



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:43 AM UTC

PDB ID : 1S1M / pdb\_00001s1m  
Title : Crystal Structure of E. Coli CTP Synthetase  
Authors : Endrizzi, J.A.; Kim, H.; Anderson, P.M.; Baldwin, E.P.  
Deposited on : 2004-01-06  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

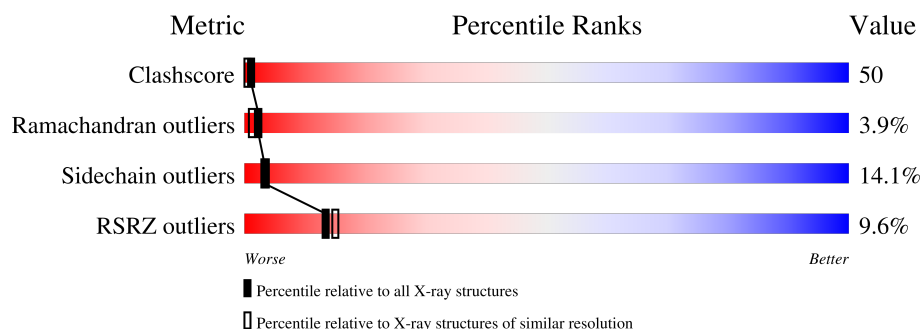
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |
| RSRZ outliers         | 180081                      | 6325 (2.30-2.30)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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     | 545    | <div> <div>9%</div> <div>44%</div> <div>41%</div> <div>12%</div> <div>..</div> </div>  |
| 1   | B     | 545    | <div> <div>10%</div> <div>42%</div> <div>41%</div> <div>12%</div> <div>..</div> </div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | IOD  | A     | 803 | -         | -        | X       | -                |
| 4   | IOD  | A     | 806 | -         | -        | X       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | IOD  | A     | 814 | -         | -        | X       | -                |
| 4   | IOD  | B     | 808 | -         | -        | X       | -                |
| 4   | IOD  | B     | 815 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

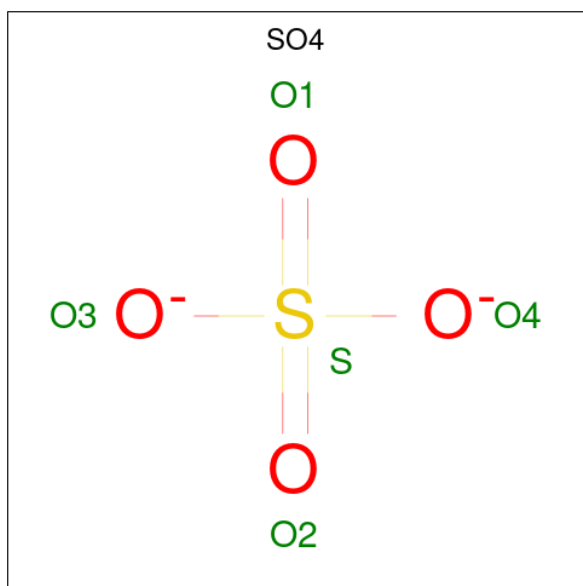
There are 6 unique types of molecules in this entry. The entry contains 8949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CTP synthase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 534      | Total | C    | N   | O   | S  | 5       | 1       | 0     |
|     |       |          | 4167  | 2633 | 729 | 784 | 21 |         |         |       |
| 1   | B     | 536      | Total | C    | N   | O   | S  | 5       | 0       | 0     |
|     |       |          | 4177  | 2640 | 730 | 786 | 21 |         |         |       |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

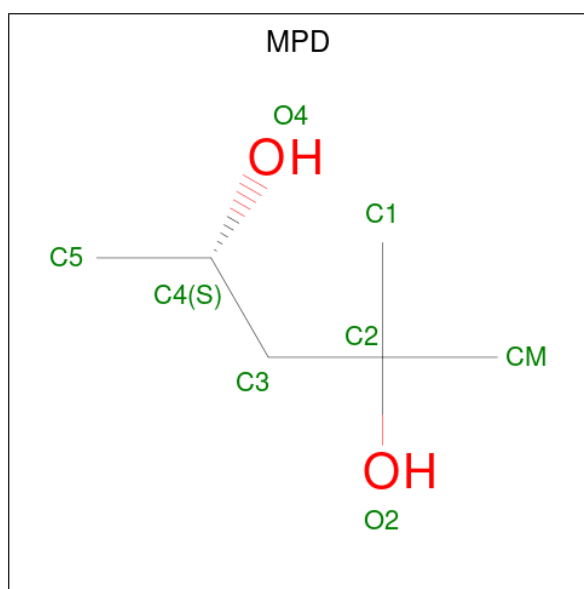
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | B     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | A     | 9        | Total | I | 0       | 0       |
|     |       |          | 9     | 9 |         |         |
| 4   | B     | 7        | Total | I | 0       | 0       |
|     |       |          | 7     | 7 |         |         |

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

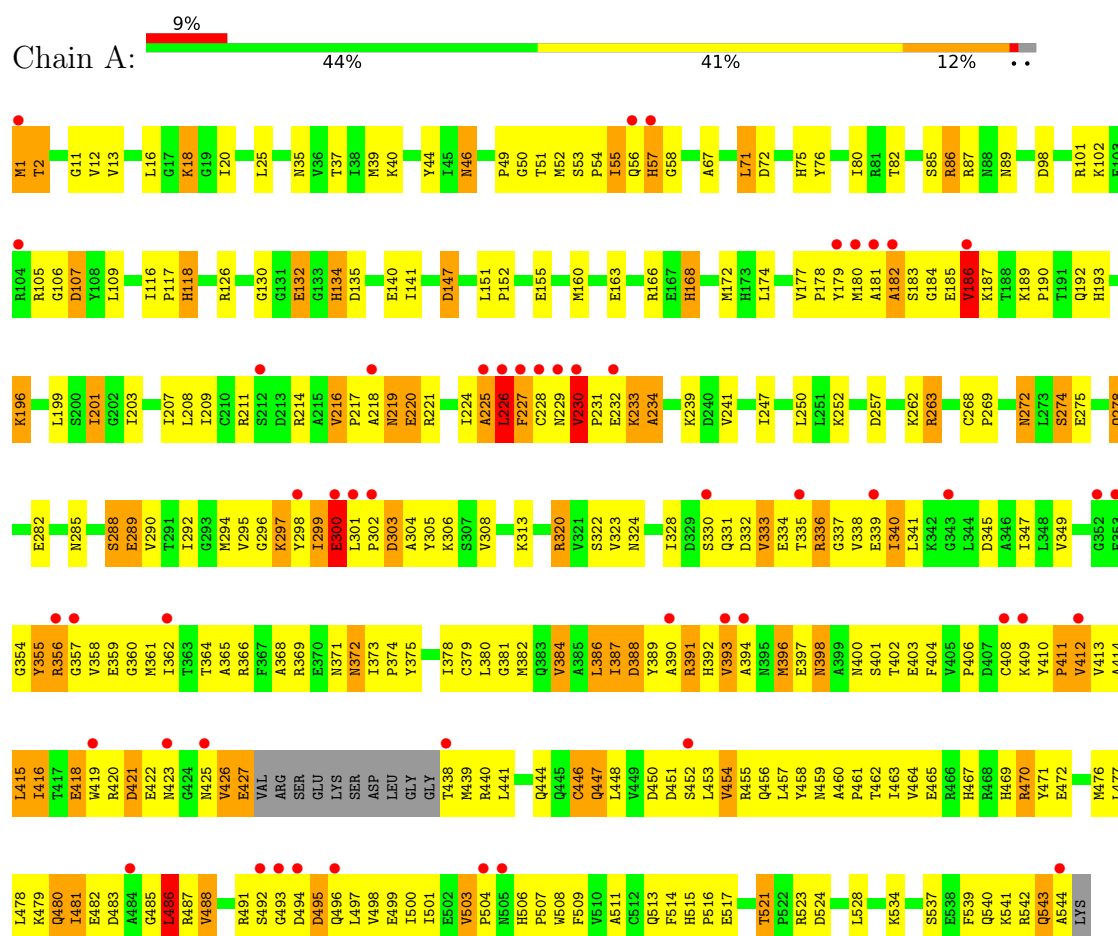
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6   | A     | 268      | Total<br>268 | O<br>268 | 0       | 0       |
| 6   | B     | 281      | Total<br>281 | O<br>281 | 0       | 0       |

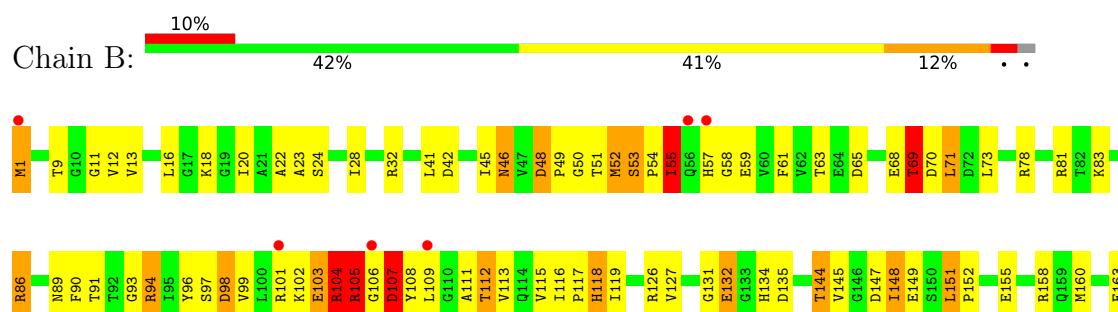
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: CTP synthase



#### • Molecule 1: CTP synthase







## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 2                                                   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 165.51Å 106.81Å 130.03Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.30<br>20.00 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (20.00-2.30)<br>98.9 (20.00-2.30)           | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.52 (at 2.29Å)                                             | Xtriage          |
| Refinement program                                                      | TNT version 5f                                              | Depositor        |
| R, $R_{free}$                                                           | 0.214 , 0.281<br>0.220 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 45.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.560                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 125.6                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 8949                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 59.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, SO4, MG, MPD

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     | 1.21         | 5/4248 (0.1%) | 1.59        | 36/5755 (0.6%)  |
| 1   | B     | 1.02         | 1/4253 (0.0%) | 1.49        | 37/5761 (0.6%)  |
| All | All   | 1.12         | 6/8501 (0.1%) | 1.54        | 73/11516 (0.6%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res   | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|-------|-------|-------------|----------|
| 1   | A     | 57[A] | HIS  | C-N   | 30.98 | 1.79        | 1.33     |
| 1   | A     | 57[B] | HIS  | C-N   | 30.98 | 1.79        | 1.33     |
| 1   | A     | 226   | LEU  | CA-C  | -6.98 | 1.46        | 1.52     |
| 1   | A     | 247   | ILE  | CA-CB | -6.37 | 1.50        | 1.54     |
| 1   | B     | 247   | ILE  | CA-CB | -5.82 | 1.51        | 1.54     |
| 1   | A     | 226   | LEU  | N-CA  | -5.15 | 1.40        | 1.46     |

All (73) bond angle outliers are listed below:

| Mol | Chain | Res   | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-------|------|------------|--------|-------------|----------|
| 1   | A     | 57[A] | HIS  | CA-C-N     | -24.06 | 87.17       | 122.06   |
| 1   | A     | 57[A] | HIS  | C-N-CA     | -24.06 | 87.17       | 122.06   |
| 1   | A     | 57[B] | HIS  | CA-C-N     | -24.06 | 87.17       | 122.06   |
| 1   | A     | 57[B] | HIS  | C-N-CA     | -24.06 | 87.17       | 122.06   |
| 1   | B     | 227   | PHE  | CA-CB-CG   | -11.46 | 102.34      | 113.80   |
| 1   | A     | 57[A] | HIS  | O-C-N      | -9.58  | 110.65      | 122.24   |
| 1   | A     | 57[B] | HIS  | O-C-N      | -9.58  | 110.65      | 122.24   |
| 1   | A     | 56    | GLN  | OE1-CD-NE2 | -9.45  | 113.15      | 122.60   |
| 1   | B     | 503   | VAL  | CA-C-N     | 9.19   | 128.80      | 119.24   |
| 1   | B     | 503   | VAL  | C-N-CA     | 9.19   | 128.80      | 119.24   |
| 1   | A     | 503   | VAL  | CA-C-N     | 8.45   | 130.41      | 119.84   |
| 1   | A     | 503   | VAL  | C-N-CA     | 8.45   | 130.41      | 119.84   |
| 1   | B     | 55    | ILE  | N-CA-C     | -8.04  | 99.10       | 109.80   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 421 | ASP  | CA-CB-CG  | 7.84  | 120.44      | 112.60   |
| 1   | B     | 495 | ASP  | N-CA-C    | -7.72 | 100.76      | 113.50   |
| 1   | A     | 333 | VAL  | N-CA-C    | -7.70 | 103.29      | 110.53   |
| 1   | B     | 69  | THR  | N-CA-CB   | -7.62 | 99.28       | 111.62   |
| 1   | B     | 118 | HIS  | CA-CB-CG  | -7.01 | 106.79      | 113.80   |
| 1   | B     | 392 | HIS  | N-CA-C    | 6.76  | 120.98      | 112.87   |
| 1   | B     | 185 | GLU  | N-CA-C    | 6.64  | 117.34      | 108.38   |
| 1   | A     | 56  | GLN  | CG-CD-NE2 | 6.55  | 126.23      | 116.40   |
| 1   | B     | 184 | GLY  | N-CA-C    | -6.50 | 104.89      | 114.90   |
| 1   | B     | 203 | ILE  | N-CA-C    | 6.45  | 117.19      | 108.17   |
| 1   | B     | 355 | TYR  | N-CA-CB   | 6.33  | 121.19      | 110.49   |
| 1   | B     | 185 | GLU  | CA-C-N    | 6.21  | 130.13      | 122.37   |
| 1   | B     | 185 | GLU  | C-N-CA    | 6.21  | 130.13      | 122.37   |
| 1   | A     | 147 | ASP  | CA-CB-CG  | 6.07  | 118.67      | 112.60   |
| 1   | B     | 98  | ASP  | CA-CB-CG  | -6.02 | 106.58      | 112.60   |
| 1   | A     | 450 | ASP  | CA-C-N    | -6.01 | 112.98      | 122.95   |
| 1   | A     | 450 | ASP  | C-N-CA    | -6.01 | 112.98      | 122.95   |
| 1   | A     | 227 | PHE  | CA-CB-CG  | -5.99 | 107.81      | 113.80   |
| 1   | A     | 225 | ALA  | CA-C-N    | -5.93 | 113.04      | 122.17   |
| 1   | A     | 225 | ALA  | C-N-CA    | -5.93 | 113.04      | 122.17   |
| 1   | B     | 186 | VAL  | N-CA-C    | 5.91  | 117.28      | 108.23   |
| 1   | B     | 426 | VAL  | N-CA-CB   | -5.73 | 105.73      | 112.32   |
| 1   | B     | 494 | ASP  | CA-C-N    | 5.71  | 128.97      | 120.17   |
| 1   | B     | 494 | ASP  | C-N-CA    | 5.71  | 128.97      | 120.17   |
| 1   | B     | 202 | GLY  | CA-C-N    | -5.64 | 116.20      | 123.19   |
| 1   | B     | 202 | GLY  | C-N-CA    | -5.64 | 116.20      | 123.19   |
| 1   | B     | 53  | SER  | CA-C-N    | 5.61  | 125.27      | 119.05   |
| 1   | B     | 53  | SER  | C-N-CA    | 5.61  | 125.27      | 119.05   |
| 1   | B     | 118 | HIS  | N-CA-C    | 5.60  | 117.83      | 111.11   |
| 1   | B     | 329 | ASP  | N-CA-C    | 5.56  | 117.79      | 108.96   |
| 1   | B     | 148 | ILE  | N-CA-CB   | 5.55  | 117.68      | 110.57   |
| 1   | B     | 544 | ALA  | CA-C-N    | 5.55  | 131.69      | 121.70   |
| 1   | B     | 544 | ALA  | C-N-CA    | 5.55  | 131.69      | 121.70   |
| 1   | A     | 35  | ASN  | CA-CB-CG  | -5.54 | 107.06      | 112.60   |
| 1   | A     | 201 | ILE  | N-CA-CB   | 5.52  | 121.35      | 112.08   |
| 1   | A     | 495 | ASP  | N-CA-C    | -5.51 | 106.63      | 113.19   |
| 1   | A     | 219 | ASN  | CA-CB-CG  | 5.51  | 118.11      | 112.60   |
| 1   | A     | 247 | ILE  | N-CA-C    | 5.48  | 119.52      | 112.67   |
| 1   | B     | 213 | ASP  | CB-CA-C   | -5.46 | 99.86       | 110.46   |
| 1   | A     | 503 | VAL  | C-N-CD    | -5.46 | 102.63      | 125.00   |
| 1   | B     | 503 | VAL  | O-C-N     | 5.40  | 124.77      | 121.37   |
| 1   | A     | 386 | LEU  | N-CA-C    | -5.39 | 105.30      | 111.07   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 72  | ASP  | CA-CB-CG | 5.38  | 117.98      | 112.60   |
| 1   | A     | 486 | LEU  | N-CA-C   | 5.37  | 117.22      | 110.24   |
| 1   | A     | 186 | VAL  | N-CA-C   | 5.36  | 115.57      | 107.80   |
| 1   | A     | 234 | ALA  | N-CA-C   | -5.33 | 106.63      | 113.02   |
| 1   | A     | 168 | HIS  | CA-CB-CG | -5.33 | 108.47      | 113.80   |
| 1   | B     | 347 | ILE  | N-CA-C   | 5.32  | 115.93      | 108.17   |
| 1   | B     | 233 | LYS  | N-CA-C   | -5.26 | 105.57      | 112.41   |
| 1   | B     | 214 | ARG  | N-CA-CB  | -5.26 | 103.25      | 111.56   |
| 1   | A     | 230 | VAL  | N-CA-C   | 5.25  | 120.23      | 108.88   |
| 1   | B     | 219 | ASN  | CA-CB-CG | -5.24 | 107.36      | 112.60   |
| 1   | A     | 323 | VAL  | N-CA-C   | 5.24  | 115.64      | 107.99   |
| 1   | B     | 426 | VAL  | N-CA-C   | 5.22  | 114.90      | 108.53   |
| 1   | A     | 134 | HIS  | N-CA-C   | -5.19 | 101.40      | 109.24   |
| 1   | B     | 69  | THR  | N-CA-C   | 5.17  | 116.84      | 109.14   |
| 1   | B     | 181 | ALA  | N-CA-C   | -5.17 | 105.10      | 111.40   |
| 1   | A     | 216 | VAL  | CA-C-N   | 5.14  | 125.30      | 119.90   |
| 1   | A     | 216 | VAL  | C-N-CA   | 5.14  | 125.30      | 119.90   |
| 1   | A     | 118 | HIS  | CA-CB-CG | -5.10 | 108.70      | 113.80   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4167  | 0        | 4178     | 411     | 0            |
| 1   | B     | 4177  | 0        | 4198     | 423     | 0            |
| 2   | A     | 10    | 0        | 0        | 0       | 0            |
| 2   | B     | 10    | 0        | 0        | 0       | 0            |
| 3   | A     | 2     | 0        | 0        | 0       | 0            |
| 3   | B     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 9     | 0        | 0        | 10      | 0            |
| 4   | B     | 7     | 0        | 0        | 8       | 0            |
| 5   | A     | 8     | 0        | 14       | 2       | 0            |
| 5   | B     | 8     | 0        | 14       | 2       | 0            |
| 6   | A     | 268   | 0        | 0        | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | B     | 281   | 0        | 0        | 25      | 0            |
| All | All   | 8949  | 0        | 8404     | 839     | 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 50.

