
| 5   | B     | 1        | Total<br>30 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |
| 5   | C     | 1        | Total<br>30 | C<br>10 | N<br>5 | O<br>12 | P<br>3 | 0       | 0       |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 6   | A     | 10       | Total O<br>10 10 | 0       | 0       |
| 6   | B     | 8        | Total O<br>8 8   | 0       | 0       |
| 6   | C     | 22       | Total O<br>22 22 | 0       | 0       |
| 6   | D     | 1        | Total O<br>1 1   | 0       | 0       |

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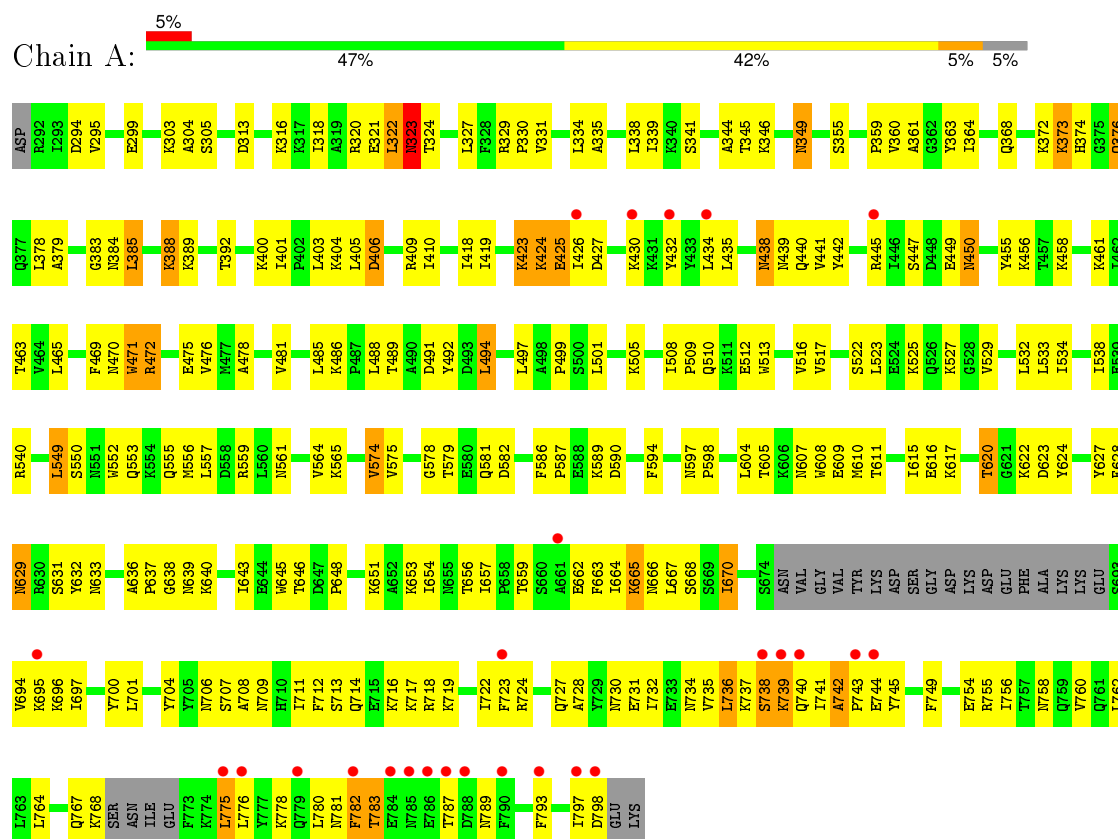
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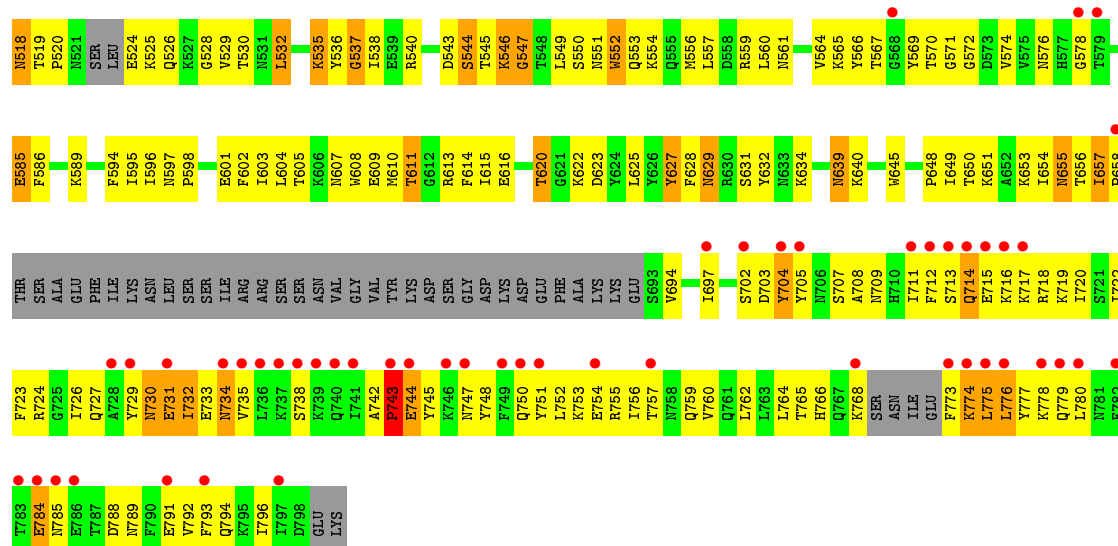
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6   | F     | 2        | Total | O | 0       | 0       |
|     |       |          | 2     | 2 |         |         |

### 3 Residue-property plots

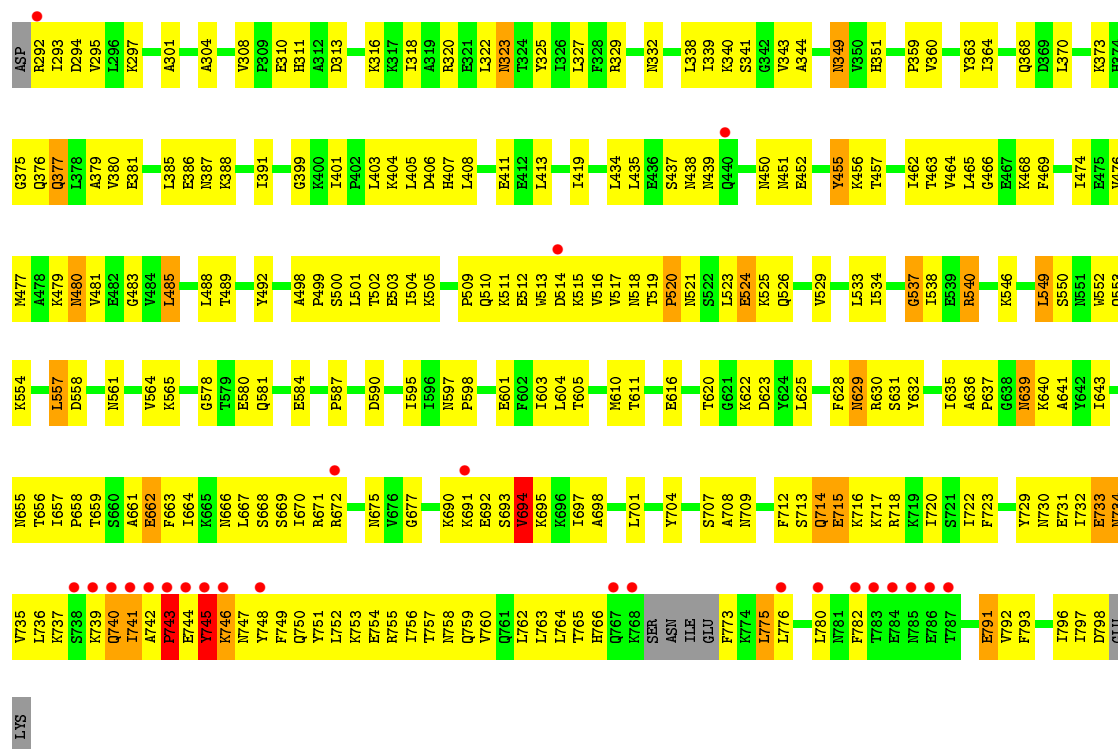
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $RSRZ > 2$ ). 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

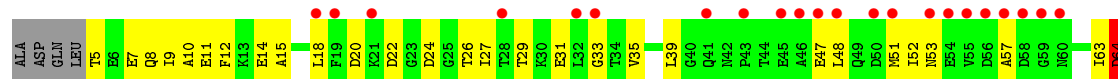
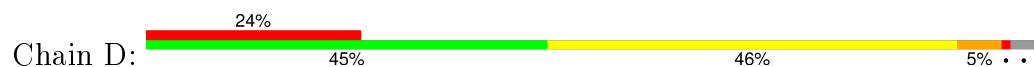


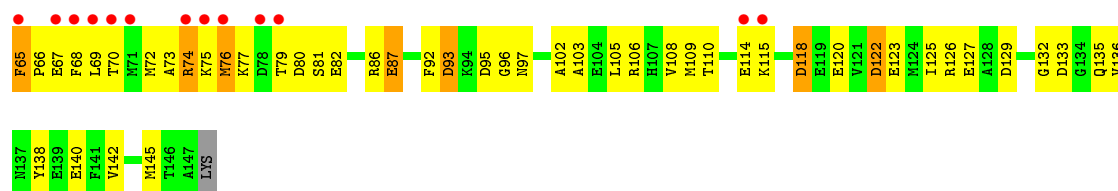


• Molecule 1: CALMODULIN-SENSITIVE ADENYLATE CYCLASE

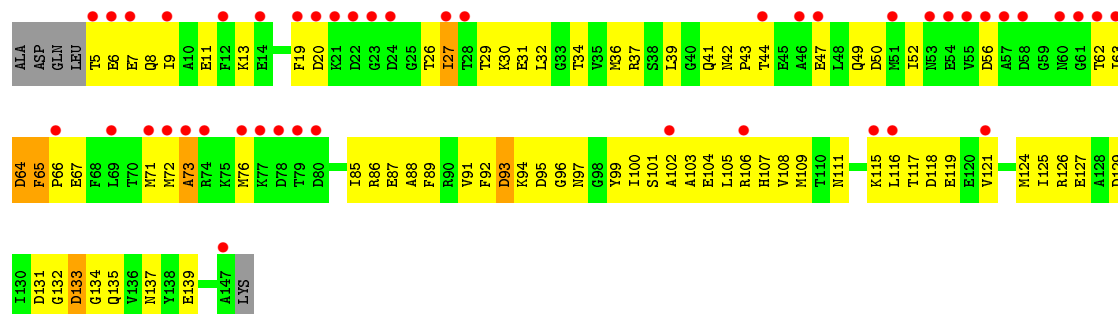
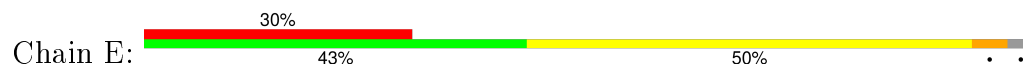


• Molecule 2: CALMODULIN

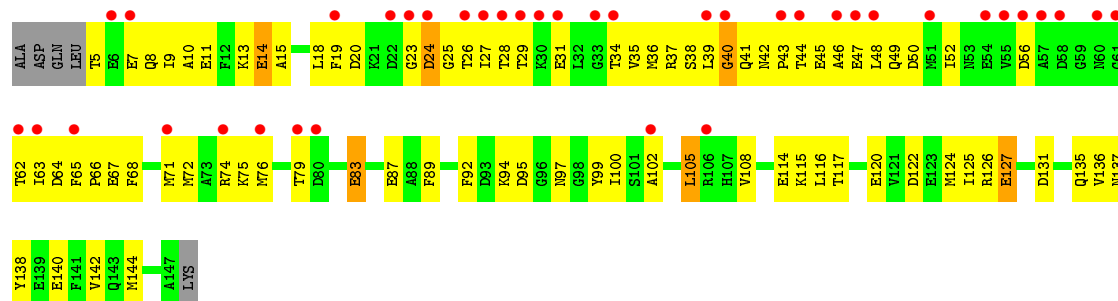
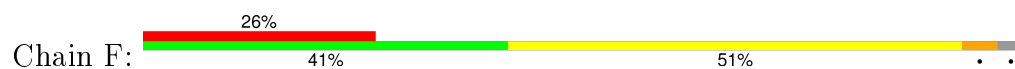




• Molecule 2: CALMODULIN



• Molecule 2: CALMODULIN





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | I 2 2 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 116.10Å 166.10Å 343.33Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 19.97 – 2.75<br>29.90 – 2.64                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.7 (19.97-2.75)<br>95.5 (29.90-2.64)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.25 (at 2.64Å)   | Xtriage          |
| Refinement program  | CNS 1.0   | Depositor        |
| R, $R_{free}$   | 0.215 , 0.286<br>0.251 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set   | No test flags present.                                      | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 66.7  | Xtriage          |
| Anisotropy  | 0.387   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 71.7   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Outliers  | 0 of 93302 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 15357   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 90.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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, YB, 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     | 0.31         | 0/4027      | 0.59        | 1/5419 (0.0%)  |
| 1   | B     | 0.30         | 0/3867      | 0.57        | 1/5204 (0.0%)  |
| 1   | C     | 0.32         | 0/4172      | 0.56        | 1/5613 (0.0%)  |
| 2   | D     | 0.29         | 0/1137      | 0.47        | 0/1527         |
| 2   | E     | 0.26         | 0/1137      | 0.45        | 0/1527         |
| 2   | F     | 0.30         | 0/1137      | 0.49        | 1/1527 (0.1%)  |
| All | All   | 0.30         | 0/15477     | 0.55        | 4/20817 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1   | A     | 738 | SER  | N-CA-C | -10.34 | 83.07       | 111.00   |
| 1   | B     | 743 | PRO  | N-CA-C | 5.65   | 126.80      | 112.10   |
| 1   | C     | 745 | TYR  | N-CA-C | -5.50  | 96.14       | 111.00   |
| 2   | F     | 40  | GLY  | N-CA-C | 5.08   | 125.81      | 113.10   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 3952  | 0        | 3999     | 257     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 3794  | 0        | 3828     | 325     | 0            |
| 1   | C     | 4094  | 0        | 4134     | 248     | 0            |
| 2   | D     | 1125  | 0        | 1049     | 64      | 0            |
| 2   | E     | 1125  | 0        | 1049     | 89      | 0            |
| 2   | F     | 1125  | 0        | 1049     | 86      | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 2     | 0        | 0        | 0       | 0            |
| 3   | F     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 30    | 0        | 12       | 2       | 0            |
| 5   | B     | 30    | 0        | 12       | 1       | 0            |
| 5   | C     | 30    | 0        | 12       | 0       | 0            |
| 6   | A     | 10    | 0        | 0        | 0       | 0            |
| 6   | B     | 8     | 0        | 0        | 1       | 0            |
| 6   | C     | 22    | 0        | 0        | 1       | 0            |
| 6   | D     | 1     | 0        | 0        | 0       | 0            |
| 6   | F     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 15357 | 0        | 15144    | 1026    | 0            |

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 34.

