



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:24 pm BST

PDB ID : 1J5S  
Title : Crystal structure of uronate isomerase (TM0064) from *Thermotoga maritima* at 2.85 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2002-07-02  
Resolution : 2.85 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.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

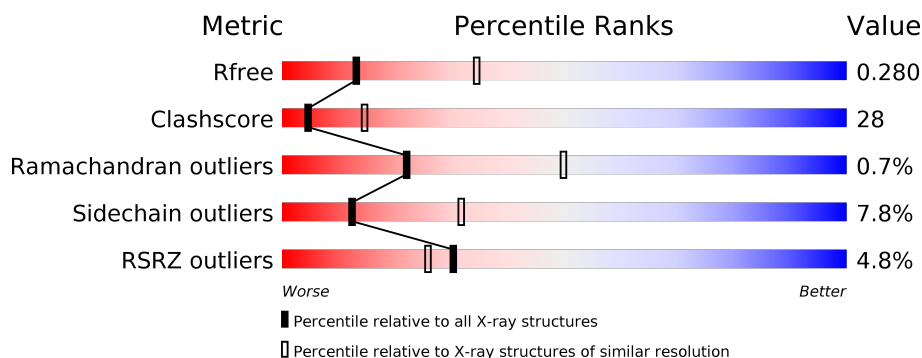
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3168 (2.90-2.82)                                      |
| Clashscore            | 141614                      | 3438 (2.90-2.82)                                      |
| Ramachandran outliers | 138981                      | 3348 (2.90-2.82)                                      |
| Sidechain outliers    | 138945                      | 3351 (2.90-2.82)                                      |
| RSRZ outliers         | 127900                      | 3103 (2.90-2.82)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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     | 463    | <div> <div>4%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>5%</div> </div> </div> |
| 1   | B     | 463    | <div> <div>5%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>5%</div> </div> </div> |
| 1   | C     | 463    | <div> <div>5%</div> <div> <div></div> <div>55%</div> <div>37%</div> <div>5%</div> </div> </div> |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11175 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 URONATE ISOMERASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 451      | Total | C    | N   | O   | S  | 81      | 0       | 0     |
|     |       |          | 3696  | 2367 | 632 | 680 | 17 |         |         |       |
| 1   | B     | 450      | Total | C    | N   | O   | S  | 86      | 0       | 0     |
|     |       |          | 3686  | 2361 | 629 | 679 | 17 |         |         |       |
| 1   | C     | 450      | Total | C    | N   | O   | S  | 83      | 0       | 0     |
|     |       |          | 3686  | 2361 | 629 | 679 | 17 |         |         |       |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment         | Reference  |
|-------|---------|----------|--------|-----------------|------------|
| A     | -11     | MET      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| A     | -10     | GLY      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| A     | -9      | SER      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| A     | -8      | ASP      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| A     | -7      | LYS      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| A     | -6      | ILE      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| A     | -5      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| A     | -4      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| A     | -3      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| A     | -2      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| A     | -1      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| A     | 0       | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| B     | -11     | MET      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| B     | -10     | GLY      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| B     | -9      | SER      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| B     | -8      | ASP      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| B     | -7      | LYS      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| B     | -6      | ILE      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| B     | -5      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| B     | -4      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| B     | -3      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| B     | -2      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| B     | -1      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |

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| Chain | Residue | Modelled | Actual | Comment         | Reference  |
|-------|---------|----------|--------|-----------------|------------|
| B     | 0       | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| C     | -11     | MET      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| C     | -10     | GLY      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| C     | -9      | SER      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| C     | -8      | ASP      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| C     | -7      | LYS      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| C     | -6      | ILE      | -      | LEADER SEQUENCE | UNP Q9WXR9 |
| C     | -5      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| C     | -4      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| C     | -3      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| C     | -2      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| C     | -1      | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |
| C     | 0       | HIS      | -      | EXPRESSION TAG  | UNP Q9WXR9 |

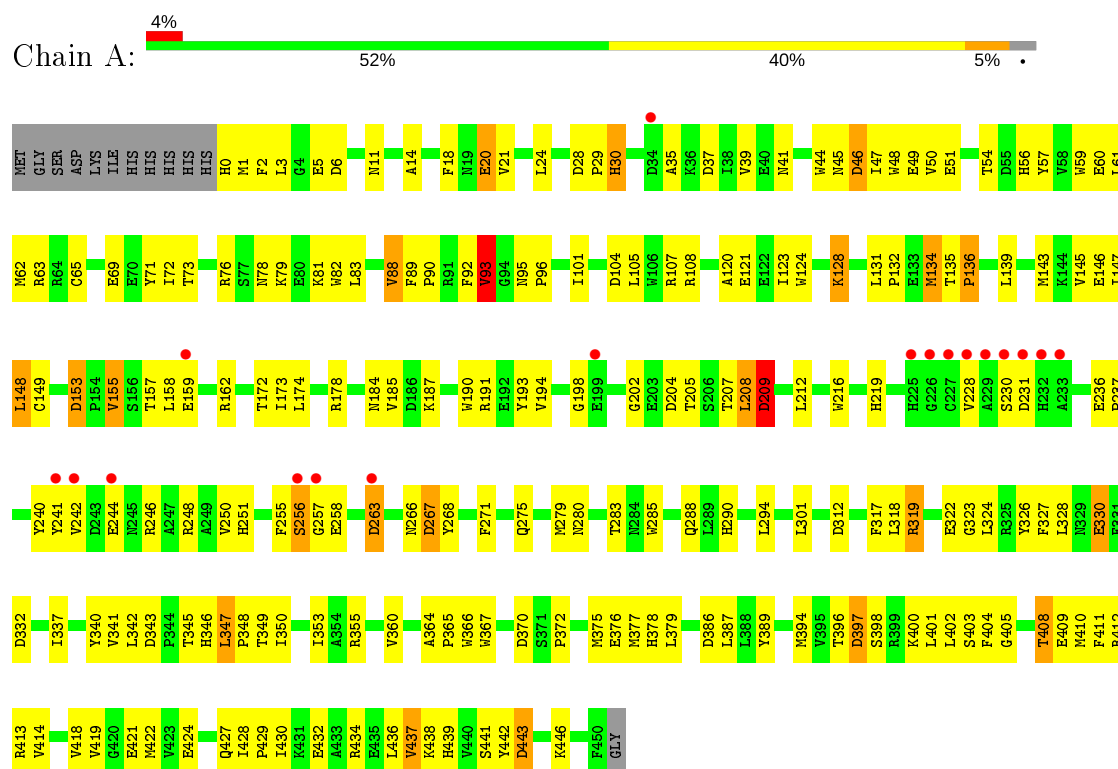
- Molecule 2 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2   | A     | 40       | Total O<br>40 40 | 0       | 0       |
| 2   | B     | 33       | Total O<br>33 33 | 0       | 0       |
| 2   | C     | 34       | Total O<br>34 34 | 0       | 0       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: URONATE ISOMERASE

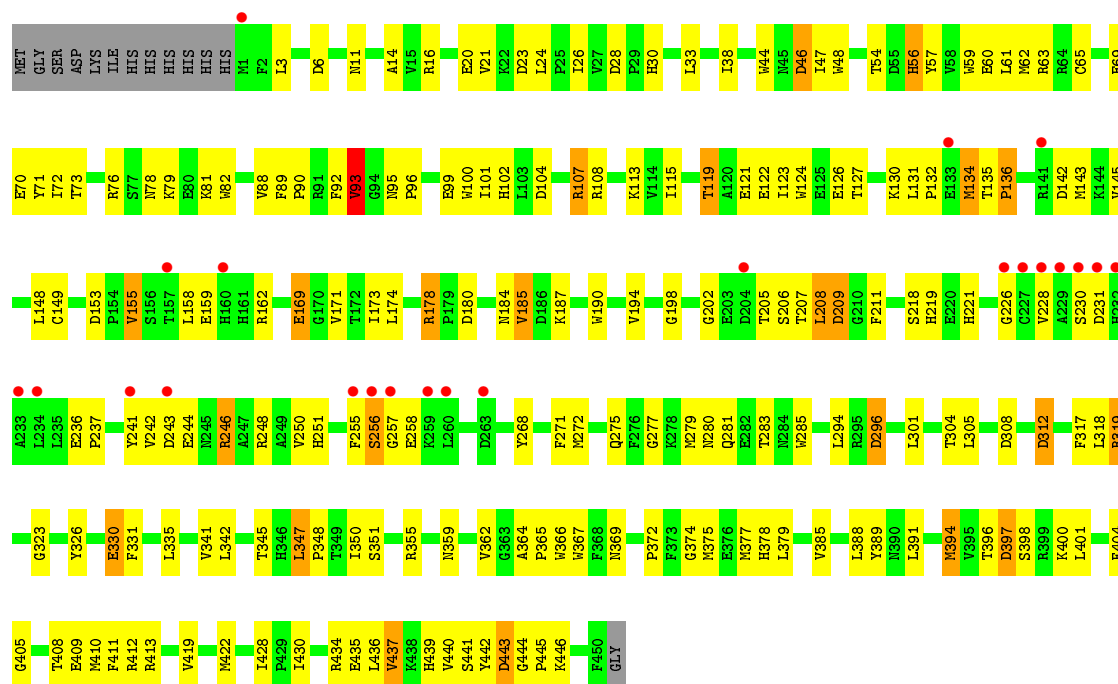


#### • Molecule 1: URONATE ISOMERASE





Chain C:  5% 55% 37% 5%



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 77.41 Å 79.96 Å 89.43 Å<br>115.73° 97.57° 110.44°           | Depositor        |
| Resolution (Å)  | 24.99 – 2.85<br>24.99 – 2.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.6 (24.99-2.85)<br>96.7 (24.99-2.75)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.07  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.91 (at 2.76 Å)  | Xtriage          |
| Refinement program  | REFMAC 5.0  | Depositor        |
| R, $R_{free}$   | 0.234 , 0.274<br>0.248 , 0.280                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4272 reflections (5.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 27.1  | Xtriage          |
| Anisotropy  | 0.297   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 63.0   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | 0.021 for k,h,-h-k-l  | Xtriage          |
| $F_o, F_c$ correlation  | 0.86  | EDS              |
| Total number of atoms   | 11175   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 34.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.52         | 0/3793      | 0.88        | 12/5136 (0.2%)  |
| 1   | B     | 0.54         | 0/3782      | 0.90        | 12/5121 (0.2%)  |
| 1   | C     | 0.54         | 0/3782      | 0.89        | 12/5121 (0.2%)  |
| All | All   | 0.54         | 0/11357     | 0.89        | 36/15378 (0.2%) |

There are no bond length outliers.