All (839) 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:A:196:LYS:NZ   | 6:A:1077:HOH:O   | 1.61                     | 1.28              |
| 4:A:807:IOD:I    | 6:A:979:HOH:O    | 2.25                     | 1.24              |
| 1:B:326:LYS:HE2  | 1:B:328:ILE:HD11 | 1.24                     | 1.16              |
| 1:A:394:ALA:HB1  | 1:A:396:MET:HE3  | 1.23                     | 1.16              |
| 1:A:439:MET:HE3  | 1:A:470:ARG:HG2  | 1.25                     | 1.11              |
| 1:B:395:ASN:HD21 | 1:B:480:GLN:NE2  | 1.46                     | 1.11              |
| 1:A:401:SER:HB2  | 1:A:413:VAL:HB   | 1.26                     | 1.10              |
| 4:B:811:IOD:I    | 6:B:1871:HOH:O   | 2.39                     | 1.10              |
| 1:A:408:CYS:H    | 1:A:420:ARG:NH2  | 1.50                     | 1.08              |
| 1:A:335:THR:HG22 | 1:A:336:ARG:HG3  | 1.34                     | 1.08              |
| 1:A:49:PRO:HA    | 1:A:52:MET:HE3   | 1.09                     | 1.05              |
| 1:A:147:ASP:HB2  | 6:A:867:HOH:O    | 1.58                     | 1.04              |
| 1:A:521:THR:HG22 | 1:A:524:ASP:H    | 1.16                     | 1.04              |
| 4:B:808:IOD:I    | 6:B:1754:HOH:O   | 2.48                     | 1.02              |
| 1:B:401:SER:HB2  | 1:B:413:VAL:HB   | 1.44                     | 1.00              |
| 1:A:396:MET:HE1  | 1:A:480:GLN:HG2  | 1.44                     | 0.99              |
| 1:A:49:PRO:HG3   | 6:A:1009:HOH:O   | 1.63                     | 0.98              |
| 1:A:382:MET:HE2  | 1:A:501:ILE:HG23 | 1.45                     | 0.96              |
| 1:B:493:GLY:HA2  | 1:B:496:GLN:NE2  | 1.82                     | 0.94              |
| 1:B:395:ASN:HD21 | 1:B:480:GLN:HE21 | 1.12                     | 0.94              |
| 1:B:198:LEU:HD12 | 1:B:205:PRO:HG3  | 1.51                     | 0.93              |
| 1:A:301:LEU:HD12 | 1:A:302:PRO:CD   | 2.00                     | 0.91              |
| 1:A:49:PRO:CA    | 1:A:52:MET:HE3   | 2.00                     | 0.90              |
| 4:B:815:IOD:I    | 6:B:1774:HOH:O   | 2.60                     | 0.90              |
| 4:A:814:IOD:I    | 1:B:193:HIS:HD2  | 2.26                     | 0.89              |
| 1:A:408:CYS:N    | 1:A:420:ARG:HH22 | 1.71                     | 0.89              |
| 1:B:49:PRO:HA    | 1:B:52:MET:CE    | 2.04                     | 0.88              |
| 1:B:189:LYS:HB3  | 1:B:190:PRO:HD3  | 1.53                     | 0.88              |
| 1:B:46:ASN:HD22  | 1:B:46:ASN:H     | 1.19                     | 0.88              |
| 1:B:294:MET:HE1  | 1:B:309:ILE:HG13 | 1.54                     | 0.88              |
| 1:B:326:LYS:CE   | 1:B:328:ILE:HD11 | 2.04                     | 0.88              |
| 1:A:178:PRO:HB3  | 4:A:806:IOD:I    | 2.45                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:468:ARG:HG2  | 1:B:468:ARG:HH11 | 1.40                     | 0.86              |
| 1:A:403:GLU:HG3  | 1:A:471:TYR:CE1  | 2.09                     | 0.86              |
| 4:A:814:IOD:I    | 1:B:193:HIS:CD2  | 2.98                     | 0.86              |
| 1:B:227:PHE:O    | 1:B:228:CYS:C    | 2.15                     | 0.86              |
| 1:B:355:TYR:CG   | 1:B:404:PHE:HB3  | 2.10                     | 0.86              |
| 1:B:408:CYS:H    | 1:B:420:ARG:HH22 | 1.23                     | 0.86              |
| 1:B:493:GLY:HA2  | 1:B:496:GLN:HE22 | 1.39                     | 0.85              |
| 1:B:344:LEU:HD12 | 1:B:347:ILE:HD11 | 1.57                     | 0.85              |
| 1:B:49:PRO:HA    | 1:B:52:MET:HE3   | 1.59                     | 0.85              |
| 1:A:301:LEU:HD12 | 1:A:302:PRO:HD2  | 1.58                     | 0.85              |
| 1:A:44:TYR:CE1   | 1:A:52:MET:HE1   | 2.11                     | 0.85              |
| 1:B:117:PRO:HD2  | 1:B:118:HIS:CE1  | 2.11                     | 0.84              |
| 1:B:46:ASN:H     | 1:B:46:ASN:ND2   | 1.69                     | 0.84              |
| 1:A:396:MET:HE1  | 1:A:480:GLN:CG   | 2.07                     | 0.84              |
| 1:B:198:LEU:CD1  | 1:B:205:PRO:HG3  | 2.08                     | 0.84              |
| 1:B:213:ASP:HB3  | 1:B:214:ARG:HE   | 1.41                     | 0.84              |
| 1:A:409:LYS:C    | 1:A:411:PRO:HD3  | 2.03                     | 0.84              |
| 1:B:86:ARG:NH1   | 1:B:89:ASN:HB3   | 1.92                     | 0.84              |
| 1:A:408:CYS:H    | 1:A:420:ARG:HH22 | 0.86                     | 0.83              |
| 1:B:334:GLU:HG2  | 1:B:360:GLY:CA   | 2.08                     | 0.83              |
| 1:B:117:PRO:HD2  | 1:B:118:HIS:ND1  | 1.93                     | 0.83              |
| 1:A:25:LEU:HD22  | 1:A:172:MET:HE1  | 1.59                     | 0.83              |
| 1:A:402:THR:HG23 | 1:A:414:ALA:HB2  | 1.61                     | 0.82              |
| 1:A:46:ASN:HB2   | 1:A:52:MET:HE2   | 1.61                     | 0.82              |
| 1:A:506:HIS:CG   | 1:A:507:PRO:HD2  | 2.13                     | 0.82              |
| 1:A:521:THR:CG2  | 1:A:524:ASP:H    | 1.92                     | 0.82              |
| 1:A:521:THR:HB   | 6:A:1001:HOH:O   | 1.77                     | 0.81              |
| 1:B:396:MET:HA   | 1:B:410:TYR:CD1  | 2.15                     | 0.81              |
| 1:B:268:CYS:HB2  | 1:B:269:PRO:HD2  | 1.62                     | 0.81              |
| 4:A:806:IOD:I    | 1:B:178:PRO:HB3  | 2.51                     | 0.81              |
| 1:A:401:SER:CB   | 1:A:413:VAL:HB   | 2.11                     | 0.80              |
| 1:B:299:ILE:HG21 | 1:B:327:LEU:HB3  | 1.64                     | 0.80              |
| 1:B:176:LEU:HD12 | 1:B:177:VAL:H    | 1.45                     | 0.79              |
| 1:B:391:ARG:HG3  | 1:B:399:ALA:HB3  | 1.62                     | 0.79              |
| 1:A:349:VAL:HG12 | 1:A:381:GLY:HA2  | 1.64                     | 0.79              |
| 1:A:345:ASP:HA   | 1:A:539:PHE:CD2  | 2.16                     | 0.79              |
| 1:B:395:ASN:ND2  | 1:B:480:GLN:HE21 | 1.79                     | 0.79              |
| 1:B:408:CYS:H    | 1:B:420:ARG:NH2  | 1.80                     | 0.79              |
| 1:B:176:LEU:HD12 | 1:B:177:VAL:N    | 1.97                     | 0.78              |
| 1:A:105:ARG:HG3  | 1:A:107:ASP:OD1  | 1.83                     | 0.78              |
| 1:A:421:ASP:CG   | 1:A:425:ASN:HB2  | 2.09                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:106:GLY:O    | 1:B:108:TYR:N    | 2.17                     | 0.78              |
| 1:A:186:VAL:HG13 | 1:A:220:GLU:HG2  | 1.65                     | 0.77              |
| 1:A:294:MET:HE3  | 1:A:308:VAL:HG11 | 1.66                     | 0.77              |
| 1:A:39:MET:HE1   | 1:A:130:GLY:HA3  | 1.64                     | 0.77              |
| 1:B:229:ASN:C    | 1:B:231:PRO:HD3  | 2.10                     | 0.77              |
| 1:A:394:ALA:CB   | 1:A:396:MET:HE3  | 2.10                     | 0.76              |
| 1:B:456:GLN:HG3  | 6:B:1857:HOH:O   | 1.84                     | 0.76              |
| 1:A:306:LYS:NZ   | 6:A:1080:HOH:O   | 2.18                     | 0.76              |
| 1:A:361:MET:HB2  | 1:A:384:VAL:HG21 | 1.68                     | 0.76              |
| 1:A:54:PRO:HA    | 1:A:58:GLY:N     | 2.00                     | 0.76              |
| 1:B:355:TYR:HB2  | 1:B:404:PHE:HD2  | 1.50                     | 0.76              |
| 1:A:25:LEU:CD2   | 1:A:172:MET:HE1  | 2.16                     | 0.76              |
| 1:A:86:ARG:HH11  | 1:A:86:ARG:CB    | 2.00                     | 0.75              |
| 1:A:349:VAL:HG12 | 1:A:381:GLY:CA   | 2.16                     | 0.75              |
| 1:A:54:PRO:O     | 1:A:58:GLY:N     | 2.20                     | 0.75              |
| 1:A:86:ARG:HH11  | 1:A:86:ARG:CA    | 2.00                     | 0.75              |
| 1:B:331:GLN:O    | 1:B:334:GLU:HG3  | 1.85                     | 0.75              |
| 1:B:506:HIS:ND1  | 1:B:507:PRO:HD2  | 2.02                     | 0.75              |
| 1:B:213:ASP:HB3  | 1:B:214:ARG:HG2  | 1.68                     | 0.75              |
| 1:A:44:TYR:HE1   | 1:A:52:MET:HE1   | 1.48                     | 0.75              |
| 1:A:448:LEU:HD11 | 1:A:463:ILE:CG2  | 2.16                     | 0.75              |
| 1:A:347:ILE:HD12 | 1:A:368:ALA:HB2  | 1.69                     | 0.74              |
| 1:A:401:SER:HB2  | 1:A:413:VAL:CB   | 2.12                     | 0.74              |
| 1:A:493:GLY:O    | 1:A:496:GLN:HG3  | 1.88                     | 0.74              |
| 1:B:348:LEU:HD23 | 1:B:349:VAL:N    | 2.02                     | 0.74              |
| 1:B:425:ASN:O    | 1:B:476:MET:HE1  | 1.87                     | 0.74              |
| 1:B:49:PRO:HG2   | 1:B:69:THR:HA    | 1.70                     | 0.74              |
| 1:B:396:MET:HB3  | 1:B:399:ALA:HB2  | 1.70                     | 0.74              |
| 1:A:423:ASN:HB2  | 1:A:425:ASN:HD22 | 1.53                     | 0.73              |
| 1:B:213:ASP:CB   | 1:B:214:ARG:HG2  | 2.18                     | 0.73              |
| 1:B:341:LEU:O    | 1:B:344:LEU:HG   | 1.88                     | 0.73              |
| 1:B:495:ASP:O    | 1:B:496:GLN:C    | 2.31                     | 0.73              |
| 1:A:447:GLN:HG3  | 1:A:462:THR:HG22 | 1.71                     | 0.73              |
| 1:B:449:VAL:HG21 | 1:B:488:VAL:O    | 1.88                     | 0.73              |
| 1:A:54:PRO:O     | 1:A:301:LEU:HD23 | 1.89                     | 0.73              |
| 1:A:347:ILE:CD1  | 1:A:368:ALA:HB2  | 2.18                     | 0.73              |
| 1:A:409:LYS:HD3  | 1:A:410:TYR:CD1  | 2.24                     | 0.73              |
| 1:A:86:ARG:NH1   | 1:A:86:ARG:N     | 2.37                     | 0.72              |
| 1:B:228:CYS:O    | 1:B:230:VAL:N    | 2.23                     | 0.72              |
| 1:A:333:VAL:HA   | 1:A:340:ILE:HD11 | 1.71                     | 0.72              |
| 1:B:395:ASN:ND2  | 1:B:480:GLN:NE2  | 2.30                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:396:MET:HE1  | 1:B:480:GLN:HB3  | 1.71                     | 0.72              |
| 1:A:1:MET:HE2    | 1:A:135:ASP:OD1  | 1.90                     | 0.71              |
| 1:B:32:ARG:HD3   | 1:B:269:PRO:O    | 1.90                     | 0.71              |
| 1:A:371:ASN:HB2  | 1:A:373:ILE:CD1  | 2.19                     | 0.71              |
| 1:B:199:LEU:HD21 | 1:B:204:GLN:NE2  | 2.05                     | 0.71              |
| 1:B:213:ASP:CB   | 1:B:214:ARG:HE   | 2.03                     | 0.71              |
| 1:A:86:ARG:HH11  | 1:A:86:ARG:N     | 1.88                     | 0.71              |
| 1:A:332:ASP:HA   | 1:A:335:THR:HB   | 1.73                     | 0.71              |
| 1:B:414:ALA:HA   | 1:B:471:TYR:HD2  | 1.54                     | 0.71              |
| 1:B:220:GLU:O    | 1:B:224:ILE:HD12 | 1.89                     | 0.71              |
| 1:B:224:ILE:C    | 1:B:229:ASN:HD22 | 1.97                     | 0.71              |
| 1:A:224:ILE:HG23 | 1:A:229:ASN:ND2  | 2.06                     | 0.71              |
| 1:B:301:LEU:HD12 | 1:B:302:PRO:HD2  | 1.73                     | 0.70              |
| 1:A:224:ILE:HG23 | 1:A:229:ASN:HD22 | 1.55                     | 0.70              |
| 1:B:326:LYS:HE2  | 1:B:328:ILE:CD1  | 2.14                     | 0.70              |
| 1:A:330:SER:OG   | 1:A:357:GLY:HA3  | 1.92                     | 0.70              |
| 1:B:313:LYS:HE3  | 6:B:1741:HOH:O   | 1.92                     | 0.70              |
| 1:B:330:SER:HB3  | 1:B:361:MET:HG3  | 1.74                     | 0.70              |
| 1:A:349:VAL:CG1  | 1:A:381:GLY:HA2  | 2.22                     | 0.70              |
| 1:A:495:ASP:HB3  | 1:A:497:LEU:CD1  | 2.21                     | 0.70              |
| 1:A:268:CYS:HB2  | 1:A:269:PRO:HD2  | 1.74                     | 0.70              |
| 1:A:408:CYS:N    | 1:A:420:ARG:NH2  | 2.34                     | 0.69              |
| 1:A:389:TYR:HD2  | 1:A:481:ILE:HG22 | 1.56                     | 0.69              |
| 1:A:294:MET:HE3  | 1:A:308:VAL:CG1  | 2.22                     | 0.69              |
| 1:A:371:ASN:HB2  | 1:A:373:ILE:HD12 | 1.74                     | 0.69              |
| 1:A:46:ASN:CB    | 1:A:52:MET:HE2   | 2.22                     | 0.69              |
| 1:A:427:GLU:HA   | 1:A:427:GLU:OE1  | 1.92                     | 0.69              |
| 1:B:402:THR:HG23 | 1:B:414:ALA:HB2  | 1.74                     | 0.69              |
| 1:A:86:ARG:NH1   | 1:A:86:ARG:H     | 1.91                     | 0.69              |
| 1:A:290:VAL:O    | 1:A:324:ASN:HB2  | 1.93                     | 0.69              |
| 1:B:108:TYR:CD2  | 1:B:118:HIS:HD2  | 2.10                     | 0.69              |
| 1:A:439:MET:CE   | 1:A:470:ARG:HG2  | 2.15                     | 0.68              |
| 1:A:448:LEU:HD11 | 1:A:463:ILE:HG21 | 1.73                     | 0.68              |
| 1:A:448:LEU:HD22 | 1:A:454:VAL:CG1  | 2.23                     | 0.68              |
| 1:B:421:ASP:HB3  | 1:B:425:ASN:H    | 1.58                     | 0.68              |
| 1:A:297:LYS:HE3  | 1:A:298:TYR:CE2  | 2.28                     | 0.68              |
| 1:B:193:HIS:NE2  | 6:B:1720:HOH:O   | 2.25                     | 0.68              |
| 1:B:334:GLU:HG2  | 1:B:360:GLY:HA3  | 1.74                     | 0.68              |
| 1:A:86:ARG:HD3   | 6:A:1016:HOH:O   | 1.92                     | 0.68              |
| 1:A:488:VAL:HG11 | 1:A:491:ARG:NE   | 2.08                     | 0.68              |
| 1:B:180:MET:HB3  | 1:B:183:SER:CB   | 2.23                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:333:VAL:HG11 | 1:B:360:GLY:O    | 1.94                     | 0.68              |
| 1:A:460:ALA:HB1  | 1:A:461:PRO:HD2  | 1.76                     | 0.68              |
| 1:B:223:LYS:O    | 1:B:227:PHE:HB2  | 1.94                     | 0.68              |
| 1:A:521:THR:HG22 | 1:A:524:ASP:N    | 1.99                     | 0.67              |
| 1:A:396:MET:CE   | 1:A:480:GLN:HG2  | 2.22                     | 0.67              |
| 1:B:224:ILE:HG23 | 1:B:229:ASN:ND2  | 2.10                     | 0.67              |
| 1:A:412:VAL:HG13 | 1:A:477:LEU:HB2  | 1.77                     | 0.67              |
| 1:B:224:ILE:O    | 1:B:229:ASN:ND2  | 2.25                     | 0.67              |
| 1:B:408:CYS:N    | 1:B:420:ARG:HH22 | 1.93                     | 0.67              |
| 1:A:355:TYR:HA   | 1:A:404:PHE:CD2  | 2.30                     | 0.67              |
| 1:B:103:GLU:O    | 1:B:105:ARG:N    | 2.27                     | 0.67              |
| 1:A:382:MET:HE3  | 1:A:511:ALA:O    | 1.94                     | 0.67              |
| 1:A:539:PHE:HA   | 1:A:542:ARG:NH2  | 2.10                     | 0.67              |
| 1:B:216:VAL:HG12 | 1:B:221:ARG:CG   | 2.24                     | 0.67              |
| 1:A:439:MET:HE2  | 1:A:469:HIS:C    | 2.20                     | 0.66              |
| 1:B:108:TYR:CE2  | 1:B:118:HIS:HD2  | 2.12                     | 0.66              |
| 1:B:220:GLU:N    | 1:B:220:GLU:OE2  | 2.29                     | 0.66              |
| 1:B:334:GLU:HG2  | 1:B:360:GLY:N    | 2.10                     | 0.66              |
| 1:A:2:THR:HG21   | 1:A:168:HIS:CE1  | 2.30                     | 0.66              |
| 1:A:345:ASP:HA   | 1:A:539:PHE:CE2  | 2.30                     | 0.66              |
| 1:B:68:GLU:O     | 1:B:86:ARG:NH2   | 2.28                     | 0.66              |
| 1:A:216:VAL:HG12 | 1:A:221:ARG:HG3  | 1.77                     | 0.66              |
| 1:A:492:SER:OG   | 1:A:493:GLY:N    | 2.28                     | 0.66              |
| 1:B:226:LEU:HG   | 1:B:227:PHE:N    | 2.01                     | 0.66              |
| 1:B:292:ILE:HG12 | 1:B:346:ALA:HB3  | 1.76                     | 0.66              |
| 1:A:301:LEU:HD11 | 1:A:303:ASP:H    | 1.60                     | 0.66              |
| 1:A:337:GLY:O    | 1:A:340:ILE:HD13 | 1.96                     | 0.66              |
| 1:A:301:LEU:HD12 | 1:A:302:PRO:N    | 2.10                     | 0.66              |
| 1:A:413:VAL:HA   | 1:A:472:GLU:O    | 1.97                     | 0.65              |
| 1:B:94:ARG:NH1   | 1:B:98:ASP:OD1   | 2.29                     | 0.65              |
| 1:B:387:ILE:O    | 1:B:390:ALA:N    | 2.29                     | 0.65              |
| 1:B:395:ASN:O    | 1:B:396:MET:C    | 2.38                     | 0.65              |
| 1:B:46:ASN:ND2   | 1:B:46:ASN:N     | 2.43                     | 0.65              |
| 1:B:331:GLN:O    | 1:B:332:ASP:C    | 2.39                     | 0.65              |
| 1:A:301:LEU:CD1  | 1:A:303:ASP:H    | 2.09                     | 0.65              |
| 1:B:53:SER:O     | 1:B:57:HIS:HB3   | 1.96                     | 0.65              |
| 1:B:396:MET:HE1  | 1:B:480:GLN:CG   | 2.26                     | 0.65              |
| 1:A:439:MET:HE3  | 1:A:470:ARG:CG   | 2.17                     | 0.65              |
| 1:B:107:ASP:N    | 1:B:107:ASP:OD2  | 2.30                     | 0.65              |
| 1:B:355:TYR:HB2  | 1:B:404:PHE:CD2  | 2.32                     | 0.65              |
| 1:A:278:GLN:NE2  | 1:A:282:GLU:OE2  | 2.29                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:372:ASN:HD22 | 1:A:506:HIS:CD2  | 2.15                     | 0.64              |
| 1:B:104:ARG:O    | 1:B:105:ARG:HB3  | 1.96                     | 0.64              |
| 1:B:180:MET:HB3  | 1:B:183:SER:HB3  | 1.78                     | 0.64              |
| 1:B:332:ASP:HA   | 1:B:335:THR:HB   | 1.79                     | 0.64              |
| 1:A:1:MET:HE1    | 1:A:134:HIS:CA   | 2.28                     | 0.64              |
| 1:B:86:ARG:HH12  | 1:B:89:ASN:HB3   | 1.58                     | 0.64              |
| 1:A:39:MET:CE    | 1:A:130:GLY:HA3  | 2.26                     | 0.64              |
| 1:A:224:ILE:O    | 1:A:229:ASN:HB2  | 1.96                     | 0.64              |
| 1:A:516:PRO:HD2  | 1:A:517:GLU:OE1  | 1.97                     | 0.64              |
| 1:A:541:LYS:O    | 1:A:542:ARG:C    | 2.40                     | 0.64              |
| 1:B:408:CYS:N    | 1:B:420:ARG:NH2  | 2.44                     | 0.64              |
| 1:B:180:MET:HE3  | 6:B:1604:HOH:O   | 1.98                     | 0.64              |