All (1026) 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:B:616:GLU:HA   | 1:B:620:THR:HG22 | 1.37                     | 1.06              |
| 1:B:489:THR:HG22 | 1:B:490:ALA:H    | 1.21                     | 1.03              |
| 1:B:325:TYR:HB2  | 1:B:498:ALA:HB3  | 1.37                     | 1.03              |
| 1:C:659:THR:HG22 | 1:C:661:ALA:H    | 1.21                     | 1.03              |
| 1:A:783:THR:HB   | 1:A:789:ASN:HD21 | 1.30                     | 0.96              |
| 1:B:324:THR:HG22 | 1:B:499:PRO:HA   | 1.48                     | 0.96              |
| 1:B:730:ASN:HD21 | 1:B:734:ASN:HB2  | 1.29                     | 0.96              |
| 1:C:691:LYS:HB2  | 1:C:694:VAL:HG13 | 1.48                     | 0.94              |
| 1:C:744:GLU:HB3  | 1:C:747:ASN:HB2  | 1.49                     | 0.94              |
| 2:F:37:ARG:HD2   | 2:F:42:ASN:HA    | 1.48                     | 0.93              |
| 1:B:597:ASN:HD21 | 1:B:601:GLU:HB2  | 1.33                     | 0.93              |
| 1:A:434:LEU:HA   | 1:A:445:ARG:HD3  | 1.52                     | 0.92              |
| 1:B:729:TYR:HE2  | 1:B:773:PHE:HE1  | 1.18                     | 0.91              |
| 1:B:353:LYS:H    | 1:B:368:GLN:NE2  | 1.68                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:327:LEU:HG   | 1:B:595:ILE:HG12 | 1.52                     | 0.91              |
| 1:B:464:VAL:HG23 | 1:B:465:LEU:H    | 1.36                     | 0.91              |
| 1:B:629:ASN:HD22 | 1:B:631:SER:H    | 1.19                     | 0.90              |
| 1:A:776:LEU:H    | 1:A:776:LEU:HD12 | 1.37                     | 0.90              |
| 1:A:722:ILE:HG23 | 1:A:760:VAL:HG13 | 1.53                     | 0.89              |
| 1:B:514:ASP:HA   | 1:B:517:VAL:HG12 | 1.55                     | 0.89              |
| 1:B:353:LYS:N    | 1:B:368:GLN:HE22 | 1.70                     | 0.88              |
| 1:C:775:LEU:HD23 | 1:C:775:LEU:H    | 1.37                     | 0.88              |
| 1:B:561:ASN:O    | 1:B:564:VAL:HG22 | 1.72                     | 0.88              |
| 2:E:26:THR:HG22  | 2:E:64:ASP:HB3   | 1.54                     | 0.88              |
| 1:C:464:VAL:HG23 | 1:C:465:LEU:HD23 | 1.56                     | 0.87              |
| 1:B:508:ILE:HG12 | 1:B:536:TYR:HD1  | 1.40                     | 0.87              |
| 1:C:605:THR:HG21 | 1:C:611:THR:HA   | 1.57                     | 0.86              |
| 1:B:526:GLN:HG3  | 2:E:124:MET:HE2  | 1.58                     | 0.86              |
| 1:C:351:HIS:HB2  | 1:C:386:GLU:HG2  | 1.58                     | 0.85              |
| 1:B:729:TYR:HE2  | 1:B:773:PHE:CE1  | 1.94                     | 0.85              |
| 1:B:543:ASP:OD1  | 1:B:544:SER:N    | 2.08                     | 0.85              |
| 1:C:714:GLN:HA   | 1:C:714:GLN:HE21 | 1.37                     | 0.85              |
| 1:A:775:LEU:HD12 | 1:A:775:LEU:H    | 1.42                     | 0.84              |
| 1:A:697:ILE:HD13 | 1:A:732:ILE:HG12 | 1.59                     | 0.84              |
| 1:B:535:LYS:HA   | 1:B:535:LYS:HE2  | 1.60                     | 0.83              |
| 2:F:138:TYR:O    | 2:F:142:VAL:HG23 | 1.77                     | 0.83              |
| 1:B:381:GLU:HG2  | 1:B:465:LEU:HD11 | 1.59                     | 0.83              |
| 1:B:489:THR:HG22 | 1:B:490:ALA:N    | 1.95                     | 0.82              |
| 1:B:509:PRO:HG2  | 1:B:512:GLU:HB3  | 1.60                     | 0.81              |
| 2:E:49:GLN:HA    | 2:E:52:ILE:HG22  | 1.61                     | 0.81              |
| 1:C:736:LEU:HD22 | 1:C:746:LYS:HG2  | 1.62                     | 0.81              |
| 1:A:797:ILE:HG23 | 1:A:798:ASP:H    | 1.45                     | 0.81              |
| 1:A:611:THR:O    | 1:A:615:ILE:HG12 | 1.81                     | 0.81              |
| 2:F:97:ASN:HD21  | 2:F:99:TYR:HB2   | 1.43                     | 0.81              |
| 2:F:76:MET:SD    | 2:F:79:THR:HG21  | 2.20                     | 0.81              |
| 1:A:456:LYS:HD3  | 1:A:471:TRP:HD1  | 1.45                     | 0.81              |
| 1:B:597:ASN:ND2  | 1:B:601:GLU:HB2  | 1.97                     | 0.80              |
| 1:B:543:ASP:HB3  | 1:B:546:LYS:O    | 1.81                     | 0.80              |
| 2:E:101:SER:HB2  | 2:E:104:GLU:HG3  | 1.64                     | 0.79              |
| 1:C:629:ASN:HD22 | 1:C:631:SER:H    | 1.30                     | 0.79              |
| 1:C:639:ASN:ND2  | 1:C:641:ALA:H    | 1.82                     | 0.78              |
| 1:A:616:GLU:HA   | 1:A:620:THR:HG22 | 1.65                     | 0.78              |
| 1:B:320:ARG:HB3  | 1:B:320:ARG:HH21 | 1.48                     | 0.78              |
| 1:B:508:ILE:HD13 | 1:B:532:LEU:HD22 | 1.66                     | 0.77              |
| 1:A:313:ASP:HA   | 1:A:316:LYS:HE2  | 1.65                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:360:VAL:HG21 | 1:B:365:PRO:HG3  | 1.66                     | 0.77              |
| 1:C:715:GLU:CD   | 1:C:715:GLU:H    | 1.86                     | 0.77              |
| 1:A:780:LEU:HD13 | 1:A:782:PHE:CZ   | 2.19                     | 0.77              |
| 2:F:5:THR:N      | 2:F:9:ILE:HG12   | 2.00                     | 0.77              |
| 1:B:730:ASN:ND2  | 1:B:734:ASN:HB2  | 1.99                     | 0.77              |
| 1:B:353:LYS:H    | 1:B:368:GLN:HE22 | 0.86                     | 0.77              |
| 1:A:629:ASN:HD22 | 1:A:631:SER:H    | 1.33                     | 0.77              |
| 1:C:629:ASN:ND2  | 1:C:631:SER:H    | 1.82                     | 0.76              |
| 2:E:103:ALA:O    | 2:E:107:HIS:HB2  | 1.85                     | 0.76              |
| 1:A:425:GLU:CD   | 1:A:445:ARG:HH12 | 1.89                     | 0.76              |
| 1:A:731:GLU:HA   | 1:A:734:ASN:HD21 | 1.48                     | 0.76              |
| 1:A:722:ILE:HD13 | 1:A:764:LEU:HD23 | 1.67                     | 0.76              |
| 1:B:518:ASN:C    | 1:B:520:PRO:HD3  | 2.06                     | 0.76              |
| 1:B:335:ALA:HB1  | 1:B:489:THR:CG2  | 2.16                     | 0.75              |
| 1:B:549:LEU:HD12 | 1:B:553:GLN:HE21 | 1.51                     | 0.75              |
| 1:B:311:HIS:HD2  | 1:B:564:VAL:HB   | 1.49                     | 0.75              |
| 1:C:351:HIS:HB2  | 1:C:386:GLU:CG   | 2.16                     | 0.75              |
| 1:B:322:LEU:O    | 1:B:324:THR:HG23 | 1.86                     | 0.74              |
| 1:C:587:PRO:HB2  | 1:C:643:ILE:HD12 | 1.69                     | 0.74              |
| 1:B:324:THR:CG2  | 1:B:499:PRO:HA   | 2.16                     | 0.74              |
| 1:A:694:VAL:HG11 | 1:A:731:GLU:CD   | 2.08                     | 0.74              |
| 1:A:440:GLN:HE21 | 1:A:441:VAL:HG23 | 1.51                     | 0.74              |
| 1:A:694:VAL:HG11 | 1:A:731:GLU:OE2  | 1.88                     | 0.74              |
| 1:B:730:ASN:HD21 | 1:B:734:ASN:CB   | 2.00                     | 0.74              |
| 1:B:629:ASN:ND2  | 1:B:631:SER:H    | 1.85                     | 0.74              |
| 1:B:720:ILE:O    | 1:B:724:ARG:HG2  | 1.87                     | 0.74              |
| 2:E:92:PHE:HD2   | 2:E:108:VAL:HG21 | 1.51                     | 0.73              |
| 1:C:419:ILE:HD12 | 1:C:435:LEU:HD22 | 1.70                     | 0.73              |
| 1:A:597:ASN:HB2  | 1:A:598:PRO:HD2  | 1.70                     | 0.73              |
| 1:B:320:ARG:HG3  | 1:B:321:GLU:N    | 2.04                     | 0.73              |
| 1:A:559:ARG:NH1  | 1:A:559:ARG:HB3  | 2.03                     | 0.73              |
| 1:C:581:GLN:HE21 | 1:C:628:PHE:HA   | 1.54                     | 0.72              |
| 1:A:629:ASN:ND2  | 1:A:631:SER:H    | 1.86                     | 0.72              |
| 1:C:313:ASP:HA   | 1:C:316:LYS:HE2  | 1.70                     | 0.72              |
| 1:C:550:SER:H    | 1:C:553:GLN:NE2  | 1.87                     | 0.72              |
| 1:C:463:THR:HG22 | 1:C:465:LEU:H    | 1.54                     | 0.72              |
| 1:C:755:ARG:HA   | 1:C:758:ASN:ND2  | 2.04                     | 0.72              |
| 1:C:690:LYS:HG2  | 1:C:691:LYS:N    | 2.05                     | 0.71              |
| 1:A:633:ASN:HD21 | 1:A:645:TRP:H    | 1.38                     | 0.71              |
| 1:C:549:LEU:H    | 1:C:549:LEU:HD12 | 1.55                     | 0.71              |
| 1:B:525:LYS:HZ3  | 2:E:116:LEU:HD21 | 1.55                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:310:GLU:OE1  | 1:C:340:LYS:HD2  | 1.90                     | 0.71              |
| 2:F:39:LEU:O     | 2:F:41:GLN:N     | 2.24                     | 0.71              |
| 1:B:717:LYS:HZ1  | 2:E:126:ARG:HG3  | 1.56                     | 0.71              |
| 1:B:653:LYS:HE2  | 1:B:755:ARG:HH12 | 1.54                     | 0.71              |
| 1:C:295:VAL:HG12 | 1:C:610:MET:SD   | 2.30                     | 0.71              |
| 1:A:581:GLN:HE21 | 1:A:628:PHE:HA   | 1.56                     | 0.71              |
| 1:B:549:LEU:HD12 | 1:B:553:GLN:NE2  | 2.04                     | 0.71              |
| 1:B:788:ASP:O    | 1:B:791:GLU:HG2  | 1.89                     | 0.70              |
| 1:C:519:THR:OG1  | 1:C:520:PRO:HD2  | 1.90                     | 0.70              |
| 1:A:697:ILE:HD11 | 1:A:731:GLU:O    | 1.92                     | 0.70              |
| 1:C:525:LYS:O    | 1:C:529:VAL:HG23 | 1.92                     | 0.70              |
| 2:F:102:ALA:HA   | 2:F:125:ILE:HG13 | 1.71                     | 0.70              |
| 2:E:99:TYR:CE2   | 2:E:137:ASN:HB3  | 2.27                     | 0.69              |
| 2:E:63:ILE:HG23  | 2:E:67:GLU:HB2   | 1.72                     | 0.69              |
| 1:A:555:GLN:O    | 1:A:559:ARG:HG2  | 1.92                     | 0.69              |
| 2:F:65:PHE:HB2   | 2:F:66:PRO:HD3   | 1.74                     | 0.69              |
| 1:B:320:ARG:HG3  | 1:B:321:GLU:H    | 1.56                     | 0.69              |
| 1:A:525:LYS:O    | 1:A:529:VAL:HG23 | 1.93                     | 0.69              |
| 1:C:797:ILE:HG13 | 1:C:798:ASP:H    | 1.57                     | 0.69              |
| 1:C:479:LYS:HB3  | 1:C:488:LEU:HD21 | 1.74                     | 0.69              |
| 2:F:26:THR:HB    | 2:F:62:THR:HB    | 1.73                     | 0.69              |
| 1:B:730:ASN:ND2  | 1:B:734:ASN:H    | 1.91                     | 0.69              |
| 1:B:320:ARG:HB3  | 1:B:320:ARG:NH2  | 2.07                     | 0.69              |
| 1:B:549:LEU:HD13 | 1:B:578:GLY:HA2  | 1.73                     | 0.69              |
| 1:B:311:HIS:CD2  | 1:B:564:VAL:HB   | 2.28                     | 0.68              |
| 1:A:706:ASN:HD21 | 1:A:708:ALA:HB3  | 1.57                     | 0.68              |
| 1:B:792:VAL:O    | 1:B:796:ILE:HG12 | 1.92                     | 0.68              |
| 1:C:526:GLN:HE22 | 2:F:144:MET:HE1  | 1.59                     | 0.68              |
| 2:E:92:PHE:CE2   | 2:E:108:VAL:HG11 | 2.28                     | 0.68              |
| 1:A:434:LEU:HG   | 1:A:445:ARG:HE   | 1.59                     | 0.67              |
| 1:C:534:ILE:HA   | 1:C:538:ILE:HB   | 1.76                     | 0.67              |
| 2:E:30:LYS:HB2   | 2:E:31:GLU:OE1   | 1.93                     | 0.67              |
| 2:D:133:ASP:OD2  | 2:D:135:GLN:HG3  | 1.95                     | 0.67              |
| 1:B:318:ILE:HG23 | 1:B:322:LEU:HD12 | 1.77                     | 0.67              |
| 1:A:731:GLU:HA   | 1:A:734:ASN:ND2  | 2.09                     | 0.67              |
| 1:C:718:ARG:HH11 | 1:C:766:HIS:HB3  | 1.60                     | 0.67              |
| 1:A:633:ASN:ND2  | 1:A:645:TRP:H    | 1.93                     | 0.67              |
| 1:A:605:THR:HG21 | 1:A:611:THR:HA   | 1.77                     | 0.67              |
| 1:B:335:ALA:HB1  | 1:B:489:THR:HG22 | 1.76                     | 0.67              |
| 1:B:333:LYS:O    | 1:B:336:THR:HG22 | 1.95                     | 0.67              |
| 1:A:696:LYS:HB2  | 1:A:731:GLU:HG2  | 1.77                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:362:GLY:O    | 1:B:489:THR:HG23 | 1.95                     | 0.66              |
| 1:A:376:GLN:NE2  | 1:B:466:GLY:HA3  | 2.11                     | 0.66              |
| 1:B:709:ASN:HD21 | 1:B:720:ILE:HD11 | 1.60                     | 0.66              |
| 2:E:102:ALA:HA   | 2:E:125:ILE:HD11 | 1.76                     | 0.66              |
| 1:C:714:GLN:CA   | 1:C:714:GLN:HE21 | 2.09                     | 0.66              |
| 2:F:97:ASN:HD22  | 2:F:99:TYR:HD1   | 1.43                     | 0.66              |
| 1:B:335:ALA:O    | 1:B:339:ILE:HG13 | 1.95                     | 0.66              |
| 1:B:320:ARG:CB   | 1:B:320:ARG:HH21 | 2.09                     | 0.66              |
| 1:C:752:LEU:O    | 1:C:756:ILE:HG12 | 1.96                     | 0.66              |
| 1:C:292:ARG:HH22 | 1:C:297:LYS:NZ   | 1.93                     | 0.66              |
| 1:B:297:LYS:HA   | 1:B:602:PHE:O    | 1.95                     | 0.66              |
| 2:F:27:ILE:HG13  | 2:F:63:ILE:HB    | 1.77                     | 0.66              |
| 2:F:89:PHE:CE1   | 2:F:100:ILE:HG12 | 2.31                     | 0.66              |
| 1:B:722:ILE:HG23 | 1:B:760:VAL:CG1  | 2.26                     | 0.65              |
| 2:F:68:PHE:O     | 2:F:72:MET:HG2   | 1.95                     | 0.65              |
| 1:B:465:LEU:O    | 1:B:467:GLU:N    | 2.29                     | 0.65              |
| 1:A:385:LEU:HD11 | 1:A:389:LYS:HE3  | 1.78                     | 0.65              |
| 1:B:722:ILE:HG12 | 1:B:760:VAL:HG13 | 1.77                     | 0.65              |
| 1:B:360:VAL:CG2  | 1:B:365:PRO:HG3  | 2.25                     | 0.65              |
| 2:D:9:ILE:H      | 2:D:9:ILE:HD12   | 1.60                     | 0.65              |
| 2:E:26:THR:HA    | 2:E:64:ASP:HA    | 1.77                     | 0.65              |
| 1:A:714:GLN:NE2  | 2:D:126:ARG:HG3  | 2.12                     | 0.65              |
| 1:C:797:ILE:HG13 | 1:C:798:ASP:N    | 2.11                     | 0.65              |
| 1:C:513:TRP:O    | 1:C:517:VAL:HG12 | 1.96                     | 0.65              |
| 1:A:659:THR:HG22 | 1:A:662:GLU:HB3  | 1.78                     | 0.65              |
| 1:A:445:ARG:HG3  | 1:A:471:TRP:CZ2  | 2.32                     | 0.65              |
| 1:B:709:ASN:ND2  | 1:B:720:ILE:HD11 | 2.12                     | 0.65              |
| 2:D:65:PHE:HB2   | 2:D:66:PRO:HD3   | 1.79                     | 0.65              |
| 1:A:492:TYR:CD2  | 1:A:574:VAL:HG13 | 2.32                     | 0.65              |
| 1:B:450:ASN:OD1  | 1:B:452:GLU:HG3  | 1.97                     | 0.65              |
| 1:C:320:ARG:HA   | 1:C:598:PRO:O    | 1.96                     | 0.64              |
| 1:B:657:ILE:HG12 | 1:B:658:PRO:HD2  | 1.78                     | 0.64              |
| 1:B:729:TYR:CE2  | 1:B:773:PHE:HE1  | 2.07                     | 0.64              |
| 1:A:670:ILE:HD12 | 1:A:745:TYR:CE1  | 2.33                     | 0.64              |
| 1:C:318:ILE:HD12 | 1:C:318:ILE:H    | 1.62                     | 0.64              |
| 1:B:556:MET:O    | 1:B:560:LEU:HG   | 1.98                     | 0.64              |
| 2:E:5:THR:OG1    | 2:E:8:GLN:HB2    | 1.97                     | 0.63              |
| 1:B:735:VAL:HG22 | 1:B:738:SER:HB2  | 1.79                     | 0.63              |
| 1:B:499:PRO:CG   | 1:B:504:ILE:HD11 | 2.28                     | 0.63              |
| 1:A:426:ILE:N    | 1:A:426:ILE:HD12 | 2.14                     | 0.63              |
| 1:A:738:SER:O    | 1:A:739:LYS:C    | 2.36                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:629:ASN:ND2  | 1:B:631:SER:HB2  | 2.13                     | 0.63              |
| 1:C:655:ASN:HA   | 1:C:758:ASN:HB2  | 1.80                     | 0.63              |
| 2:E:131:ASP:HB2  | 2:E:133:ASP:OD2  | 1.98                     | 0.63              |
| 1:C:595:ILE:HB   | 1:C:603:ILE:HB   | 1.80                     | 0.63              |
| 1:B:716:LYS:O    | 1:B:720:ILE:HG12 | 1.99                     | 0.63              |
| 2:D:26:THR:HG22  | 2:D:64:ASP:OD1   | 1.99                     | 0.63              |
| 1:B:391:ILE:HD11 | 1:B:400:LYS:HG2  | 1.80                     | 0.63              |
| 1:C:659:THR:H    | 1:C:662:GLU:HB2  | 1.64                     | 0.63              |
| 1:B:514:ASP:HA   | 1:B:517:VAL:CG1  | 2.26                     | 0.63              |
| 1:A:440:GLN:O    | 1:A:458:LYS:HD3  | 1.99                     | 0.62              |
| 1:C:339:ILE:HD13 | 1:C:492:TYR:HE1  | 1.64                     | 0.62              |
| 1:C:690:LYS:HG2  | 1:C:691:LYS:H    | 1.62                     | 0.62              |
| 1:C:639:ASN:C    | 1:C:639:ASN:HD22 | 2.01                     | 0.62              |
| 1:B:714:GLN:OE1  | 1:B:715:GLU:HG3  | 2.00                     | 0.62              |
| 1:A:434:LEU:CA   | 1:A:445:ARG:HD3  | 2.26                     | 0.62              |
| 2:E:52:ILE:O     | 2:E:56:ASP:HB3   | 1.98                     | 0.62              |
| 1:B:777:TYR:HD1  | 1:B:780:LEU:HD12 | 1.64                     | 0.62              |
| 1:A:741:ILE:O    | 1:A:742:ALA:C    | 2.38                     | 0.62              |
| 1:A:299:GLU:HG3  | 1:A:303:LYS:NZ   | 2.15                     | 0.62              |
| 2:E:115:LYS:HB3  | 2:E:115:LYS:HZ2  | 1.65                     | 0.62              |
| 2:E:115:LYS:NZ   | 2:E:115:LYS:HB3  | 2.15                     | 0.62              |
| 2:E:7:GLU:O      | 2:E:11:GLU:HG3   | 1.98                     | 0.62              |
| 1:B:714:GLN:HA   | 1:B:717:LYS:HD2  | 1.82                     | 0.62              |
| 2:E:124:MET:O    | 2:E:127:GLU:HB2  | 1.99                     | 0.62              |
| 1:A:559:ARG:HH11 | 1:A:559:ARG:HB3  | 1.64                     | 0.62              |
| 1:B:349:ASN:OD1  | 1:B:350:VAL:HG23 | 2.00                     | 0.62              |
| 1:B:750:GLN:O    | 1:B:754:GLU:HG3  | 2.00                     | 0.61              |
| 1:A:550:SER:H    | 1:A:553:GLN:NE2  | 1.97                     | 0.61              |
| 2:E:39:LEU:O     | 2:E:39:LEU:HD23  | 1.99                     | 0.61              |
| 2:F:37:ARG:HG2   | 2:F:43:PRO:HD2   | 1.82                     | 0.61              |
| 1:C:351:HIS:CB   | 1:C:386:GLU:HG2  | 2.29                     | 0.61              |
| 1:C:731:GLU:O    | 1:C:735:VAL:HG23 | 2.00                     | 0.61              |
| 1:A:492:TYR:HD2  | 1:A:574:VAL:HG13 | 1.65                     | 0.61              |
| 1:A:426:ILE:H    | 1:A:426:ILE:HD12 | 1.65                     | 0.61              |
| 1:B:615:ILE:HD12 | 1:B:645:TRP:HH2  | 1.64                     | 0.61              |
| 2:F:114:GLU:HG3  | 2:F:116:LEU:CD1  | 2.30                     | 0.61              |
| 1:A:517:VAL:HG13 | 2:D:114:GLU:OE2  | 2.00                     | 0.61              |
| 1:A:589:LYS:HE3  | 1:A:608:TRP:CG   | 2.36                     | 0.61              |
| 1:B:327:LEU:HG   | 1:B:595:ILE:CG1  | 2.29                     | 0.61              |
| 1:A:657:ILE:HG22 | 1:A:756:ILE:HA   | 1.81                     | 0.61              |
| 1:B:538:ILE:CD1  | 1:B:625:LEU:HD11 | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:722:ILE:HD13 | 1:C:764:LEU:HD23 | 1.83                     | 0.61              |
| 1:A:322:LEU:O    | 1:A:323:ASN:C    | 2.38                     | 0.61              |
| 1:B:332:ASN:C    | 1:B:332:ASN:HD22 | 2.04                     | 0.61              |
| 1:A:561:ASN:O    | 1:A:565:LYS:HG3  | 2.01                     | 0.61              |
| 1:C:661:ALA:C    | 1:C:663:PHE:H    | 2.03                     | 0.60              |
| 1:A:439:ASN:ND2  | 1:A:442:TYR:H    | 1.98                     | 0.60              |
| 1:A:327:LEU:HD12 | 1:A:327:LEU:N    | 2.16                     | 0.60              |
| 1:B:305:SER:HB3  | 1:B:594:PHE:CD1  | 2.36                     | 0.60              |
| 1:C:325:TYR:HB2  | 1:C:498:ALA:HB3  | 1.82                     | 0.60              |
| 1:B:366:PHE:HD1  | 1:B:477:MET:CE   | 2.14                     | 0.60              |
| 1:B:777:TYR:CD1  | 1:B:780:LEU:HD12 | 2.36                     | 0.60              |
| 1:A:664:ILE:C    | 1:A:666:ASN:H    | 2.05                     | 0.60              |
| 1:A:400:LYS:HE2  | 1:A:475:GLU:OE2  | 2.02                     | 0.60              |
| 1:C:736:LEU:HD21 | 1:C:749:PHE:HB2  | 1.83                     | 0.60              |
| 1:C:716:LYS:O    | 1:C:720:ILE:HG12 | 2.01                     | 0.60              |
| 1:C:733:GLU:HG2  | 1:C:753:LYS:HE2  | 1.83                     | 0.60              |
| 1:A:295:VAL:HG23 | 1:A:605:THR:HA   | 1.82                     | 0.60              |
| 1:A:334:LEU:HD13 | 1:A:361:ALA:HB1  | 1.82                     | 0.60              |
| 1:B:616:GLU:HA   | 1:B:620:THR:CG2  | 2.25                     | 0.60              |
| 2:F:28:THR:OG1   | 2:F:31:GLU:HG2   | 2.01                     | 0.60              |
| 1:C:744:GLU:HB3  | 1:C:747:ASN:CB   | 2.30                     | 0.60              |
| 1:B:656:THR:O    | 1:B:657:ILE:HB   | 2.02                     | 0.60              |
| 1:A:706:ASN:ND2  | 1:A:708:ALA:HB3  | 2.17                     | 0.60              |
| 1:C:722:ILE:HD13 | 1:C:764:LEU:CD2  | 2.32                     | 0.60              |
| 1:B:364:ILE:HB   | 1:B:477:MET:HB2  | 1.84                     | 0.60              |
| 1:B:697:ILE:HD13 | 1:B:732:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:664:ILE:HA   | 1:A:667:LEU:HD12 | 1.84                     | 0.59              |
| 1:A:738:SER:O    | 1:A:740:GLN:N    | 2.34                     | 0.59              |
| 1:A:497:LEU:HD12 | 1:A:553:GLN:HG2  | 1.83                     | 0.59              |
| 1:A:438:ASN:HD22 | 1:A:438:ASN:N    | 2.00                     | 0.59              |
| 1:B:726:ILE:HD13 | 1:B:780:LEU:HD13 | 1.82                     | 0.59              |
| 2:D:9:ILE:N      | 2:D:9:ILE:HD12   | 2.17                     | 0.59              |
| 1:A:324:THR:HG21 | 1:A:556:MET:HE1  | 1.83                     | 0.59              |
| 1:C:373:LYS:HD2  | 1:C:379:ALA:HB1  | 1.84                     | 0.59              |
| 1:A:463:THR:HG22 | 1:A:465:LEU:H    | 1.66                     | 0.59              |
| 1:C:664:ILE:HG21 | 2:F:15:ALA:HB2   | 1.83                     | 0.59              |