All (36) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 243 | ASP  | N-CA-CB   | -9.25 | 93.94       | 110.60   |
| 1   | B     | 243 | ASP  | CB-CG-OD2 | 8.96  | 126.37      | 118.30   |
| 1   | A     | 104 | ASP  | CB-CG-OD2 | 7.03  | 124.62      | 118.30   |
| 1   | A     | 132 | PRO  | CA-N-CD   | -6.98 | 101.72      | 111.50   |
| 1   | B     | 23  | ASP  | CB-CG-OD2 | 6.65  | 124.29      | 118.30   |
| 1   | B     | 34  | ASP  | CB-CG-OD2 | 6.15  | 123.84      | 118.30   |
| 1   | C     | 443 | ASP  | CB-CG-OD2 | 6.10  | 123.79      | 118.30   |
| 1   | C     | 46  | ASP  | CB-CG-OD2 | 6.07  | 123.77      | 118.30   |
| 1   | C     | 6   | ASP  | CB-CG-OD2 | 6.03  | 123.72      | 118.30   |
| 1   | C     | 104 | ASP  | CB-CG-OD2 | 5.98  | 123.68      | 118.30   |
| 1   | A     | 332 | ASP  | CB-CG-OD2 | 5.81  | 123.53      | 118.30   |
| 1   | C     | 23  | ASP  | CB-CG-OD2 | 5.81  | 123.53      | 118.30   |
| 1   | A     | 6   | ASP  | CB-CG-OD2 | 5.75  | 123.47      | 118.30   |
| 1   | B     | 443 | ASP  | CB-CG-OD2 | 5.70  | 123.43      | 118.30   |
| 1   | C     | 142 | ASP  | CB-CG-OD2 | 5.67  | 123.40      | 118.30   |
| 1   | C     | 308 | ASP  | CB-CG-OD2 | 5.65  | 123.39      | 118.30   |
| 1   | B     | 267 | ASP  | CB-CG-OD2 | 5.61  | 123.35      | 118.30   |
| 1   | B     | 186 | ASP  | CB-CG-OD2 | 5.33  | 123.09      | 118.30   |
| 1   | C     | 209 | ASP  | CB-CG-OD2 | 5.31  | 123.08      | 118.30   |
| 1   | A     | 267 | ASP  | CB-CG-OD2 | 5.30  | 123.07      | 118.30   |
| 1   | B     | 6   | ASP  | CB-CG-OD2 | 5.28  | 123.06      | 118.30   |
| 1   | C     | 312 | ASP  | CB-CG-OD2 | 5.27  | 123.04      | 118.30   |
| 1   | B     | 231 | ASP  | CB-CG-OD2 | 5.22  | 123.00      | 118.30   |
| 1   | A     | 263 | ASP  | CB-CG-OD2 | 5.18  | 122.96      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 308 | ASP  | CB-CG-OD2 | 5.16  | 122.94      | 118.30   |
| 1   | A     | 312 | ASP  | CB-CG-OD2 | 5.14  | 122.92      | 118.30   |
| 1   | C     | 243 | ASP  | CB-CG-OD2 | 5.13  | 122.92      | 118.30   |
| 1   | A     | 153 | ASP  | CB-CG-OD2 | 5.13  | 122.91      | 118.30   |
| 1   | C     | 169 | GLU  | CA-C-N    | 5.11  | 126.42      | 116.20   |
| 1   | A     | 443 | ASP  | CB-CG-OD2 | 5.10  | 122.89      | 118.30   |
| 1   | B     | 386 | ASP  | CB-CG-OD2 | 5.10  | 122.89      | 118.30   |
| 1   | A     | 148 | LEU  | CB-CA-C   | -5.09 | 100.53      | 110.20   |
| 1   | A     | 209 | ASP  | CB-CG-OD2 | 5.09  | 122.88      | 118.30   |
| 1   | B     | 37  | ASP  | CB-CG-OD2 | 5.06  | 122.86      | 118.30   |
| 1   | A     | 37  | ASP  | CB-CG-OD2 | 5.06  | 122.85      | 118.30   |
| 1   | C     | 180 | ASP  | CB-CG-OD2 | 5.04  | 122.84      | 118.30   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3696  | 0        | 3621     | 217     | 7            |
| 1   | B     | 3686  | 0        | 3614     | 202     | 11           |
| 1   | C     | 3686  | 0        | 3614     | 223     | 4            |
| 2   | A     | 40    | 0        | 0        | 3       | 0            |
| 2   | B     | 33    | 0        | 0        | 4       | 0            |
| 2   | C     | 34    | 0        | 0        | 5       | 0            |
| All | All   | 11175 | 0        | 10849    | 603     | 11           |

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 28.