| 1:B:289:GLU:HG3  | 1:B:324:ASN:HD21 | 1.63                     | 0.64              |
| 1:B:468:ARG:HG2  | 1:B:468:ARG:NH1  | 2.06                     | 0.64              |
| 1:A:369:ARG:NH2  | 1:A:388:ASP:OD2  | 2.30                     | 0.64              |
| 1:A:1:MET:HE1    | 1:A:134:HIS:C    | 2.23                     | 0.64              |
| 1:A:403:GLU:HG3  | 1:A:471:TYR:CZ   | 2.32                     | 0.64              |
| 1:A:439:MET:HG3  | 1:A:440:ARG:N    | 2.12                     | 0.64              |
| 1:A:85:SER:OG    | 1:A:87:ARG:HG2   | 1.98                     | 0.63              |
| 1:A:409:LYS:H    | 1:A:420:ARG:HH21 | 1.43                     | 0.63              |
| 1:A:373:ILE:HG23 | 1:A:374:PRO:HD2  | 1.81                     | 0.63              |
| 1:B:105:ARG:HG3  | 1:B:107:ASP:OD2  | 1.98                     | 0.63              |
| 1:A:389:TYR:CD2  | 1:A:481:ILE:HG22 | 2.33                     | 0.63              |
| 1:B:408:CYS:O    | 1:B:420:ARG:NH2  | 2.28                     | 0.63              |
| 1:A:126:ARG:NH1  | 6:A:934:HOH:O    | 2.30                     | 0.62              |
| 1:A:189:LYS:HB3  | 1:A:190:PRO:HD3  | 1.81                     | 0.62              |
| 1:B:482:GLU:O    | 1:B:485:GLY:N    | 2.29                     | 0.62              |
| 1:B:189:LYS:HB2  | 4:B:808:IOD:I    | 2.69                     | 0.62              |
| 1:A:230:VAL:HG12 | 1:A:230:VAL:O    | 2.00                     | 0.62              |
| 1:B:503:VAL:HG13 | 1:B:504:PRO:HD2  | 1.81                     | 0.62              |
| 1:A:444:GLN:HG2  | 6:A:1022:HOH:O   | 1.99                     | 0.62              |
| 1:B:151:LEU:HB2  | 1:B:152:PRO:HD3  | 1.82                     | 0.62              |
| 1:B:332:ASP:O    | 1:B:336:ARG:N    | 2.26                     | 0.62              |
| 1:A:421:ASP:OD1  | 1:A:425:ASN:HB2  | 1.99                     | 0.61              |
| 1:B:211:ARG:NH1  | 1:B:238:LEU:O    | 2.32                     | 0.61              |
| 1:B:333:VAL:HG12 | 1:B:360:GLY:HA2  | 1.82                     | 0.61              |
| 1:A:285:ASN:O    | 1:A:320:ARG:HD2  | 2.01                     | 0.61              |
| 1:A:486:LEU:HG   | 1:A:487:ARG:N    | 2.14                     | 0.61              |
| 1:B:112:THR:N    | 6:B:1838:HOH:O   | 2.31                     | 0.61              |
| 1:B:395:ASN:ND2  | 1:B:410:TYR:OH   | 2.27                     | 0.61              |
| 1:B:327:LEU:N    | 1:B:327:LEU:HD23 | 2.13                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:382:MET:HE1  | 1:B:499:GLU:O    | 2.00                     | 0.61              |
| 1:B:396:MET:HE1  | 1:B:480:GLN:CB   | 2.31                     | 0.61              |
| 1:B:69:THR:HG21  | 1:B:73:LEU:HD22  | 1.81                     | 0.61              |
| 1:B:183:SER:CB   | 1:B:185:GLU:HG2  | 2.31                     | 0.61              |
| 1:B:183:SER:HB3  | 1:B:185:GLU:HG2  | 1.80                     | 0.61              |
| 1:B:396:MET:HA   | 1:B:410:TYR:CG   | 2.36                     | 0.61              |
| 1:A:410:TYR:N    | 1:A:411:PRO:HD3  | 2.14                     | 0.61              |
| 1:A:478:LEU:HD21 | 1:A:498:VAL:HG21 | 1.81                     | 0.61              |
| 1:B:148:ILE:HG22 | 1:B:151:LEU:HD11 | 1.83                     | 0.61              |
| 1:A:402:THR:CG2  | 1:A:414:ALA:HB2  | 2.31                     | 0.60              |
| 1:B:371:ASN:N    | 1:B:371:ASN:HD22 | 1.99                     | 0.60              |
| 1:A:387:ILE:O    | 1:A:388:ASP:C    | 2.42                     | 0.60              |
| 1:A:335:THR:HG22 | 1:A:336:ARG:CG   | 2.21                     | 0.60              |
| 1:A:355:TYR:O    | 1:A:356:ARG:C    | 2.44                     | 0.60              |
| 1:A:426:VAL:O    | 1:A:427:GLU:HB2  | 2.02                     | 0.60              |
| 1:A:252:LYS:HE3  | 6:A:817:HOH:O    | 2.02                     | 0.60              |
| 1:B:224:ILE:O    | 1:B:229:ASN:HB2  | 2.02                     | 0.60              |
| 1:B:409:LYS:HE2  | 1:B:422:GLU:HB2  | 1.82                     | 0.60              |
| 1:A:174:LEU:HG   | 1:A:209:ILE:HB   | 1.82                     | 0.60              |
| 1:B:395:ASN:HD21 | 1:B:480:GLN:HE22 | 1.44                     | 0.60              |
| 1:B:395:ASN:O    | 1:B:397:GLU:N    | 2.34                     | 0.60              |
| 1:B:517:GLU:OE2  | 1:B:517:GLU:N    | 2.31                     | 0.60              |
| 1:B:541:LYS:HE3  | 6:B:1742:HOH:O   | 2.01                     | 0.60              |
| 1:A:390:ALA:HB2  | 1:A:481:ILE:CD1  | 2.32                     | 0.60              |
| 1:A:413:VAL:HG12 | 1:A:471:TYR:HB3  | 1.82                     | 0.60              |
| 1:B:68:GLU:OE2   | 1:B:468:ARG:NE   | 2.26                     | 0.60              |
| 1:B:148:ILE:HG22 | 1:B:151:LEU:CD1  | 2.32                     | 0.60              |
| 1:B:333:VAL:HG12 | 1:B:334:GLU:N    | 2.16                     | 0.60              |
| 1:B:415:LEU:HD23 | 1:B:471:TYR:CD2  | 2.37                     | 0.60              |
| 1:A:289:GLU:HB2  | 1:A:322:SER:HB3  | 1.84                     | 0.59              |
| 1:A:439:MET:HB2  | 1:A:470:ARG:NH1  | 2.16                     | 0.59              |
| 1:B:46:ASN:HD22  | 1:B:46:ASN:N     | 1.96                     | 0.59              |
| 1:A:313:LYS:NZ   | 6:A:1045:HOH:O   | 2.30                     | 0.59              |
| 1:A:1:MET:O      | 1:A:2:THR:C      | 2.46                     | 0.59              |
| 1:B:295:VAL:HG13 | 1:B:328:ILE:HG22 | 1.82                     | 0.59              |
| 1:A:193:HIS:HB3  | 6:B:1720:HOH:O   | 2.01                     | 0.59              |
| 1:A:382:MET:CE   | 1:A:501:ILE:HG23 | 2.28                     | 0.59              |
| 1:A:495:ASP:HB3  | 1:A:497:LEU:HD11 | 1.83                     | 0.59              |
| 1:B:387:ILE:O    | 1:B:388:ASP:C    | 2.44                     | 0.59              |
| 1:A:408:CYS:O    | 1:A:410:TYR:N    | 2.34                     | 0.59              |
| 1:B:331:GLN:O    | 1:B:334:GLU:N    | 2.36                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:333:VAL:HA   | 1:B:340:ILE:HD11 | 1.84                     | 0.59              |
| 1:B:355:TYR:CD1  | 1:B:358:VAL:HB   | 2.38                     | 0.59              |
| 1:A:387:ILE:HG22 | 1:A:388:ASP:N    | 2.17                     | 0.59              |
| 1:A:408:CYS:SG   | 1:A:411:PRO:HB3  | 2.43                     | 0.59              |
| 1:A:481:ILE:O    | 1:A:482:GLU:C    | 2.45                     | 0.59              |
| 1:B:216:VAL:HG12 | 1:B:221:ARG:HG3  | 1.85                     | 0.59              |
| 1:A:39:MET:HE1   | 1:A:130:GLY:CA   | 2.33                     | 0.59              |
| 1:B:217:PRO:O    | 1:B:220:GLU:N    | 2.35                     | 0.59              |
| 1:A:542:ARG:O    | 1:A:544:ALA:N    | 2.29                     | 0.58              |
| 1:B:71:LEU:C     | 1:B:71:LEU:HD12  | 2.28                     | 0.58              |
| 1:A:331:GLN:O    | 1:A:334:GLU:HB2  | 2.04                     | 0.58              |
| 1:A:71:LEU:HD12  | 1:A:71:LEU:C     | 2.28                     | 0.58              |
| 1:A:337:GLY:O    | 1:A:339:GLU:N    | 2.37                     | 0.58              |
| 1:A:379:CYS:O    | 1:A:382:MET:N    | 2.34                     | 0.58              |
| 1:B:325:ILE:HG22 | 1:B:327:LEU:CD2  | 2.34                     | 0.58              |
| 1:A:46:ASN:H     | 1:A:46:ASN:HD22  | 1.51                     | 0.58              |
| 1:A:98:ASP:OD2   | 1:A:126:ARG:NH1  | 2.35                     | 0.58              |
| 1:A:116:ILE:HD11 | 1:A:155:GLU:HG2  | 1.85                     | 0.58              |
| 1:B:155:GLU:CD   | 1:B:158:ARG:HH21 | 2.11                     | 0.58              |
| 1:A:439:MET:HE2  | 1:A:469:HIS:CA   | 2.34                     | 0.58              |
| 1:B:330:SER:O    | 1:B:360:GLY:HA3  | 2.03                     | 0.58              |
| 1:B:332:ASP:O    | 1:B:333:VAL:C    | 2.47                     | 0.58              |
| 1:B:396:MET:HE1  | 1:B:480:GLN:CD   | 2.29                     | 0.58              |
| 1:B:401:SER:HA   | 1:B:413:VAL:O    | 2.04                     | 0.57              |
| 1:B:41:LEU:HG    | 1:B:90:PHE:CZ    | 2.39                     | 0.57              |
| 1:B:447:GLN:HE22 | 1:B:493:GLY:H    | 1.53                     | 0.57              |
| 1:B:447:GLN:HE22 | 1:B:493:GLY:N    | 2.03                     | 0.57              |
| 1:A:355:TYR:CD1  | 1:A:404:PHE:HB3  | 2.40                     | 0.57              |
| 1:A:226:LEU:O    | 1:A:227:PHE:C    | 2.44                     | 0.57              |
| 1:A:361:MET:CB   | 1:A:384:VAL:HG21 | 2.34                     | 0.57              |
| 1:A:374:PRO:HA   | 1:A:508:TRP:O    | 2.05                     | 0.57              |
| 1:A:426:VAL:HA   | 1:A:476:MET:HE1  | 1.87                     | 0.57              |
| 1:B:99:VAL:HG21  | 1:B:119:ILE:HD13 | 1.86                     | 0.57              |
| 1:B:238:LEU:HD21 | 5:B:1601:MPD:H51 | 1.86                     | 0.57              |
| 1:B:330:SER:HB2  | 1:B:357:GLY:O    | 2.05                     | 0.57              |
| 1:B:241:VAL:HA   | 4:B:810:IOD:I    | 2.75                     | 0.57              |
| 1:A:186:VAL:HG13 | 1:A:220:GLU:CG   | 2.35                     | 0.56              |
| 1:A:183:SER:OG   | 1:A:185:GLU:HG2  | 2.05                     | 0.56              |
| 1:B:102:LYS:HB3  | 1:B:108:TYR:CE1  | 2.39                     | 0.56              |
| 1:B:473:VAL:HB   | 6:B:1622:HOH:O   | 2.05                     | 0.56              |
| 1:B:52:MET:HB3   | 1:B:57:HIS:CG    | 2.41                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:288:SER:HB2  | 6:B:1778:HOH:O   | 2.05                     | 0.56              |
| 1:A:358:VAL:HG21 | 1:A:404:PHE:CE2  | 2.41                     | 0.56              |
| 1:B:301:LEU:HD12 | 1:B:301:LEU:C    | 2.29                     | 0.56              |
| 1:A:408:CYS:O    | 1:A:409:LYS:HB3  | 2.06                     | 0.56              |
| 1:B:333:VAL:HG12 | 1:B:360:GLY:CA   | 2.35                     | 0.56              |
| 1:A:452:SER:OG   | 1:A:455:ARG:HB2  | 2.06                     | 0.56              |
| 1:B:213:ASP:HB3  | 1:B:214:ARG:NE   | 2.16                     | 0.56              |
| 1:A:379:CYS:O    | 1:A:380:LEU:C    | 2.49                     | 0.56              |
| 1:B:391:ARG:CG   | 1:B:399:ALA:HB3  | 2.35                     | 0.56              |
| 1:B:460:ALA:HB1  | 1:B:461:PRO:HD2  | 1.88                     | 0.56              |
| 1:A:117:PRO:HD2  | 1:A:118:HIS:CE1  | 2.41                     | 0.55              |
| 1:A:409:LYS:N    | 1:A:420:ARG:HH21 | 2.02                     | 0.55              |
| 1:A:421:ASP:OD2  | 1:A:425:ASN:HB2  | 2.06                     | 0.55              |
| 1:A:464:VAL:C    | 1:A:465:GLU:HG2  | 2.31                     | 0.55              |
| 1:B:387:ILE:O    | 1:B:389:TYR:N    | 2.39                     | 0.55              |
| 1:A:186:VAL:CG1  | 1:A:220:GLU:HG2  | 2.34                     | 0.55              |
| 1:A:313:LYS:NZ   | 1:A:313:LYS:HB3  | 2.21                     | 0.55              |
| 1:A:337:GLY:C    | 1:A:339:GLU:H    | 2.15                     | 0.55              |
| 1:B:277:GLU:HG3  | 6:B:1699:HOH:O   | 2.06                     | 0.55              |
| 1:B:290:VAL:HG22 | 1:B:321:VAL:CG1  | 2.37                     | 0.55              |
| 1:B:224:ILE:O    | 1:B:225:ALA:C    | 2.46                     | 0.55              |
| 1:B:355:TYR:CD2  | 1:B:404:PHE:HB3  | 2.42                     | 0.55              |
| 1:A:347:ILE:HD12 | 1:A:368:ALA:CB   | 2.37                     | 0.55              |
| 1:A:440:ARG:HH21 | 1:A:469:HIS:CE1  | 2.25                     | 0.55              |
| 1:A:441:LEU:HA   | 1:A:467:HIS:O    | 2.06                     | 0.55              |
| 1:B:455:ARG:HD2  | 1:B:455:ARG:O    | 2.06                     | 0.55              |
| 1:B:488:VAL:HG11 | 1:B:491:ARG:CZ   | 2.36                     | 0.55              |
| 1:B:186:VAL:HG21 | 1:B:220:GLU:HG2  | 1.89                     | 0.55              |
| 1:B:211:ARG:HB3  | 1:B:211:ARG:CZ   | 2.37                     | 0.55              |
| 1:B:273:LEU:O    | 1:B:277:GLU:HG2  | 2.07                     | 0.55              |
| 1:B:421:ASP:CB   | 1:B:425:ASN:H    | 2.18                     | 0.55              |
| 1:A:272:ASN:C    | 1:A:272:ASN:HD22 | 2.12                     | 0.55              |
| 1:A:332:ASP:O    | 1:A:336:ARG:N    | 2.37                     | 0.55              |
| 1:B:289:GLU:CG   | 1:B:324:ASN:HD21 | 2.19                     | 0.55              |
| 1:A:151:LEU:N    | 1:A:152:PRO:HD2  | 2.22                     | 0.55              |
| 1:A:294:MET:HE1  | 1:A:305:TYR:HB3  | 1.88                     | 0.55              |
| 1:A:297:LYS:O    | 1:A:300:GLU:OE2  | 2.25                     | 0.54              |
| 1:A:398:ASN:N    | 1:A:398:ASN:OD1  | 2.39                     | 0.54              |
| 1:B:409:LYS:HD3  | 1:B:410:TYR:CE1  | 2.42                     | 0.54              |
| 1:B:539:PHE:CE2  | 1:B:543:GLN:HG3  | 2.43                     | 0.54              |
| 1:A:275:GLU:OE1  | 1:A:523:ARG:HD2  | 2.07                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:331:GLN:HG2  | 1:A:334:GLU:OE1  | 2.08                     | 0.54              |
| 1:B:49:PRO:HA    | 1:B:52:MET:HE1   | 1.88                     | 0.54              |
| 1:B:216:VAL:CG1  | 1:B:221:ARG:HG2  | 2.37                     | 0.54              |
| 1:A:336:ARG:NH2  | 1:A:340:ILE:HG22 | 2.23                     | 0.54              |
| 1:B:180:MET:HG2  | 1:B:183:SER:H    | 1.72                     | 0.54              |
| 1:A:177:VAL:CG1  | 1:A:186:VAL:HG23 | 2.36                     | 0.54              |
| 1:B:539:PHE:O    | 1:B:543:GLN:HG2  | 2.07                     | 0.54              |
| 1:A:391:ARG:O    | 1:A:393:VAL:N    | 2.41                     | 0.54              |
| 1:A:486:LEU:HG   | 1:A:487:ARG:H    | 1.72                     | 0.54              |
| 1:B:91:THR:N     | 6:B:1759:HOH:O   | 2.25                     | 0.54              |
| 1:B:226:LEU:O    | 1:B:228:CYS:O    | 2.25                     | 0.54              |
| 1:A:390:ALA:O    | 1:A:394:ALA:HB3  | 2.07                     | 0.54              |
| 1:B:329:ASP:O    | 1:B:330:SER:C    | 2.50                     | 0.54              |
| 1:A:40:LYS:HB3   | 1:A:89:ASN:ND2   | 2.22                     | 0.54              |
| 1:A:46:ASN:HB2   | 1:A:52:MET:CE    | 2.35                     | 0.54              |
| 1:B:415:LEU:HD21 | 1:B:471:TYR:CE1  | 2.42                     | 0.54              |
| 1:B:506:HIS:CG   | 1:B:507:PRO:HD2  | 2.42                     | 0.54              |
| 1:A:199:LEU:HD23 | 1:A:203:ILE:O    | 2.08                     | 0.54              |
| 1:A:422:GLU:OE2  | 1:A:422:GLU:N    | 2.29                     | 0.54              |
| 1:B:49:PRO:HG2   | 1:B:69:THR:CA    | 2.38                     | 0.54              |
| 1:A:54:PRO:CA    | 1:A:58:GLY:N     | 2.71                     | 0.53              |
| 1:A:355:TYR:O    | 1:A:358:VAL:HG23 | 2.08                     | 0.53              |
| 1:A:420:ARG:HG3  | 1:A:421:ASP:H    | 1.71                     | 0.53              |
| 1:B:403:GLU:HG3  | 1:B:471:TYR:CE1  | 2.43                     | 0.53              |
| 1:A:416:ILE:HG23 | 1:A:419:TRP:CH2  | 2.43                     | 0.53              |
| 1:B:179:TYR:CD2  | 1:B:214:ARG:NH2  | 2.75                     | 0.53              |
| 1:B:227:PHE:C    | 1:B:228:CYS:O    | 2.46                     | 0.53              |
| 1:B:516:PRO:HD2  | 1:B:517:GLU:OE2  | 2.07                     | 0.53              |
| 1:A:18:LYS:HE3   | 1:A:141:ILE:O    | 2.07                     | 0.53              |
| 1:A:241:VAL:HA   | 4:A:812:IOD:I    | 2.79                     | 0.53              |
| 1:A:333:VAL:HA   | 1:A:340:ILE:CD1  | 2.37                     | 0.53              |
| 1:B:331:GLN:HA   | 1:B:334:GLU:OE2  | 2.08                     | 0.53              |
| 1:B:379:CYS:O    | 1:B:380:LEU:C    | 2.50                     | 0.53              |
| 1:A:409:LYS:O    | 1:A:422:GLU:HA   | 2.09                     | 0.53              |
| 1:B:488:VAL:HG11 | 1:B:491:ARG:NE   | 2.23                     | 0.53              |
| 1:A:20:ILE:HG13  | 6:A:908:HOH:O    | 2.08                     | 0.53              |
| 1:B:486:LEU:HG   | 1:B:487:ARG:N    | 2.22                     | 0.53              |
| 1:A:86:ARG:HH11  | 1:A:86:ARG:CG    | 2.22                     | 0.53              |
| 1:A:211:ARG:CZ   | 5:A:601:MPD:H53  | 2.38                     | 0.53              |
| 1:B:216:VAL:HG12 | 1:B:221:ARG:HG2  | 1.90                     | 0.53              |
| 1:B:216:VAL:O    | 1:B:221:ARG:NH1  | 2.38                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:393:VAL:HG12 | 1:B:393:VAL:O     | 2.09                     | 0.53              |
| 1:B:441:LEU:CD2  | 1:B:468:ARG:HD2   | 2.39                     | 0.53              |
| 1:A:288:SER:HB3  | 6:A:999:HOH:O     | 2.08                     | 0.53              |
| 1:B:166:ARG:NH2  | 6:B:1830:HOH:O    | 2.42                     | 0.53              |
| 1:A:46:ASN:H     | 1:A:46:ASN:ND2    | 2.06                     | 0.52              |
| 1:B:325:ILE:HG22 | 1:B:327:LEU:HD23  | 1.90                     | 0.52              |
| 1:B:450:ASP:O    | 1:B:451:ASP:HB2   | 2.09                     | 0.52              |
| 1:A:53:SER:O     | 1:A:57[B]:HIS:HB3 | 2.09                     | 0.52              |
| 1:A:494:ASP:C    | 1:A:496:GLN:H     | 2.17                     | 0.52              |
| 1:A:401:SER:HA   | 1:A:413:VAL:O     | 2.08                     | 0.52              |
| 1:B:416:ILE:HD11 | 1:B:497:LEU:HD21  | 1.91                     | 0.52              |
| 1:A:409:LYS:O    | 1:A:411:PRO:HD3   | 2.09                     | 0.52              |
| 1:A:444:GLN:HB2  | 1:A:467:HIS:ND1   | 2.24                     | 0.52              |
| 1:B:111:ALA:HB1  | 6:B:1838:HOH:O    | 2.09                     | 0.52              |
| 1:B:229:ASN:C    | 1:B:230:VAL:HG23  | 2.35                     | 0.52              |
| 1:A:355:TYR:O    | 1:A:356:ARG:O     | 2.27                     | 0.52              |