| 2:E:92:PHE:CD2   | 2:E:108:VAL:HG21 | 2.36                     | 0.59              |
| 1:A:653:LYS:O    | 1:A:755:ARG:HD3  | 2.01                     | 0.59              |
| 1:A:418:ILE:HG22 | 1:A:419:ILE:HG23 | 1.84                     | 0.59              |
| 1:B:499:PRO:HG2  | 1:B:625:LEU:HB3  | 1.84                     | 0.59              |
| 1:C:739:LYS:C    | 1:C:741:ILE:H    | 2.05                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:376:GLN:HB2  | 1:B:379:ALA:HB3  | 1.84                     | 0.59              |
| 1:B:744:GLU:OE1  | 1:B:744:GLU:HA   | 2.01                     | 0.59              |
| 1:B:597:ASN:HB2  | 1:B:598:PRO:HD2  | 1.85                     | 0.59              |
| 1:B:375:GLY:HA2  | 1:B:464:VAL:HG11 | 1.84                     | 0.59              |
| 1:C:457:THR:HG21 | 1:C:468:LYS:HA   | 1.84                     | 0.59              |
| 1:A:587:PRO:HB2  | 1:A:643:ILE:HD12 | 1.85                     | 0.59              |
| 1:B:744:GLU:O    | 1:B:748:TYR:N    | 2.36                     | 0.59              |
| 1:B:460:GLY:HA2  | 1:B:468:LYS:HZ3  | 1.67                     | 0.59              |
| 1:B:464:VAL:HG23 | 1:B:465:LEU:N    | 2.14                     | 0.59              |
| 1:A:722:ILE:HD13 | 1:A:764:LEU:CD2  | 2.32                     | 0.59              |
| 1:A:783:THR:CB   | 1:A:789:ASN:HD21 | 2.11                     | 0.59              |
| 1:A:666:ASN:O    | 1:A:670:ILE:HB   | 2.02                     | 0.59              |
| 1:A:663:PHE:O    | 1:A:667:LEU:HG   | 2.03                     | 0.59              |
| 1:C:546:LYS:HB3  | 1:C:549:LEU:HD21 | 1.84                     | 0.58              |
| 1:C:722:ILE:HG23 | 1:C:760:VAL:HG13 | 1.85                     | 0.58              |
| 1:B:526:GLN:HE21 | 2:E:124:MET:HE3  | 1.68                     | 0.58              |
| 1:B:546:LYS:HG3  | 1:B:576:ASN:O    | 2.02                     | 0.58              |
| 1:A:736:LEU:HD21 | 1:A:749:PHE:HB2  | 1.85                     | 0.58              |
| 1:C:526:GLN:HB2  | 2:F:124:MET:CE   | 2.34                     | 0.58              |
| 2:F:44:THR:HG23  | 2:F:46:ALA:HB3   | 1.84                     | 0.58              |
| 2:D:92:PHE:CD2   | 2:D:108:VAL:HG21 | 2.39                     | 0.58              |
| 1:A:534:ILE:HA   | 1:A:538:ILE:HD13 | 1.85                     | 0.58              |
| 2:F:97:ASN:ND2   | 2:F:99:TYR:HD1   | 2.00                     | 0.58              |
| 1:C:669:SER:HA   | 1:C:672:ARG:HG2  | 1.85                     | 0.58              |
| 1:A:349:ASN:N    | 1:A:349:ASN:HD22 | 2.02                     | 0.58              |
| 2:F:10:ALA:O     | 2:F:14:GLU:HB2   | 2.03                     | 0.58              |
| 2:D:5:THR:OG1    | 2:D:8:GLN:HG3    | 2.03                     | 0.58              |
| 1:B:508:ILE:HG12 | 1:B:536:TYR:CD1  | 2.30                     | 0.58              |
| 1:A:734:ASN:O    | 1:A:737:LYS:HB2  | 2.04                     | 0.58              |
| 1:A:629:ASN:HD22 | 1:A:631:SER:N    | 1.99                     | 0.58              |
| 2:F:52:ILE:HD11  | 2:F:63:ILE:HD11  | 1.84                     | 0.58              |
| 1:B:450:ASN:O    | 1:B:451:ASN:HB2  | 2.03                     | 0.58              |
| 1:C:368:GLN:HG2  | 1:C:387:ASN:ND2  | 2.19                     | 0.58              |
| 1:B:538:ILE:HD13 | 1:B:625:LEU:HD11 | 1.86                     | 0.57              |
| 1:A:586:PHE:CE2  | 1:A:638:GLY:HA3  | 2.39                     | 0.57              |
| 1:A:481:VAL:HG21 | 1:A:486:LYS:HD2  | 1.86                     | 0.57              |
| 1:B:722:ILE:HG23 | 1:B:760:VAL:HG11 | 1.85                     | 0.57              |
| 2:E:95:ASP:OD2   | 2:E:97:ASN:HB3   | 2.04                     | 0.57              |
| 2:D:29:THR:OG1   | 2:D:52:ILE:HG12  | 2.04                     | 0.57              |
| 2:F:97:ASN:ND2   | 2:F:99:TYR:HB2   | 2.18                     | 0.57              |
| 1:C:338:LEU:O    | 1:C:343:VAL:HG23 | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:726:ILE:HA   | 1:B:729:TYR:HB2  | 1.85                     | 0.57              |
| 1:A:636:ALA:O    | 1:A:640:LYS:HA   | 2.04                     | 0.57              |
| 2:F:45:GLU:HA    | 2:F:48:LEU:HD12  | 1.86                     | 0.57              |
| 1:A:372:LYS:NZ   | 5:A:902:3AT:O2G  | 2.33                     | 0.57              |
| 1:A:758:ASN:O    | 1:A:762:LEU:HB2  | 2.05                     | 0.57              |
| 1:B:514:ASP:CA   | 1:B:517:VAL:HG12 | 2.32                     | 0.57              |
| 1:A:440:GLN:NE2  | 1:A:441:VAL:HG23 | 2.18                     | 0.57              |
| 1:B:754:GLU:O    | 1:B:757:THR:HB   | 2.05                     | 0.57              |
| 1:A:735:VAL:C    | 1:A:737:LYS:H    | 2.08                     | 0.57              |
| 1:C:293:ILE:HG22 | 1:C:295:VAL:HG13 | 1.87                     | 0.57              |
| 2:F:115:LYS:O    | 2:F:116:LEU:HD12 | 2.05                     | 0.57              |
| 1:B:497:LEU:HD13 | 1:B:556:MET:HG2  | 1.86                     | 0.57              |
| 1:C:636:ALA:HB3  | 1:C:639:ASN:HD21 | 1.70                     | 0.57              |
| 2:F:26:THR:HA    | 2:F:63:ILE:O     | 2.05                     | 0.57              |
| 2:E:44:THR:HG23  | 2:E:47:GLU:H     | 1.70                     | 0.57              |
| 1:C:723:PHE:HB2  | 1:C:793:PHE:CE2  | 2.40                     | 0.57              |
| 1:A:778:LYS:C    | 1:A:780:LEU:H    | 2.07                     | 0.57              |
| 1:B:629:ASN:HD21 | 1:B:631:SER:HB2  | 1.70                     | 0.56              |
| 1:C:629:ASN:HD22 | 1:C:631:SER:N    | 2.00                     | 0.56              |
| 2:E:99:TYR:CD2   | 2:E:137:ASN:HB3  | 2.39                     | 0.56              |
| 1:A:440:GLN:HG2  | 1:A:461:LYS:HE2  | 1.87                     | 0.56              |
| 1:A:323:ASN:HD22 | 1:A:323:ASN:C    | 2.08                     | 0.56              |
| 1:C:670:ILE:HD11 | 1:C:745:TYR:HA   | 1.87                     | 0.56              |
| 2:E:64:ASP:OD1   | 2:E:66:PRO:HD2   | 2.05                     | 0.56              |
| 2:E:89:PHE:HE1   | 2:E:100:ILE:HG13 | 1.70                     | 0.56              |
| 1:B:716:LYS:HA   | 1:B:719:LYS:HE2  | 1.87                     | 0.56              |
| 1:C:546:LYS:HG2  | 1:C:549:LEU:HD21 | 1.87                     | 0.56              |
| 2:F:49:GLN:HA    | 2:F:52:ILE:HG22  | 1.88                     | 0.56              |
| 1:B:744:GLU:O    | 1:B:745:TYR:C    | 2.44                     | 0.56              |
| 1:B:296:LEU:HB2  | 1:B:604:LEU:HB3  | 1.87                     | 0.56              |
| 2:D:53:ASN:O     | 2:D:57:ALA:HB2   | 2.05                     | 0.56              |
| 2:F:63:ILE:N     | 2:F:63:ILE:HD12  | 2.20                     | 0.56              |
| 1:B:732:ILE:HG22 | 1:B:732:ILE:O    | 2.06                     | 0.56              |
| 1:A:540:ARG:NH2  | 2:D:87:GLU:OE1   | 2.39                     | 0.56              |
| 1:A:718:ARG:O    | 1:A:722:ILE:HG13 | 2.06                     | 0.56              |
| 1:B:462:ILE:HG12 | 1:B:468:LYS:HE3  | 1.87                     | 0.56              |
| 1:A:305:SER:HB3  | 1:A:594:PHE:CD1  | 2.41                     | 0.56              |
| 1:B:657:ILE:CG1  | 1:B:658:PRO:HD2  | 2.35                     | 0.56              |
| 2:F:37:ARG:HD2   | 2:F:42:ASN:CA    | 2.31                     | 0.56              |
| 1:C:775:LEU:H    | 1:C:775:LEU:CD2  | 2.15                     | 0.56              |
| 1:B:509:PRO:HD2  | 1:B:536:TYR:CE1  | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:105:LEU:HD12 | 2:F:125:ILE:CD1  | 2.36                     | 0.56              |
| 2:E:71:MET:C     | 2:E:73:ALA:H     | 2.09                     | 0.56              |
| 2:F:49:GLN:HA    | 2:F:52:ILE:CG2   | 2.36                     | 0.56              |
| 2:D:79:THR:C     | 2:D:81:SER:H     | 2.07                     | 0.56              |
| 1:B:528:GLY:O    | 1:B:532:LEU:HB2  | 2.05                     | 0.56              |
| 2:F:122:ASP:HB3  | 2:F:126:ARG:HH22 | 1.71                     | 0.56              |
| 1:C:329:ARG:HD2  | 1:C:590:ASP:OD2  | 2.06                     | 0.56              |
| 1:B:729:TYR:CE2  | 1:B:773:PHE:CE1  | 2.85                     | 0.56              |
| 1:C:697:ILE:HD13 | 1:C:732:ILE:HG12 | 1.88                     | 0.56              |
| 1:B:538:ILE:O    | 1:B:540:ARG:HD3  | 2.06                     | 0.55              |
| 1:A:368:GLN:HG3  | 1:A:383:GLY:C    | 2.26                     | 0.55              |
| 1:A:668:SER:HB2  | 2:D:11:GLU:HA    | 1.88                     | 0.55              |
| 2:F:92:PHE:CB    | 2:F:100:ILE:HD12 | 2.36                     | 0.55              |
| 1:A:529:VAL:HG11 | 2:D:109:MET:SD   | 2.47                     | 0.55              |
| 1:C:780:LEU:HB3  | 1:C:782:PHE:HE1  | 1.71                     | 0.55              |
| 1:B:742:ALA:HB1  | 1:B:743:PRO:HD2  | 1.87                     | 0.55              |
| 2:E:99:TYR:HB3   | 2:E:135:GLN:HB3  | 1.89                     | 0.55              |
| 1:B:416:ASN:HB2  | 1:B:418:ILE:HG12 | 1.87                     | 0.55              |
| 1:C:691:LYS:HB2  | 1:C:694:VAL:CG1  | 2.29                     | 0.55              |
| 1:B:733:GLU:O    | 1:B:735:VAL:N    | 2.31                     | 0.55              |
| 1:A:617:LYS:HD2  | 1:A:617:LYS:O    | 2.05                     | 0.55              |
| 1:B:489:THR:CG2  | 1:B:490:ALA:H    | 2.04                     | 0.55              |
| 1:B:359:PRO:HB3  | 1:B:405:LEU:HD11 | 1.88                     | 0.55              |
| 2:E:41:GLN:HB3   | 2:E:43:PRO:HD3   | 1.89                     | 0.55              |
| 1:C:663:PHE:CZ   | 1:C:667:LEU:HD11 | 2.42                     | 0.55              |
| 2:F:35:VAL:O     | 2:F:39:LEU:HG    | 2.06                     | 0.55              |
| 1:A:434:LEU:HG   | 1:A:445:ARG:NE   | 2.20                     | 0.55              |
| 1:A:659:THR:HG23 | 1:A:662:GLU:H    | 1.72                     | 0.55              |
| 1:B:401:ILE:HG21 | 1:B:485:LEU:HB3  | 1.88                     | 0.55              |
| 1:C:308:VAL:HG23 | 1:C:492:TYR:OH   | 2.06                     | 0.55              |
| 1:A:709:ASN:HD21 | 1:A:724:ARG:NH1  | 2.05                     | 0.55              |
| 2:D:68:PHE:O     | 2:D:72:MET:HG2   | 2.07                     | 0.55              |
| 1:B:639:ASN:HD22 | 1:B:640:LYS:N    | 2.05                     | 0.55              |
| 1:C:526:GLN:OE1  | 2:F:144:MET:HE2  | 2.07                     | 0.55              |
| 1:C:502:THR:O    | 1:C:505:LYS:HB3  | 2.07                     | 0.55              |
| 1:B:639:ASN:C    | 1:B:639:ASN:HD22 | 2.09                     | 0.55              |
| 2:D:102:ALA:HA   | 2:D:125:ILE:HG13 | 1.88                     | 0.55              |
| 1:C:540:ARG:HH22 | 2:F:87:GLU:CD    | 2.11                     | 0.54              |
| 2:F:136:VAL:HA   | 2:F:140:GLU:OE1  | 2.07                     | 0.54              |
| 1:B:629:ASN:HD22 | 1:B:631:SER:N    | 1.98                     | 0.54              |
| 2:F:62:THR:C     | 2:F:63:ILE:HD12  | 2.27                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:697:ILE:HD13 | 1:B:732:ILE:CD1  | 2.38                     | 0.54              |
| 1:B:585:GLU:HB3  | 1:B:586:PHE:CD1  | 2.42                     | 0.54              |
| 1:A:607:ASN:ND2  | 1:A:610:MET:H    | 2.03                     | 0.54              |
| 1:B:756:ILE:O    | 1:B:760:VAL:HG23 | 2.06                     | 0.54              |
| 2:E:13:LYS:HG2   | 2:E:65:PHE:CE1   | 2.43                     | 0.54              |
| 1:B:526:GLN:HE21 | 2:E:124:MET:CE   | 2.19                     | 0.54              |
| 1:B:403:LEU:HD13 | 1:B:476:VAL:HG21 | 1.90                     | 0.54              |
| 2:E:37:ARG:HA    | 2:E:41:GLN:O     | 2.08                     | 0.54              |
| 1:C:623:ASP:OD1  | 2:F:94:LYS:HD3   | 2.07                     | 0.54              |
| 1:B:752:LEU:O    | 1:B:756:ILE:HG13 | 2.08                     | 0.54              |
| 1:C:775:LEU:HG   | 1:C:776:LEU:CD1  | 2.37                     | 0.54              |
| 2:F:72:MET:O     | 2:F:76:MET:HB3   | 2.08                     | 0.54              |
| 1:C:759:GLN:O    | 1:C:762:LEU:HB3  | 2.08                     | 0.54              |
| 2:D:9:ILE:HG23   | 2:D:69:LEU:HD22  | 1.90                     | 0.54              |
| 1:C:360:VAL:HG22 | 1:C:363:TYR:HB2  | 1.88                     | 0.54              |
| 1:C:667:LEU:HA   | 1:C:670:ILE:HG22 | 1.89                     | 0.54              |
| 1:A:657:ILE:HD11 | 1:A:704:TYR:CD1  | 2.42                     | 0.54              |
| 1:C:746:LYS:HD2  | 1:C:746:LYS:O    | 2.08                     | 0.54              |
| 1:C:639:ASN:HD22 | 1:C:640:LYS:N    | 2.04                     | 0.54              |
| 1:A:629:ASN:ND2  | 1:A:631:SER:HB2  | 2.22                     | 0.54              |
| 1:A:318:ILE:O    | 1:A:322:LEU:HG   | 2.08                     | 0.54              |
| 1:C:729:TYR:HB2  | 1:C:756:ILE:HG21 | 1.88                     | 0.54              |
| 2:D:12:PHE:HB3   | 2:D:68:PHE:HE2   | 1.73                     | 0.54              |
| 1:A:499:PRO:HD3  | 1:A:552:TRP:CH2  | 2.43                     | 0.54              |
| 1:A:540:ARG:HH22 | 2:D:87:GLU:CD    | 2.11                     | 0.54              |
| 1:A:329:ARG:HD2  | 1:A:590:ASP:OD2  | 2.08                     | 0.54              |
| 1:A:797:ILE:HG23 | 1:A:798:ASP:N    | 2.16                     | 0.54              |
| 2:F:27:ILE:CG1   | 2:F:63:ILE:HB    | 2.37                     | 0.54              |
| 1:C:318:ILE:N    | 1:C:318:ILE:HD12 | 2.22                     | 0.54              |
| 1:B:366:PHE:HD1  | 1:B:477:MET:HE1  | 1.73                     | 0.54              |
| 1:C:791:GLU:OE1  | 1:C:791:GLU:N    | 2.36                     | 0.54              |
| 1:C:659:THR:HG22 | 1:C:661:ALA:N    | 2.06                     | 0.54              |
| 1:B:535:LYS:HE2  | 1:B:535:LYS:CA   | 2.35                     | 0.54              |
| 2:F:68:PHE:HA    | 2:F:71:MET:HE3   | 1.90                     | 0.54              |
| 2:E:100:ILE:HA   | 2:E:104:GLU:OE1  | 2.08                     | 0.54              |
| 1:C:722:ILE:HG12 | 1:C:763:LEU:HB2  | 1.90                     | 0.54              |
| 1:C:657:ILE:HG13 | 1:C:759:GLN:CB   | 2.38                     | 0.54              |
| 1:C:730:ASN:ND2  | 1:C:782:PHE:HB2  | 2.23                     | 0.54              |
| 1:B:368:GLN:HG3  | 1:B:383:GLY:HA3  | 1.89                     | 0.54              |
| 1:B:733:GLU:C    | 1:B:735:VAL:H    | 2.10                     | 0.54              |
| 1:A:368:GLN:HG3  | 1:A:383:GLY:HA3  | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:425:GLU:CD   | 1:A:445:ARG:NH1  | 2.59                     | 0.54              |
| 1:C:480:ASN:HD21 | 1:C:483:GLY:CA   | 2.20                     | 0.54              |
| 1:B:322:LEU:HD13 | 1:B:556:MET:CE   | 2.38                     | 0.53              |
| 1:B:560:LEU:O    | 1:B:564:VAL:HG13 | 2.07                     | 0.53              |
| 1:C:456:LYS:HA   | 1:C:469:PHE:CE1  | 2.43                     | 0.53              |
| 2:D:63:ILE:HA    | 2:D:67:GLU:OE2   | 2.08                     | 0.53              |
| 1:A:616:GLU:HA   | 1:A:620:THR:CG2  | 2.37                     | 0.53              |
| 1:A:670:ILE:O    | 1:A:670:ILE:HD13 | 2.08                     | 0.53              |
| 1:B:424:LYS:HE2  | 1:B:433:TYR:OH   | 2.08                     | 0.53              |
| 2:F:37:ARG:C     | 2:F:39:LEU:H     | 2.12                     | 0.53              |
| 2:E:63:ILE:HG13  | 2:E:67:GLU:OE2   | 2.08                     | 0.53              |
| 1:C:698:ALA:O    | 1:C:701:LEU:HB2  | 2.08                     | 0.53              |
| 1:A:360:VAL:HG23 | 1:A:403:LEU:HD22 | 1.91                     | 0.53              |
| 1:C:657:ILE:HG13 | 1:C:759:GLN:CG   | 2.39                     | 0.53              |
| 1:B:445:ARG:HB3  | 1:B:471:TRP:CH2  | 2.43                     | 0.53              |
| 1:C:751:TYR:O    | 1:C:754:GLU:HB3  | 2.09                     | 0.53              |
| 1:B:299:GLU:C    | 1:B:303:LYS:HZ3  | 2.12                     | 0.53              |
| 1:A:335:ALA:O    | 1:A:339:ILE:HG13 | 2.09                     | 0.53              |
| 1:C:301:ALA:HB1  | 1:C:604:LEU:HB2  | 1.91                     | 0.53              |
| 1:B:519:THR:N    | 1:B:520:PRO:HD3  | 2.24                     | 0.53              |
| 1:C:501:LEU:O    | 1:C:504:ILE:HG12 | 2.08                     | 0.53              |
| 1:C:450:ASN:O    | 1:C:451:ASN:HB2  | 2.09                     | 0.53              |
| 2:F:75:LYS:HG2   | 2:F:75:LYS:O     | 2.09                     | 0.53              |
| 1:B:762:LEU:O    | 1:B:766:HIS:HB2  | 2.09                     | 0.53              |
| 1:B:564:VAL:HG11 | 1:B:574:VAL:HG11 | 1.90                     | 0.53              |
| 1:A:656:THR:O    | 1:A:755:ARG:HD2  | 2.08                     | 0.53              |
| 1:C:349:ASN:N    | 1:C:349:ASN:HD22 | 2.05                     | 0.53              |
| 1:A:440:GLN:H    | 1:A:440:GLN:CD   | 2.12                     | 0.52              |
| 1:A:385:LEU:CD1  | 1:A:389:LYS:HE3  | 2.39                     | 0.52              |
| 1:B:705:TYR:CE1  | 2:E:139:GLU:HB3  | 2.44                     | 0.52              |
| 2:F:52:ILE:O     | 2:F:56:ASP:HB3   | 2.09                     | 0.52              |
| 1:A:657:ILE:CG2  | 1:A:756:ILE:HA   | 2.39                     | 0.52              |
| 2:E:44:THR:HG22  | 2:E:47:GLU:OE1   | 2.09                     | 0.52              |
| 1:A:540:ARG:HD3  | 1:A:627:TYR:OH   | 2.09                     | 0.52              |
| 1:C:509:PRO:O    | 1:C:511:LYS:N    | 2.39                     | 0.52              |
| 1:C:512:GLU:O    | 1:C:516:VAL:HG23 | 2.09                     | 0.52              |
| 1:B:327:LEU:N    | 1:B:327:LEU:HD12 | 2.25                     | 0.52              |
| 1:B:724:ARG:O    | 1:B:727:GLN:HB3  | 2.10                     | 0.52              |
| 1:C:695:LYS:HD2  | 2:F:18:LEU:HB3   | 1.92                     | 0.52              |
| 2:D:15:ALA:HB1   | 2:D:35:VAL:HG13  | 1.90                     | 0.52              |
| 2:F:25:GLY:O     | 2:F:64:ASP:HA    | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:722:ILE:HG23 | 1:A:760:VAL:CG1  | 2.32                     | 0.52              |
| 1:C:597:ASN:HB2  | 1:C:598:PRO:HD2  | 1.91                     | 0.52              |
| 1:A:513:TRP:O    | 1:A:517:VAL:HG23 | 2.09                     | 0.52              |
| 1:C:515:LYS:O    | 1:C:515:LYS:HG2  | 2.09                     | 0.52              |
| 2:F:41:GLN:HB3   | 2:F:43:PRO:HD3   | 1.92                     | 0.52              |
| 1:B:419:ILE:HD12 | 1:B:419:ILE:O    | 2.09                     | 0.52              |
| 1:C:616:GLU:HA   | 1:C:620:THR:OG1  | 2.09                     | 0.52              |
| 1:A:533:LEU:HG   | 1:A:538:ILE:HD11 | 1.92                     | 0.52              |
| 1:A:304:ALA:HB3  | 1:A:604:LEU:HD13 | 1.92                     | 0.52              |
| 1:B:368:GLN:HG3  | 1:B:383:GLY:C    | 2.31                     | 0.52              |
| 1:B:546:LYS:O    | 1:B:547:GLY:O    | 2.28                     | 0.52              |
| 1:B:752:LEU:CD2  | 1:B:756:ILE:HD11 | 2.40                     | 0.52              |
| 2:D:80:ASP:C     | 2:D:82:GLU:H     | 2.13                     | 0.52              |
| 1:B:334:LEU:HD22 | 1:B:334:LEU:N    | 2.25                     | 0.52              |
| 2:E:29:THR:HG23  | 2:E:32:LEU:HD22  | 1.91                     | 0.52              |
| 1:A:456:LYS:HD3  | 1:A:471:TRP:CD1  | 2.34                     | 0.51              |
| 1:C:775:LEU:HG   | 1:C:776:LEU:HD12 | 1.92                     | 0.51              |
| 2:F:95:ASP:OD1   | 2:F:97:ASN:OD1   | 2.29                     | 0.51              |
| 1:B:789:ASN:OD1  | 1:B:792:VAL:HB   | 2.10                     | 0.51              |
| 1:C:755:ARG:HA   | 1:C:758:ASN:HD22 | 1.74                     | 0.51              |
| 2:D:52:ILE:HD11  | 2:D:63:ILE:HG12  | 1.92                     | 0.51              |
| 1:C:744:GLU:C    | 1:C:746:LYS:N    | 2.59                     | 0.51              |
| 2:D:12:PHE:HD1   | 2:D:39:LEU:HD21  | 1.75                     | 0.51              |
| 1:B:607:ASN:ND2  | 1:B:609:GLU:HB2  | 2.26                     | 0.51              |
| 1:C:747:ASN:HA   | 1:C:750:GLN:CD   | 2.31                     | 0.51              |
| 1:B:752:LEU:O    | 1:B:752:LEU:HD23 | 2.10                     | 0.51              |
| 2:E:63:ILE:HD12  | 2:E:63:ILE:N     | 2.26                     | 0.51              |
| 1:C:561:ASN:O    | 1:C:564:VAL:HG22 | 2.11                     | 0.51              |
| 1:B:565:LYS:NZ   | 1:B:572:GLY:HA2  | 2.25                     | 0.51              |
| 1:C:639:ASN:C    | 1:C:639:ASN:ND2  | 2.63                     | 0.51              |
| 1:B:360:VAL:HG22 | 1:B:360:VAL:O    | 2.09                     | 0.51              |
| 1:B:711:ILE:HG13 | 1:B:712:PHE:CD1  | 2.45                     | 0.51              |
| 1:C:747:ASN:HD22 | 1:C:750:GLN:NE2  | 2.09                     | 0.51              |
| 2:F:37:ARG:C     | 2:F:39:LEU:N     | 2.62                     | 0.51              |
| 1:B:760:VAL:HG11 | 1:B:773:PHE:HE2  | 1.75                     | 0.51              |
| 1:A:657:ILE:HD11 | 1:A:704:TYR:CG   | 2.46                     | 0.51              |
| 1:C:504:ILE:HG21 | 1:C:625:LEU:HD22 | 1.93                     | 0.51              |
| 1:A:449:GLU:N    | 1:A:449:GLU:OE1  | 2.44                     | 0.51              |
| 1:A:456:LYS:HB2  | 1:A:470:ASN:HA   | 1.93                     | 0.51              |
| 1:A:648:PRO:HA   | 1:A:651:LYS:CD   | 2.41                     | 0.51              |
| 1:B:655:ASN:HB3  | 1:B:759:GLN:NE2  | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:549:LEU:HD12 | 1:A:549:LEU:N    | 2.26                     | 0.51              |
| 1:A:404:LYS:HE2  | 1:A:450:ASN:O    | 2.10                     | 0.51              |
| 1:B:540:ARG:CZ   | 1:B:627:TYR:CE1  | 2.94                     | 0.51              |
| 1:B:632:TYR:O    | 1:B:634:LYS:HG3  | 2.10                     | 0.51              |
| 1:A:478:ALA:HA   | 1:A:488:LEU:HG   | 1.92                     | 0.51              |
| 1:B:711:ILE:HG13 | 1:B:712:PHE:HD1  | 1.76                     | 0.51              |