All (603) 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:194:VAL:HG12 | 1:A:205:THR:CG2 | 1.53                     | 1.34              |
| 1:A:251:HIS:ND1  | 2:A:454:HOH:O   | 1.65                     | 1.21              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:62:MET:CE    | 1:B:72:ILE:HG12  | 1.73                     | 1.19              |
| 1:A:194:VAL:CG1  | 1:A:205:THR:CG2  | 2.22                     | 1.17              |
| 1:C:400:LYS:HD3  | 2:C:458:HOH:O    | 1.40                     | 1.17              |
| 1:C:143:MET:HE1  | 1:C:404:PHE:HB2  | 1.22                     | 1.16              |
| 1:A:194:VAL:HG12 | 1:A:205:THR:HG21 | 1.12                     | 1.10              |
| 1:A:194:VAL:CG1  | 1:A:205:THR:HG21 | 1.79                     | 1.10              |
| 1:A:41:ASN:CG    | 1:A:135:THR:HG21 | 1.71                     | 1.09              |
| 1:C:400:LYS:CD   | 2:C:458:HOH:O    | 1.96                     | 1.04              |
| 1:B:62:MET:HE3   | 1:B:72:ILE:HG12  | 1.33                     | 1.03              |
| 1:C:47:ILE:HD11  | 1:C:82:TRP:CE2   | 1.92                     | 1.03              |
| 1:A:424:GLU:HA   | 1:B:1:MET:SD     | 1.97                     | 1.03              |
| 1:C:21:VAL:HG13  | 1:C:24:LEU:HD12  | 1.37                     | 1.02              |
| 1:C:400:LYS:CE   | 2:C:458:HOH:O    | 2.03                     | 1.02              |
| 1:A:194:VAL:HG12 | 1:A:205:THR:HG22 | 1.38                     | 1.00              |
| 1:C:47:ILE:HD11  | 1:C:82:TRP:CD2   | 1.98                     | 0.98              |
| 1:C:219:HIS:CE1  | 1:C:285:TRP:CZ3  | 2.52                     | 0.97              |
| 1:A:251:HIS:CE1  | 2:A:454:HOH:O    | 2.07                     | 0.97              |
| 1:C:409:GLU:OE2  | 1:C:413:ARG:NH1  | 1.97                     | 0.97              |
| 1:A:46:ASP:OD2   | 1:A:78:ASN:ND2   | 1.99                     | 0.96              |
| 1:A:41:ASN:OD1   | 1:A:135:THR:CG2  | 2.13                     | 0.96              |
| 1:C:194:VAL:CG1  | 1:C:205:THR:HG22 | 1.95                     | 0.94              |
| 1:A:424:GLU:O    | 1:B:1:MET:SD     | 2.25                     | 0.94              |
| 1:C:246:ARG:HH11 | 1:C:246:ARG:HG3  | 1.33                     | 0.93              |
| 1:A:41:ASN:OD1   | 1:A:135:THR:HG21 | 1.67                     | 0.92              |
| 1:C:209:ASP:OD1  | 1:C:248:ARG:NH2  | 2.04                     | 0.90              |
| 1:C:143:MET:CE   | 1:C:404:PHE:HB2  | 2.02                     | 0.89              |
| 1:A:105:LEU:CD1  | 1:A:123:ILE:HD11 | 2.01                     | 0.89              |
| 1:C:256:SER:O    | 1:C:258:GLU:N    | 2.07                     | 0.88              |
| 1:A:256:SER:O    | 1:A:258:GLU:N    | 2.07                     | 0.88              |
| 1:C:119:THR:CG2  | 1:C:123:ILE:HD11 | 2.03                     | 0.88              |
| 1:A:194:VAL:CG1  | 1:A:205:THR:HG22 | 1.99                     | 0.87              |
| 1:B:412:ARG:O    | 1:B:416:SER:OG   | 1.92                     | 0.87              |
| 1:B:119:THR:CG2  | 1:B:123:ILE:HD11 | 2.05                     | 0.86              |
| 1:A:135:THR:HG23 | 1:A:136:PRO:HD2  | 1.56                     | 0.86              |
| 1:B:256:SER:O    | 1:B:258:GLU:N    | 2.07                     | 0.86              |
| 1:C:143:MET:HE1  | 1:C:404:PHE:CB   | 2.06                     | 0.85              |
| 1:A:20:GLU:OE2   | 1:A:434:ARG:HB3  | 1.77                     | 0.85              |
| 1:A:389:TYR:CE2  | 1:A:439:HIS:CE1  | 2.65                     | 0.85              |
| 1:C:194:VAL:HG12 | 1:C:205:THR:HG22 | 1.56                     | 0.84              |
| 1:C:153:ASP:OD1  | 1:C:155:VAL:HG23 | 1.76                     | 0.84              |
| 1:A:105:LEU:HD11 | 1:A:123:ILE:HD11 | 1.59                     | 0.83              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:131:LEU:N    | 1:B:132:PRO:CD   | 2.40                     | 0.83              |
| 1:C:244:GLU:O    | 1:C:248:ARG:HG3  | 1.77                     | 0.83              |
| 1:B:135:THR:OG1  | 1:B:136:PRO:HD2  | 1.78                     | 0.83              |
| 1:C:119:THR:CG2  | 1:C:123:ILE:CD1  | 2.57                     | 0.83              |
| 1:C:145:VAL:HG11 | 1:C:148:LEU:HD21 | 1.61                     | 0.83              |
| 1:C:241:TYR:HD1  | 1:C:326:TYR:OH   | 1.62                     | 0.83              |
| 1:B:165:LYS:O    | 2:B:466:HOH:O    | 1.95                     | 0.82              |
| 1:C:241:TYR:HD1  | 1:C:326:TYR:HH   | 0.83                     | 0.82              |
| 1:A:428:ILE:HG23 | 1:B:93:VAL:CG2   | 2.10                     | 0.82              |
| 1:B:119:THR:CG2  | 1:B:123:ILE:CD1  | 2.58                     | 0.81              |
| 1:A:241:TYR:HD1  | 1:A:326:TYR:OH   | 1.62                     | 0.81              |
| 1:A:143:MET:CE   | 1:A:405:GLY:H    | 1.93                     | 0.80              |
| 1:B:71:TYR:CE2   | 1:B:76:ARG:HD3   | 2.17                     | 0.80              |
| 1:C:159:GLU:HA   | 1:C:159:GLU:OE1  | 1.82                     | 0.79              |
| 1:A:93:VAL:CG2   | 1:C:428:ILE:HG23 | 2.13                     | 0.79              |
| 1:A:241:TYR:HD1  | 1:A:326:TYR:HH   | 0.81                     | 0.79              |
| 1:B:131:LEU:N    | 1:B:132:PRO:HD3  | 1.99                     | 0.78              |
| 1:B:243:ASP:N    | 1:B:243:ASP:OD1  | 2.10                     | 0.78              |
| 1:B:20:GLU:OE2   | 1:B:434:ARG:HB3  | 1.83                     | 0.78              |
| 1:A:228:VAL:O    | 1:A:228:VAL:HG12 | 1.84                     | 0.77              |
| 1:A:205:THR:O    | 1:A:205:THR:HG22 | 1.82                     | 0.77              |
| 1:A:62:MET:HE3   | 1:A:72:ILE:HG12  | 1.67                     | 0.77              |
| 1:A:424:GLU:CA   | 1:B:1:MET:SD     | 2.72                     | 0.77              |
| 1:B:146:GLU:OE1  | 1:B:446:LYS:NZ   | 2.18                     | 0.77              |
| 1:B:21:VAL:HG12  | 1:B:412:ARG:HD3  | 1.66                     | 0.77              |
| 1:A:244:GLU:O    | 1:A:248:ARG:HG3  | 1.84                     | 0.77              |
| 1:A:71:TYR:CE2   | 1:A:76:ARG:HD3   | 2.20                     | 0.77              |
| 1:C:219:HIS:CE1  | 1:C:285:TRP:CH2  | 2.73                     | 0.77              |
| 1:B:58:VAL:O     | 1:B:62:MET:HG3   | 1.86                     | 0.76              |
| 1:A:409:GLU:OE2  | 1:A:413:ARG:NH1  | 2.18                     | 0.76              |
| 1:C:219:HIS:CE1  | 1:C:285:TRP:CE3  | 2.73                     | 0.76              |
| 1:B:409:GLU:OE2  | 1:B:413:ARG:NH1  | 2.19                     | 0.75              |
| 1:A:365:PRO:CD   | 1:A:378:HIS:HD2  | 1.99                     | 0.75              |
| 1:B:184:ASN:HB3  | 1:B:187:LYS:HG2  | 1.69                     | 0.75              |
| 1:C:71:TYR:CE2   | 1:C:76:ARG:HD3   | 2.20                     | 0.75              |
| 1:A:208:LEU:N    | 1:A:251:HIS:CD2  | 2.54                     | 0.75              |
| 1:B:143:MET:CE   | 1:B:405:GLY:H    | 1.98                     | 0.75              |
| 1:B:41:ASN:HD21  | 1:B:135:THR:HG21 | 1.50                     | 0.75              |
| 1:B:21:VAL:HG21  | 1:B:437:VAL:HG13 | 1.67                     | 0.75              |
| 1:B:62:MET:HE2   | 1:B:72:ILE:HG12  | 1.66                     | 0.74              |
| 1:C:21:VAL:HG21  | 1:C:437:VAL:HG13 | 1.69                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:347:LEU:HD23 | 1:C:350:ILE:HD11 | 1.68                     | 0.74              |
| 1:B:153:ASP:OD1  | 1:B:155:VAL:HG23 | 1.87                     | 0.74              |
| 1:A:442:TYR:HD2  | 1:A:443:ASP:OD1  | 1.71                     | 0.73              |
| 1:A:347:LEU:HD11 | 1:A:378:HIS:ND1  | 2.04                     | 0.73              |
| 1:C:16:ARG:HH11  | 1:C:430:ILE:CD1  | 2.01                     | 0.73              |
| 1:B:185:VAL:HG21 | 1:B:268:TYR:CD2  | 2.23                     | 0.73              |
| 1:B:228:VAL:O    | 1:B:228:VAL:HG12 | 1.87                     | 0.73              |
| 1:C:47:ILE:CD1   | 1:C:82:TRP:CE2   | 2.72                     | 0.73              |
| 1:A:153:ASP:OD1  | 1:A:193:TYR:OH   | 2.06                     | 0.73              |
| 1:A:271:PHE:CZ   | 1:A:275:GLN:NE2  | 2.57                     | 0.72              |
| 1:A:120:ALA:O    | 1:A:123:ILE:HG22 | 1.89                     | 0.72              |
| 1:A:158:LEU:O    | 1:A:162:ARG:HG3  | 1.90                     | 0.72              |
| 1:A:41:ASN:OD1   | 1:A:135:THR:HG22 | 1.89                     | 0.72              |
| 1:B:36:LYS:HB2   | 1:B:160:HIS:CD2  | 2.25                     | 0.71              |
| 1:C:44:TRP:HH2   | 1:C:401:LEU:HD12 | 1.56                     | 0.71              |
| 1:B:145:VAL:HG11 | 1:B:148:LEU:HD21 | 1.72                     | 0.71              |
| 1:C:79:LYS:HE3   | 1:C:124:TRP:CD1  | 2.26                     | 0.71              |
| 1:A:93:VAL:HG22  | 1:C:428:ILE:HG23 | 1.73                     | 0.70              |
| 1:B:198:GLY:HA3  | 1:B:205:THR:HG23 | 1.72                     | 0.70              |
| 1:A:79:LYS:NZ    | 1:A:121:GLU:OE2  | 2.22                     | 0.70              |
| 1:B:430:ILE:O    | 1:B:434:ARG:HG3  | 1.92                     | 0.70              |
| 1:B:46:ASP:OD2   | 1:B:78:ASN:ND2   | 2.25                     | 0.70              |
| 1:C:46:ASP:OD2   | 1:C:78:ASN:ND2   | 2.24                     | 0.70              |
| 1:A:135:THR:HG23 | 1:A:136:PRO:CD   | 2.21                     | 0.70              |
| 1:A:21:VAL:HG21  | 1:A:437:VAL:HG13 | 1.74                     | 0.69              |
| 1:B:436:LEU:HD22 | 1:C:93:VAL:CG1   | 2.21                     | 0.69              |
| 1:C:283:THR:HG21 | 1:C:285:TRP:NE1  | 2.07                     | 0.69              |
| 1:C:47:ILE:HD12  | 1:C:82:TRP:CH2   | 2.28                     | 0.69              |
| 1:A:131:LEU:HA   | 1:A:134:MET:HG3  | 1.75                     | 0.69              |
| 1:B:185:VAL:CG2  | 1:B:268:TYR:CD2  | 2.75                     | 0.69              |
| 1:C:208:LEU:N    | 1:C:251:HIS:HD2  | 1.90                     | 0.68              |
| 1:C:79:LYS:NZ    | 1:C:121:GLU:OE2  | 2.25                     | 0.68              |
| 1:C:131:LEU:N    | 1:C:132:PRO:CD   | 2.56                     | 0.68              |
| 1:A:28:ASP:OD2   | 1:A:396:THR:OG1  | 2.10                     | 0.68              |
| 1:B:271:PHE:CE2  | 1:B:275:GLN:OE1  | 2.45                     | 0.68              |