| 1:A:488:VAL:HG11 | 1:A:491:ARG:CZ    | 2.39                     | 0.52              |
| 1:B:1:MET:HE2    | 1:B:135:ASP:OD1   | 2.10                     | 0.52              |
| 1:B:415:LEU:HD21 | 1:B:471:TYR:CD1   | 2.44                     | 0.52              |
| 1:A:233:LYS:HB3  | 6:A:1067:HOH:O    | 2.09                     | 0.52              |
| 1:A:295:VAL:HA   | 1:A:328:ILE:O     | 2.10                     | 0.52              |
| 1:A:369:ARG:HH21 | 1:A:388:ASP:CG    | 2.18                     | 0.52              |
| 1:B:331:GLN:O    | 1:B:333:VAL:N     | 2.43                     | 0.52              |
| 1:B:98:ASP:OD2   | 1:B:126:ARG:NH2   | 2.35                     | 0.52              |
| 1:B:183:SER:OG   | 1:B:185:GLU:OE2   | 2.27                     | 0.52              |
| 1:A:362:ILE:HG13 | 1:A:384:VAL:HG22  | 1.92                     | 0.51              |
| 1:A:453:LEU:O    | 1:A:456:GLN:HB2   | 2.10                     | 0.51              |
| 1:B:515:HIS:HB3  | 1:B:517:GLU:CD    | 2.35                     | 0.51              |
| 1:A:420:ARG:HG3  | 1:A:421:ASP:N     | 2.24                     | 0.51              |
| 1:B:355:TYR:HD1  | 1:B:358:VAL:HB    | 1.75                     | 0.51              |
| 1:B:492:SER:O    | 1:B:493:GLY:O     | 2.29                     | 0.51              |
| 1:B:412:VAL:HG13 | 1:B:413:VAL:HG23  | 1.92                     | 0.51              |
| 1:B:301:LEU:HD12 | 1:B:302:PRO:CD    | 2.40                     | 0.51              |
| 1:B:390:ALA:HB1  | 1:B:396:MET:HG2   | 1.91                     | 0.51              |
| 1:A:160:MET:HG2  | 4:A:803:IOD:I     | 2.80                     | 0.51              |
| 1:A:233:LYS:O    | 1:A:233:LYS:HG2   | 2.10                     | 0.51              |
| 1:A:389:TYR:HD2  | 1:A:481:ILE:CG2   | 2.23                     | 0.51              |
| 1:B:493:GLY:HA2  | 1:B:496:GLN:CD    | 2.33                     | 0.51              |
| 1:B:155:GLU:OE2  | 1:B:158:ARG:NH2   | 2.36                     | 0.51              |
| 1:B:495:ASP:O    | 1:B:496:GLN:O     | 2.29                     | 0.51              |
| 1:A:355:TYR:CD1  | 1:A:404:PHE:CG    | 2.99                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:131:GLY:O    | 1:B:134:HIS:HD2  | 1.93                     | 0.51              |
| 1:B:268:CYS:HB2  | 1:B:269:PRO:CD   | 2.35                     | 0.51              |
| 1:A:357:GLY:O    | 1:A:360:GLY:N    | 2.43                     | 0.51              |
| 1:A:448:LEU:HD22 | 1:A:454:VAL:HG13 | 1.93                     | 0.51              |
| 1:B:361:MET:HB3  | 1:B:384:VAL:HG21 | 1.93                     | 0.51              |
| 1:B:409:LYS:O    | 1:B:411:PRO:HD3  | 2.11                     | 0.51              |
| 1:B:53:SER:O     | 1:B:55:ILE:O     | 2.29                     | 0.51              |
| 1:B:147:ASP:HB2  | 6:B:1785:HOH:O   | 2.10                     | 0.51              |
| 1:B:225:ALA:O    | 1:B:230:VAL:N    | 2.44                     | 0.51              |
| 1:B:425:ASN:C    | 1:B:476:MET:HE1  | 2.36                     | 0.51              |
| 1:B:499:GLU:O    | 1:B:512:CYS:HA   | 2.11                     | 0.50              |
| 1:A:396:MET:O    | 1:A:397:GLU:C    | 2.53                     | 0.50              |
| 1:B:355:TYR:CB   | 1:B:404:PHE:CD2  | 2.94                     | 0.50              |
| 1:B:426:VAL:CG1  | 1:B:427:GLU:N    | 2.74                     | 0.50              |
| 1:A:86:ARG:HH11  | 1:A:86:ARG:H     | 1.53                     | 0.50              |
| 1:A:179:TYR:CD2  | 1:A:214:ARG:NH2  | 2.80                     | 0.50              |
| 1:A:478:LEU:O    | 1:A:482:GLU:HG3  | 2.10                     | 0.50              |
| 1:A:289:GLU:CB   | 1:A:322:SER:HB3  | 2.42                     | 0.50              |
| 1:B:108:TYR:CD2  | 1:B:118:HIS:CD2  | 2.98                     | 0.50              |
| 1:B:366:ARG:HA   | 1:B:388:ASP:OD2  | 2.12                     | 0.50              |
| 1:A:458:TYR:O    | 1:A:459:ASN:C    | 2.52                     | 0.50              |
| 1:B:48:ASP:OD1   | 1:B:50:GLY:N     | 2.42                     | 0.50              |
| 1:B:405:VAL:HG12 | 1:B:405:VAL:O    | 2.12                     | 0.50              |
| 1:B:413:VAL:O    | 1:B:414:ALA:HB2  | 2.10                     | 0.50              |
| 1:A:166:ARG:HB2  | 1:A:263:ARG:HH21 | 1.76                     | 0.50              |
| 1:A:331:GLN:O    | 1:A:335:THR:N    | 2.36                     | 0.50              |
| 1:A:331:GLN:HG2  | 6:A:1069:HOH:O   | 2.11                     | 0.50              |
| 1:B:45:ILE:O     | 1:B:46:ASN:C     | 2.51                     | 0.50              |
| 1:B:295:VAL:HA   | 1:B:328:ILE:O    | 2.10                     | 0.50              |
| 1:A:179:TYR:CE1  | 1:A:214:ARG:NH1  | 2.80                     | 0.50              |
| 1:B:212:SER:HB3  | 1:B:214:ARG:O    | 2.12                     | 0.50              |
| 1:A:268:CYS:CB   | 1:A:269:PRO:HD2  | 2.41                     | 0.50              |
| 1:A:272:ASN:C    | 1:A:272:ASN:ND2  | 2.70                     | 0.50              |
| 1:A:409:LYS:HD3  | 1:A:410:TYR:CE1  | 2.47                     | 0.50              |
| 1:B:395:ASN:ND2  | 1:B:410:TYR:CZ   | 2.80                     | 0.50              |
| 1:B:447:GLN:NE2  | 1:B:493:GLY:H    | 2.09                     | 0.50              |
| 1:A:341:LEU:HD23 | 1:A:341:LEU:N    | 2.26                     | 0.50              |
| 1:B:179:TYR:CE1  | 1:B:214:ARG:NH1  | 2.80                     | 0.50              |
| 1:B:299:ILE:HG22 | 1:B:299:ILE:O    | 2.11                     | 0.50              |
| 1:B:371:ASN:N    | 1:B:371:ASN:ND2  | 2.58                     | 0.50              |
| 1:B:382:MET:HE3  | 1:B:512:CYS:CA   | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:420:ARG:HA   | 1:B:425:ASN:O    | 2.11                     | 0.50              |
| 1:B:86:ARG:NH1   | 1:B:89:ASN:O     | 2.45                     | 0.49              |
| 1:A:355:TYR:CD1  | 1:A:404:PHE:CD2  | 2.99                     | 0.49              |
| 1:A:403:GLU:HB2  | 1:A:471:TYR:CE2  | 2.47                     | 0.49              |
| 1:B:389:TYR:CE2  | 1:B:486:LEU:HB2  | 2.47                     | 0.49              |
| 1:A:177:VAL:HG12 | 1:A:186:VAL:HG23 | 1.93                     | 0.49              |
| 1:A:179:TYR:HE2  | 1:A:181:ALA:HA   | 1.78                     | 0.49              |
| 1:A:201:ILE:CD1  | 1:A:203:ILE:HD12 | 2.42                     | 0.49              |
| 1:B:392:HIS:CD2  | 1:B:392:HIS:N    | 2.80                     | 0.49              |
| 1:A:469:HIS:CE1  | 1:A:513:GLN:NE2  | 2.79                     | 0.49              |
| 1:B:369:ARG:NH1  | 1:B:393:VAL:HG21 | 2.26                     | 0.49              |
| 1:B:388:ASP:OD1  | 1:B:389:TYR:N    | 2.45                     | 0.49              |
| 1:A:336:ARG:HH21 | 1:A:340:ILE:HG22 | 1.76                     | 0.49              |
| 1:A:413:VAL:CG1  | 1:A:471:TYR:HB3  | 2.42                     | 0.49              |
| 1:B:415:LEU:HD23 | 1:B:415:LEU:N    | 2.26                     | 0.49              |
| 1:A:488:VAL:HG11 | 1:A:491:ARG:HE   | 1.77                     | 0.49              |
| 1:B:115:VAL:O    | 1:B:119:ILE:HB   | 2.13                     | 0.49              |
| 1:A:301:LEU:O    | 1:A:301:LEU:HG   | 2.10                     | 0.49              |
| 1:B:494:ASP:CG   | 1:B:495:ASP:N    | 2.70                     | 0.49              |
| 1:A:415:LEU:HG   | 1:A:418:GLU:CD   | 2.37                     | 0.49              |
| 1:B:299:ILE:CG2  | 1:B:327:LEU:HB3  | 2.41                     | 0.49              |
| 1:B:373:ILE:HG23 | 1:B:374:PRO:HD2  | 1.95                     | 0.49              |
| 1:A:302:PRO:C    | 1:A:304:ALA:N    | 2.71                     | 0.49              |
| 1:B:179:TYR:CD2  | 1:B:179:TYR:C    | 2.90                     | 0.49              |
| 1:B:69:THR:CG2   | 1:B:73:LEU:HD22  | 2.43                     | 0.49              |
| 1:B:382:MET:HE3  | 1:B:512:CYS:HA   | 1.95                     | 0.49              |
| 1:A:448:LEU:HD11 | 1:A:463:ILE:HG23 | 1.93                     | 0.48              |
| 1:B:378:ILE:CD1  | 1:B:516:PRO:HD2  | 2.42                     | 0.48              |
| 1:A:454:VAL:HG22 | 1:A:528:LEU:HD21 | 1.96                     | 0.48              |
| 1:A:494:ASP:C    | 1:A:496:GLN:N    | 2.71                     | 0.48              |
| 1:B:415:LEU:CD2  | 1:B:471:TYR:CD2  | 2.97                     | 0.48              |
| 1:A:355:TYR:CD1  | 1:A:404:PHE:CB   | 2.96                     | 0.48              |
| 1:A:517:GLU:OE1  | 1:A:517:GLU:N    | 2.46                     | 0.48              |
| 1:B:380:LEU:O    | 1:B:383:GLN:HB2  | 2.13                     | 0.48              |
| 1:A:229:ASN:C    | 1:A:231:PRO:HD3  | 2.38                     | 0.48              |
| 1:A:361:MET:HB2  | 1:A:384:VAL:CG2  | 2.42                     | 0.48              |
| 1:A:396:MET:HE1  | 1:A:480:GLN:CB   | 2.44                     | 0.48              |
| 1:B:12:VAL:HG11  | 1:B:176:LEU:HB3  | 1.94                     | 0.48              |
| 1:A:179:TYR:OH   | 1:A:184:GLY:HA2  | 2.13                     | 0.48              |
| 1:A:296:GLY:C    | 1:A:299:ILE:HG12 | 2.39                     | 0.48              |
| 1:B:189:LYS:HB3  | 1:B:190:PRO:CD   | 2.35                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:413:VAL:O    | 1:A:414:ALA:HB2  | 2.13                     | 0.48              |
| 1:A:416:ILE:HA   | 1:A:419:TRP:CE2  | 2.49                     | 0.48              |
| 1:B:81:ARG:HB2   | 6:B:1816:HOH:O   | 2.14                     | 0.48              |
| 1:A:503:VAL:HA   | 1:A:504:PRO:HD3  | 1.68                     | 0.48              |
| 1:B:227:PHE:O    | 1:B:228:CYS:O    | 2.31                     | 0.48              |
| 1:A:49:PRO:C     | 1:A:51:THR:H     | 2.22                     | 0.48              |
| 1:B:172:MET:HG2  | 1:B:209:ILE:HD12 | 1.96                     | 0.48              |
| 1:A:302:PRO:C    | 1:A:304:ALA:H    | 2.21                     | 0.48              |
| 1:B:369:ARG:NH1  | 1:B:393:VAL:CG2  | 2.77                     | 0.48              |
| 1:B:493:GLY:O    | 1:B:494:ASP:OD1  | 2.32                     | 0.48              |
| 1:A:298:TYR:O    | 1:A:300:GLU:N    | 2.47                     | 0.48              |
| 1:A:403:GLU:HB2  | 1:A:471:TYR:CD2  | 2.48                     | 0.48              |
| 1:A:415:LEU:HD21 | 1:A:471:TYR:CE2  | 2.49                     | 0.48              |
| 1:B:97:SER:O     | 1:B:101:ARG:HD2  | 2.14                     | 0.48              |
| 1:B:398:ASN:O    | 1:B:399:ALA:C    | 2.56                     | 0.48              |
| 1:A:375:TYR:HB3  | 1:A:509:PHE:CD1  | 2.49                     | 0.47              |
| 1:B:63:THR:OG1   | 1:B:65:ASP:OD1   | 2.29                     | 0.47              |
| 1:B:492:SER:HB2  | 1:B:499:GLU:OE2  | 2.14                     | 0.47              |
| 1:A:75:HIS:O     | 1:A:76:TYR:C     | 2.53                     | 0.47              |
| 1:A:347:ILE:HD13 | 1:A:368:ALA:HB2  | 1.92                     | 0.47              |
| 1:A:355:TYR:HD1  | 1:A:404:PHE:CD2  | 2.32                     | 0.47              |
| 1:A:420:ARG:CG   | 1:A:421:ASP:N    | 2.77                     | 0.47              |
| 1:B:211:ARG:NE   | 5:B:1601:MPD:H53 | 2.29                     | 0.47              |
| 1:B:172:MET:HG2  | 1:B:209:ILE:CD1  | 2.44                     | 0.47              |
| 1:B:506:HIS:CE1  | 1:B:507:PRO:HD2  | 2.49                     | 0.47              |
| 1:A:471:TYR:C    | 1:A:472:GLU:HG2  | 2.40                     | 0.47              |
| 1:B:301:LEU:HD11 | 1:B:303:ASP:HB2  | 1.97                     | 0.47              |
| 1:B:421:ASP:N    | 1:B:476:MET:HE1  | 2.30                     | 0.47              |
| 1:A:506:HIS:CD2  | 1:A:507:PRO:HD2  | 2.50                     | 0.47              |
| 1:B:378:ILE:HD13 | 1:B:516:PRO:CD   | 2.44                     | 0.47              |
| 1:B:441:LEU:HA   | 1:B:467:HIS:O    | 2.14                     | 0.47              |
| 1:A:163:GLU:HG2  | 4:A:803:IOD:I    | 2.85                     | 0.47              |
| 1:A:272:ASN:ND2  | 1:A:274:SER:H    | 2.13                     | 0.47              |
| 1:A:495:ASP:HB3  | 1:A:497:LEU:HD12 | 1.94                     | 0.47              |
| 1:A:67:ALA:HB2   | 1:A:86:ARG:CB    | 2.45                     | 0.47              |
| 1:A:221:ARG:O    | 1:A:224:ILE:N    | 2.48                     | 0.47              |
| 1:A:285:ASN:O    | 1:A:320:ARG:NH1  | 2.47                     | 0.47              |
| 1:B:101:ARG:O    | 1:B:102:LYS:C    | 2.58                     | 0.47              |
| 1:B:151:LEU:HB2  | 1:B:152:PRO:CD   | 2.45                     | 0.47              |
| 1:B:277:GLU:HG2  | 1:B:277:GLU:H    | 1.62                     | 0.47              |
| 1:A:106:GLY:O    | 1:A:109:LEU:HD23 | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:49:PRO:C     | 1:B:51:THR:H     | 2.23                     | 0.47              |
| 1:B:54:PRO:HA    | 1:B:58:GLY:O     | 2.14                     | 0.47              |
| 1:A:151:LEU:N    | 1:A:152:PRO:CD   | 2.78                     | 0.47              |
| 1:A:297:LYS:HG2  | 6:A:1048:HOH:O   | 2.15                     | 0.47              |
| 1:A:444:GLN:HB2  | 1:A:467:HIS:CE1  | 2.50                     | 0.47              |
| 1:B:144:THR:O    | 1:B:145:VAL:C    | 2.57                     | 0.47              |
| 1:B:355:TYR:CB   | 1:B:404:PHE:HD2  | 2.25                     | 0.47              |
| 1:A:382:MET:HE1  | 1:A:499:GLU:C    | 2.40                     | 0.47              |
| 1:A:372:ASN:ND2  | 1:A:506:HIS:CD2  | 2.82                     | 0.46              |
| 1:A:483:ASP:C    | 1:A:485:GLY:H    | 2.24                     | 0.46              |
| 1:B:13:VAL:HG23  | 1:B:16:LEU:HG    | 1.97                     | 0.46              |
| 1:B:390:ALA:C    | 1:B:396:MET:HB2  | 2.41                     | 0.46              |
| 1:A:263:ARG:O    | 1:A:263:ARG:HG3  | 2.10                     | 0.46              |
| 1:A:297:LYS:C    | 1:A:299:ILE:H    | 2.23                     | 0.46              |
| 1:A:302:PRO:O    | 1:A:304:ALA:N    | 2.48                     | 0.46              |
| 1:A:341:LEU:CD1  | 1:A:364:THR:HG23 | 2.45                     | 0.46              |
| 1:B:289:GLU:HG3  | 1:B:324:ASN:ND2  | 2.29                     | 0.46              |
| 1:B:379:CYS:HB3  | 1:B:380:LEU:H    | 1.43                     | 0.46              |
| 1:B:389:TYR:O    | 1:B:390:ALA:C    | 2.58                     | 0.46              |
| 1:B:426:VAL:HG13 | 1:B:427:GLU:H    | 1.80                     | 0.46              |
| 1:B:42:ASP:O     | 1:B:91:THR:HA    | 2.15                     | 0.46              |
| 1:B:227:PHE:O    | 1:B:229:ASN:ND2  | 2.48                     | 0.46              |
| 1:A:55:ILE:CD1   | 1:A:55:ILE:N     | 2.79                     | 0.46              |
| 1:A:207:ILE:HA   | 1:A:234:ALA:HB1  | 1.96                     | 0.46              |
| 1:B:296:GLY:O    | 1:B:329:ASP:HA   | 2.16                     | 0.46              |
| 1:B:402:THR:CG2  | 1:B:414:ALA:HB2  | 2.42                     | 0.46              |
| 1:B:93:GLY:O     | 1:B:97:SER:HB2   | 2.15                     | 0.46              |
| 1:B:503:VAL:O    | 1:B:503:VAL:HG12 | 2.13                     | 0.46              |
| 1:A:13:VAL:HG23  | 1:A:16:LEU:HD21  | 1.97                     | 0.46              |
| 1:A:40:LYS:HB3   | 1:A:89:ASN:HD22  | 1.81                     | 0.46              |
| 1:A:313:LYS:HB3  | 1:A:313:LYS:HZ3  | 1.81                     | 0.46              |
| 1:A:543:GLN:O    | 1:A:544:ALA:HB2  | 2.16                     | 0.46              |
| 1:B:230:VAL:HG12 | 1:B:230:VAL:O    | 2.16                     | 0.46              |
| 1:B:382:MET:HE1  | 1:B:499:GLU:C    | 2.41                     | 0.46              |
| 1:B:106:GLY:O    | 1:B:109:LEU:N    | 2.35                     | 0.46              |
| 1:B:224:ILE:CA   | 1:B:229:ASN:HD22 | 2.28                     | 0.46              |
| 1:B:495:ASP:HB3  | 1:B:497:LEU:HG   | 1.98                     | 0.46              |
| 1:A:537:SER:O    | 1:A:541:LYS:HG3  | 2.16                     | 0.45              |
| 1:B:9:THR:O      | 1:B:173:HIS:HA   | 2.16                     | 0.45              |
| 1:B:86:ARG:HA    | 1:B:86:ARG:HD3   | 1.68                     | 0.45              |
| 1:A:18:LYS:HE2   | 1:A:140:GLU:HG2  | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:300:GLU:O    | 1:A:302:PRO:HD3  | 2.16                     | 0.45              |
| 1:A:362:ILE:HA   | 1:A:384:VAL:HG13 | 1.97                     | 0.45              |
| 1:A:409:LYS:H    | 1:A:420:ARG:NH2  | 2.13                     | 0.45              |
| 1:B:355:TYR:HA   | 1:B:404:PHE:CD2  | 2.51                     | 0.45              |
| 1:A:382:MET:CE   | 1:A:500:ILE:HA   | 2.46                     | 0.45              |
| 1:B:78:ARG:NH1   | 1:B:307:SER:OG   | 2.48                     | 0.45              |
| 1:B:488:VAL:CG1  | 1:B:491:ARG:NH2  | 2.79                     | 0.45              |
| 1:A:54:PRO:C     | 1:A:58:GLY:N     | 2.74                     | 0.45              |
| 1:A:272:ASN:ND2  | 1:A:274:SER:OG   | 2.36                     | 0.45              |
| 1:A:340:ILE:HG12 | 1:A:341:LEU:N    | 2.31                     | 0.45              |
| 1:A:537:SER:O    | 1:A:540:GLN:HB3  | 2.16                     | 0.45              |
| 1:A:189:LYS:N    | 1:A:190:PRO:CD   | 2.79                     | 0.45              |
| 1:A:414:ALA:HB1  | 1:A:418:GLU:OE1  | 2.17                     | 0.45              |
| 1:B:189:LYS:N    | 1:B:190:PRO:CD   | 2.80                     | 0.45              |
| 1:A:301:LEU:HD21 | 1:A:303:ASP:HB2  | 1.97                     | 0.45              |
| 1:A:86:ARG:HH22  | 1:A:87:ARG:HH11  | 1.64                     | 0.45              |
| 1:A:230:VAL:N    | 1:A:231:PRO:CD   | 2.80                     | 0.45              |
| 1:B:163:GLU:HG2  | 4:B:804:IOD:I    | 2.87                     | 0.45              |
| 1:B:220:GLU:N    | 1:B:220:GLU:CD   | 2.75                     | 0.45              |
| 1:B:252:LYS:HE3  | 1:B:271:ALA:HB3  | 1.97                     | 0.45              |