| 1:A:338:LEU:O    | 1:A:341:SER:HB3  | 2.11                     | 0.51              |
| 1:B:381:GLU:CG   | 1:B:465:LEU:HD21 | 2.40                     | 0.50              |
| 1:C:640:LYS:HE2  | 6:C:36:HOH:O     | 2.11                     | 0.50              |
| 2:E:47:GLU:HA    | 2:E:50:ASP:OD1   | 2.11                     | 0.50              |
| 1:B:549:LEU:HD11 | 1:B:553:GLN:HB3  | 1.93                     | 0.50              |
| 1:C:339:ILE:HD13 | 1:C:492:TYR:CE1  | 2.44                     | 0.50              |
| 1:C:521:ASN:HB2  | 1:C:524:GLU:HB2  | 1.94                     | 0.50              |
| 2:F:64:ASP:OD1   | 2:F:67:GLU:HG3   | 2.11                     | 0.50              |
| 1:B:730:ASN:ND2  | 1:B:734:ASN:N    | 2.58                     | 0.50              |
| 1:B:773:PHE:O    | 1:B:777:TYR:N    | 2.45                     | 0.50              |
| 1:B:499:PRO:HD2  | 1:B:625:LEU:O    | 2.12                     | 0.50              |
| 2:E:125:ILE:O    | 2:E:129:ASP:HB2  | 2.10                     | 0.50              |
| 1:C:376:GLN:O    | 1:C:380:VAL:HG23 | 2.11                     | 0.50              |
| 1:B:743:PRO:O    | 1:B:747:ASN:CB   | 2.60                     | 0.50              |
| 1:C:666:ASN:HD22 | 1:C:666:ASN:N    | 2.08                     | 0.50              |
| 1:B:537:GLY:O    | 1:B:625:LEU:HD21 | 2.11                     | 0.50              |
| 1:B:778:LYS:C    | 1:B:780:LEU:H    | 2.14                     | 0.50              |
| 1:B:704:TYR:HD1  | 1:B:724:ARG:HB2  | 1.77                     | 0.50              |
| 1:C:668:SER:O    | 1:C:671:ARG:HB3  | 2.11                     | 0.50              |
| 2:D:95:ASP:OD2   | 2:D:97:ASN:HB3   | 2.12                     | 0.50              |
| 1:C:523:LEU:HD11 | 2:F:144:MET:HG2  | 1.94                     | 0.50              |
| 1:B:331:VAL:O    | 1:B:332:ASN:C    | 2.50                     | 0.50              |
| 2:E:87:GLU:O     | 2:E:91:VAL:HG23  | 2.11                     | 0.50              |
| 1:A:406:ASP:O    | 1:A:410:ILE:HG12 | 2.11                     | 0.50              |
| 1:A:740:GLN:O    | 1:A:741:ILE:HG12 | 2.12                     | 0.50              |
| 1:B:424:LYS:HG2  | 1:B:433:TYR:CE2  | 2.47                     | 0.50              |
| 2:D:15:ALA:HA    | 2:D:18:LEU:HD12  | 1.94                     | 0.50              |
| 1:B:605:THR:HG21 | 1:B:611:THR:OG1  | 2.11                     | 0.50              |
| 1:B:332:ASN:HD22 | 1:B:333:LYS:N    | 2.10                     | 0.50              |
| 1:A:299:GLU:O    | 1:A:303:LYS:HG3  | 2.12                     | 0.50              |
| 1:C:387:ASN:O    | 1:C:391:ILE:HG12 | 2.12                     | 0.50              |
| 1:C:437:SER:C    | 1:C:439:ASN:H    | 2.15                     | 0.50              |
| 1:A:781:ASN:HB3  | 1:A:789:ASN:ND2  | 2.27                     | 0.50              |
| 1:B:735:VAL:CG2  | 1:B:738:SER:HB2  | 2.42                     | 0.50              |
| 1:A:505:LYS:HE3  | 1:A:513:TRP:CD2  | 2.47                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:712:PHE:HB3  | 1:C:716:LYS:HG2  | 1.93                     | 0.50              |
| 2:F:83:GLU:O     | 2:F:87:GLU:HG3   | 2.11                     | 0.50              |
| 1:B:793:PHE:HA   | 1:B:796:ILE:HG12 | 1.94                     | 0.49              |
| 1:C:657:ILE:CD1  | 1:C:759:GLN:HG2  | 2.42                     | 0.49              |
| 1:B:366:PHE:CD1  | 1:B:400:LYS:HD3  | 2.47                     | 0.49              |
| 1:B:459:GLU:O    | 1:B:461:LYS:N    | 2.44                     | 0.49              |
| 1:B:775:LEU:O    | 1:B:776:LEU:HG   | 2.12                     | 0.49              |
| 1:A:321:GLU:HG2  | 1:A:322:LEU:HD23 | 1.94                     | 0.49              |
| 2:D:24:ASP:O     | 2:D:65:PHE:HE1   | 1.94                     | 0.49              |
| 1:B:318:ILE:N    | 1:B:318:ILE:HD12 | 2.28                     | 0.49              |
| 2:E:63:ILE:HG21  | 2:E:71:MET:CE    | 2.42                     | 0.49              |
| 1:A:349:ASN:ND2  | 1:A:349:ASN:H    | 2.10                     | 0.49              |
| 1:B:743:PRO:O    | 1:B:747:ASN:HB2  | 2.11                     | 0.49              |
| 1:B:585:GLU:HB3  | 1:B:586:PHE:CE1  | 2.46                     | 0.49              |
| 1:B:299:GLU:O    | 1:B:303:LYS:HG3  | 2.13                     | 0.49              |
| 1:C:537:GLY:O    | 1:C:625:LEU:HD21 | 2.13                     | 0.49              |
| 1:B:653:LYS:O    | 1:B:755:ARG:HD3  | 2.13                     | 0.49              |
| 1:A:392:THR:HG21 | 1:C:635:ILE:HG13 | 1.93                     | 0.49              |
| 1:A:694:VAL:HG12 | 1:A:696:LYS:HB2  | 1.95                     | 0.49              |
| 2:D:48:LEU:O     | 2:D:52:ILE:HG22  | 2.13                     | 0.49              |
| 1:B:730:ASN:HD21 | 1:B:734:ASN:N    | 2.10                     | 0.49              |
| 1:B:300:LYS:HA   | 1:B:303:LYS:NZ   | 2.28                     | 0.49              |
| 1:B:530:THR:C    | 1:B:532:LEU:H    | 2.16                     | 0.49              |
| 1:C:376:GLN:HB2  | 1:C:379:ALA:HB3  | 1.93                     | 0.49              |
| 1:C:304:ALA:HB3  | 1:C:604:LEU:HD13 | 1.95                     | 0.49              |
| 1:C:364:ILE:HB   | 1:C:477:MET:HB2  | 1.95                     | 0.49              |
| 1:C:636:ALA:HB3  | 1:C:639:ASN:ND2  | 2.28                     | 0.49              |
| 1:A:564:VAL:HG23 | 1:A:565:LYS:N    | 2.27                     | 0.49              |
| 1:B:315:PHE:HE2  | 1:B:560:LEU:HB3  | 1.78                     | 0.49              |
| 1:C:523:LEU:HB2  | 2:F:127:GLU:OE2  | 2.13                     | 0.49              |
| 1:C:657:ILE:HD12 | 1:C:704:TYR:CE1  | 2.48                     | 0.49              |
| 1:A:538:ILE:H    | 1:A:538:ILE:HD12 | 1.78                     | 0.49              |
| 2:E:52:ILE:HG13  | 2:E:52:ILE:O     | 2.12                     | 0.49              |
| 2:E:19:PHE:CE2   | 2:E:34:THR:HG21  | 2.48                     | 0.49              |
| 1:A:349:ASN:N    | 1:A:349:ASN:ND2  | 2.61                     | 0.49              |
| 1:B:296:LEU:O    | 1:B:603:ILE:HA   | 2.13                     | 0.49              |
| 1:A:346:LYS:HD3  | 1:A:364:ILE:HG12 | 1.94                     | 0.49              |
| 1:C:292:ARG:HH22 | 1:C:297:LYS:HZ2  | 1.57                     | 0.48              |
| 2:D:27:ILE:HB    | 2:D:31:GLU:CG    | 2.42                     | 0.48              |
| 2:E:106:ARG:NH2  | 2:E:118:ASP:HA   | 2.27                     | 0.48              |
| 1:C:667:LEU:HA   | 1:C:670:ILE:CG2  | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:463:THR:O    | 1:C:466:GLY:N    | 2.34                     | 0.48              |
| 1:C:581:GLN:NE2  | 1:C:628:PHE:HA   | 2.27                     | 0.48              |
| 1:C:550:SER:H    | 1:C:553:GLN:HE21 | 1.60                     | 0.48              |
| 2:F:114:GLU:HG3  | 2:F:116:LEU:HD11 | 1.94                     | 0.48              |
| 1:C:671:ARG:HD3  | 1:C:672:ARG:HH21 | 1.76                     | 0.48              |
| 1:C:451:ASN:N    | 1:C:451:ASN:HD22 | 2.11                     | 0.48              |
| 1:B:368:GLN:HG3  | 1:B:384:ASN:N    | 2.28                     | 0.48              |
| 1:A:559:ARG:CB   | 1:A:559:ARG:HH11 | 2.24                     | 0.48              |
| 1:B:419:ILE:C    | 1:B:419:ILE:HD12 | 2.34                     | 0.48              |
| 2:E:37:ARG:HG2   | 2:E:42:ASN:HA    | 1.96                     | 0.48              |
| 1:A:718:ARG:HG3  | 2:D:132:GLY:O    | 2.13                     | 0.48              |
| 1:B:549:LEU:HD21 | 1:B:557:LEU:HD22 | 1.94                     | 0.48              |
| 1:C:655:ASN:N    | 1:C:655:ASN:ND2  | 2.60                     | 0.48              |
| 1:B:774:LYS:O    | 1:B:774:LYS:CG   | 2.62                     | 0.48              |
| 1:B:499:PRO:HG2  | 1:B:504:ILE:HD11 | 1.94                     | 0.48              |
| 1:C:747:ASN:HD22 | 1:C:750:GLN:CD   | 2.16                     | 0.48              |
| 1:C:763:LEU:HD21 | 2:F:131:ASP:HB2  | 1.95                     | 0.48              |
| 1:B:460:GLY:HA2  | 1:B:468:LYS:NZ   | 2.28                     | 0.48              |
| 1:C:511:LYS:O    | 1:C:514:ASP:HB2  | 2.13                     | 0.48              |
| 2:F:102:ALA:CA   | 2:F:125:ILE:HG13 | 2.40                     | 0.48              |
| 2:F:24:ASP:O     | 2:F:26:THR:HG23  | 2.13                     | 0.48              |
| 1:B:350:VAL:CG2  | 1:B:398:ILE:HG12 | 2.43                     | 0.48              |
| 1:A:508:ILE:HG23 | 1:A:532:LEU:HD22 | 1.96                     | 0.48              |
| 1:C:712:PHE:HB3  | 1:C:716:LYS:CG   | 2.44                     | 0.48              |
| 1:C:691:LYS:HE2  | 1:C:741:ILE:CD1  | 2.44                     | 0.48              |
| 1:A:372:LYS:C    | 1:A:374:HIS:H    | 2.17                     | 0.48              |
| 1:B:339:ILE:HD11 | 1:B:490:ALA:O    | 2.13                     | 0.48              |
| 1:B:311:HIS:HD2  | 1:B:564:VAL:CB   | 2.23                     | 0.48              |
| 2:F:13:LYS:HG3   | 2:F:65:PHE:CD2   | 2.49                     | 0.48              |
| 1:C:753:LYS:NZ   | 1:C:753:LYS:HB3  | 2.29                     | 0.48              |
| 2:D:120:GLU:O    | 2:D:123:GLU:N    | 2.47                     | 0.48              |
| 1:C:691:LYS:O    | 1:C:694:VAL:HG22 | 2.13                     | 0.48              |
| 1:B:773:PHE:C    | 1:B:775:LEU:H    | 2.17                     | 0.48              |
| 1:B:377:GLN:O    | 1:B:381:GLU:HG3  | 2.14                     | 0.48              |
| 1:C:693:SER:O    | 1:C:697:ILE:HG13 | 2.14                     | 0.48              |
| 1:C:636:ALA:O    | 1:C:640:LYS:HA   | 2.14                     | 0.48              |
| 2:E:105:LEU:O    | 2:E:109:MET:HG2  | 2.14                     | 0.48              |
| 1:A:438:ASN:ND2  | 1:A:438:ASN:N    | 2.62                     | 0.48              |
| 1:A:324:THR:CB   | 1:A:499:PRO:HA   | 2.44                     | 0.48              |
| 1:C:723:PHE:HB2  | 1:C:793:PHE:CD2  | 2.49                     | 0.48              |
| 1:A:368:GLN:HG3  | 1:A:383:GLY:CA   | 2.44                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:310:GLU:HB3  | 1:B:567:THR:CG2  | 2.44                     | 0.48              |
| 1:C:747:ASN:O    | 1:C:750:GLN:HG2  | 2.14                     | 0.47              |
| 1:B:450:ASN:CG   | 1:B:452:GLU:HG3  | 2.34                     | 0.47              |
| 1:C:664:ILE:CG2  | 2:F:15:ALA:HB2   | 2.44                     | 0.47              |
| 1:C:597:ASN:HD21 | 1:C:601:GLU:HB2  | 1.78                     | 0.47              |
| 2:F:92:PHE:HB2   | 2:F:100:ILE:HD12 | 1.96                     | 0.47              |
| 1:C:669:SER:C    | 1:C:671:ARG:H    | 2.16                     | 0.47              |
| 1:A:604:LEU:O    | 1:A:604:LEU:HD23 | 2.14                     | 0.47              |
| 1:A:512:GLU:O    | 1:A:516:VAL:HG23 | 2.15                     | 0.47              |
| 1:B:596:ILE:HG12 | 1:B:602:PHE:CD2  | 2.49                     | 0.47              |
| 1:C:550:SER:O    | 1:C:554:LYS:HG3  | 2.13                     | 0.47              |
| 1:B:355:SER:HB2  | 1:B:371:SER:HA   | 1.96                     | 0.47              |
| 1:B:326:ILE:C    | 1:B:327:LEU:HD12 | 2.34                     | 0.47              |
| 1:A:775:LEU:H    | 1:A:775:LEU:CD1  | 2.20                     | 0.47              |
| 1:B:550:SER:H    | 1:B:553:GLN:HE21 | 1.63                     | 0.47              |
| 1:C:587:PRO:HB2  | 1:C:643:ILE:CD1  | 2.43                     | 0.47              |
| 1:C:763:LEU:O    | 1:C:766:HIS:HB2  | 2.15                     | 0.47              |
| 1:C:292:ARG:HH12 | 1:C:297:LYS:HE2  | 1.80                     | 0.47              |
| 1:C:597:ASN:ND2  | 1:C:601:GLU:HB2  | 2.29                     | 0.47              |
| 1:B:570:THR:O    | 1:B:572:GLY:N    | 2.48                     | 0.47              |
| 1:A:345:THR:HB   | 1:A:491:ASP:HB3  | 1.96                     | 0.47              |
| 1:C:434:LEU:HD22 | 1:C:434:LEU:N    | 2.30                     | 0.47              |
| 2:D:93:ASP:OD2   | 2:D:96:GLY:N     | 2.47                     | 0.47              |
| 2:F:20:ASP:OD2   | 2:F:27:ILE:HG23  | 2.15                     | 0.47              |
| 1:C:292:ARG:HH22 | 1:C:297:LYS:CE   | 2.27                     | 0.47              |
| 1:B:308:VAL:HB   | 1:B:311:HIS:ND1  | 2.30                     | 0.47              |
| 1:B:722:ILE:O    | 1:B:726:ILE:HG13 | 2.15                     | 0.47              |
| 2:E:92:PHE:HE2   | 2:E:108:VAL:HG11 | 1.79                     | 0.47              |
| 2:F:97:ASN:ND2   | 2:F:99:TYR:CD1   | 2.83                     | 0.47              |
| 1:C:657:ILE:HG23 | 1:C:658:PRO:HD2  | 1.97                     | 0.47              |
| 2:D:102:ALA:CA   | 2:D:125:ILE:HG13 | 2.45                     | 0.47              |
| 1:B:310:GLU:CD   | 1:B:310:GLU:H    | 2.18                     | 0.47              |
| 1:B:649:ILE:O    | 1:B:649:ILE:HG22 | 2.15                     | 0.47              |
| 1:C:622:LYS:HD3  | 1:C:622:LYS:HA   | 1.71                     | 0.47              |
| 1:B:338:LEU:HD21 | 1:B:409:ARG:CZ   | 2.44                     | 0.47              |
| 2:F:99:TYR:CD2   | 2:F:137:ASN:HB3  | 2.50                     | 0.46              |
| 1:B:784:GLU:HG2  | 1:B:788:ASP:OD2  | 2.15                     | 0.46              |
| 1:A:492:TYR:CD2  | 1:A:574:VAL:CG1  | 2.98                     | 0.46              |
| 2:D:29:THR:HG22  | 2:D:29:THR:O     | 2.16                     | 0.46              |
| 1:C:713:SER:OG   | 1:C:715:GLU:HG2  | 2.15                     | 0.46              |
| 1:B:723:PHE:HB2  | 1:B:793:PHE:CE2  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:92:PHE:CD2   | 2:F:108:VAL:HG21 | 2.50                     | 0.46              |
| 1:B:401:ILE:HG22 | 1:B:485:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:711:ILE:HG13 | 1:A:712:PHE:N    | 2.31                     | 0.46              |
| 1:A:501:LEU:HD23 | 1:A:623:ASP:C    | 2.35                     | 0.46              |
| 1:B:353:LYS:HE2  | 1:B:353:LYS:HA   | 1.97                     | 0.46              |
| 1:C:546:LYS:CB   | 1:C:549:LEU:HD21 | 2.46                     | 0.46              |
| 1:B:456:LYS:HG3  | 1:B:457:THR:N    | 2.30                     | 0.46              |
| 1:A:694:VAL:HG11 | 1:A:731:GLU:CG   | 2.45                     | 0.46              |
| 1:A:581:GLN:NE2  | 1:A:629:ASN:H    | 2.14                     | 0.46              |
| 1:B:709:ASN:OD1  | 1:B:717:LYS:HG2  | 2.15                     | 0.46              |
| 1:C:655:ASN:HD22 | 1:C:655:ASN:N    | 2.13                     | 0.46              |
| 1:C:697:ILE:HD11 | 1:C:735:VAL:HG21 | 1.96                     | 0.46              |
| 2:F:47:GLU:HA    | 2:F:50:ASP:HB3   | 1.96                     | 0.46              |
| 1:B:589:LYS:HE2  | 1:B:608:TRP:CD1  | 2.51                     | 0.46              |
| 1:A:754:GLU:HG2  | 1:A:758:ASN:HD21 | 1.81                     | 0.46              |
| 1:B:530:THR:HG22 | 2:E:92:PHE:CZ    | 2.51                     | 0.46              |
| 1:B:346:LYS:HD3  | 1:B:364:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:615:ILE:HD12 | 1:B:645:TRP:CH2  | 2.49                     | 0.46              |
| 1:A:359:PRO:HB2  | 1:A:405:LEU:HD11 | 1.97                     | 0.46              |
| 1:A:723:PHE:HB2  | 1:A:793:PHE:CE2  | 2.50                     | 0.46              |
| 1:A:456:LYS:HA   | 1:A:469:PHE:CE1  | 2.50                     | 0.46              |
| 2:F:92:PHE:HB2   | 2:F:100:ILE:CD1  | 2.45                     | 0.46              |
| 1:A:781:ASN:HB3  | 1:A:789:ASN:CG   | 2.35                     | 0.46              |
| 1:A:434:LEU:HD23 | 1:A:435:LEU:N    | 2.30                     | 0.46              |
| 1:A:768:LYS:HB2  | 1:A:797:ILE:CD1  | 2.46                     | 0.46              |
| 1:C:437:SER:O    | 1:C:439:ASN:N    | 2.48                     | 0.46              |
| 1:B:338:LEU:HD21 | 1:B:409:ARG:NE   | 2.29                     | 0.46              |
| 2:D:86:ARG:HA    | 2:D:138:TYR:CE1  | 2.50                     | 0.46              |
| 1:A:664:ILE:HD12 | 2:D:39:LEU:HD13  | 1.97                     | 0.46              |
| 1:A:587:PRO:HB2  | 1:A:643:ILE:CD1  | 2.46                     | 0.46              |
| 1:C:455:TYR:HB3  | 1:C:474:ILE:HD11 | 1.97                     | 0.46              |
| 1:B:368:GLN:HG3  | 1:B:383:GLY:CA   | 2.46                     | 0.46              |
| 2:E:109:MET:C    | 2:E:111:ASN:H    | 2.20                     | 0.46              |
| 1:B:723:PHE:O    | 1:B:727:GLN:N    | 2.44                     | 0.46              |
| 1:A:329:ARG:HB3  | 1:A:330:PRO:CD   | 2.46                     | 0.46              |
| 1:C:456:LYS:HA   | 1:C:469:PHE:HE1  | 1.81                     | 0.46              |
| 1:C:406:ASP:OD1  | 1:C:408:LEU:N    | 2.49                     | 0.46              |
| 2:D:20:ASP:C     | 2:D:22:ASP:H     | 2.18                     | 0.46              |
| 2:E:107:HIS:O    | 2:E:111:ASN:ND2  | 2.49                     | 0.46              |
| 2:F:23:GLY:C     | 2:F:25:GLY:H     | 2.19                     | 0.46              |
| 1:A:359:PRO:O    | 1:A:405:LEU:HD11 | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:378:LEU:HB2  | 1:C:377:GLN:HE22 | 1.81                     | 0.46              |
| 1:C:730:ASN:HD21 | 1:C:782:PHE:HB2  | 1.81                     | 0.45              |
| 1:C:748:TYR:O    | 1:C:751:TYR:HB3  | 2.16                     | 0.45              |
| 1:A:344:ALA:O    | 1:A:489:THR:HG22 | 2.16                     | 0.45              |
| 1:B:707:SER:C    | 1:B:709:ASN:H    | 2.18                     | 0.45              |
| 1:C:520:PRO:HG2  | 1:C:521:ASN:H    | 1.80                     | 0.45              |
| 2:D:27:ILE:O     | 2:D:63:ILE:HB    | 2.17                     | 0.45              |
| 1:B:373:LYS:O    | 1:B:374:HIS:C    | 2.54                     | 0.45              |
| 1:C:740:GLN:O    | 1:C:741:ILE:C    | 2.54                     | 0.45              |
| 1:A:299:GLU:HG3  | 1:A:303:LYS:CE   | 2.47                     | 0.45              |
| 1:A:432:TYR:CD2  | 1:A:447:SER:HA   | 2.52                     | 0.45              |
| 1:C:747:ASN:ND2  | 1:C:750:GLN:NE2  | 2.65                     | 0.45              |
| 1:B:653:LYS:HE2  | 1:B:755:ARG:NH1  | 2.28                     | 0.45              |
| 1:A:438:ASN:ND2  | 1:A:438:ASN:H    | 2.15                     | 0.45              |
| 1:A:695:LYS:HD2  | 2:D:18:LEU:HB3   | 1.99                     | 0.45              |
| 1:B:607:ASN:HD21 | 1:B:609:GLU:HB2  | 1.82                     | 0.45              |
| 1:B:501:LEU:HG   | 1:B:623:ASP:O    | 2.16                     | 0.45              |
| 1:A:670:ILE:HG23 | 1:A:745:TYR:CZ   | 2.51                     | 0.45              |
| 2:D:92:PHE:CE2   | 2:D:108:VAL:HG11 | 2.50                     | 0.45              |
| 1:B:603:ILE:HD13 | 1:B:614:PHE:HE1  | 1.80                     | 0.45              |
| 1:B:703:ASP:O    | 1:B:704:TYR:C    | 2.54                     | 0.45              |
| 1:B:792:VAL:HG12 | 1:B:796:ILE:HD11 | 1.98                     | 0.45              |
| 2:F:29:THR:OG1   | 2:F:52:ILE:HG12  | 2.16                     | 0.45              |
| 1:C:505:LYS:HE3  | 1:C:513:TRP:CE2  | 2.52                     | 0.45              |
| 1:A:299:GLU:HG3  | 1:A:303:LYS:HE2  | 1.99                     | 0.45              |
| 1:B:359:PRO:C    | 1:B:361:ALA:H    | 2.20                     | 0.45              |
| 2:E:117:THR:C    | 2:E:119:GLU:H    | 2.20                     | 0.45              |
| 1:B:455:TYR:CD2  | 1:B:474:ILE:HG12 | 2.51                     | 0.45              |
| 1:C:344:ALA:O    | 1:C:489:THR:HG22 | 2.16                     | 0.45              |
| 1:A:364:ILE:N    | 1:A:364:ILE:HD12 | 2.31                     | 0.45              |
| 1:A:782:PHE:O    | 1:A:783:THR:C    | 2.54                     | 0.45              |
| 1:C:375:GLY:HA2  | 1:C:464:VAL:HG11 | 1.99                     | 0.45              |
| 1:C:323:ASN:HD22 | 1:C:598:PRO:CB   | 2.29                     | 0.45              |
| 1:C:792:VAL:O    | 1:C:796:ILE:HG12 | 2.17                     | 0.45              |
| 1:B:793:PHE:HA   | 1:B:796:ILE:CG1  | 2.47                     | 0.45              |
| 1:B:785:ASN:OD1  | 1:B:788:ASP:HB2  | 2.17                     | 0.45              |
| 1:B:391:ILE:HD11 | 1:B:400:LYS:CG   | 2.45                     | 0.45              |
| 1:A:587:PRO:HG3  | 1:A:636:ALA:HB2  | 1.99                     | 0.45              |
| 1:C:744:GLU:C    | 1:C:747:ASN:H    | 2.20                     | 0.45              |
| 1:C:462:ILE:HD11 | 1:C:466:GLY:C    | 2.37                     | 0.45              |
| 1:B:507:GLN:HG2  | 1:B:536:TYR:HB3  | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:308:VAL:HG13 | 1:C:340:LYS:HD3  | 1.99                     | 0.45              |
| 2:D:15:ALA:O     | 2:D:18:LEU:HB2   | 2.16                     | 0.45              |
| 1:B:302:LEU:C    | 1:B:304:ALA:H    | 2.20                     | 0.45              |
| 1:B:322:LEU:HD11 | 1:B:559:ARG:HD3  | 1.97                     | 0.44              |
| 1:A:706:ASN:C    | 1:A:708:ALA:H    | 2.20                     | 0.44              |
| 1:B:744:GLU:OE2  | 1:B:748:TYR:HB2  | 2.18                     | 0.44              |
| 1:A:534:ILE:HA   | 1:A:538:ILE:CD1  | 2.47                     | 0.44              |
| 1:C:791:GLU:CD   | 1:C:791:GLU:H    | 2.17                     | 0.44              |
| 2:E:29:THR:HA    | 2:E:32:LEU:HB2   | 1.99                     | 0.44              |
| 1:C:403:LEU:HD13 | 1:C:476:VAL:HG11 | 1.99                     | 0.44              |
| 1:C:524:GLU:HA   | 1:C:524:GLU:OE1  | 2.17                     | 0.44              |
| 2:F:115:LYS:HD3  | 2:F:116:LEU:N    | 2.33                     | 0.44              |
| 2:F:38:SER:C     | 2:F:39:LEU:HD23  | 2.38                     | 0.44              |
| 1:C:462:ILE:HG13 | 1:C:463:THR:N    | 2.33                     | 0.44              |
| 2:F:137:ASN:OD1  | 2:F:137:ASN:C    | 2.56                     | 0.44              |
| 1:A:440:GLN:C    | 1:A:458:LYS:HD3  | 2.37                     | 0.44              |
| 1:B:716:LYS:HA   | 1:B:719:LYS:HB3  | 2.00                     | 0.44              |