| 1:B:32:HIS:NE2   | 2:B:452:HOH:O    | 1.78                     | 0.68              |
| 1:C:21:VAL:HG12  | 1:C:412:ARG:HD3  | 1.76                     | 0.68              |
| 1:C:228:VAL:HG12 | 1:C:228:VAL:O    | 1.92                     | 0.68              |
| 1:C:271:PHE:CE2  | 1:C:275:GLN:OE1  | 2.47                     | 0.68              |
| 1:A:153:ASP:OD1  | 1:A:155:VAL:HG23 | 1.93                     | 0.68              |
| 1:A:44:TRP:HH2   | 1:A:401:LEU:HD12 | 1.59                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:436:LEU:HD22 | 1:B:93:VAL:CG1   | 2.24                     | 0.68              |
| 1:B:155:VAL:O    | 1:B:200:ARG:NH1  | 2.25                     | 0.68              |
| 1:A:271:PHE:CE2  | 1:A:275:GLN:NE2  | 2.61                     | 0.67              |
| 1:A:145:VAL:HG11 | 1:A:148:LEU:HD21 | 1.77                     | 0.67              |
| 1:A:322:GLU:OE1  | 1:B:294:LEU:HD11 | 1.94                     | 0.67              |
| 1:A:190:TRP:O    | 1:A:194:VAL:HG23 | 1.94                     | 0.67              |
| 1:B:71:TYR:CZ    | 1:B:76:ARG:HD3   | 2.28                     | 0.67              |
| 1:A:194:VAL:HG13 | 1:A:205:THR:CG2  | 2.23                     | 0.67              |
| 1:B:209:ASP:OD2  | 1:B:248:ARG:CZ   | 2.42                     | 0.67              |
| 1:A:21:VAL:HG12  | 1:A:21:VAL:O     | 1.94                     | 0.67              |
| 1:A:208:LEU:N    | 1:A:251:HIS:HD2  | 1.93                     | 0.67              |
| 1:C:56:HIS:HE1   | 1:C:57:TYR:CE2   | 2.12                     | 0.67              |
| 1:C:419:VAL:HA   | 1:C:422:MET:HE2  | 1.77                     | 0.67              |
| 1:C:246:ARG:HH11 | 1:C:246:ARG:CG   | 2.03                     | 0.66              |
| 1:C:119:THR:HG21 | 1:C:123:ILE:HD11 | 1.78                     | 0.66              |
| 1:C:283:THR:CG2  | 1:C:285:TRP:NE1  | 2.58                     | 0.66              |
| 1:A:347:LEU:HD23 | 1:A:350:ILE:HD11 | 1.78                     | 0.66              |
| 1:B:71:TYR:OH    | 1:B:76:ARG:NH1   | 2.29                     | 0.66              |
| 1:C:194:VAL:HG13 | 1:C:205:THR:HG22 | 1.74                     | 0.66              |
| 1:A:41:ASN:ND2   | 1:A:135:THR:HG21 | 2.10                     | 0.65              |
| 1:C:208:LEU:N    | 1:C:251:HIS:CD2  | 2.64                     | 0.65              |
| 1:A:424:GLU:C    | 1:B:1:MET:SD     | 2.75                     | 0.65              |
| 1:A:212:LEU:HD21 | 1:A:275:GLN:OE1  | 1.95                     | 0.65              |
| 1:A:135:THR:CG2  | 1:A:136:PRO:HD2  | 2.27                     | 0.65              |
| 1:B:394:MET:HG2  | 2:B:458:HOH:O    | 1.97                     | 0.65              |
| 1:C:145:VAL:HG11 | 1:C:148:LEU:CD2  | 2.26                     | 0.65              |
| 1:C:219:HIS:CD2  | 1:C:279:MET:HB3  | 2.32                     | 0.65              |
| 1:A:135:THR:CG2  | 1:A:136:PRO:CD   | 2.75                     | 0.65              |
| 1:B:319:ARG:HG3  | 1:C:317:PHE:CD2  | 2.31                     | 0.65              |
| 1:B:62:MET:HE3   | 1:B:72:ILE:CG1   | 2.19                     | 0.65              |
| 1:A:135:THR:HG22 | 1:A:136:PRO:N    | 2.10                     | 0.64              |
| 1:C:131:LEU:O    | 1:C:134:MET:HB2  | 1.96                     | 0.64              |
| 1:C:16:ARG:NH1   | 1:C:430:ILE:CD1  | 2.60                     | 0.64              |
| 1:C:283:THR:HG22 | 1:C:285:TRP:CD1  | 2.31                     | 0.64              |
| 1:A:430:ILE:O    | 1:A:434:ARG:HG3  | 1.97                     | 0.64              |
| 1:B:63:ARG:NE    | 1:B:69:GLU:OE2   | 2.25                     | 0.64              |
| 1:B:44:TRP:HH2   | 1:B:401:LEU:HD12 | 1.63                     | 0.64              |
| 1:C:135:THR:HB   | 1:C:136:PRO:HD2  | 1.79                     | 0.64              |
| 1:A:438:LYS:HE2  | 1:A:443:ASP:OD2  | 1.97                     | 0.64              |
| 1:C:122:GLU:HG2  | 1:C:126:GLU:OE2  | 1.97                     | 0.64              |
| 1:A:71:TYR:CZ    | 1:A:76:ARG:HD3   | 2.33                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:82:TRP:HZ2   | 1:A:123:ILE:HG21 | 1.63                     | 0.63              |
| 1:C:178:ARG:HG3  | 1:C:231:ASP:HB3  | 1.79                     | 0.63              |
| 1:C:47:ILE:CD1   | 1:C:82:TRP:CD2   | 2.77                     | 0.63              |
| 1:B:198:GLY:CA   | 1:B:205:THR:CG2  | 2.76                     | 0.63              |
| 1:C:16:ARG:HD3   | 1:C:430:ILE:HD11 | 1.81                     | 0.63              |
| 1:C:21:VAL:HG12  | 1:C:21:VAL:O     | 1.98                     | 0.63              |
| 1:C:47:ILE:HD12  | 1:C:82:TRP:CZ3   | 2.33                     | 0.63              |
| 1:A:21:VAL:HG13  | 1:A:24:LEU:HD12  | 1.79                     | 0.62              |
| 1:B:442:TYR:HD2  | 1:B:443:ASP:OD1  | 1.81                     | 0.62              |
| 1:A:365:PRO:CG   | 1:A:378:HIS:HD2  | 2.13                     | 0.62              |
| 1:A:205:THR:O    | 1:A:205:THR:CG2  | 2.48                     | 0.62              |
| 1:C:30:HIS:NE2   | 1:C:397:ASP:OD1  | 2.32                     | 0.62              |
| 1:A:366:TRP:CD1  | 1:A:366:TRP:C    | 2.73                     | 0.62              |
| 1:B:119:THR:HG23 | 1:B:123:ILE:CD1  | 2.30                     | 0.62              |
| 1:B:198:GLY:N    | 1:B:205:THR:HG21 | 2.14                     | 0.62              |
| 1:B:319:ARG:HG3  | 1:C:317:PHE:CE2  | 2.34                     | 0.62              |
| 1:A:365:PRO:HG3  | 1:A:378:HIS:CD2  | 2.35                     | 0.62              |
| 1:B:109:PHE:CE2  | 1:B:134:MET:HE1  | 2.35                     | 0.62              |
| 1:C:442:TYR:HD2  | 1:C:443:ASP:OD1  | 1.83                     | 0.62              |
| 1:C:194:VAL:HG12 | 1:C:205:THR:CG2  | 2.30                     | 0.62              |
| 1:A:419:VAL:HA   | 1:A:422:MET:CE   | 2.29                     | 0.61              |
| 1:A:319:ARG:HG3  | 1:B:317:PHE:CD2  | 2.35                     | 0.61              |
| 1:B:135:THR:HG23 | 1:B:138:LYS:H    | 1.65                     | 0.61              |
| 1:B:242:VAL:O    | 1:B:271:PHE:HD1  | 1.82                     | 0.61              |
| 1:C:119:THR:HG22 | 1:C:123:ILE:CD1  | 2.30                     | 0.61              |
| 1:C:400:LYS:NZ   | 2:C:458:HOH:O    | 2.05                     | 0.61              |
| 1:A:105:LEU:HD13 | 1:A:123:ILE:HD11 | 1.83                     | 0.61              |
| 1:C:347:LEU:HD21 | 1:C:378:HIS:CE1  | 2.36                     | 0.61              |
| 1:A:69:GLU:OE2   | 1:A:72:ILE:HD12  | 2.01                     | 0.61              |
| 1:B:198:GLY:HA3  | 1:B:205:THR:CG2  | 2.31                     | 0.61              |
| 1:C:143:MET:CE   | 1:C:405:GLY:H    | 2.14                     | 0.61              |
| 1:A:157:THR:OG1  | 1:A:159:GLU:CG   | 2.49                     | 0.60              |
| 1:B:88:VAL:CG1   | 1:B:88:VAL:O     | 2.49                     | 0.60              |
| 1:B:65:CYS:SG    | 1:B:88:VAL:CG1   | 2.89                     | 0.60              |
| 1:C:251:HIS:HB2  | 1:C:268:TYR:HE1  | 1.67                     | 0.60              |
| 1:C:56:HIS:CE1   | 1:C:57:TYR:CE2   | 2.89                     | 0.60              |
| 1:C:131:LEU:N    | 1:C:132:PRO:HD3  | 2.17                     | 0.60              |
| 1:B:347:LEU:HD23 | 1:B:350:ILE:HD11 | 1.84                     | 0.60              |
| 1:C:119:THR:HG22 | 1:C:123:ILE:HD12 | 1.84                     | 0.60              |
| 1:A:143:MET:HE2  | 1:A:405:GLY:N    | 2.17                     | 0.59              |
| 1:B:428:ILE:HG23 | 1:C:93:VAL:CG2   | 2.32                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:428:ILE:HG23 | 1:B:93:VAL:HG22  | 1.82                     | 0.59              |
| 1:A:319:ARG:HG3  | 1:B:317:PHE:CE2  | 2.37                     | 0.59              |
| 1:C:219:HIS:ND1  | 1:C:285:TRP:CH2  | 2.70                     | 0.59              |
| 1:C:136:PRO:HA   | 1:C:401:LEU:CD1  | 2.33                     | 0.59              |
| 1:C:88:VAL:CG1   | 1:C:88:VAL:O     | 2.48                     | 0.59              |
| 1:A:347:LEU:HD21 | 1:A:378:HIS:CE1  | 2.36                     | 0.59              |
| 1:B:158:LEU:O    | 1:B:162:ARG:HG3  | 2.03                     | 0.59              |
| 1:B:365:PRO:HG2  | 1:B:375:MET:HG2  | 1.83                     | 0.59              |
| 1:B:428:ILE:HG23 | 1:C:93:VAL:HG22  | 1.84                     | 0.59              |
| 1:C:143:MET:CE   | 1:C:404:PHE:CB   | 2.75                     | 0.59              |
| 1:C:372:PRO:HD3  | 1:C:410:MET:SD   | 2.43                     | 0.59              |
| 1:A:135:THR:CG2  | 1:A:136:PRO:N    | 2.65                     | 0.59              |
| 1:A:143:MET:HE2  | 1:A:405:GLY:H    | 1.66                     | 0.59              |
| 1:A:93:VAL:HG21  | 1:C:428:ILE:HG23 | 1.85                     | 0.58              |
| 1:C:47:ILE:CD1   | 1:C:82:TRP:CZ2   | 2.86                     | 0.58              |
| 1:B:88:VAL:HG12  | 1:B:88:VAL:O     | 2.01                     | 0.58              |
| 1:B:119:THR:HG22 | 1:B:123:ILE:HD12 | 1.85                     | 0.58              |
| 1:C:100:TRP:NE1  | 1:C:410:MET:CE   | 2.66                     | 0.58              |
| 1:B:242:VAL:CG1  | 1:B:271:PHE:HB2  | 2.34                     | 0.58              |
| 1:A:30:HIS:C     | 1:A:30:HIS:CD2   | 2.76                     | 0.58              |
| 1:B:242:VAL:O    | 1:B:271:PHE:CD1  | 2.56                     | 0.58              |
| 1:C:194:VAL:CG1  | 1:C:205:THR:CG2  | 2.78                     | 0.58              |
| 1:A:145:VAL:HG11 | 1:A:148:LEU:CD2  | 2.34                     | 0.58              |
| 1:A:71:TYR:OH    | 1:A:76:ARG:NH1   | 2.37                     | 0.58              |
| 1:B:268:TYR:O    | 1:B:272:MET:HG2  | 2.04                     | 0.58              |
| 1:C:95:ASN:OD1   | 1:C:96:PRO:HD2   | 2.04                     | 0.58              |
| 1:A:194:VAL:HG13 | 1:A:205:THR:HG21 | 1.82                     | 0.57              |
| 1:B:41:ASN:ND2   | 1:B:135:THR:HG21 | 2.19                     | 0.57              |
| 1:C:435:GLU:OE2  | 2:C:474:HOH:O    | 2.17                     | 0.57              |
| 1:C:158:LEU:O    | 1:C:162:ARG:HG3  | 2.04                     | 0.57              |
| 1:C:11:ASN:OD1   | 1:C:14:ALA:N     | 2.30                     | 0.57              |
| 1:C:65:CYS:HG    | 1:C:92:PHE:HE1   | 1.52                     | 0.57              |
| 1:C:47:ILE:CG2   | 1:C:127:THR:OG1  | 2.52                     | 0.57              |