| 1:A:359:GLU:HA   | 1:A:362:ILE:HD12 | 1.98                     | 0.45              |
| 1:A:506:HIS:ND1  | 1:A:507:PRO:HD2  | 2.32                     | 0.45              |
| 1:B:348:LEU:HD23 | 1:B:348:LEU:C    | 2.42                     | 0.45              |
| 1:A:390:ALA:CB   | 1:A:481:ILE:HD13 | 2.47                     | 0.45              |
| 1:B:258:ASP:O    | 1:B:259:TYR:C    | 2.58                     | 0.45              |
| 1:B:341:LEU:HB2  | 1:B:367:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:186:VAL:HG13 | 1:A:220:GLU:CD   | 2.42                     | 0.45              |
| 1:B:216:VAL:HA   | 1:B:217:PRO:HD3  | 1.74                     | 0.45              |
| 1:B:355:TYR:CD1  | 1:B:404:PHE:HB3  | 2.50                     | 0.45              |
| 1:A:396:MET:HE1  | 1:A:480:GLN:HB3  | 1.99                     | 0.44              |
| 1:A:420:ARG:CG   | 1:A:421:ASP:H    | 2.28                     | 0.44              |
| 1:B:106:GLY:O    | 1:B:107:ASP:C    | 2.60                     | 0.44              |
| 1:B:244:ILE:HG23 | 6:B:1763:HOH:O   | 2.17                     | 0.44              |
| 1:B:338:VAL:O    | 1:B:338:VAL:HG13 | 2.17                     | 0.44              |
| 1:B:421:ASP:N    | 1:B:476:MET:CE   | 2.80                     | 0.44              |
| 1:A:382:MET:HE1  | 1:A:499:GLU:O    | 2.17                     | 0.44              |
| 1:B:69:THR:HG23  | 1:B:70:ASP:N     | 2.33                     | 0.44              |
| 1:B:103:GLU:OE1  | 1:B:104:ARG:HG2  | 2.17                     | 0.44              |
| 1:B:217:PRO:O    | 1:B:218:ALA:C    | 2.60                     | 0.44              |
| 1:A:86:ARG:NH1   | 1:A:86:ARG:CG    | 2.80                     | 0.44              |
| 1:A:181:ALA:O    | 1:A:182:ALA:O    | 2.34                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:167:GLU:HB2  | 6:B:1789:HOH:O   | 2.17                     | 0.44              |
| 1:B:373:ILE:C    | 1:B:506:HIS:HE1  | 2.25                     | 0.44              |
| 1:B:421:ASP:CB   | 1:B:425:ASN:N    | 2.80                     | 0.44              |
| 1:B:426:VAL:HG13 | 1:B:427:GLU:N    | 2.33                     | 0.44              |
| 1:B:506:HIS:ND1  | 1:B:507:PRO:CD   | 2.78                     | 0.44              |
| 1:A:402:THR:OG1  | 1:A:418:GLU:OE1  | 2.29                     | 0.44              |
| 1:B:127:VAL:HG11 | 1:B:160:MET:HE1  | 2.00                     | 0.44              |
| 1:B:228:CYS:HB2  | 6:B:1722:HOH:O   | 2.17                     | 0.44              |
| 1:A:400:ASN:O    | 1:A:411:PRO:HA   | 2.18                     | 0.44              |
| 1:A:414:ALA:HA   | 1:A:471:TYR:HD2  | 1.83                     | 0.44              |
| 1:B:218:ALA:O    | 1:B:219:ASN:C    | 2.59                     | 0.44              |
| 1:B:366:ARG:HB2  | 1:B:388:ASP:OD2  | 2.18                     | 0.44              |
| 1:B:478:LEU:O    | 1:B:481:ILE:N    | 2.50                     | 0.44              |
| 1:A:219:ASN:HB2  | 6:A:942:HOH:O    | 2.16                     | 0.44              |
| 1:A:382:MET:HA   | 1:A:511:ALA:HB1  | 1.98                     | 0.44              |
| 1:A:415:LEU:HD21 | 1:A:471:TYR:CZ   | 2.53                     | 0.44              |
| 1:B:118:HIS:ND1  | 1:B:118:HIS:N    | 2.56                     | 0.44              |
| 1:B:267:ASN:O    | 1:B:268:CYS:HB3  | 2.17                     | 0.44              |
| 1:A:239:LYS:HD3  | 4:A:801:IOD:I    | 2.88                     | 0.44              |
| 1:B:52:MET:HE3   | 1:B:52:MET:HB2   | 1.84                     | 0.44              |
| 1:B:396:MET:CA   | 1:B:410:TYR:CD1  | 2.96                     | 0.44              |
| 1:B:494:ASP:CG   | 1:B:495:ASP:HB2  | 2.43                     | 0.44              |
| 1:A:229:ASN:C    | 1:A:231:PRO:CD   | 2.91                     | 0.44              |
| 1:B:341:LEU:O    | 1:B:344:LEU:CG   | 2.64                     | 0.44              |
| 1:A:408:CYS:C    | 1:A:410:TYR:N    | 2.76                     | 0.43              |
| 1:A:540:GLN:OE1  | 1:A:541:LYS:HG2  | 2.17                     | 0.43              |
| 1:B:301:LEU:HD12 | 1:B:303:ASP:H    | 1.83                     | 0.43              |
| 5:A:601:MPD:O4   | 5:A:601:MPD:O2   | 2.30                     | 0.43              |
| 1:B:1:MET:HG3    | 1:B:135:ASP:OD1  | 2.18                     | 0.43              |
| 1:B:224:ILE:CG2  | 1:B:229:ASN:ND2  | 2.79                     | 0.43              |
| 1:A:208:LEU:HD12 | 1:A:231:PRO:HG2  | 1.99                     | 0.43              |
| 1:B:171:PHE:N    | 1:B:206:ASP:OD2  | 2.50                     | 0.43              |
| 1:B:294:MET:HB3  | 1:B:327:LEU:HD22 | 1.99                     | 0.43              |
| 1:B:492:SER:C    | 1:B:493:GLY:O    | 2.60                     | 0.43              |
| 1:B:545:LYS:HB3  | 6:B:1809:HOH:O   | 2.19                     | 0.43              |
| 1:A:182:ALA:C    | 1:A:184:GLY:H    | 2.26                     | 0.43              |
| 1:A:303:ASP:OD2  | 1:A:303:ASP:N    | 2.52                     | 0.43              |
| 1:A:349:VAL:HG12 | 1:A:381:GLY:HA3  | 1.95                     | 0.43              |
| 1:A:389:TYR:O    | 1:A:390:ALA:C    | 2.61                     | 0.43              |
| 1:B:11:GLY:C     | 1:B:12:VAL:HG23  | 2.42                     | 0.43              |
| 1:B:61:PHE:HB3   | 1:B:69:THR:HG22  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:86:ARG:HD3   | 1:B:86:ARG:O     | 2.17                     | 0.43              |
| 1:B:276:TRP:O    | 1:B:280:ILE:HG13 | 2.18                     | 0.43              |
| 1:B:468:ARG:NH1  | 1:B:468:ARG:CG   | 2.77                     | 0.43              |
| 1:B:487:ARG:HG3  | 6:B:1855:HOH:O   | 2.18                     | 0.43              |
| 1:A:294:MET:HE1  | 1:A:308:VAL:HB   | 2.00                     | 0.43              |
| 1:A:335:THR:HG22 | 1:A:336:ARG:N    | 2.33                     | 0.43              |
| 1:B:378:ILE:HD12 | 1:B:516:PRO:HD2  | 1.99                     | 0.43              |
| 1:B:386:LEU:HD12 | 1:B:386:LEU:HA   | 1.81                     | 0.43              |
| 1:A:345:ASP:HA   | 1:A:539:PHE:HD2  | 1.78                     | 0.43              |
| 1:A:362:ILE:HG12 | 1:A:387:ILE:HG21 | 2.00                     | 0.43              |
| 1:A:378:ILE:HG23 | 1:A:514:PHE:O    | 2.18                     | 0.43              |
| 1:B:189:LYS:O    | 1:B:192:GLN:HB2  | 2.19                     | 0.43              |
| 1:B:262:LYS:O    | 1:B:263:ARG:C    | 2.61                     | 0.43              |
| 1:B:397:GLU:N    | 1:B:410:TYR:CD1  | 2.87                     | 0.43              |
| 1:A:224:ILE:O    | 1:A:225:ALA:C    | 2.62                     | 0.43              |
| 1:A:388:ASP:O    | 1:A:389:TYR:C    | 2.62                     | 0.43              |
| 1:A:402:THR:CG2  | 1:A:414:ALA:CB   | 2.97                     | 0.43              |
| 1:B:109:LEU:C    | 1:B:111:ALA:N    | 2.77                     | 0.43              |
| 1:B:325:ILE:HG22 | 1:B:327:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:420:ARG:HG3  | 1:B:421:ASP:O    | 2.19                     | 0.43              |
| 1:A:1:MET:HE1    | 1:A:134:HIS:HA   | 2.01                     | 0.43              |
| 1:B:102:LYS:HB3  | 1:B:108:TYR:HE1  | 1.84                     | 0.43              |
| 1:B:113:VAL:HG13 | 1:B:118:HIS:CG   | 2.54                     | 0.43              |
| 1:B:383:GLN:C    | 1:B:385:ALA:N    | 2.76                     | 0.43              |
| 1:B:396:MET:HA   | 1:B:410:TYR:CE1  | 2.54                     | 0.43              |
| 1:B:421:ASP:N    | 1:B:425:ASN:O    | 2.50                     | 0.43              |
| 1:A:2:THR:HG21   | 1:A:168:HIS:NE2  | 2.34                     | 0.43              |
| 1:A:166:ARG:HB2  | 1:A:263:ARG:NH2  | 2.34                     | 0.43              |
| 1:A:178:PRO:HD2  | 1:A:187:LYS:O    | 2.18                     | 0.42              |
| 1:A:179:TYR:CG   | 1:A:214:ARG:CZ   | 3.02                     | 0.42              |
| 1:A:390:ALA:HA   | 1:A:481:ILE:HG23 | 2.01                     | 0.42              |
| 1:B:86:ARG:HH12  | 1:B:89:ASN:CB    | 2.30                     | 0.42              |
| 1:B:148:ILE:HG13 | 1:B:149:GLU:OE1  | 2.19                     | 0.42              |
| 1:A:216:VAL:HG12 | 1:A:221:ARG:CG   | 2.47                     | 0.42              |
| 1:A:408:CYS:SG   | 1:A:411:PRO:CB   | 3.07                     | 0.42              |
| 1:B:379:CYS:O    | 1:B:382:MET:N    | 2.46                     | 0.42              |
| 1:B:454:VAL:HG12 | 1:B:528:LEU:HD21 | 2.00                     | 0.42              |
| 1:A:207:ILE:HG12 | 1:A:234:ALA:HB1  | 2.00                     | 0.42              |
| 1:A:421:ASP:OD2  | 1:A:425:ASN:N    | 2.47                     | 0.42              |
| 1:B:209:ILE:HG13 | 1:B:236:ILE:HB   | 2.00                     | 0.42              |
| 1:B:230:VAL:N    | 1:B:231:PRO:CD   | 2.82                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:388:ASP:O    | 1:B:392:HIS:N    | 2.53                     | 0.42              |
| 1:A:294:MET:CE   | 1:A:308:VAL:HG11 | 2.44                     | 0.42              |
| 1:A:386:LEU:HD12 | 1:A:386:LEU:HA   | 1.82                     | 0.42              |
| 1:A:391:ARG:C    | 1:A:393:VAL:H    | 2.27                     | 0.42              |
| 1:A:515:HIS:HB3  | 1:A:517:GLU:CD   | 2.45                     | 0.42              |
| 1:B:94:ARG:NH1   | 1:B:97:SER:HB3   | 2.33                     | 0.42              |
| 1:B:389:TYR:HD2  | 1:B:481:ILE:HG22 | 1.85                     | 0.42              |
| 1:B:449:VAL:O    | 1:B:450:ASP:C    | 2.62                     | 0.42              |
| 1:B:466:ARG:HG3  | 4:B:815:IOD:I    | 2.90                     | 0.42              |
| 1:A:217:PRO:O    | 1:A:219:ASN:N    | 2.52                     | 0.42              |
| 1:A:408:CYS:C    | 1:A:410:TYR:H    | 2.25                     | 0.42              |
| 1:A:487:ARG:O    | 1:A:501:ILE:HA   | 2.20                     | 0.42              |
| 1:A:335:THR:CG2  | 1:A:336:ARG:HG3  | 2.26                     | 0.42              |
| 1:A:354:GLY:O    | 1:A:355:TYR:C    | 2.61                     | 0.42              |
| 1:B:295:VAL:HG22 | 1:B:328:ILE:CG2  | 2.50                     | 0.42              |
| 1:A:177:VAL:CG1  | 1:A:186:VAL:CG2  | 2.98                     | 0.42              |
| 1:A:199:LEU:HD23 | 1:A:199:LEU:HA   | 1.62                     | 0.42              |
| 1:A:217:PRO:C    | 1:A:219:ASN:N    | 2.78                     | 0.42              |
| 1:B:131:GLY:O    | 1:B:132:GLU:C    | 2.63                     | 0.42              |
| 1:B:179:TYR:CD1  | 1:B:214:ARG:NH1  | 2.87                     | 0.42              |
| 1:B:330:SER:HB3  | 1:B:361:MET:CG   | 2.47                     | 0.42              |
| 1:A:98:ASP:OD2   | 6:A:934:HOH:O    | 2.22                     | 0.42              |
| 1:A:179:TYR:CE2  | 1:A:181:ALA:HA   | 2.55                     | 0.42              |
| 1:A:192:GLN:HG2  | 1:A:228:CYS:HB3  | 2.01                     | 0.42              |
| 1:B:179:TYR:CG   | 1:B:214:ARG:CZ   | 3.03                     | 0.42              |
| 1:B:515:HIS:HA   | 1:B:516:PRO:HD2  | 1.90                     | 0.42              |
| 1:B:528:LEU:HA   | 1:B:528:LEU:HD23 | 1.69                     | 0.42              |
| 1:B:474:ASN:OD1  | 1:B:476:MET:HB2  | 2.20                     | 0.42              |
| 1:A:76:TYR:N     | 1:A:76:TYR:CD2   | 2.86                     | 0.42              |
| 1:A:420:ARG:O    | 1:A:476:MET:SD   | 2.78                     | 0.42              |
| 1:A:446:CYS:SG   | 1:A:447:GLN:N    | 2.92                     | 0.42              |
| 1:B:24:SER:O     | 1:B:28:ILE:HG13  | 2.19                     | 0.42              |
| 1:B:268:CYS:CB   | 1:B:269:PRO:CD   | 2.96                     | 0.42              |
| 1:B:378:ILE:HD13 | 1:B:516:PRO:CG   | 2.49                     | 0.42              |
| 1:A:37:THR:HB    | 1:A:134:HIS:CE1  | 2.54                     | 0.41              |
| 1:A:241:VAL:HG11 | 1:A:250:LEU:CD1  | 2.50                     | 0.41              |
| 1:A:371:ASN:CB   | 1:A:373:ILE:HD12 | 2.47                     | 0.41              |
| 1:B:91:THR:HG23  | 6:B:1759:HOH:O   | 2.20                     | 0.41              |
| 1:B:441:LEU:HD21 | 1:B:468:ARG:HD2  | 2.02                     | 0.41              |
| 1:B:458:TYR:CE1  | 1:B:528:LEU:HG   | 2.55                     | 0.41              |
| 1:A:366:ARG:NH1  | 6:A:890:HOH:O    | 2.52                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:411:PRO:HG3  | 1:A:420:ARG:NH2  | 2.35                     | 0.41              |
| 1:A:457:LEU:HD23 | 1:A:457:LEU:HA   | 1.78                     | 0.41              |
| 1:B:151:LEU:CB   | 1:B:152:PRO:CD   | 2.98                     | 0.41              |
| 1:B:301:LEU:CD1  | 1:B:302:PRO:HD2  | 2.46                     | 0.41              |
| 1:A:320:ARG:HD2  | 1:A:320:ARG:HH11 | 1.73                     | 0.41              |
| 1:B:172:MET:HG3  | 1:B:207:ILE:HB   | 2.02                     | 0.41              |
| 1:B:290:VAL:HG22 | 1:B:321:VAL:HG11 | 2.02                     | 0.41              |
| 1:B:348:LEU:HA   | 1:B:376:LEU:O    | 2.21                     | 0.41              |
| 1:B:539:PHE:CD2  | 1:B:539:PHE:C    | 2.98                     | 0.41              |
| 1:A:54:PRO:O     | 1:A:55:ILE:C     | 2.60                     | 0.41              |
| 1:A:262:LYS:HD2  | 4:A:805:IOD:I    | 2.90                     | 0.41              |
| 1:A:364:THR:O    | 1:A:365:ALA:C    | 2.63                     | 0.41              |
| 1:B:22:ALA:O     | 1:B:23:ALA:C     | 2.63                     | 0.41              |
| 1:B:488:VAL:CG1  | 1:B:491:ARG:CZ   | 2.99                     | 0.41              |
| 1:B:96:TYR:O     | 1:B:97:SER:C     | 2.63                     | 0.41              |
| 1:B:226:LEU:O    | 1:B:228:CYS:N    | 2.53                     | 0.41              |
| 1:B:297:LYS:HZ3  | 1:B:354:GLY:HA3  | 1.84                     | 0.41              |
| 1:B:360:GLY:O    | 1:B:363:THR:HB   | 2.21                     | 0.41              |
| 1:B:449:VAL:HG23 | 1:B:489:ALA:C    | 2.45                     | 0.41              |
| 1:A:241:VAL:CG1  | 1:A:250:LEU:HD11 | 2.51                     | 0.41              |
| 1:A:354:GLY:O    | 1:A:356:ARG:N    | 2.53                     | 0.41              |
| 1:A:454:VAL:HG11 | 1:A:500:ILE:HD13 | 2.03                     | 0.41              |
| 1:A:455:ARG:O    | 1:A:455:ARG:HD3  | 2.20                     | 0.41              |
| 1:B:368:ALA:HB1  | 1:B:375:TYR:HB2  | 2.01                     | 0.41              |
| 1:B:390:ALA:HB1  | 1:B:396:MET:CB   | 2.51                     | 0.41              |
| 1:A:542:ARG:HH11 | 1:A:542:ARG:HD3  | 1.74                     | 0.41              |
| 1:B:192:GLN:HG2  | 6:B:1722:HOH:O   | 2.20                     | 0.41              |
| 1:A:337:GLY:C    | 1:A:339:GLU:N    | 2.78                     | 0.41              |
| 1:A:341:LEU:HD11 | 1:A:364:THR:HG23 | 2.02                     | 0.41              |
| 1:A:401:SER:C    | 1:A:403:GLU:N    | 2.77                     | 0.41              |
| 1:B:415:LEU:CD2  | 1:B:471:TYR:CG   | 3.03                     | 0.41              |
| 1:B:421:ASP:HB2  | 1:B:425:ASN:HB2  | 2.03                     | 0.41              |
| 1:A:116:ILE:CD1  | 1:A:155:GLU:HG2  | 2.50                     | 0.41              |
| 1:A:183:SER:HB2  | 1:A:185:GLU:CD   | 2.46                     | 0.41              |
| 1:A:390:ALA:HB2  | 1:A:481:ILE:HD12 | 2.03                     | 0.41              |
| 1:A:415:LEU:HD23 | 1:A:415:LEU:N    | 2.35                     | 0.41              |
| 1:A:491:ARG:HA   | 1:A:497:LEU:O    | 2.21                     | 0.41              |
| 1:A:539:PHE:O    | 1:A:540:GLN:C    | 2.64                     | 0.41              |
| 1:B:396:MET:CE   | 1:B:480:GLN:HB3  | 2.47                     | 0.41              |
| 1:B:482:GLU:C    | 1:B:484:ALA:N    | 2.76                     | 0.41              |
| 1:A:80:ILE:HD12  | 1:A:82:THR:HB    | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:402:THR:HG23 | 1:A:402:THR:H    | 1.61                     | 0.41              |
| 1:B:172:MET:SD   | 1:B:209:ILE:HD11 | 2.61                     | 0.41              |
| 1:B:195:VAL:HG11 | 1:B:229:ASN:HA   | 2.02                     | 0.41              |
| 1:B:220:GLU:O    | 1:B:223:LYS:HB3  | 2.21                     | 0.41              |
| 1:B:358:VAL:O    | 1:B:362:ILE:HD12 | 2.21                     | 0.41              |
| 1:A:2:THR:HG21   | 1:A:168:HIS:CD2  | 2.56                     | 0.40              |
| 1:A:334:GLU:HG3  | 1:A:360:GLY:CA   | 2.51                     | 0.40              |
| 1:A:406:PRO:O    | 1:A:420:ARG:NH1  | 2.27                     | 0.40              |
| 1:B:116:ILE:HA   | 1:B:117:PRO:HA   | 1.83                     | 0.40              |
| 1:B:355:TYR:OH   | 1:B:359:GLU:OE2  | 2.39                     | 0.40              |
| 1:B:402:THR:CG2  | 1:B:414:ALA:CB   | 2.99                     | 0.40              |
| 1:B:515:HIS:HB3  | 1:B:517:GLU:OE1  | 2.22                     | 0.40              |
| 1:A:298:TYR:C    | 1:A:300:GLU:N    | 2.78                     | 0.40              |
| 1:B:239:LYS:HB3  | 4:B:802:IOD:I    | 2.92                     | 0.40              |
| 1:B:383:GLN:O    | 1:B:384:VAL:C    | 2.60                     | 0.40              |
| 1:A:11:GLY:C     | 1:A:12:VAL:HG23  | 2.46                     | 0.40              |
| 1:A:86:ARG:CA    | 1:A:86:ARG:NH1   | 2.75                     | 0.40              |
| 1:A:224:ILE:CG2  | 1:A:229:ASN:HD22 | 2.29                     | 0.40              |
| 1:A:460:ALA:HB1  | 1:A:461:PRO:CD   | 2.48                     | 0.40              |
| 1:B:109:LEU:C    | 1:B:111:ALA:H    | 2.30                     | 0.40              |
| 1:B:172:MET:SD   | 1:B:209:ILE:CD1  | 3.10                     | 0.40              |
| 1:B:334:GLU:HG3  | 1:B:334:GLU:H    | 1.50                     | 0.40              |
| 1:B:415:LEU:HD23 | 1:B:471:TYR:CG   | 2.56                     | 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     | 531/545 (97%) | 469 (88%) | 45 (8%) | 17 (3%)  | 3           | 2 |
| 1   | B     | 532/545 (98%) | 467 (88%) | 41 (8%) | 24 (4%)  | 2           | 1 |