| 1:C:656:THR:O    | 1:C:755:ARG:HD2  | 2.18                     | 0.44              |
| 1:C:764:LEU:C    | 1:C:766:HIS:H    | 2.20                     | 0.44              |
| 2:E:129:ASP:OD1  | 2:E:132:GLY:N    | 2.37                     | 0.44              |
| 1:B:425:GLU:N    | 1:B:432:TYR:O    | 2.47                     | 0.44              |
| 2:D:136:VAL:HA   | 2:D:140:GLU:OE1  | 2.17                     | 0.44              |
| 1:B:345:THR:HB   | 1:B:491:ASP:HB3  | 1.98                     | 0.44              |
| 1:B:530:THR:C    | 1:B:532:LEU:N    | 2.70                     | 0.44              |
| 2:E:89:PHE:HD1   | 2:E:100:ILE:HD11 | 1.83                     | 0.44              |
| 1:C:581:GLN:O    | 1:C:629:ASN:HA   | 2.17                     | 0.44              |
| 1:C:636:ALA:CB   | 1:C:639:ASN:HD21 | 2.30                     | 0.44              |
| 1:A:505:LYS:HE3  | 1:A:513:TRP:CG   | 2.52                     | 0.44              |
| 1:A:700:TYR:CD1  | 1:A:727:GLN:HB3  | 2.53                     | 0.44              |
| 2:E:29:THR:HG23  | 2:E:32:LEU:CD2   | 2.48                     | 0.44              |
| 1:B:649:ILE:CD1  | 2:E:86:ARG:HG3   | 2.47                     | 0.44              |
| 2:D:75:LYS:C     | 2:D:77:LYS:H     | 2.21                     | 0.44              |
| 1:C:385:LEU:HD22 | 1:C:385:LEU:O    | 2.18                     | 0.44              |
| 1:A:423:LYS:HG2  | 1:A:423:LYS:O    | 2.17                     | 0.44              |
| 1:B:376:GLN:O    | 1:B:379:ALA:N    | 2.49                     | 0.44              |
| 1:B:613:ARG:O    | 1:B:616:GLU:HG2  | 2.18                     | 0.44              |
| 1:B:325:TYR:HB3  | 1:B:327:LEU:HD11 | 2.00                     | 0.44              |
| 1:A:781:ASN:O    | 1:A:783:THR:N    | 2.51                     | 0.44              |
| 1:B:764:LEU:HD22 | 1:B:768:LYS:HD3  | 2.00                     | 0.44              |
| 1:A:697:ILE:HD13 | 1:A:732:ILE:CG1  | 2.37                     | 0.44              |
| 1:B:529:VAL:HG11 | 2:E:109:MET:CE   | 2.48                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:9:ILE:H      | 2:D:9:ILE:CD1    | 2.28                     | 0.44              |
| 1:B:400:LYS:HA   | 1:B:476:VAL:O    | 2.17                     | 0.44              |
| 1:A:523:LEU:HD13 | 2:D:127:GLU:HB3  | 1.99                     | 0.44              |
| 1:C:308:VAL:HB   | 1:C:311:HIS:CG   | 2.52                     | 0.44              |
| 1:C:717:LYS:HA   | 1:C:720:ILE:HD11 | 1.99                     | 0.44              |
| 2:D:10:ALA:O     | 2:D:14:GLU:HG2   | 2.18                     | 0.44              |
| 1:A:731:GLU:O    | 1:A:735:VAL:HG23 | 2.18                     | 0.44              |
| 1:C:718:ARG:O    | 1:C:722:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:426:ILE:HA   | 1:A:430:LYS:O    | 2.17                     | 0.44              |
| 1:A:400:LYS:HE2  | 1:A:475:GLU:CD   | 2.39                     | 0.44              |
| 1:A:522:SER:OG   | 2:D:127:GLU:HG3  | 2.17                     | 0.44              |
| 1:B:525:LYS:NZ   | 2:E:116:LEU:HD21 | 2.30                     | 0.44              |
| 1:A:549:LEU:H    | 1:A:549:LEU:HD12 | 1.83                     | 0.44              |
| 1:B:310:GLU:HB3  | 1:B:567:THR:HG21 | 2.00                     | 0.44              |
| 2:F:117:THR:OG1  | 2:F:120:GLU:HG3  | 2.18                     | 0.44              |
| 1:A:557:LEU:HG   | 1:A:575:VAL:HG12 | 1.99                     | 0.44              |
| 2:D:47:GLU:O     | 2:D:51:MET:HG3   | 2.18                     | 0.44              |
| 1:B:730:ASN:HD22 | 1:B:730:ASN:HA   | 1.62                     | 0.43              |
| 2:F:36:MET:O     | 2:F:41:GLN:HB2   | 2.18                     | 0.43              |
| 1:B:776:LEU:HD23 | 1:B:776:LEU:HA   | 1.87                     | 0.43              |
| 1:B:629:ASN:HB3  | 1:B:632:TYR:CE2  | 2.53                     | 0.43              |
| 1:A:697:ILE:O    | 1:A:701:LEU:HG   | 2.18                     | 0.43              |
| 1:A:540:ARG:HD2  | 1:A:582:ASP:OD1  | 2.17                     | 0.43              |
| 1:C:465:LEU:N    | 1:C:465:LEU:HD23 | 2.33                     | 0.43              |
| 1:C:629:ASN:HB3  | 1:C:632:TYR:CD2  | 2.53                     | 0.43              |
| 2:E:62:THR:C     | 2:E:63:ILE:HD12  | 2.39                     | 0.43              |
| 1:A:549:LEU:HB2  | 1:A:553:GLN:HE21 | 1.83                     | 0.43              |
| 1:B:376:GLN:HE21 | 1:B:376:GLN:HB3  | 1.70                     | 0.43              |
| 1:A:636:ALA:HA   | 1:A:637:PRO:HD3  | 1.90                     | 0.43              |
| 2:E:85:ILE:O     | 2:E:88:ALA:HB3   | 2.17                     | 0.43              |
| 1:B:760:VAL:CG1  | 1:B:773:PHE:HE2  | 2.31                     | 0.43              |
| 1:C:732:ILE:HD13 | 1:C:752:LEU:HD12 | 2.00                     | 0.43              |
| 2:D:66:PRO:O     | 2:D:70:THR:HB    | 2.19                     | 0.43              |
| 2:E:6:GLU:C      | 2:E:8:GLN:N      | 2.69                     | 0.43              |
| 1:A:700:TYR:CE1  | 1:A:727:GLN:HB3  | 2.54                     | 0.43              |
| 1:B:774:LYS:HG3  | 1:B:774:LYS:O    | 2.18                     | 0.43              |
| 1:A:373:LYS:HG2  | 1:A:379:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:513:TRP:O    | 1:B:517:VAL:HG12 | 2.18                     | 0.43              |
| 1:B:508:ILE:HG23 | 1:B:509:PRO:HD2  | 1.99                     | 0.43              |
| 1:B:530:THR:HG22 | 2:E:92:PHE:HZ    | 1.82                     | 0.43              |
| 1:B:543:ASP:OD2  | 1:B:554:LYS:HE2  | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:664:ILE:C    | 1:A:666:ASN:N    | 2.69                     | 0.43              |
| 1:C:318:ILE:HG23 | 1:C:322:LEU:HD12 | 2.01                     | 0.43              |
| 2:E:115:LYS:CB   | 2:E:115:LYS:NZ   | 2.81                     | 0.43              |
| 2:F:114:GLU:HG3  | 2:F:116:LEU:HD13 | 1.98                     | 0.43              |
| 1:B:418:ILE:HG22 | 1:B:419:ILE:HG23 | 2.01                     | 0.43              |
| 1:B:437:SER:C    | 1:B:439:ASN:H    | 2.21                     | 0.43              |
| 1:B:552:TRP:C    | 1:B:552:TRP:CD1  | 2.90                     | 0.43              |
| 1:B:547:GLY:HA3  | 5:B:903:3AT:N1   | 2.34                     | 0.43              |
| 1:A:376:GLN:HE22 | 1:B:466:GLY:HA3  | 1.80                     | 0.43              |
| 1:C:657:ILE:HG23 | 1:C:756:ILE:CD1  | 2.48                     | 0.43              |
| 1:A:742:ALA:O    | 1:A:744:GLU:N    | 2.52                     | 0.43              |
| 1:A:505:LYS:O    | 1:A:508:ILE:N    | 2.51                     | 0.43              |
| 1:A:651:LYS:O    | 1:A:654:ILE:HG22 | 2.18                     | 0.43              |
| 2:D:118:ASP:O    | 2:D:122:ASP:OD1  | 2.36                     | 0.43              |
| 1:B:596:ILE:HA   | 1:B:601:GLU:O    | 2.17                     | 0.43              |
| 1:B:657:ILE:HG12 | 1:B:658:PRO:CD   | 2.44                     | 0.43              |
| 2:D:33:GLY:C     | 2:D:35:VAL:H     | 2.22                     | 0.43              |
| 1:B:605:THR:HG22 | 1:B:607:ASN:H    | 1.84                     | 0.43              |
| 1:B:505:LYS:O    | 1:B:508:ILE:N    | 2.47                     | 0.43              |
| 2:F:7:GLU:O      | 2:F:11:GLU:HG3   | 2.19                     | 0.43              |
| 1:C:661:ALA:C    | 1:C:663:PHE:N    | 2.71                     | 0.43              |
| 1:C:629:ASN:HB3  | 1:C:632:TYR:CE2  | 2.54                     | 0.43              |
| 1:A:581:GLN:O    | 1:A:629:ASN:HA   | 2.19                     | 0.43              |
| 1:B:336:THR:HG23 | 1:B:337:ASN:N    | 2.34                     | 0.43              |
| 1:C:695:LYS:HB2  | 2:F:18:LEU:HD22  | 2.00                     | 0.43              |
| 1:A:478:ALA:HB1  | 1:A:486:LYS:O    | 2.18                     | 0.43              |
| 1:A:665:LYS:HG2  | 2:D:11:GLU:CD    | 2.39                     | 0.43              |
| 1:B:435:LEU:HD11 | 1:B:446:ILE:HB   | 2.01                     | 0.43              |
| 1:A:778:LYS:C    | 1:A:780:LEU:N    | 2.72                     | 0.43              |
| 1:C:714:GLN:CA   | 1:C:714:GLN:NE2  | 2.81                     | 0.43              |
| 1:A:716:LYS:O    | 1:A:717:LYS:C    | 2.57                     | 0.43              |
| 1:C:549:LEU:N    | 1:C:549:LEU:HD12 | 2.27                     | 0.43              |
| 1:C:329:ARG:HD3  | 1:C:580:GLU:HG2  | 2.00                     | 0.43              |
| 1:C:584:GLU:OE2  | 1:C:630:ARG:HB2  | 2.19                     | 0.43              |
| 1:B:390:SER:O    | 1:B:394:HIS:HB2  | 2.19                     | 0.43              |
| 1:B:648:PRO:C    | 1:B:650:THR:N    | 2.72                     | 0.43              |
| 2:D:103:ALA:O    | 2:D:106:ARG:HB3  | 2.18                     | 0.43              |
| 2:E:102:ALA:CA   | 2:E:125:ILE:HD11 | 2.45                     | 0.43              |
| 1:A:509:PRO:HG3  | 1:A:512:GLU:OE1  | 2.19                     | 0.43              |
| 1:B:322:LEU:O    | 1:B:503:GLU:HG3  | 2.18                     | 0.42              |
| 1:B:538:ILE:HD11 | 1:B:625:LEU:HD11 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:550:SER:H    | 1:B:553:GLN:NE2  | 2.16                     | 0.42              |
| 1:C:401:ILE:HG21 | 1:C:485:LEU:HB3  | 2.01                     | 0.42              |
| 1:A:533:LEU:HG   | 1:A:538:ILE:CD1  | 2.49                     | 0.42              |
| 1:B:470:ASN:CG   | 1:B:471:TRP:H    | 2.22                     | 0.42              |
| 1:B:565:LYS:C    | 1:B:567:THR:N    | 2.73                     | 0.42              |
| 1:A:780:LEU:HD13 | 1:A:782:PHE:CE1  | 2.53                     | 0.42              |
| 1:A:372:LYS:CE   | 5:A:902:3AT:O2G  | 2.67                     | 0.42              |
| 1:C:499:PRO:HG2  | 1:C:625:LEU:HB3  | 1.99                     | 0.42              |
| 2:F:71:MET:O     | 2:F:74:ARG:HB2   | 2.18                     | 0.42              |
| 1:A:299:GLU:HG3  | 1:A:303:LYS:HZ3  | 1.85                     | 0.42              |
| 2:D:7:GLU:O      | 2:D:11:GLU:HG3   | 2.20                     | 0.42              |
| 1:A:424:LYS:O    | 1:A:425:GLU:HB2  | 2.19                     | 0.42              |
| 1:B:320:ARG:CG   | 1:B:321:GLU:H    | 2.27                     | 0.42              |
| 1:C:391:ILE:HD12 | 1:C:399:GLY:HA2  | 2.01                     | 0.42              |
| 1:B:311:HIS:HE2  | 1:B:569:TYR:HB2  | 1.84                     | 0.42              |
| 2:E:132:GLY:C    | 2:E:134:GLY:H    | 2.21                     | 0.42              |
| 2:E:5:THR:CB     | 2:E:8:GLN:HB2    | 2.49                     | 0.42              |
| 1:B:751:TYR:HA   | 1:B:754:GLU:OE2  | 2.20                     | 0.42              |
| 1:A:538:ILE:N    | 1:A:538:ILE:HD12 | 2.33                     | 0.42              |
| 2:F:34:THR:HG22  | 2:F:34:THR:O     | 2.20                     | 0.42              |
| 1:A:378:LEU:HD23 | 1:A:378:LEU:HA   | 1.83                     | 0.42              |
| 1:A:716:LYS:O    | 1:A:719:LYS:HB2  | 2.19                     | 0.42              |
| 2:F:68:PHE:HA    | 2:F:71:MET:CE    | 2.49                     | 0.42              |
| 1:C:479:LYS:HG3  | 1:C:481:VAL:HG22 | 2.00                     | 0.42              |
| 1:C:701:LEU:O    | 1:C:704:TYR:HB3  | 2.19                     | 0.42              |
| 1:C:318:ILE:CD1  | 1:C:318:ILE:H    | 2.30                     | 0.42              |
| 1:A:768:LYS:HB2  | 1:A:797:ILE:HD13 | 2.02                     | 0.42              |
| 2:F:5:THR:N      | 2:F:8:GLN:HB3    | 2.35                     | 0.42              |
| 2:E:9:ILE:C      | 2:E:11:GLU:H     | 2.23                     | 0.42              |
| 1:A:540:ARG:HD3  | 1:A:627:TYR:CZ   | 2.54                     | 0.42              |
| 2:E:42:ASN:N     | 2:E:43:PRO:CD    | 2.82                     | 0.42              |
| 1:C:385:LEU:HA   | 1:C:388:LYS:HE3  | 2.00                     | 0.42              |
| 1:C:692:GLU:C    | 1:C:734:ASN:HD21 | 2.23                     | 0.42              |
| 1:A:776:LEU:H    | 1:A:776:LEU:CD1  | 2.14                     | 0.42              |
| 2:E:49:GLN:HA    | 2:E:52:ILE:CG2   | 2.40                     | 0.42              |
| 1:A:713:SER:O    | 1:A:717:LYS:N    | 2.47                     | 0.42              |
| 1:B:733:GLU:C    | 1:B:735:VAL:N    | 2.70                     | 0.42              |
| 1:A:360:VAL:HG22 | 1:A:363:TYR:HB2  | 2.02                     | 0.42              |
| 1:B:718:ARG:O    | 1:B:722:ILE:HG13 | 2.19                     | 0.42              |
| 2:E:19:PHE:CE1   | 2:E:31:GLU:HB3   | 2.55                     | 0.42              |
| 2:E:9:ILE:C      | 2:E:11:GLU:N     | 2.73                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:614:PHE:CD2  | 1:B:614:PHE:C    | 2.92                     | 0.42              |
| 1:B:774:LYS:HD2  | 1:B:774:LYS:HA   | 1.73                     | 0.42              |
| 1:C:408:LEU:O    | 1:C:411:GLU:HB3  | 2.20                     | 0.42              |
| 1:A:787:THR:O    | 1:A:787:THR:HG22 | 2.20                     | 0.42              |
| 1:B:327:LEU:N    | 1:B:327:LEU:CD1  | 2.83                     | 0.42              |
| 1:A:494:LEU:HD21 | 1:A:497:LEU:HD21 | 2.00                     | 0.42              |
| 2:D:138:TYR:O    | 2:D:142:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:302:LEU:HD11 | 1:B:312:ALA:CB   | 2.50                     | 0.42              |
| 1:B:776:LEU:HD13 | 1:B:779:GLN:CD   | 2.41                     | 0.41              |
| 1:A:719:LYS:HE2  | 1:A:797:ILE:HG21 | 2.02                     | 0.41              |
| 1:A:320:ARG:HA   | 1:A:598:PRO:O    | 2.20                     | 0.41              |
| 2:D:72:MET:O     | 2:D:74:ARG:N     | 2.53                     | 0.41              |
| 1:A:494:LEU:HB3  | 1:A:579:THR:HG22 | 2.02                     | 0.41              |
| 2:E:117:THR:C    | 2:E:119:GLU:N    | 2.73                     | 0.41              |
| 1:A:426:ILE:HG22 | 1:A:427:ASP:N    | 2.34                     | 0.41              |
| 1:C:540:ARG:HH12 | 1:C:630:ARG:NH2  | 2.18                     | 0.41              |
| 1:B:622:LYS:O    | 1:B:623:ASP:HB2  | 2.20                     | 0.41              |
| 2:D:110:THR:HG23 | 2:D:115:LYS:HD2  | 2.02                     | 0.41              |
| 1:C:500:SER:O    | 1:C:503:GLU:HB3  | 2.19                     | 0.41              |
| 2:D:145:MET:HB2  | 2:D:145:MET:HE2  | 1.90                     | 0.41              |
| 1:C:742:ALA:O    | 1:C:743:PRO:C    | 2.58                     | 0.41              |
| 1:B:540:ARG:CZ   | 1:B:627:TYR:HE1  | 2.33                     | 0.41              |
| 2:E:65:PHE:N     | 2:E:66:PRO:CD    | 2.83                     | 0.41              |
| 1:A:629:ASN:HD21 | 1:A:631:SER:HB2  | 1.84                     | 0.41              |
| 1:A:323:ASN:ND2  | 1:A:624:TYR:CE2  | 2.88                     | 0.41              |
| 2:F:13:LYS:HG3   | 2:F:65:PHE:HD2   | 1.84                     | 0.41              |
| 1:B:415:GLU:C    | 1:B:417:GLY:H    | 2.23                     | 0.41              |
| 1:B:764:LEU:O    | 1:B:768:LYS:HB2  | 2.20                     | 0.41              |
| 1:A:760:VAL:C    | 1:A:762:LEU:H    | 2.23                     | 0.41              |
| 1:C:657:ILE:HG13 | 1:C:759:GLN:HG2  | 2.01                     | 0.41              |
| 1:B:731:GLU:HG3  | 1:B:732:ILE:H    | 1.84                     | 0.41              |
| 2:F:44:THR:HG22  | 2:F:47:GLU:OE1   | 2.20                     | 0.41              |
| 1:B:374:HIS:HB3  | 6:B:14:HOH:O     | 2.20                     | 0.41              |
| 1:A:470:ASN:O    | 1:A:471:TRP:C    | 2.59                     | 0.41              |
| 1:A:735:VAL:C    | 1:A:737:LYS:N    | 2.73                     | 0.41              |
| 1:A:323:ASN:ND2  | 1:A:598:PRO:HB3  | 2.35                     | 0.41              |
| 1:B:750:GLN:O    | 1:B:753:LYS:HB3  | 2.21                     | 0.41              |
| 1:B:731:GLU:HG2  | 1:B:731:GLU:H    | 1.34                     | 0.41              |
| 1:A:586:PHE:HA   | 1:A:639:ASN:ND2  | 2.35                     | 0.41              |
| 1:B:762:LEU:HA   | 1:B:765:THR:OG1  | 2.20                     | 0.41              |
| 1:A:401:ILE:O    | 1:A:476:VAL:HG22 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:109:MET:HG3  | 2:E:116:LEU:CD1  | 2.50                     | 0.41              |
| 2:E:63:ILE:HG21  | 2:E:71:MET:HE3   | 2.02                     | 0.41              |
| 1:C:479:LYS:O    | 1:C:485:LEU:HD12 | 2.20                     | 0.41              |
| 2:D:9:ILE:HA     | 2:D:12:PHE:CD2   | 2.55                     | 0.41              |
| 1:C:517:VAL:HG13 | 1:C:518:ASN:N    | 2.35                     | 0.41              |
| 1:B:366:PHE:CE1  | 1:B:391:ILE:HD12 | 2.55                     | 0.41              |
| 1:B:565:LYS:O    | 1:B:567:THR:N    | 2.53                     | 0.41              |
| 1:C:370:LEU:HD11 | 1:C:455:TYR:CE1  | 2.55                     | 0.41              |
| 1:B:650:THR:O    | 1:B:651:LYS:C    | 2.59                     | 0.41              |
| 2:E:93:ASP:OD2   | 2:E:96:GLY:HA2   | 2.19                     | 0.41              |
| 2:E:20:ASP:CG    | 2:E:27:ILE:HG22  | 2.41                     | 0.41              |
| 1:C:757:THR:HG23 | 1:C:773:PHE:CD2  | 2.55                     | 0.41              |
| 2:E:89:PHE:CE1   | 2:E:100:ILE:HG13 | 2.54                     | 0.41              |
| 1:B:654:ILE:HA   | 1:B:755:ARG:HD2  | 2.01                     | 0.41              |
| 1:A:540:ARG:NH2  | 2:D:87:GLU:CD    | 2.73                     | 0.41              |
| 1:A:718:ARG:HD2  | 1:A:767:GLN:HG3  | 2.03                     | 0.41              |
| 1:A:629:ASN:HB3  | 1:A:632:TYR:CE2  | 2.56                     | 0.41              |
| 1:B:714:GLN:HB3  | 2:E:126:ARG:HD2  | 2.03                     | 0.41              |
| 2:D:129:ASP:OD1  | 2:D:133:ASP:N    | 2.53                     | 0.41              |
| 1:A:360:VAL:O    | 1:A:361:ALA:C    | 2.57                     | 0.41              |
| 1:A:709:ASN:HD21 | 1:A:724:ARG:HH12 | 1.69                     | 0.41              |
| 1:A:607:ASN:ND2  | 1:A:609:GLU:HB2  | 2.36                     | 0.41              |
| 1:C:499:PRO:HD3  | 1:C:552:TRP:CH2  | 2.56                     | 0.41              |
| 1:B:334:LEU:H    | 1:B:334:LEU:HD22 | 1.83                     | 0.41              |
| 1:B:323:ASN:OD1  | 1:B:500:SER:HB3  | 2.21                     | 0.41              |
| 1:A:704:TYR:CD2  | 1:A:704:TYR:C    | 2.94                     | 0.41              |
| 2:F:15:ALA:O     | 2:F:18:LEU:HB2   | 2.21                     | 0.41              |
| 1:B:603:ILE:HG21 | 1:B:614:PHE:CE1  | 2.56                     | 0.41              |
| 1:C:349:ASN:H    | 1:C:349:ASN:HD22 | 1.69                     | 0.41              |
| 1:B:648:PRO:O    | 1:B:650:THR:N    | 2.54                     | 0.41              |
| 1:A:728:ALA:C    | 1:A:730:ASN:N    | 2.74                     | 0.41              |
| 1:A:384:ASN:O    | 1:A:388:LYS:HD3  | 2.21                     | 0.41              |
| 1:A:728:ALA:C    | 1:A:730:ASN:H    | 2.23                     | 0.41              |
| 1:C:327:LEU:HD12 | 1:C:327:LEU:N    | 2.36                     | 0.41              |
| 1:A:472:ARG:HB2  | 1:A:472:ARG:HH11 | 1.86                     | 0.41              |
| 1:C:744:GLU:OE1  | 1:C:747:ASN:HB2  | 2.21                     | 0.41              |
| 1:C:636:ALA:HA   | 1:C:637:PRO:HD3  | 1.84                     | 0.41              |
| 1:B:628:PHE:CD2  | 1:B:645:TRP:CD1  | 3.09                     | 0.41              |
| 1:B:524:GLU:O    | 1:B:524:GLU:HG3  | 2.21                     | 0.41              |
| 1:B:551:ASN:ND2  | 1:B:551:ASN:H    | 2.19                     | 0.41              |
| 1:C:557:LEU:O    | 1:C:558:ASP:C    | 2.59                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:105:LEU:HD12 | 2:F:125:ILE:HD13 | 2.03                     | 0.40              |
| 1:A:331:VAL:HG21 | 1:A:492:TYR:HD1  | 1.85                     | 0.40              |
| 2:D:52:ILE:HD12  | 2:D:52:ILE:HA    | 1.95                     | 0.40              |
| 2:E:36:MET:O     | 2:E:41:GLN:HB2   | 2.21                     | 0.40              |
| 1:C:692:GLU:O    | 1:C:734:ASN:ND2  | 2.55                     | 0.40              |
| 1:C:709:ASN:HD22 | 1:C:709:ASN:N    | 2.18                     | 0.40              |
| 1:B:778:LYS:C    | 1:B:780:LEU:N    | 2.75                     | 0.40              |
| 2:E:92:PHE:HA    | 2:E:108:VAL:HG21 | 2.02                     | 0.40              |
| 2:E:71:MET:O     | 2:E:73:ALA:N     | 2.54                     | 0.40              |
| 1:C:407:HIS:H    | 1:C:407:HIS:CD2  | 2.35                     | 0.40              |
| 1:A:355:SER:CB   | 1:A:360:VAL:HG13 | 2.51                     | 0.40              |
| 1:A:724:ARG:O    | 1:A:727:GLN:HB2  | 2.21                     | 0.40              |
| 1:C:404:LYS:HA   | 1:C:451:ASN:O    | 2.22                     | 0.40              |
| 1:A:527:LYS:HG3  | 2:D:145:MET:SD   | 2.61                     | 0.40              |
| 1:B:472:ARG:HB3  | 1:B:473:ASN:H    | 1.53                     | 0.40              |
| 1:B:722:ILE:HD13 | 1:B:764:LEU:CD2  | 2.52                     | 0.40              |
| 1:B:529:VAL:HG21 | 2:E:109:MET:SD   | 2.61                     | 0.40              |
| 1:C:413:LEU:HB3  | 1:C:419:ILE:HG12 | 2.03                     | 0.40              |
| 1:C:753:LYS:NZ   | 1:C:753:LYS:CB   | 2.85                     | 0.40              |
| 1:C:477:MET:HE2  | 1:C:477:MET:HA   | 2.03                     | 0.40              |
| 2:E:106:ARG:HE   | 2:E:121:VAL:HG21 | 1.85                     | 0.40              |
| 1:C:707:SER:C    | 1:C:709:ASN:H    | 2.24                     | 0.40              |
| 1:B:294:ASP:HB3  | 1:B:610:MET:HE1  | 2.03                     | 0.40              |
| 1:C:359:PRO:HB2  | 1:C:405:LEU:HD11 | 2.04                     | 0.40              |
| 1:C:736:LEU:HD21 | 1:C:749:PHE:CB   | 2.51                     | 0.40              |
| 2:E:71:MET:C     | 2:E:73:ALA:N     | 2.72                     | 0.40              |
| 1:A:360:VAL:HA   | 1:A:403:LEU:HD21 | 2.02                     | 0.40              |
| 1:C:450:ASN:CG   | 1:C:452:GLU:HG3  | 2.41                     | 0.40              |