| 1:B:65:CYS:SG    | 1:B:88:VAL:HG11  | 2.45                     | 0.57              |
| 1:A:365:PRO:HD3  | 1:A:378:HIS:HD2  | 1.68                     | 0.57              |
| 1:A:327:PHE:HE2  | 1:A:337:ILE:HD13 | 1.69                     | 0.57              |
| 1:B:135:THR:OG1  | 1:B:136:PRO:CD   | 2.52                     | 0.57              |
| 1:B:198:GLY:CA   | 1:B:205:THR:HG21 | 2.35                     | 0.57              |
| 1:A:387:LEU:HD22 | 1:B:92:PHE:HA    | 1.86                     | 0.57              |
| 1:C:143:MET:HE3  | 1:C:405:GLY:H    | 1.69                     | 0.57              |
| 1:A:149:CYS:HA   | 1:A:174:LEU:O    | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:143:MET:HE2  | 1:B:405:GLY:N    | 2.20                     | 0.56              |
| 1:B:60:GLU:OE2   | 1:B:310:GLY:HA2  | 2.04                     | 0.56              |
| 1:B:119:THR:HG23 | 1:B:123:ILE:HD11 | 1.84                     | 0.56              |
| 1:B:65:CYS:CB    | 1:B:88:VAL:HG11  | 2.35                     | 0.56              |
| 1:C:102:HIS:CE1  | 1:C:115:ILE:HD12 | 2.40                     | 0.56              |
| 1:A:317:PHE:CD2  | 1:C:319:ARG:HG3  | 2.40                     | 0.56              |
| 1:C:33:LEU:CD2   | 1:C:38:ILE:HD11  | 2.36                     | 0.56              |
| 1:A:241:TYR:CD1  | 1:A:326:TYR:OH   | 2.45                     | 0.56              |
| 1:A:246:ARG:HD3  | 1:A:267:ASP:OD2  | 2.05                     | 0.56              |
| 1:A:283:THR:HG21 | 1:A:285:TRP:NE1  | 2.20                     | 0.56              |
| 1:C:148:LEU:HD12 | 1:C:173:ILE:HG12 | 1.88                     | 0.56              |
| 1:A:178:ARG:CG   | 1:A:231:ASP:HB3  | 2.36                     | 0.56              |
| 1:A:209:ASP:OD1  | 1:A:248:ARG:NH2  | 2.38                     | 0.56              |
| 1:A:327:PHE:HE2  | 1:A:337:ILE:CD1  | 2.17                     | 0.56              |
| 1:A:185:VAL:HG21 | 1:A:268:TYR:CD2  | 2.39                     | 0.56              |
| 1:B:242:VAL:HG11 | 1:B:271:PHE:HB2  | 1.88                     | 0.56              |
| 1:B:389:TYR:CE2  | 1:B:439:HIS:CE1  | 2.93                     | 0.56              |
| 1:B:419:VAL:HA   | 1:B:422:MET:HE2  | 1.88                     | 0.56              |
| 1:B:109:PHE:CE2  | 1:B:134:MET:CE   | 2.89                     | 0.55              |
| 1:B:326:TYR:O    | 1:B:330:GLU:HB2  | 2.05                     | 0.55              |
| 1:C:159:GLU:CA   | 1:C:159:GLU:OE1  | 2.53                     | 0.55              |
| 1:A:205:THR:C    | 1:A:207:THR:H    | 2.10                     | 0.55              |
| 1:C:89:PHE:CZ    | 1:C:101:ILE:HD12 | 2.40                     | 0.55              |
| 1:B:21:VAL:O     | 1:B:21:VAL:HG12  | 2.05                     | 0.55              |
| 1:B:244:GLU:O    | 1:B:248:ARG:HG3  | 2.07                     | 0.55              |
| 1:C:419:VAL:HA   | 1:C:422:MET:CE   | 2.35                     | 0.55              |
| 1:A:136:PRO:HA   | 1:A:401:LEU:HD13 | 1.89                     | 0.55              |
| 1:A:136:PRO:HA   | 1:A:401:LEU:CD1  | 2.37                     | 0.55              |
| 1:B:242:VAL:O    | 1:B:242:VAL:HG12 | 2.06                     | 0.55              |
| 1:C:184:ASN:HB3  | 1:C:187:LYS:HG2  | 1.88                     | 0.55              |
| 1:A:93:VAL:HG22  | 1:C:428:ILE:HG12 | 1.88                     | 0.54              |
| 1:C:136:PRO:HA   | 1:C:401:LEU:HD13 | 1.88                     | 0.54              |
| 1:A:11:ASN:OD1   | 1:A:14:ALA:N     | 2.38                     | 0.54              |
| 1:C:149:CYS:HA   | 1:C:174:LEU:O    | 2.08                     | 0.54              |
| 1:B:136:PRO:HA   | 1:B:401:LEU:CD1  | 2.36                     | 0.54              |
| 1:A:326:TYR:O    | 1:A:330:GLU:HB2  | 2.08                     | 0.54              |
| 1:A:93:VAL:CG1   | 1:C:436:LEU:HD22 | 2.37                     | 0.54              |
| 1:B:149:CYS:HA   | 1:B:174:LEU:O    | 2.08                     | 0.54              |
| 1:B:283:THR:HG21 | 1:B:285:TRP:NE1  | 2.22                     | 0.54              |
| 1:C:59:TRP:O     | 1:C:63:ARG:HG3   | 2.08                     | 0.54              |
| 1:B:119:THR:HG21 | 1:B:123:ILE:HD11 | 1.88                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:241:TYR:CE2  | 1:B:243:ASP:OD1  | 2.61                     | 0.54              |
| 1:B:119:THR:HG22 | 1:B:123:ILE:CD1  | 2.37                     | 0.53              |
| 1:A:394:MET:HB2  | 1:A:411:PHE:CE2  | 2.43                     | 0.53              |
| 1:C:3:LEU:O      | 1:C:107:ARG:NH2  | 2.41                     | 0.53              |
| 1:B:442:TYR:O    | 1:B:445:PRO:HD2  | 2.08                     | 0.53              |
| 1:B:57:TYR:O     | 1:B:61:LEU:HG    | 2.09                     | 0.53              |
| 1:C:16:ARG:HH11  | 1:C:430:ILE:HD11 | 1.73                     | 0.53              |
| 1:B:114:VAL:O    | 1:B:119:THR:HG21 | 2.09                     | 0.53              |
| 1:B:130:LYS:C    | 1:B:132:PRO:HD2  | 2.29                     | 0.53              |
| 1:C:394:MET:HB2  | 1:C:411:PHE:CE2  | 2.44                     | 0.53              |
| 1:A:240:TYR:OH   | 1:A:266:ASN:HB3  | 2.09                     | 0.53              |
| 1:A:283:THR:HG22 | 1:A:285:TRP:CD1  | 2.44                     | 0.53              |
| 1:B:145:VAL:HG11 | 1:B:148:LEU:CD2  | 2.39                     | 0.53              |
| 1:B:219:HIS:NE2  | 1:B:285:TRP:CZ3  | 2.77                     | 0.53              |
| 1:A:428:ILE:CG2  | 1:B:93:VAL:HG22  | 2.38                     | 0.53              |
| 1:A:48:TRP:CZ2   | 1:A:81:LYS:HD3   | 2.44                     | 0.53              |
| 1:B:236:GLU:HG2  | 1:B:318:LEU:HD12 | 1.90                     | 0.52              |
| 1:C:47:ILE:HG23  | 1:C:127:THR:OG1  | 2.09                     | 0.52              |
| 1:C:219:HIS:HE1  | 1:C:285:TRP:CD2  | 2.27                     | 0.52              |
| 1:C:30:HIS:C     | 1:C:30:HIS:CD2   | 2.83                     | 0.52              |
| 1:A:178:ARG:HG2  | 1:A:231:ASP:HB3  | 1.91                     | 0.52              |
| 1:A:283:THR:CG2  | 1:A:285:TRP:NE1  | 2.72                     | 0.52              |
| 1:A:376:GLU:HG2  | 1:A:414:VAL:HG13 | 1.91                     | 0.52              |
| 1:B:198:GLY:CA   | 1:B:205:THR:HG23 | 2.39                     | 0.52              |
| 1:B:48:TRP:CE2   | 1:B:81:LYS:HD3   | 2.44                     | 0.52              |
| 1:C:72:ILE:HG22  | 1:C:73:THR:HG23  | 1.91                     | 0.52              |
| 1:B:237:PRO:O    | 1:B:323:GLY:HA3  | 2.09                     | 0.52              |
| 1:B:209:ASP:OD1  | 1:B:248:ARG:NH2  | 2.43                     | 0.52              |
| 1:A:418:VAL:O    | 1:A:422:MET:HE2  | 2.09                     | 0.52              |
| 1:B:122:GLU:HG2  | 1:B:126:GLU:OE2  | 2.10                     | 0.52              |
| 1:C:119:THR:HG23 | 1:C:123:ILE:HG13 | 1.91                     | 0.52              |
| 1:A:21:VAL:HG13  | 1:A:24:LEU:CD1   | 2.40                     | 0.51              |
| 1:C:100:TRP:NE1  | 1:C:410:MET:HE3  | 2.25                     | 0.51              |
| 1:A:317:PHE:CD2  | 1:C:319:ARG:CG   | 2.93                     | 0.51              |
| 1:B:44:TRP:HZ3   | 1:B:139:LEU:CD1  | 2.23                     | 0.51              |
| 1:C:119:THR:HG23 | 1:C:123:ILE:CD1  | 2.40                     | 0.51              |
| 1:B:419:VAL:HA   | 1:B:422:MET:CE   | 2.41                     | 0.51              |
| 1:C:242:VAL:O    | 1:C:271:PHE:CD1  | 2.63                     | 0.51              |
| 1:C:56:HIS:CE1   | 1:C:57:TYR:CD2   | 2.98                     | 0.51              |
| 1:B:283:THR:HG22 | 1:B:283:THR:O    | 2.09                     | 0.51              |
| 1:C:44:TRP:CH2   | 1:C:401:LEU:HD12 | 2.42                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:105:LEU:HD11 | 1:A:123:ILE:CD1  | 2.37                     | 0.51              |
| 1:B:178:ARG:HG2  | 1:B:231:ASP:HB3  | 1.92                     | 0.51              |
| 1:C:347:LEU:CD2  | 1:C:350:ILE:HD11 | 2.36                     | 0.51              |
| 1:C:89:PHE:HZ    | 1:C:101:ILE:HD12 | 1.75                     | 0.51              |
| 1:A:228:VAL:CG1  | 1:A:228:VAL:O    | 2.55                     | 0.51              |
| 1:A:365:PRO:CG   | 1:A:378:HIS:CD2  | 2.94                     | 0.51              |
| 1:C:237:PRO:O    | 1:C:323:GLY:HA3  | 2.11                     | 0.51              |
| 1:C:47:ILE:CD1   | 1:C:82:TRP:CE3   | 2.94                     | 0.51              |
| 1:A:386:ASP:CG   | 1:A:387:LEU:H    | 2.14                     | 0.51              |
| 1:C:246:ARG:CG   | 1:C:246:ARG:NH1  | 2.68                     | 0.51              |
| 1:C:30:HIS:CD2   | 1:C:397:ASP:OD1  | 2.64                     | 0.51              |
| 1:C:283:THR:HG22 | 1:C:283:THR:O    | 2.10                     | 0.51              |
| 1:B:219:HIS:NE2  | 1:B:285:TRP:CE3  | 2.79                     | 0.51              |
| 1:C:21:VAL:HG11  | 1:C:441:SER:CB   | 2.41                     | 0.51              |
| 1:A:205:THR:C    | 1:A:207:THR:N    | 2.63                     | 0.51              |
| 1:A:319:ARG:CG   | 1:B:317:PHE:CD2  | 2.94                     | 0.51              |
| 1:B:366:TRP:C    | 1:B:366:TRP:CD1  | 2.84                     | 0.51              |
| 1:C:143:MET:HE2  | 1:C:405:GLY:N    | 2.26                     | 0.51              |
| 1:B:345:THR:HG23 | 1:C:345:THR:CG2  | 2.41                     | 0.50              |
| 1:C:70:GLU:OE1   | 1:C:76:ARG:NE    | 2.44                     | 0.50              |
| 1:A:45:ASN:HB2   | 1:A:49:GLU:OE1   | 2.11                     | 0.50              |
| 1:C:209:ASP:OD2  | 1:C:248:ARG:CZ   | 2.59                     | 0.50              |
| 1:C:185:VAL:CG2  | 1:C:268:TYR:CD2  | 2.95                     | 0.50              |
| 1:B:36:LYS:CB    | 1:B:160:HIS:CD2  | 2.94                     | 0.50              |
| 1:C:16:ARG:HB3   | 1:C:434:ARG:HH21 | 1.75                     | 0.50              |
| 1:A:89:PHE:CZ    | 1:A:101:ILE:HD12 | 2.46                     | 0.50              |
| 1:A:21:VAL:HG11  | 1:A:441:SER:CB   | 2.41                     | 0.50              |
| 1:C:130:LYS:O    | 1:C:134:MET:SD   | 2.69                     | 0.50              |
| 1:C:143:MET:CE   | 1:C:405:GLY:N    | 2.74                     | 0.50              |
| 1:C:326:TYR:O    | 1:C:330:GLU:HB2  | 2.11                     | 0.50              |