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| Mol | Chain | Analysed        | Favoured  | Allowed | Outliers | Percentiles       |
|-----|-------|-----------------|-----------|---------|----------|-------------------|
| All | All   | 1063/1090 (98%) | 936 (88%) | 86 (8%) | 41 (4%)  | <b>2</b> <b>1</b> |

All (41) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 182 | ALA  |
| 1   | A     | 230 | VAL  |
| 1   | A     | 232 | GLU  |
| 1   | A     | 338 | VAL  |
| 1   | A     | 356 | ARG  |
| 1   | A     | 391 | ARG  |
| 1   | A     | 392 | HIS  |
| 1   | A     | 411 | PRO  |
| 1   | B     | 105 | ARG  |
| 1   | B     | 107 | ASP  |
| 1   | B     | 151 | LEU  |
| 1   | B     | 355 | TYR  |
| 1   | B     | 356 | ARG  |
| 1   | B     | 396 | MET  |
| 1   | B     | 494 | ASP  |
| 1   | A     | 299 | ILE  |
| 1   | A     | 300 | GLU  |
| 1   | A     | 387 | ILE  |
| 1   | A     | 543 | GLN  |
| 1   | B     | 103 | GLU  |
| 1   | B     | 104 | ARG  |
| 1   | B     | 227 | PHE  |
| 1   | B     | 229 | ASN  |
| 1   | B     | 331 | GLN  |
| 1   | B     | 387 | ILE  |
| 1   | B     | 388 | ASP  |
| 1   | B     | 391 | ARG  |
| 1   | B     | 397 | GLU  |
| 1   | B     | 399 | ALA  |
| 1   | B     | 493 | GLY  |
| 1   | A     | 132 | GLU  |
| 1   | A     | 218 | ALA  |
| 1   | A     | 355 | TYR  |
| 1   | B     | 132 | GLU  |
| 1   | B     | 332 | ASP  |
| 1   | B     | 338 | VAL  |
| 1   | B     | 335 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 496 | GLN  |
| 1   | A     | 50  | GLY  |
| 1   | A     | 303 | ASP  |
| 1   | B     | 230 | 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     | 453/461 (98%) | 398 (88%) | 55 (12%)  | 5           | 5 |
| 1   | B     | 454/461 (98%) | 381 (84%) | 73 (16%)  | 2           | 2 |
| All | All   | 907/922 (98%) | 779 (86%) | 128 (14%) | 3           | 3 |