There are no symmetry-related clashes.

## 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     | 479/510 (94%)   | 411 (86%)  | 52 (11%)  | 16 (3%)  | 5           | 14 |
| 1   | B     | 457/510 (90%)   | 364 (80%)  | 66 (14%)  | 27 (6%)  | 2           | 4  |
| 1   | C     | 499/510 (98%)   | 423 (85%)  | 60 (12%)  | 16 (3%)  | 5           | 15 |
| 2   | D     | 141/148 (95%)   | 111 (79%)  | 24 (17%)  | 6 (4%)   | 3           | 9  |
| 2   | E     | 141/148 (95%)   | 107 (76%)  | 29 (21%)  | 5 (4%)   | 4           | 13 |
| 2   | F     | 141/148 (95%)   | 116 (82%)  | 23 (16%)  | 2 (1%)   | 14          | 38 |
| All | All   | 1858/1974 (94%) | 1532 (82%) | 254 (14%) | 72 (4%)  | 4           | 11 |

All (72) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 323 | ASN  |
| 1   | A     | 739 | LYS  |
| 2   | D     | 64  | ASP  |
| 1   | B     | 466 | GLY  |
| 2   | E     | 73  | ALA  |
| 1   | C     | 520 | PRO  |
| 1   | C     | 694 | VAL  |
| 1   | C     | 741 | ILE  |
| 2   | F     | 40  | GLY  |
| 1   | A     | 294 | ASP  |
| 1   | A     | 471 | TRP  |
| 1   | A     | 578 | GLY  |
| 1   | A     | 707 | SER  |
| 2   | D     | 73  | ALA  |
| 2   | D     | 74  | ARG  |
| 2   | D     | 93  | ASP  |
| 1   | B     | 460 | GLY  |
| 1   | B     | 464 | VAL  |
| 1   | B     | 537 | GLY  |
| 1   | B     | 547 | GLY  |
| 1   | B     | 571 | GLY  |
| 1   | B     | 732 | ILE  |
| 1   | B     | 776 | LEU  |
| 2   | E     | 93  | ASP  |
| 1   | C     | 438 | ASN  |
| 1   | C     | 510 | GLN  |
| 1   | C     | 675 | ASN  |
| 1   | A     | 424 | LYS  |
| 1   | A     | 782 | PHE  |
| 2   | D     | 65  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 702 | SER  |
| 1   | B     | 734 | ASN  |
| 2   | E     | 72  | MET  |
| 1   | C     | 332 | ASN  |
| 1   | C     | 743 | PRO  |
| 2   | F     | 24  | ASP  |
| 1   | A     | 376 | GLN  |
| 1   | A     | 425 | GLU  |
| 1   | A     | 665 | LYS  |
| 1   | A     | 743 | PRO  |
| 1   | A     | 783 | THR  |
| 2   | D     | 76  | MET  |
| 1   | B     | 406 | ASP  |
| 1   | B     | 566 | TYR  |
| 1   | B     | 794 | GLN  |
| 2   | E     | 133 | ASP  |
| 1   | C     | 662 | GLU  |
| 1   | C     | 677 | GLY  |
| 1   | C     | 740 | GLN  |
| 1   | A     | 510 | GLN  |
| 1   | A     | 736 | LEU  |
| 1   | A     | 742 | ALA  |
| 1   | B     | 438 | ASN  |
| 1   | B     | 459 | GLU  |
| 1   | B     | 535 | LYS  |
| 1   | B     | 694 | VAL  |
| 1   | B     | 704 | TYR  |
| 1   | B     | 708 | ALA  |
| 1   | B     | 713 | SER  |
| 1   | B     | 774 | LYS  |
| 1   | C     | 294 | ASP  |
| 1   | B     | 303 | LYS  |
| 1   | B     | 377 | GLN  |
| 1   | C     | 708 | ALA  |
| 1   | C     | 765 | THR  |
| 1   | C     | 578 | GLY  |
| 1   | B     | 743 | PRO  |
| 2   | E     | 27  | ILE  |
| 1   | C     | 537 | GLY  |
| 1   | B     | 309 | PRO  |
| 1   | B     | 657 | ILE  |
| 1   | B     | 295 | VAL  |