| 1:B:345:THR:HG23 | 1:C:345:THR:HG23 | 1.94                     | 0.50              |
| 1:A:60:GLU:HG2   | 2:A:476:HOH:O    | 2.11                     | 0.50              |
| 1:B:21:VAL:O     | 1:B:21:VAL:CG1   | 2.60                     | 0.50              |
| 1:C:123:ILE:O    | 1:C:127:THR:HG23 | 2.12                     | 0.50              |
| 1:A:184:ASN:HB3  | 1:A:187:LYS:HG2  | 1.94                     | 0.49              |
| 1:A:157:THR:OG1  | 1:A:159:GLU:HG3  | 2.12                     | 0.49              |
| 1:B:198:GLY:O    | 1:B:202:GLY:N    | 2.45                     | 0.49              |
| 1:B:157:THR:OG1  | 1:B:159:GLU:HG3  | 2.12                     | 0.49              |
| 1:B:177:TRP:CZ3  | 1:B:179:PRO:HG3  | 2.47                     | 0.49              |
| 1:A:237:PRO:O    | 1:A:323:GLY:HA3  | 2.13                     | 0.49              |
| 1:A:345:THR:HG21 | 1:C:345:THR:CG2  | 2.43                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:48:TRP:CZ2   | 1:B:81:LYS:HD3   | 2.47                     | 0.49              |
| 1:A:428:ILE:HG12 | 1:B:93:VAL:HG22  | 1.94                     | 0.49              |
| 1:C:16:ARG:NH1   | 1:C:430:ILE:HD13 | 2.28                     | 0.49              |
| 1:C:230:SER:OG   | 1:C:280:ASN:ND2  | 2.43                     | 0.49              |
| 1:B:290:HIS:HB3  | 1:B:366:TRP:CH2  | 2.48                     | 0.49              |
| 1:A:230:SER:OG   | 1:A:280:ASN:ND2  | 2.46                     | 0.49              |
| 1:A:317:PHE:CE2  | 1:C:319:ARG:HG3  | 2.47                     | 0.49              |
| 1:B:344:PRO:HD3  | 1:B:369:ASN:OD1  | 2.13                     | 0.49              |
| 1:C:366:TRP:C    | 1:C:366:TRP:CD1  | 2.86                     | 0.49              |
| 1:A:21:VAL:CG1   | 1:A:21:VAL:O     | 2.60                     | 0.49              |
| 1:B:151:THR:HG23 | 1:B:178:ARG:HG3  | 1.94                     | 0.49              |
| 1:A:72:ILE:HG22  | 1:A:73:THR:HG23  | 1.94                     | 0.48              |
| 1:C:198:GLY:O    | 1:C:202:GLY:N    | 2.45                     | 0.48              |
| 1:A:61:LEU:HB2   | 1:A:92:PHE:CE2   | 2.48                     | 0.48              |
| 1:B:306:GLY:O    | 1:B:309:SER:OG   | 2.25                     | 0.48              |
| 1:C:185:VAL:HG21 | 1:C:268:TYR:CD2  | 2.47                     | 0.48              |
| 1:A:219:HIS:CD2  | 1:A:279:MET:HB3  | 2.48                     | 0.48              |
| 1:A:375:MET:O    | 1:A:379:LEU:HG   | 2.14                     | 0.48              |
| 1:A:143:MET:HE1  | 1:A:401:LEU:O    | 2.13                     | 0.48              |
| 1:C:430:ILE:O    | 1:C:434:ARG:HG3  | 2.12                     | 0.48              |
| 1:A:342:LEU:CD1  | 1:A:367:TRP:HB3  | 2.43                     | 0.48              |
| 1:B:185:VAL:CG2  | 1:B:268:TYR:CE2  | 2.97                     | 0.48              |
| 1:A:57:TYR:OH    | 1:A:367:TRP:CD1  | 2.63                     | 0.48              |
| 1:C:21:VAL:CG1   | 1:C:21:VAL:O     | 2.61                     | 0.48              |
| 1:C:436:LEU:O    | 1:C:440:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:408:THR:O    | 1:A:412:ARG:HG3  | 2.14                     | 0.48              |
| 1:B:143:MET:CE   | 1:B:405:GLY:N    | 2.70                     | 0.48              |
| 1:B:21:VAL:CG1   | 1:B:412:ARG:HD3  | 2.40                     | 0.48              |
| 1:B:178:ARG:CG   | 1:B:231:ASP:HB3  | 2.44                     | 0.48              |
| 1:A:428:ILE:CG2  | 1:B:93:VAL:CG2   | 2.86                     | 0.48              |
| 1:A:194:VAL:O    | 1:A:205:THR:HG21 | 2.14                     | 0.48              |
| 1:C:130:LYS:C    | 1:C:132:PRO:HD2  | 2.34                     | 0.48              |
| 1:C:283:THR:CG2  | 1:C:285:TRP:CD1  | 2.95                     | 0.48              |
| 1:C:33:LEU:HD23  | 1:C:38:ILE:HD11  | 1.96                     | 0.48              |
| 1:A:21:VAL:HG11  | 1:A:441:SER:OG   | 2.14                     | 0.48              |
| 1:A:92:PHE:O     | 1:A:93:VAL:C     | 2.53                     | 0.48              |
| 1:B:219:HIS:CD2  | 1:B:285:TRP:CZ3  | 3.02                     | 0.47              |
| 1:C:242:VAL:O    | 1:C:271:PHE:HD1  | 1.97                     | 0.47              |
| 1:C:342:LEU:CD1  | 1:C:367:TRP:HB3  | 2.43                     | 0.47              |
| 1:A:105:LEU:CD1  | 1:A:123:ILE:CD1  | 2.84                     | 0.47              |
| 1:B:21:VAL:HG13  | 1:B:24:LEU:HD12  | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:205:THR:C    | 1:C:207:THR:H    | 2.17                     | 0.47              |
| 1:C:48:TRP:CZ2   | 1:C:81:LYS:HD3   | 2.50                     | 0.47              |
| 1:A:89:PHE:N     | 1:A:90:PRO:CD    | 2.76                     | 0.47              |
| 1:A:5:GLU:O      | 1:A:413:ARG:NH2  | 2.48                     | 0.47              |
| 1:B:143:MET:HE2  | 1:B:405:GLY:H    | 1.73                     | 0.47              |
| 1:A:207:THR:C    | 1:A:251:HIS:HE2  | 2.18                     | 0.47              |
| 1:B:290:HIS:HD2  | 1:B:366:TRP:CE2  | 2.32                     | 0.47              |
| 1:C:219:HIS:HD2  | 1:C:279:MET:HB3  | 1.80                     | 0.47              |
| 1:C:364:ALA:HB1  | 1:C:365:PRO:HD2  | 1.97                     | 0.47              |
| 1:A:365:PRO:HG3  | 1:A:378:HIS:HD2  | 1.70                     | 0.47              |
| 1:A:436:LEU:HD22 | 1:B:93:VAL:HG13  | 1.96                     | 0.47              |
| 1:C:379:LEU:HD22 | 1:C:388:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:146:GLU:OE1  | 1:A:446:LYS:NZ   | 2.37                     | 0.47              |
| 1:A:208:LEU:CA   | 1:A:251:HIS:CD2  | 2.98                     | 0.47              |
| 1:A:327:PHE:CE2  | 1:A:337:ILE:HD13 | 2.49                     | 0.47              |
| 1:A:349:THR:O    | 1:A:353:ILE:HG13 | 2.15                     | 0.47              |
| 1:C:21:VAL:CG2   | 1:C:437:VAL:HG13 | 2.42                     | 0.47              |
| 1:A:427:GLN:HG2  | 1:B:99:GLU:OE1   | 2.15                     | 0.46              |
| 1:B:304:THR:HG22 | 1:B:305:LEU:HG   | 1.97                     | 0.46              |
| 1:C:158:LEU:HD12 | 1:C:221:HIS:CD2  | 2.50                     | 0.46              |
| 1:C:283:THR:HG22 | 1:C:285:TRP:NE1  | 2.27                     | 0.46              |
| 1:B:394:MET:HB2  | 1:B:411:PHE:CE2  | 2.50                     | 0.46              |
| 1:C:69:GLU:OE2   | 1:C:72:ILE:HD12  | 2.15                     | 0.46              |
| 1:A:409:GLU:O    | 1:A:413:ARG:HG3  | 2.16                     | 0.46              |
| 1:B:147:ILE:HG12 | 1:B:172:THR:HB   | 1.97                     | 0.46              |
| 1:B:148:LEU:HD12 | 1:B:173:ILE:HG12 | 1.96                     | 0.46              |
| 1:B:283:THR:HG22 | 1:B:285:TRP:CD1  | 2.51                     | 0.46              |
| 1:B:72:ILE:O     | 1:B:81:LYS:HE2   | 2.16                     | 0.46              |
| 1:C:113:LYS:CD   | 1:C:122:GLU:OE1  | 2.63                     | 0.46              |
| 1:C:304:THR:HG22 | 1:C:305:LEU:HG   | 1.96                     | 0.46              |
| 1:B:221:HIS:CE1  | 1:B:225:HIS:HE1  | 2.33                     | 0.46              |
| 1:A:204:ASP:O    | 1:A:207:THR:OG1  | 2.32                     | 0.46              |
| 1:B:109:PHE:CD2  | 1:B:134:MET:HE1  | 2.50                     | 0.46              |
| 1:C:194:VAL:HG13 | 1:C:205:THR:CG2  | 2.43                     | 0.46              |
| 1:C:65:CYS:SG    | 1:C:88:VAL:CG1   | 3.04                     | 0.46              |
| 1:A:185:VAL:CG2  | 1:A:268:TYR:CD2  | 2.98                     | 0.46              |
| 1:B:290:HIS:CD2  | 1:B:366:TRP:CE2  | 3.04                     | 0.46              |
| 1:A:364:ALA:HB1  | 1:A:365:PRO:HD2  | 1.97                     | 0.46              |
| 1:B:85:LEU:HD11  | 1:B:89:PHE:CD1   | 2.51                     | 0.46              |
| 1:C:362:VAL:O    | 1:C:391:LEU:HD12 | 2.15                     | 0.46              |
| 1:C:208:LEU:CA   | 1:C:251:HIS:CD2  | 2.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:59:TRP:O     | 1:A:63:ARG:HG3   | 2.16                     | 0.45              |
| 1:A:360:VAL:O    | 1:B:64:ARG:NH1   | 2.41                     | 0.45              |
| 1:C:219:HIS:HE1  | 1:C:285:TRP:CE3  | 2.23                     | 0.45              |
| 1:C:88:VAL:O     | 1:C:88:VAL:HG13  | 2.14                     | 0.45              |
| 1:A:419:VAL:HA   | 1:A:422:MET:HE2  | 1.96                     | 0.45              |
| 1:B:190:TRP:O    | 1:B:194:VAL:HG23 | 2.16                     | 0.45              |
| 1:B:30:HIS:NE2   | 1:B:397:ASP:OD1  | 2.50                     | 0.45              |
| 1:B:26:ILE:HG12  | 1:B:408:THR:HG21 | 1.99                     | 0.45              |
| 1:A:123:ILE:HG23 | 1:A:124:TRP:N    | 2.32                     | 0.45              |
| 1:B:343:ASP:HB3  | 1:B:346:HIS:CE1  | 2.52                     | 0.45              |
| 1:A:35:ALA:O     | 1:A:39:VAL:HG23  | 2.16                     | 0.45              |
| 1:B:394:MET:HB2  | 1:B:411:PHE:CD2  | 2.52                     | 0.45              |
| 1:A:82:TRP:CZ2   | 1:A:123:ILE:HG21 | 2.48                     | 0.45              |
| 1:A:143:MET:CE   | 1:A:405:GLY:N    | 2.68                     | 0.45              |
| 1:A:372:PRO:HD3  | 1:A:410:MET:SD   | 2.57                     | 0.45              |
| 1:A:50:VAL:HG11  | 1:A:402:LEU:HD12 | 1.98                     | 0.45              |
| 1:B:432:GLU:HB2  | 1:C:93:VAL:HG21  | 1.99                     | 0.45              |
| 1:C:389:TYR:CE2  | 1:C:439:HIS:CD2  | 3.05                     | 0.45              |
| 1:A:343:ASP:HB3  | 1:A:346:HIS:ND1  | 2.32                     | 0.45              |
| 1:B:342:LEU:CD1  | 1:B:367:TRP:HB3  | 2.47                     | 0.45              |
| 1:B:74:GLY:O     | 1:B:81:LYS:NZ    | 2.33                     | 0.45              |
| 1:C:355:ARG:HG2  | 1:C:355:ARG:O    | 2.16                     | 0.45              |
| 1:A:400:LYS:HG3  | 1:A:403:SER:OG   | 2.18                     | 0.44              |
| 1:B:288:GLN:NE2  | 1:B:340:TYR:OH   | 2.50                     | 0.44              |
| 1:C:194:VAL:O    | 1:C:205:THR:HG21 | 2.17                     | 0.44              |
| 1:C:92:PHE:O     | 1:C:93:VAL:C     | 2.55                     | 0.44              |
| 1:A:365:PRO:CD   | 1:A:378:HIS:CD2  | 2.90                     | 0.44              |
| 1:A:65:CYS:SG    | 1:A:88:VAL:HG13  | 2.57                     | 0.44              |
| 1:B:427:GLN:HG2  | 1:C:99:GLU:OE1   | 2.17                     | 0.44              |