All (128) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 2   | THR  |
| 1   | A     | 18  | LYS  |
| 1   | A     | 46  | ASN  |
| 1   | A     | 55  | ILE  |
| 1   | A     | 71  | LEU  |
| 1   | A     | 86  | ARG  |
| 1   | A     | 101 | ARG  |
| 1   | A     | 102 | LYS  |
| 1   | A     | 107 | ASP  |
| 1   | A     | 132 | GLU  |
| 1   | A     | 180 | MET  |
| 1   | A     | 186 | VAL  |
| 1   | A     | 196 | LYS  |
| 1   | A     | 220 | GLU  |
| 1   | A     | 226 | LEU  |
| 1   | A     | 233 | LYS  |
| 1   | A     | 257 | ASP  |
| 1   | A     | 263 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 272 | ASN  |
| 1   | A     | 274 | SER  |
| 1   | A     | 278 | GLN  |
| 1   | A     | 288 | SER  |
| 1   | A     | 289 | GLU  |
| 1   | A     | 292 | ILE  |
| 1   | A     | 297 | LYS  |
| 1   | A     | 300 | GLU  |
| 1   | A     | 320 | ARG  |
| 1   | A     | 336 | ARG  |
| 1   | A     | 340 | ILE  |
| 1   | A     | 372 | ASN  |
| 1   | A     | 384 | VAL  |
| 1   | A     | 388 | ASP  |
| 1   | A     | 393 | VAL  |
| 1   | A     | 396 | MET  |
| 1   | A     | 398 | ASN  |
| 1   | A     | 412 | VAL  |
| 1   | A     | 415 | LEU  |
| 1   | A     | 416 | ILE  |
| 1   | A     | 418 | GLU  |
| 1   | A     | 426 | VAL  |
| 1   | A     | 427 | GLU  |
| 1   | A     | 438 | THR  |
| 1   | A     | 446 | CYS  |
| 1   | A     | 447 | GLN  |
| 1   | A     | 451 | ASP  |
| 1   | A     | 454 | VAL  |
| 1   | A     | 470 | ARG  |
| 1   | A     | 479 | LYS  |
| 1   | A     | 480 | GLN  |
| 1   | A     | 481 | ILE  |
| 1   | A     | 486 | LEU  |
| 1   | A     | 488 | VAL  |
| 1   | A     | 521 | THR  |
| 1   | A     | 534 | LYS  |
| 1   | B     | 1   | MET  |
| 1   | B     | 18  | LYS  |
| 1   | B     | 20  | ILE  |
| 1   | B     | 46  | ASN  |
| 1   | B     | 48  | ASP  |
| 1   | B     | 52  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 55  | ILE  |
| 1   | B     | 59  | GLU  |
| 1   | B     | 69  | THR  |
| 1   | B     | 71  | LEU  |
| 1   | B     | 83  | LYS  |
| 1   | B     | 86  | ARG  |
| 1   | B     | 94  | ARG  |
| 1   | B     | 104 | ARG  |
| 1   | B     | 105 | ARG  |
| 1   | B     | 107 | ASP  |
| 1   | B     | 112 | THR  |
| 1   | B     | 144 | THR  |
| 1   | B     | 166 | ARG  |
| 1   | B     | 180 | MET  |
| 1   | B     | 183 | SER  |
| 1   | B     | 186 | VAL  |
| 1   | B     | 200 | SER  |
| 1   | B     | 207 | ILE  |
| 1   | B     | 209 | ILE  |
| 1   | B     | 213 | ASP  |
| 1   | B     | 214 | ARG  |
| 1   | B     | 220 | GLU  |
| 1   | B     | 226 | LEU  |
| 1   | B     | 227 | PHE  |
| 1   | B     | 228 | CYS  |
| 1   | B     | 233 | LYS  |
| 1   | B     | 243 | SER  |
| 1   | B     | 265 | SER  |
| 1   | B     | 277 | GLU  |
| 1   | B     | 288 | SER  |
| 1   | B     | 301 | LEU  |
| 1   | B     | 306 | LYS  |
| 1   | B     | 309 | ILE  |
| 1   | B     | 313 | LYS  |
| 1   | B     | 327 | LEU  |
| 1   | B     | 328 | ILE  |
| 1   | B     | 330 | SER  |
| 1   | B     | 332 | ASP  |
| 1   | B     | 333 | VAL  |
| 1   | B     | 334 | GLU  |
| 1   | B     | 338 | VAL  |
| 1   | B     | 340 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 342 | LYS  |
| 1   | B     | 347 | ILE  |
| 1   | B     | 356 | ARG  |
| 1   | B     | 362 | ILE  |
| 1   | B     | 366 | ARG  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 378 | ILE  |
| 1   | B     | 379 | CYS  |
| 1   | B     | 384 | VAL  |
| 1   | B     | 388 | ASP  |
| 1   | B     | 392 | HIS  |
| 1   | B     | 397 | GLU  |
| 1   | B     | 403 | GLU  |
| 1   | B     | 416 | ILE  |
| 1   | B     | 417 | THR  |
| 1   | B     | 426 | VAL  |
| 1   | B     | 428 | VAL  |
| 1   | B     | 438 | THR  |
| 1   | B     | 446 | CYS  |
| 1   | B     | 447 | GLN  |
| 1   | B     | 451 | ASP  |
| 1   | B     | 468 | ARG  |
| 1   | B     | 481 | ILE  |
| 1   | B     | 487 | ARG  |
| 1   | B     | 496 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 46  | ASN  |
| 1   | A     | 134 | HIS  |
| 1   | A     | 229 | ASN  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 371 | ASN  |
| 1   | A     | 372 | ASN  |
| 1   | A     | 383 | GLN  |
| 1   | A     | 425 | ASN  |
| 1   | A     | 469 | HIS  |
| 1   | A     | 513 | GLN  |
| 1   | B     | 46  | ASN  |
| 1   | B     | 75  | HIS  |
| 1   | B     | 118 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 134 | HIS  |
| 1   | B     | 193 | HIS  |
| 1   | B     | 204 | GLN  |
| 1   | B     | 229 | ASN  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 324 | ASN  |
| 1   | B     | 371 | ASN  |
| 1   | B     | 392 | HIS  |
| 1   | B     | 447 | GLN  |
| 1   | B     | 469 | HIS  |
| 1   | B     | 480 | GLN  |
| 1   | B     | 496 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 26 ligands modelled in this entry, 20 are monoatomic - leaving 6 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | MPD  | B     | 1601 | -    | 7,7,7        | 0.59 | 0           | 9,10,10     | 0.42 | 0           |
| 5   | MPD  | A     | 601  | -    | 7,7,7        | 0.68 | 0           | 9,10,10     | 0.68 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | SO4  | A     | 602  | 3    | 4,4,4        | 0.49 | 0        | 6,6,6       | 0.10 | 0        |
| 2   | SO4  | B     | 1603 | 3    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.06 | 0        |
| 2   | SO4  | B     | 1602 | 3    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.19 | 0        |
| 2   | SO4  | A     | 603  | 3    | 4,4,4        | 0.42 | 0        | 6,6,6       | 0.13 | 0        |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|-------|
| 5   | MPD  | B     | 1601 | -    | -       | 3/5/5/5  | -     |
| 5   | MPD  | A     | 601  | -    | -       | 0/5/5/5  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 5   | B     | 1601 | MPD  | O2-C2-C3-C4 |
| 5   | B     | 1601 | MPD  | C1-C2-C3-C4 |
| 5   | B     | 1601 | MPD  | CM-C2-C3-C4 |