### 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     | 433/455 (95%)   | 410 (95%)  | 23 (5%)  | 28          | 58 |
| 1   | B     | 414/455 (91%)   | 382 (92%)  | 32 (8%)  | 16          | 38 |
| 1   | C     | 448/455 (98%)   | 421 (94%)  | 27 (6%)  | 24          | 53 |
| 2   | D     | 121/126 (96%)   | 115 (95%)  | 6 (5%)   | 30          | 61 |
| 2   | E     | 121/126 (96%)   | 117 (97%)  | 4 (3%)   | 45          | 77 |
| 2   | F     | 121/126 (96%)   | 115 (95%)  | 6 (5%)   | 30          | 61 |
| All | All   | 1658/1743 (95%) | 1560 (94%) | 98 (6%)  | 24          | 53 |

All (98) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 322 | LEU  |
| 1   | A     | 323 | ASN  |
| 1   | A     | 349 | ASN  |
| 1   | A     | 373 | LYS  |
| 1   | A     | 385 | LEU  |
| 1   | A     | 388 | LYS  |
| 1   | A     | 406 | ASP  |
| 1   | A     | 409 | ARG  |
| 1   | A     | 423 | LYS  |
| 1   | A     | 438 | ASN  |
| 1   | A     | 450 | ASN  |
| 1   | A     | 455 | TYR  |
| 1   | A     | 472 | ARG  |
| 1   | A     | 485 | LEU  |
| 1   | A     | 494 | LEU  |
| 1   | A     | 549 | LEU  |
| 1   | A     | 574 | VAL  |
| 1   | A     | 620 | THR  |
| 1   | A     | 622 | LYS  |
| 1   | A     | 629 | ASN  |
| 1   | A     | 646 | THR  |
| 1   | A     | 670 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 775 | LEU  |
| 2   | D     | 64  | ASP  |
| 2   | D     | 76  | MET  |
| 2   | D     | 87  | GLU  |
| 2   | D     | 105 | LEU  |
| 2   | D     | 118 | ASP  |
| 2   | D     | 122 | ASP  |
| 1   | B     | 320 | ARG  |
| 1   | B     | 332 | ASN  |
| 1   | B     | 351 | HIS  |
| 1   | B     | 353 | LYS  |
| 1   | B     | 391 | ILE  |
| 1   | B     | 406 | ASP  |
| 1   | B     | 415 | GLU  |
| 1   | B     | 426 | ILE  |
| 1   | B     | 439 | ASN  |
| 1   | B     | 440 | GLN  |
| 1   | B     | 485 | LEU  |
| 1   | B     | 510 | GLN  |
| 1   | B     | 518 | ASN  |
| 1   | B     | 532 | LEU  |
| 1   | B     | 544 | SER  |
| 1   | B     | 545 | THR  |
| 1   | B     | 546 | LYS  |
| 1   | B     | 552 | TRP  |
| 1   | B     | 585 | GLU  |
| 1   | B     | 611 | THR  |
| 1   | B     | 620 | THR  |
| 1   | B     | 627 | TYR  |
| 1   | B     | 629 | ASN  |
| 1   | B     | 639 | ASN  |
| 1   | B     | 655 | ASN  |
| 1   | B     | 714 | GLN  |
| 1   | B     | 730 | ASN  |
| 1   | B     | 731 | GLU  |
| 1   | B     | 743 | PRO  |
| 1   | B     | 744 | GLU  |
| 1   | B     | 775 | LEU  |
| 1   | B     | 784 | GLU  |
| 2   | E     | 64  | ASP  |
| 2   | E     | 65  | PHE  |
| 2   | E     | 76  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 94  | LYS  |
| 1   | C     | 323 | ASN  |
| 1   | C     | 341 | SER  |
| 1   | C     | 349 | ASN  |
| 1   | C     | 377 | GLN  |
| 1   | C     | 381 | GLU  |
| 1   | C     | 455 | TYR  |
| 1   | C     | 480 | ASN  |
| 1   | C     | 485 | LEU  |
| 1   | C     | 524 | GLU  |
| 1   | C     | 533 | LEU  |
| 1   | C     | 540 | ARG  |
| 1   | C     | 549 | LEU  |
| 1   | C     | 557 | LEU  |
| 1   | C     | 565 | LYS  |
| 1   | C     | 629 | ASN  |
| 1   | C     | 639 | ASN  |
| 1   | C     | 694 | VAL  |
| 1   | C     | 714 | GLN  |
| 1   | C     | 715 | GLU  |
| 1   | C     | 733 | GLU  |
| 1   | C     | 734 | ASN  |
| 1   | C     | 737 | LYS  |
| 1   | C     | 743 | PRO  |
| 1   | C     | 745 | TYR  |
| 1   | C     | 746 | LYS  |
| 1   | C     | 775 | LEU  |
| 1   | C     | 791 | GLU  |
| 2   | F     | 14  | GLU  |
| 2   | F     | 19  | PHE  |
| 2   | F     | 83  | GLU  |
| 2   | F     | 105 | LEU  |
| 2   | F     | 127 | GLU  |
| 2   | F     | 135 | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 323 | ASN  |
| 1   | A     | 337 | ASN  |
| 1   | A     | 349 | ASN  |
| 1   | A     | 351 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 376 | GLN  |
| 1   | A     | 394 | HIS  |
| 1   | A     | 416 | ASN  |
| 1   | A     | 438 | ASN  |
| 1   | A     | 439 | ASN  |
| 1   | A     | 440 | GLN  |
| 1   | A     | 507 | GLN  |
| 1   | A     | 518 | ASN  |
| 1   | A     | 526 | GLN  |
| 1   | A     | 531 | ASN  |
| 1   | A     | 553 | GLN  |
| 1   | A     | 581 | GLN  |
| 1   | A     | 607 | ASN  |
| 1   | A     | 629 | ASN  |
| 1   | A     | 633 | ASN  |
| 1   | A     | 706 | ASN  |
| 1   | A     | 714 | GLN  |
| 1   | A     | 727 | GLN  |
| 1   | A     | 758 | ASN  |
| 1   | A     | 789 | ASN  |
| 1   | A     | 794 | GLN  |
| 2   | D     | 41  | GLN  |
| 2   | D     | 42  | ASN  |
| 1   | B     | 332 | ASN  |
| 1   | B     | 368 | GLN  |
| 1   | B     | 376 | GLN  |
| 1   | B     | 377 | GLN  |
| 1   | B     | 407 | HIS  |
| 1   | B     | 439 | ASN  |
| 1   | B     | 451 | ASN  |
| 1   | B     | 507 | GLN  |
| 1   | B     | 518 | ASN  |
| 1   | B     | 526 | GLN  |
| 1   | B     | 551 | ASN  |
| 1   | B     | 553 | GLN  |
| 1   | B     | 555 | GLN  |
| 1   | B     | 629 | ASN  |
| 1   | B     | 639 | ASN  |
| 1   | B     | 655 | ASN  |
| 1   | B     | 709 | ASN  |
| 1   | B     | 730 | ASN  |
| 1   | B     | 734 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 747 | ASN  |
| 1   | B     | 759 | GLN  |
| 1   | B     | 761 | GLN  |
| 1   | B     | 794 | GLN  |
| 2   | E     | 107 | HIS  |
| 2   | E     | 135 | GLN  |
| 2   | E     | 143 | GLN  |
| 1   | C     | 323 | ASN  |
| 1   | C     | 349 | ASN  |
| 1   | C     | 376 | GLN  |
| 1   | C     | 440 | GLN  |
| 1   | C     | 451 | ASN  |
| 1   | C     | 480 | ASN  |
| 1   | C     | 507 | GLN  |
| 1   | C     | 510 | GLN  |
| 1   | C     | 518 | ASN  |
| 1   | C     | 553 | GLN  |
| 1   | C     | 555 | GLN  |
| 1   | C     | 577 | HIS  |
| 1   | C     | 581 | GLN  |
| 1   | C     | 629 | ASN  |
| 1   | C     | 639 | ASN  |
| 1   | C     | 655 | ASN  |
| 1   | C     | 666 | ASN  |
| 1   | C     | 709 | ASN  |
| 1   | C     | 714 | GLN  |
| 1   | C     | 727 | GLN  |
| 1   | C     | 734 | ASN  |
| 1   | C     | 747 | ASN  |
| 1   | C     | 758 | ASN  |
| 1   | C     | 794 | GLN  |
| 2   | F     | 111 | ASN  |
| 2   | F     | 143 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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     | 902 | 4    | 24,32,32     | 1.38 | 4 (16%)     | 26,50,50    | 1.24 | 1 (3%)      |
| 5   | 3AT  | B     | 903 | 4    | 24,32,32     | 1.38 | 5 (20%)     | 26,50,50    | 1.25 | 2 (7%)      |
| 5   | 3AT  | C     | 904 | 4    | 24,32,32     | 1.41 | 6 (25%)     | 26,50,50    | 1.21 | 1 (3%)      |