| 1:C:148:LEU:HD22 | 1:C:404:PHE:CE2  | 2.53                     | 0.44              |
| 1:C:296:ASP:OD1  | 1:C:296:ASP:N    | 2.47                     | 0.44              |
| 1:A:157:THR:OG1  | 1:A:159:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:148:LEU:HD22 | 1:A:404:PHE:CE2  | 2.52                     | 0.44              |
| 1:A:153:ASP:OD1  | 1:A:155:VAL:CG2  | 2.64                     | 0.44              |
| 1:B:208:LEU:HD11 | 1:B:247:ALA:HB1  | 1.99                     | 0.44              |
| 1:A:242:VAL:O    | 1:A:271:PHE:HD1  | 2.00                     | 0.44              |
| 1:B:71:TYR:CZ    | 1:B:76:ARG:CD    | 3.00                     | 0.44              |
| 1:C:89:PHE:N     | 1:C:90:PRO:CD    | 2.80                     | 0.44              |
| 1:A:148:LEU:HD12 | 1:A:173:ILE:HG12 | 1.98                     | 0.44              |
| 1:A:347:LEU:HD21 | 1:A:378:HIS:HE1  | 1.78                     | 0.44              |
| 1:B:239:VAL:HG11 | 1:B:327:PHE:HB2  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:46:ASP:HB2   | 1:B:49:GLU:H     | 1.83                     | 0.44              |
| 1:C:268:TYR:O    | 1:C:272:MET:HG2  | 2.17                     | 0.44              |
| 1:A:365:PRO:HG2  | 1:A:375:MET:HG2  | 2.00                     | 0.44              |
| 1:B:293:ALA:HB3  | 1:B:295:ARG:HE   | 1.83                     | 0.44              |
| 1:B:347:LEU:N    | 1:B:348:PRO:CD   | 2.81                     | 0.44              |
| 1:B:349:THR:O    | 1:B:353:ILE:HG13 | 2.18                     | 0.44              |
| 1:A:44:TRP:CH2   | 1:A:401:LEU:HD12 | 2.48                     | 0.43              |
| 1:B:131:LEU:N    | 1:B:132:PRO:HD2  | 2.29                     | 0.43              |
| 1:B:157:THR:OG1  | 1:B:159:GLU:CG   | 2.66                     | 0.43              |
| 1:B:319:ARG:CG   | 1:C:317:PHE:CD2  | 2.99                     | 0.43              |
| 1:A:216:TRP:HE3  | 1:A:279:MET:HG2  | 1.83                     | 0.43              |
| 1:A:71:TYR:CZ    | 1:A:76:ARG:CD    | 3.01                     | 0.43              |
| 1:B:88:VAL:HG13  | 1:B:91:ARG:HD3   | 1.99                     | 0.43              |
| 1:A:250:VAL:HG11 | 1:A:268:TYR:HB2  | 2.00                     | 0.43              |
| 1:B:184:ASN:HB3  | 1:B:187:LYS:CG   | 2.42                     | 0.43              |
| 1:C:119:THR:HG23 | 1:C:123:ILE:CG1  | 2.48                     | 0.43              |
| 1:C:342:LEU:HB2  | 1:C:366:TRP:CZ3  | 2.54                     | 0.43              |
| 1:B:206:SER:HA   | 1:B:255:PHE:CE1  | 2.54                     | 0.43              |
| 1:C:442:TYR:O    | 1:C:445:PRO:HD2  | 2.18                     | 0.43              |
| 1:B:47:ILE:HD13  | 1:B:82:TRP:CH2   | 2.54                     | 0.43              |
| 1:C:442:TYR:OH   | 1:C:446:LYS:NZ   | 2.49                     | 0.43              |
| 1:A:198:GLY:O    | 1:A:202:GLY:N    | 2.48                     | 0.43              |
| 1:A:244:GLU:O    | 1:A:248:ARG:N    | 2.44                     | 0.43              |
| 1:C:159:GLU:OE1  | 1:C:162:ARG:HD2  | 2.18                     | 0.43              |
| 1:C:26:ILE:HG12  | 1:C:408:THR:HG21 | 2.00                     | 0.43              |
| 1:A:347:LEU:N    | 1:A:348:PRO:CD   | 2.81                     | 0.43              |
| 1:A:2:PHE:CE1    | 1:A:3:LEU:HD13   | 2.54                     | 0.43              |
| 1:A:0:HIS:CD2    | 1:A:1:MET:N      | 2.87                     | 0.42              |
| 1:A:242:VAL:O    | 1:A:271:PHE:CD1  | 2.71                     | 0.42              |
| 1:A:30:HIS:NE2   | 1:A:397:ASP:OD1  | 2.52                     | 0.42              |
| 1:B:290:HIS:HA   | 1:B:340:TYR:HB2  | 2.01                     | 0.42              |
| 1:C:89:PHE:CE2   | 1:C:115:ILE:HD12 | 2.54                     | 0.42              |
| 1:C:250:VAL:HG11 | 1:C:268:TYR:HB2  | 2.00                     | 0.42              |
| 1:A:355:ARG:O    | 1:A:355:ARG:HG2  | 2.19                     | 0.42              |
| 1:B:11:ASN:OD1   | 1:B:14:ALA:N     | 2.44                     | 0.42              |
| 1:A:105:LEU:HD13 | 1:A:123:ILE:CD1  | 2.48                     | 0.42              |
| 1:A:327:PHE:CE2  | 1:A:337:ILE:CD1  | 3.00                     | 0.42              |
| 1:B:209:ASP:OD2  | 1:B:248:ARG:NH2  | 2.52                     | 0.42              |
| 1:A:147:ILE:HG12 | 1:A:172:THR:HB   | 2.01                     | 0.42              |
| 1:C:190:TRP:O    | 1:C:194:VAL:HG23 | 2.18                     | 0.42              |
| 1:C:244:GLU:O    | 1:C:248:ARG:N    | 2.43                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:312:ASP:HB2  | 1:C:367:TRP:HH2  | 1.84                     | 0.42              |
| 1:B:244:GLU:O    | 1:B:248:ARG:N    | 2.47                     | 0.42              |
| 1:C:277:GLY:HA3  | 1:C:331:PHE:CZ   | 2.53                     | 0.42              |
| 1:C:47:ILE:HD12  | 1:C:82:TRP:CZ2   | 2.54                     | 0.42              |
| 1:B:3:LEU:O      | 1:B:107:ARG:NH2  | 2.52                     | 0.42              |
| 1:C:206:SER:HA   | 1:C:255:PHE:CE1  | 2.54                     | 0.42              |
| 1:A:51:GLU:OE1   | 1:A:400:LYS:NZ   | 2.31                     | 0.42              |
| 1:B:119:THR:HG23 | 1:B:123:ILE:HG13 | 2.02                     | 0.42              |
| 1:B:296:ASP:OD1  | 1:B:296:ASP:N    | 2.53                     | 0.42              |
| 1:B:283:THR:CG2  | 1:B:285:TRP:NE1  | 2.82                     | 0.42              |
| 1:C:335:LEU:O    | 1:C:359:ASN:HB2  | 2.19                     | 0.42              |
| 1:A:283:THR:HG22 | 1:A:283:THR:O    | 2.20                     | 0.42              |
| 1:A:288:GLN:NE2  | 1:A:340:TYR:OH   | 2.52                     | 0.42              |
| 1:A:324:LEU:HB3  | 1:A:328:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:93:VAL:HG22  | 1:C:428:ILE:CG2  | 2.45                     | 0.42              |
| 1:B:113:LYS:HD2  | 1:B:122:GLU:OE1  | 2.20                     | 0.42              |
| 1:A:62:MET:CE    | 1:A:72:ILE:HG12  | 2.45                     | 0.41              |
| 1:B:19:ASN:OD1   | 1:B:22:LYS:HE2   | 2.19                     | 0.41              |
| 1:C:28:ASP:OD2   | 1:C:396:THR:OG1  | 2.31                     | 0.41              |
| 1:C:355:ARG:NE   | 1:C:385:VAL:O    | 2.44                     | 0.41              |
| 1:C:62:MET:HB2   | 1:C:62:MET:HE2   | 1.82                     | 0.41              |
| 1:A:135:THR:O    | 1:A:139:LEU:N    | 2.47                     | 0.41              |
| 1:A:18:PHE:CE1   | 1:A:413:ARG:HG2  | 2.55                     | 0.41              |
| 1:A:88:VAL:O     | 1:A:88:VAL:HG13  | 2.21                     | 0.41              |
| 1:C:350:ILE:HG13 | 1:C:351:SER:N    | 2.34                     | 0.41              |
| 1:B:373:PHE:N    | 2:B:484:HOH:O    | 2.43                     | 0.41              |
| 1:C:347:LEU:N    | 1:C:348:PRO:CD   | 2.84                     | 0.41              |
| 1:A:389:TYR:O    | 1:A:389:TYR:CD2  | 2.74                     | 0.41              |
| 1:B:362:VAL:O    | 1:B:391:LEU:HD12 | 2.20                     | 0.41              |
| 1:C:190:TRP:HH2  | 1:C:251:HIS:ND1  | 2.19                     | 0.41              |
| 1:B:355:ARG:HD3  | 1:C:60:GLU:OE1   | 2.20                     | 0.41              |
| 1:B:155:VAL:CG2  | 1:B:193:TYR:CE1  | 3.03                     | 0.41              |
| 1:C:246:ARG:HG3  | 1:C:246:ARG:NH1  | 2.14                     | 0.41              |
| 1:A:47:ILE:HD13  | 1:A:82:TRP:CH2   | 2.56                     | 0.41              |
| 1:B:136:PRO:HA   | 1:B:401:LEU:HD13 | 2.02                     | 0.41              |
| 1:C:218:SER:O    | 1:C:221:HIS:HB3  | 2.21                     | 0.41              |
| 1:B:122:GLU:O    | 1:B:126:GLU:HG3  | 2.21                     | 0.41              |
| 1:A:283:THR:CG2  | 1:A:285:TRP:CD1  | 3.04                     | 0.41              |
| 1:A:290:HIS:CD2  | 1:A:340:TYR:CG   | 3.09                     | 0.41              |
| 1:B:428:ILE:HG22 | 1:B:429:PRO:O    | 2.20                     | 0.41              |
| 1:C:365:PRO:HG3  | 1:C:378:HIS:CB   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:A:155:VAL:CG2  | 1:A:193:TYR:CE1 | 3.04                     | 0.41              |
| 1:A:428:ILE:HG22 | 1:A:429:PRO:O   | 2.21                     | 0.41              |
| 1:B:283:THR:CG2  | 1:B:285:TRP:CD1 | 3.04                     | 0.41              |
| 1:C:369:ASN:O    | 1:C:374:GLY:HA3 | 2.20                     | 0.41              |
| 1:A:79:LYS:O     | 1:A:83:LEU:HG   | 2.21                     | 0.41              |
| 1:B:130:LYS:C    | 1:B:132:PRO:CD  | 2.87                     | 0.41              |
| 1:C:394:MET:HB2  | 1:C:411:PHE:CD2 | 2.56                     | 0.41              |
| 1:B:386:ASP:CG   | 1:B:387:LEU:H   | 2.24                     | 0.40              |
| 1:B:85:LEU:CD1   | 1:B:89:PHE:HD1  | 2.34                     | 0.40              |
| 1:C:219:HIS:HE1  | 1:C:285:TRP:CE2 | 2.39                     | 0.40              |
| 1:C:365:PRO:HG3  | 1:C:378:HIS:CG  | 2.57                     | 0.40              |
| 1:C:71:TYR:CZ    | 1:C:76:ARG:HD3  | 2.54                     | 0.40              |
| 1:A:95:ASN:OD1   | 1:A:96:PRO:HD2  | 2.20                     | 0.40              |
| 1:B:121:GLU:O    | 1:B:125:GLU:HG3 | 2.22                     | 0.40              |
| 1:B:355:ARG:O    | 1:B:355:ARG:HG2 | 2.20                     | 0.40              |
| 1:C:174:LEU:HD13 | 1:C:226:GLY:O   | 2.21                     | 0.40              |
| 1:B:251:HIS:HB2  | 1:B:268:TYR:HE1 | 1.87                     | 0.40              |
| 1:B:89:PHE:N     | 1:B:90:PRO:CD   | 2.84                     | 0.40              |
| 1:C:100:TRP:CD1  | 1:C:410:MET:HE3 | 2.56                     | 0.40              |
| 1:C:205:THR:HG23 | 1:C:211:PHE:CD1 | 2.57                     | 0.40              |
| 1:C:439:HIS:CE1  | 1:C:444:GLY:HA2 | 2.56                     | 0.40              |
| 1:C:65:CYS:SG    | 1:C:88:VAL:HG13 | 2.62                     | 0.40              |
| 1:C:61:LEU:HB2   | 1:C:92:PHE:CE2  | 2.57                     | 0.40              |
| 1:A:139:LEU:HD22 | 1:A:402:LEU:CD2 | 2.51                     | 0.40              |
| 1:B:92:PHE:O     | 1:B:93:VAL:C    | 2.58                     | 0.40              |
| 1:C:113:LYS:NZ   | 1:C:122:GLU:OE1 | 2.49                     | 0.40              |
| 1:C:375:MET:HE1  | 1:C:410:MET:HG2 | 2.03                     | 0.40              |