There are no ring outliers.

2 monomers are involved in 4 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | B     | 1601 | MPD  | 2       | 0            |
| 5   | A     | 601  | MPD  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:



| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | A     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 57:HIS    | C      | 58:GLY    | N      | 1.79         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                      | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|------------------------------|-----------------------|--------|
| 1   | A     | 534/545 (97%)   | 0.50   | 50 (9%) <b>14</b> <b>15</b>  | 31, 55, 93, 100       | 2 (0%) |
| 1   | B     | 536/545 (98%)   | 0.55   | 53 (9%) <b>13</b> <b>14</b>  | 32, 54, 93, 100       | 1 (0%) |
| All | All   | 1070/1090 (98%) | 0.53   | 103 (9%) <b>13</b> <b>15</b> | 31, 54, 93, 100       | 3 (0%) |

All (103) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | A     | 227   | PHE  | 10.3 |
| 1   | B     | 494   | ASP  | 6.4  |
| 1   | B     | 493   | GLY  | 6.0  |
| 1   | A     | 228   | CYS  | 5.9  |
| 1   | A     | 493   | GLY  | 5.9  |
| 1   | B     | 184   | GLY  | 5.3  |
| 1   | B     | 544   | ALA  | 5.0  |
| 1   | A     | 504   | PRO  | 4.8  |
| 1   | B     | 438   | THR  | 4.5  |
| 1   | B     | 181   | ALA  | 4.2  |
| 1   | A     | 438   | THR  | 4.2  |
| 1   | B     | 335   | THR  | 4.2  |
| 1   | A     | 335   | THR  | 4.1  |
| 1   | B     | 1     | MET  | 4.1  |
| 1   | B     | 394   | ALA  | 4.1  |
| 1   | B     | 182   | ALA  | 4.0  |
| 1   | B     | 412   | VAL  | 4.0  |
| 1   | A     | 57[A] | HIS  | 4.0  |
| 1   | B     | 230   | VAL  | 3.9  |
| 1   | A     | 408   | CYS  | 3.9  |
| 1   | A     | 352   | GLY  | 3.9  |
| 1   | B     | 395   | ASN  | 3.9  |
| 1   | A     | 230   | VAL  | 3.8  |
| 1   | A     | 544   | ALA  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 228 | CYS  | 3.6  |
| 1   | B     | 408 | CYS  | 3.6  |
| 1   | B     | 299 | ILE  | 3.6  |
| 1   | B     | 337 | GLY  | 3.5  |
| 1   | B     | 101 | ARG  | 3.5  |
| 1   | B     | 300 | GLU  | 3.5  |
| 1   | B     | 424 | GLY  | 3.4  |
| 1   | B     | 352 | GLY  | 3.4  |
| 1   | B     | 179 | TYR  | 3.3  |
| 1   | A     | 330 | SER  | 3.3  |
| 1   | B     | 227 | PHE  | 3.3  |
| 1   | B     | 57  | HIS  | 3.2  |
| 1   | A     | 412 | VAL  | 3.2  |
| 1   | B     | 411 | PRO  | 3.1  |
| 1   | B     | 492 | SER  | 3.0  |
| 1   | B     | 183 | SER  | 3.0  |
| 1   | B     | 298 | TYR  | 2.9  |
| 1   | A     | 353 | PHE  | 2.9  |
| 1   | B     | 180 | MET  | 2.9  |
| 1   | B     | 355 | TYR  | 2.9  |
| 1   | B     | 428 | VAL  | 2.9  |
| 1   | A     | 1   | MET  | 2.9  |
| 1   | A     | 225 | ALA  | 2.9  |
| 1   | B     | 426 | VAL  | 2.8  |
| 1   | A     | 300 | GLU  | 2.8  |
| 1   | A     | 301 | LEU  | 2.8  |
| 1   | A     | 393 | VAL  | 2.8  |
| 1   | B     | 353 | PHE  | 2.8  |
| 1   | A     | 232 | GLU  | 2.8  |
| 1   | B     | 425 | ASN  | 2.7  |
| 1   | A     | 339 | GLU  | 2.7  |
| 1   | B     | 233 | LYS  | 2.7  |
| 1   | A     | 218 | ALA  | 2.7  |
| 1   | A     | 357 | GLY  | 2.7  |
| 1   | A     | 409 | LYS  | 2.7  |
| 1   | A     | 179 | TYR  | 2.6  |
| 1   | B     | 504 | PRO  | 2.6  |
| 1   | B     | 106 | GLY  | 2.6  |
| 1   | A     | 181 | ALA  | 2.6  |
| 1   | A     | 182 | ALA  | 2.5  |
| 1   | A     | 425 | ASN  | 2.5  |
| 1   | B     | 342 | LYS  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 419 | TRP  | 2.5  |
| 1   | A     | 298 | TYR  | 2.5  |
| 1   | A     | 362 | ILE  | 2.4  |
| 1   | B     | 218 | ALA  | 2.4  |
| 1   | B     | 301 | LEU  | 2.4  |
| 1   | A     | 229 | ASN  | 2.4  |
| 1   | A     | 356 | ARG  | 2.4  |
| 1   | A     | 302 | PRO  | 2.4  |
| 1   | B     | 545 | LYS  | 2.4  |
| 1   | B     | 338 | VAL  | 2.4  |
| 1   | B     | 56  | GLN  | 2.4  |
| 1   | A     | 212 | SER  | 2.4  |
| 1   | A     | 492 | SER  | 2.4  |
| 1   | A     | 56  | GLN  | 2.4  |
| 1   | B     | 329 | ASP  | 2.3  |
| 1   | B     | 339 | GLU  | 2.3  |
| 1   | A     | 104 | ARG  | 2.3  |
| 1   | A     | 343 | GLY  | 2.3  |
| 1   | A     | 496 | GLN  | 2.3  |
| 1   | A     | 390 | ALA  | 2.2  |
| 1   | B     | 232 | GLU  | 2.2  |
| 1   | A     | 394 | ALA  | 2.2  |
| 1   | B     | 231 | PRO  | 2.2  |
| 1   | A     | 484 | ALA  | 2.2  |
| 1   | B     | 356 | ARG  | 2.1  |
| 1   | A     | 494 | ASP  | 2.1  |
| 1   | A     | 505 | ASN  | 2.1  |
| 1   | B     | 421 | ASP  | 2.1  |
| 1   | B     | 417 | THR  | 2.1  |
| 1   | B     | 109 | LEU  | 2.1  |
| 1   | A     | 186 | VAL  | 2.1  |
| 1   | B     | 357 | GLY  | 2.1  |
| 1   | A     | 452 | SER  | 2.0  |
| 1   | A     | 180 | MET  | 2.0  |
| 1   | B     | 419 | TRP  | 2.0  |
| 1   | A     | 226 | LEU  | 2.0  |
| 1   | A     | 423 | ASN  | 2.0  |

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

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

### 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 6.4 Ligands ⓘ

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. 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  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | IOD  | A     | 814  | 1/1   | 0.83 | 0.18 | 89,89,89,89                 | 1     |
| 5   | MPD  | B     | 1601 | 8/8   | 0.84 | 0.16 | 57,79,87,88                 | 0     |
| 5   | MPD  | A     | 601  | 8/8   | 0.86 | 0.16 | 50,80,92,100                | 0     |
| 4   | IOD  | A     | 816  | 1/1   | 0.90 | 0.12 | 90,90,90,90                 | 1     |
| 3   | MG   | B     | 704  | 1/1   | 0.91 | 0.40 | 91,91,91,91                 | 0     |
| 3   | MG   | A     | 703  | 1/1   | 0.92 | 0.21 | 92,92,92,92                 | 0     |
| 2   | SO4  | B     | 1602 | 5/5   | 0.92 | 0.14 | 54,60,70,89                 | 0     |
| 2   | SO4  | A     | 603  | 5/5   | 0.93 | 0.10 | 68,83,90,91                 | 0     |
| 4   | IOD  | B     | 810  | 1/1   | 0.95 | 0.09 | 76,76,76,76                 | 1     |
| 4   | IOD  | A     | 807  | 1/1   | 0.95 | 0.08 | 63,63,63,63                 | 1     |
| 4   | IOD  | B     | 809  | 1/1   | 0.95 | 0.10 | 77,77,77,77                 | 1     |
| 4   | IOD  | A     | 806  | 1/1   | 0.96 | 0.06 | 72,72,72,72                 | 1     |
| 2   | SO4  | A     | 602  | 5/5   | 0.96 | 0.13 | 65,72,82,88                 | 0     |
| 3   | MG   | B     | 701  | 1/1   | 0.96 | 0.15 | 64,64,64,64                 | 0     |
| 2   | SO4  | B     | 1603 | 5/5   | 0.96 | 0.11 | 57,65,92,93                 | 0     |
| 4   | IOD  | B     | 815  | 1/1   | 0.97 | 0.09 | 76,76,76,76                 | 1     |
| 4   | IOD  | A     | 812  | 1/1   | 0.97 | 0.05 | 72,72,72,72                 | 1     |
| 4   | IOD  | A     | 813  | 1/1   | 0.97 | 0.06 | 69,69,69,69                 | 1     |
| 4   | IOD  | A     | 801  | 1/1   | 0.98 | 0.05 | 72,72,72,72                 | 0     |
| 4   | IOD  | B     | 811  | 1/1   | 0.98 | 0.05 | 72,72,72,72                 | 1     |
| 4   | IOD  | B     | 802  | 1/1   | 0.98 | 0.05 | 69,69,69,69                 | 0     |
| 4   | IOD  | B     | 808  | 1/1   | 0.98 | 0.05 | 73,73,73,73                 | 1     |
| 3   | MG   | A     | 702  | 1/1   | 0.98 | 0.17 | 47,47,47,47                 | 0     |
| 4   | IOD  | A     | 803  | 1/1   | 0.99 | 0.03 | 72,72,72,72                 | 0     |
| 4   | IOD  | B     | 804  | 1/1   | 0.99 | 0.04 | 73,73,73,73                 | 0     |
| 4   | IOD  | A     | 805  | 1/1   | 0.99 | 0.03 | 64,64,64,64                 | 1     |

### 6.5 Other polymers ⓘ

There are no such residues in this entry.