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     | 902 | 4    | -       | 0/18/34/34 | 0/3/3/3 |
| 5   | 3AT  | B     | 903 | 4    | -       | 0/18/34/34 | 0/3/3/3 |
| 5   | 3AT  | C     | 904 | 4    | -       | 0/18/34/34 | 0/3/3/3 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | A     | 902 | 3AT  | PG-O2G | -3.03 | 1.43        | 1.54     |
| 5   | B     | 903 | 3AT  | PG-O2G | -2.60 | 1.45        | 1.54     |
| 5   | C     | 904 | 3AT  | PG-O3G | -2.49 | 1.45        | 1.54     |
| 5   | C     | 904 | 3AT  | PB-O2B | -2.42 | 1.44        | 1.54     |
| 5   | C     | 904 | 3AT  | PG-O2G | -2.38 | 1.46        | 1.54     |
| 5   | B     | 903 | 3AT  | PB-O2B | -2.37 | 1.44        | 1.54     |
| 5   | B     | 903 | 3AT  | C8-N7  | -2.22 | 1.30        | 1.34     |
| 5   | A     | 902 | 3AT  | PB-O2B | -2.18 | 1.45        | 1.54     |
| 5   | C     | 904 | 3AT  | C2-N3  | 2.08  | 1.35        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 5   | C     | 904 | 3AT  | C4-N3   | 2.20 | 1.38        | 1.35     |
| 5   | A     | 902 | 3AT  | C2-N3   | 2.24 | 1.36        | 1.32     |
| 5   | A     | 902 | 3AT  | O4'-C1' | 2.26 | 1.44        | 1.41     |
| 5   | B     | 903 | 3AT  | C4-N3   | 2.34 | 1.39        | 1.35     |
| 5   | C     | 904 | 3AT  | O4'-C1' | 2.38 | 1.44        | 1.41     |
| 5   | B     | 903 | 3AT  | O4'-C1' | 2.82 | 1.44        | 1.41     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 5   | B     | 903 | 3AT  | C4-C5-N7   | 2.16 | 111.46      | 109.48   |
| 5   | A     | 902 | 3AT  | O3G-PG-O2G | 2.62 | 117.38      | 107.38   |
| 5   | B     | 903 | 3AT  | O3G-PG-O2G | 2.66 | 117.51      | 107.38   |
| 5   | C     | 904 | 3AT  | O3G-PG-O2G | 2.70 | 117.65      | 107.38   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 902 | 3AT  | 2       | 0            |
| 5   | B     | 903 | 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(Å²)          | Q<0.9   |
|-----|-------|-----------------|--------|-----------|----|----|-------------------|---------|
| 1   | A     | 485/510 (95%)   | 0.07   | 26 (5%)   | 29 | 22 | 24, 64, 145, 174  | 16 (3%) |
| 1   | B     | 457/510 (89%)   | 0.58   | 60 (13%)  | 5  | 3  | 29, 79, 172, 191  | 12 (2%) |
| 1   | C     | 491/510 (96%)   | 0.13   | 25 (5%)   | 32 | 24 | 17, 62, 151, 177  | 19 (3%) |
| 2   | D     | 143/148 (96%)   | 1.18   | 35 (24%)  | 1  | 0  | 39, 134, 185, 193 | 0       |
| 2   | E     | 143/148 (96%)   | 1.72   | 45 (31%)  | 1  | 0  | 61, 159, 199, 199 | 0       |
| 2   | F     | 143/148 (96%)   | 1.23   | 39 (27%)  | 1  | 0  | 43, 145, 188, 198 | 0       |
| All | All   | 1862/1974 (94%) | 0.51   | 230 (12%) | 5  | 3  | 17, 76, 181, 199  | 47 (2%) |

All (230) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 19  | PHE  | 17.2 |
| 2   | D     | 57  | ALA  | 12.5 |
| 2   | E     | 62  | THR  | 10.9 |
| 1   | B     | 697 | ILE  | 10.7 |
| 2   | F     | 62  | THR  | 10.6 |
| 1   | C     | 741 | ILE  | 10.5 |
| 1   | A     | 798 | ASP  | 9.4  |
| 2   | F     | 30  | LYS  | 8.8  |
| 1   | B     | 774 | LYS  | 8.3  |
| 2   | E     | 55  | VAL  | 7.6  |
| 1   | B     | 741 | ILE  | 7.5  |
| 2   | E     | 76  | MET  | 7.5  |
| 1   | B     | 736 | LEU  | 7.4  |
| 2   | D     | 58  | ASP  | 7.3  |
| 2   | D     | 19  | PHE  | 7.2  |
| 2   | D     | 75  | LYS  | 6.8  |
| 1   | B     | 739 | LYS  | 6.7  |
| 1   | B     | 779 | GLN  | 6.7  |
| 2   | F     | 56  | ASP  | 6.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 61  | GLY  | 6.6  |
| 2   | E     | 80  | ASP  | 6.6  |
| 2   | D     | 59  | GLY  | 6.4  |
| 2   | D     | 46  | ALA  | 6.4  |
| 1   | B     | 782 | PHE  | 6.2  |
| 1   | B     | 773 | PHE  | 6.2  |
| 2   | E     | 79  | THR  | 6.2  |
| 1   | B     | 776 | LEU  | 6.2  |
| 2   | E     | 57  | ALA  | 6.1  |
| 2   | E     | 51  | MET  | 6.1  |
| 2   | F     | 55  | VAL  | 6.0  |
| 2   | F     | 46  | ALA  | 5.9  |
| 1   | B     | 713 | SER  | 5.8  |
| 1   | B     | 658 | PRO  | 5.8  |
| 1   | B     | 740 | GLN  | 5.7  |
| 2   | F     | 29  | THR  | 5.7  |
| 2   | D     | 69  | LEU  | 5.7  |
| 2   | D     | 55  | VAL  | 5.6  |
| 2   | D     | 56  | ASP  | 5.6  |
| 1   | B     | 775 | LEU  | 5.5  |
| 2   | E     | 71  | MET  | 5.4  |
| 1   | C     | 786 | GLU  | 5.3  |
| 2   | F     | 63  | ILE  | 5.3  |
| 2   | F     | 28  | THR  | 5.2  |
| 1   | B     | 783 | THR  | 5.1  |
| 1   | B     | 793 | PHE  | 5.1  |
| 2   | F     | 44  | THR  | 5.0  |
| 2   | E     | 21  | LYS  | 4.9  |
| 2   | E     | 77  | LYS  | 4.9  |
| 1   | B     | 734 | ASN  | 4.9  |
| 1   | C     | 787 | THR  | 4.8  |
| 2   | F     | 19  | PHE  | 4.7  |
| 2   | E     | 69  | LEU  | 4.7  |
| 2   | E     | 72  | MET  | 4.6  |
| 2   | D     | 18  | LEU  | 4.6  |
| 1   | B     | 786 | GLU  | 4.6  |
| 2   | E     | 7   | GLU  | 4.5  |
| 1   | B     | 738 | SER  | 4.5  |
| 2   | E     | 5   | THR  | 4.4  |
| 1   | B     | 711 | ILE  | 4.4  |
| 1   | C     | 742 | ALA  | 4.4  |
| 2   | F     | 24  | ASP  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 74  | ARG  | 4.3  |
| 2   | F     | 43  | PRO  | 4.2  |
| 1   | A     | 785 | ASN  | 4.2  |
| 2   | D     | 74  | ARG  | 4.2  |
| 2   | E     | 63  | ILE  | 4.2  |
| 1   | B     | 747 | ASN  | 4.1  |
| 2   | D     | 53  | ASN  | 4.0  |
| 2   | D     | 47  | GLU  | 4.0  |
| 1   | C     | 785 | ASN  | 3.9  |
| 2   | E     | 60  | ASN  | 3.9  |
| 1   | C     | 740 | GLN  | 3.9  |
| 2   | F     | 6   | GLU  | 3.8  |
| 2   | F     | 23  | GLY  | 3.8  |
| 1   | B     | 735 | VAL  | 3.8  |
| 2   | F     | 61  | GLY  | 3.8  |
| 2   | E     | 28  | THR  | 3.8  |
| 1   | A     | 432 | TYR  | 3.7  |
| 1   | A     | 744 | GLU  | 3.7  |
| 2   | E     | 78  | ASP  | 3.7  |
| 2   | F     | 79  | THR  | 3.7  |
| 1   | B     | 737 | LYS  | 3.7  |
| 2   | D     | 114 | GLU  | 3.6  |
| 2   | E     | 12  | PHE  | 3.6  |
| 1   | B     | 702 | SER  | 3.6  |
| 1   | B     | 780 | LEU  | 3.6  |
| 1   | A     | 793 | PHE  | 3.6  |
| 1   | C     | 739 | LYS  | 3.6  |
| 2   | E     | 56  | ASP  | 3.6  |
| 1   | B     | 757 | THR  | 3.5  |
| 1   | A     | 790 | PHE  | 3.5  |
| 1   | A     | 740 | GLN  | 3.5  |
| 2   | E     | 54  | GLU  | 3.4  |
| 2   | D     | 50  | ASP  | 3.4  |
| 1   | A     | 445 | ARG  | 3.4  |
| 2   | D     | 71  | MET  | 3.4  |
| 2   | F     | 57  | ALA  | 3.4  |
| 1   | A     | 786 | GLU  | 3.3  |
| 2   | E     | 20  | ASP  | 3.3  |
| 1   | B     | 785 | ASN  | 3.3  |
| 2   | D     | 115 | LYS  | 3.3  |
| 1   | B     | 496 | ALA  | 3.3  |
| 1   | B     | 716 | LYS  | 3.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 728 | ALA  | 3.3  |
| 2   | E     | 6   | GLU  | 3.3  |
| 1   | B     | 797 | ILE  | 3.2  |
| 2   | E     | 22  | ASP  | 3.2  |
| 1   | B     | 754 | GLU  | 3.2  |
| 1   | A     | 784 | GLU  | 3.2  |
| 1   | C     | 691 | LYS  | 3.2  |
| 2   | F     | 47  | GLU  | 3.2  |
| 2   | F     | 102 | ALA  | 3.2  |
| 1   | B     | 729 | TYR  | 3.2  |
| 1   | B     | 731 | GLU  | 3.2  |
| 2   | F     | 31  | GLU  | 3.2  |
| 1   | C     | 743 | PRO  | 3.1  |
| 1   | B     | 578 | GLY  | 3.1  |
| 2   | D     | 33  | GLY  | 3.1  |
| 2   | F     | 34  | THR  | 3.1  |
| 2   | F     | 106 | ARG  | 3.1  |
| 2   | D     | 68  | PHE  | 3.1  |
| 2   | E     | 47  | GLU  | 3.1  |
| 2   | F     | 33  | GLY  | 3.1  |
| 2   | F     | 76  | MET  | 3.1  |
| 2   | F     | 48  | LEU  | 3.1  |
| 1   | B     | 749 | PHE  | 3.1  |
| 2   | D     | 45  | GLU  | 3.1  |
| 2   | E     | 27  | ILE  | 3.1  |
| 2   | E     | 14  | GLU  | 3.1  |
| 2   | E     | 121 | VAL  | 3.1  |
| 2   | E     | 102 | ALA  | 3.0  |
| 1   | C     | 292 | ARG  | 3.0  |
| 1   | B     | 778 | LYS  | 3.0  |
| 2   | F     | 54  | GLU  | 3.0  |
| 2   | D     | 67  | GLU  | 3.0  |
| 1   | C     | 672 | ARG  | 2.9  |
| 1   | B     | 714 | GLN  | 2.9  |
| 1   | B     | 746 | LYS  | 2.9  |
| 2   | F     | 7   | GLU  | 2.9  |
| 2   | F     | 22  | ASP  | 2.9  |
| 2   | F     | 39  | LEU  | 2.9  |
| 1   | A     | 782 | PHE  | 2.9  |
| 2   | F     | 27  | ILE  | 2.9  |
| 1   | C     | 780 | LEU  | 2.9  |
| 1   | B     | 516 | VAL  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 775 | LEU  | 2.8  |
| 1   | C     | 776 | LEU  | 2.8  |
| 1   | C     | 440 | GLN  | 2.8  |
| 2   | F     | 80  | ASP  | 2.8  |
| 1   | C     | 767 | GLN  | 2.8  |
| 1   | C     | 738 | SER  | 2.8  |
| 1   | C     | 784 | GLU  | 2.8  |
| 2   | E     | 24  | ASP  | 2.8  |
| 1   | B     | 712 | PHE  | 2.8  |
| 2   | D     | 41  | GLN  | 2.8  |
| 2   | D     | 54  | GLU  | 2.7  |
| 1   | B     | 568 | GLY  | 2.7  |
| 2   | D     | 70  | THR  | 2.7  |
| 1   | B     | 579 | THR  | 2.7  |
| 1   | A     | 434 | LEU  | 2.7  |
| 2   | D     | 28  | THR  | 2.7  |
| 1   | C     | 783 | THR  | 2.6  |
| 1   | A     | 779 | GLN  | 2.6  |
| 1   | A     | 739 | LYS  | 2.6  |
| 1   | A     | 661 | ALA  | 2.6  |
| 2   | E     | 58  | ASP  | 2.6  |
| 2   | F     | 40  | GLY  | 2.6  |
| 2   | E     | 46  | ALA  | 2.6  |
| 1   | B     | 744 | GLU  | 2.6  |
| 1   | B     | 751 | TYR  | 2.5  |
| 2   | D     | 79  | THR  | 2.5  |
| 1   | B     | 493 | ASP  | 2.5  |
| 1   | B     | 704 | TYR  | 2.5  |
| 1   | A     | 797 | ILE  | 2.5  |
| 2   | D     | 51  | MET  | 2.4  |
| 1   | A     | 787 | THR  | 2.4  |
| 1   | A     | 788 | ASP  | 2.4  |
| 1   | A     | 743 | PRO  | 2.4  |
| 1   | B     | 784 | GLU  | 2.4  |
| 2   | E     | 9   | ILE  | 2.4  |
| 2   | D     | 43  | PRO  | 2.4  |
| 2   | F     | 71  | MET  | 2.4  |
| 1   | C     | 782 | PHE  | 2.3  |
| 1   | A     | 738 | SER  | 2.3  |
| 2   | F     | 60  | ASN  | 2.3  |
| 2   | D     | 65  | PHE  | 2.3  |
| 1   | B     | 750 | GLN  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 489 | THR  | 2.3  |
| 1   | B     | 791 | GLU  | 2.3  |
| 1   | A     | 723 | PHE  | 2.3  |
| 2   | E     | 147 | ALA  | 2.3  |
| 2   | E     | 23  | GLY  | 2.3  |
| 1   | C     | 768 | LYS  | 2.3  |
| 1   | B     | 743 | PRO  | 2.3  |
| 1   | B     | 715 | GLU  | 2.2  |
| 1   | C     | 745 | TYR  | 2.2  |
| 2   | D     | 48  | LEU  | 2.2  |
| 1   | C     | 746 | LYS  | 2.2  |
| 1   | B     | 321 | GLU  | 2.2  |
| 1   | B     | 705 | TYR  | 2.2  |
| 2   | E     | 73  | ALA  | 2.2  |
| 1   | B     | 434 | LEU  | 2.2  |
| 1   | B     | 497 | LEU  | 2.2  |
| 2   | D     | 32  | LEU  | 2.2  |
| 2   | E     | 53  | ASN  | 2.2  |
| 2   | E     | 106 | ARG  | 2.2  |
| 2   | F     | 65  | PHE  | 2.2  |
| 1   | A     | 776 | LEU  | 2.1  |
| 1   | A     | 430 | LYS  | 2.1  |
| 2   | D     | 21  | LYS  | 2.1  |
| 1   | C     | 514 | ASP  | 2.1  |
| 2   | F     | 58  | ASP  | 2.1  |
| 2   | F     | 51  | MET  | 2.1  |
| 2   | F     | 74  | ARG  | 2.1  |
| 1   | A     | 426 | ILE  | 2.1  |
| 2   | D     | 78  | ASP  | 2.1  |
| 2   | D     | 60  | ASN  | 2.1  |
| 2   | F     | 26  | THR  | 2.1  |
| 2   | E     | 115 | LYS  | 2.1  |
| 1   | B     | 717 | LYS  | 2.1  |
| 1   | A     | 695 | LYS  | 2.0  |
| 1   | B     | 768 | LYS  | 2.0  |
| 2   | E     | 66  | PRO  | 2.0  |
| 1   | C     | 748 | TYR  | 2.0  |
| 1   | B     | 322 | LEU  | 2.0  |
| 1   | B     | 491 | ASP  | 2.0  |
| 1   | C     | 744 | GLU  | 2.0  |
| 2   | E     | 116 | LEU  | 2.0  |
| 2   | D     | 76  | MET  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 44  | THR  | 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( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 3   | CA   | F     | 804 | 1/1   | 0.98 | 0.16 | 0.55  | 67,67,67,67                 | 0     |
| 5   | 3AT  | A     | 902 | 30/30 | 0.96 | 0.20 | 0.40  | 23,44,55,55                 | 0     |
| 5   | 3AT  | B     | 903 | 30/30 | 0.96 | 0.22 | -0.02 | 43,54,61,65                 | 0     |
| 5   | 3AT  | C     | 904 | 30/30 | 0.96 | 0.17 | -0.27 | 28,44,53,58                 | 0     |
| 3   | CA   | D     | 801 | 1/1   | 0.96 | 0.12 | -0.38 | 59,59,59,59                 | 0     |
| 3   | CA   | D     | 800 | 1/1   | 0.97 | 0.14 | -1.02 | 53,53,53,53                 | 0     |
| 3   | CA   | E     | 802 | 1/1   | 0.96 | 0.13 | -1.27 | 105,105,105,105             | 0     |
| 3   | CA   | E     | 803 | 1/1   | 0.96 | 0.07 | -1.41 | 83,83,83,83                 | 0     |
| 3   | CA   | F     | 805 | 1/1   | 0.98 | 0.05 | -4.09 | 63,63,63,63                 | 0     |
| 4   | YB   | B     | 902 | 1/1   | 0.99 | 0.18 | -     | 47,47,47,47                 | 0     |
| 4   | YB   | C     | 903 | 1/1   | 0.99 | 0.17 | -     | 38,38,38,38                 | 0     |
| 4   | YB   | A     | 901 | 1/1   | 1.00 | 0.18 | -     | 38,38,38,38                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.