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:A:204:ASP:OD2 | 1:B:112:LYS:NZ[1_655]  | 0.84                     | 1.36              |
| 1:A:128:LYS:NZ  | 1:B:169:GLU:OE2[1_665] | 1.20                     | 1.00              |
| 1:B:128:LYS:NZ  | 1:C:169:GLU:CD[1_556]  | 1.49                     | 0.71              |
| 1:B:128:LYS:NZ  | 1:C:169:GLU:OE2[1_556] | 1.51                     | 0.69              |
| 1:A:255:PHE:O   | 1:B:5:GLU:OE2[1_655]   | 1.58                     | 0.62              |
| 1:A:204:ASP:CG  | 1:B:112:LYS:NZ[1_655]  | 1.89                     | 0.31              |
| 1:B:206:SER:O   | 1:C:16:ARG:NH2[1_545]  | 1.95                     | 0.25              |
| 1:A:128:LYS:NZ  | 1:B:169:GLU:CD[1_665]  | 1.98                     | 0.22              |

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| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:A:191:ARG:NH2 | 1:B:5:GLU:OE1[1_655]  | 2.03                     | 0.17              |
| 1:A:255:PHE:C   | 1:B:5:GLU:OE2[1_655]  | 2.08                     | 0.12              |
| 1:B:128:LYS:NZ  | 1:C:169:GLU:CG[1_556] | 2.08                     | 0.12              |

## 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     | 449/463 (97%)   | 425 (95%)  | 20 (4%) | 4 (1%)   | 17          | 43 |
| 1   | B     | 448/463 (97%)   | 420 (94%)  | 25 (6%) | 3 (1%)   | 22          | 50 |
| 1   | C     | 448/463 (97%)   | 422 (94%)  | 23 (5%) | 3 (1%)   | 22          | 50 |
| All | All   | 1345/1389 (97%) | 1267 (94%) | 68 (5%) | 10 (1%)  | 22          | 50 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 257 | GLY  |
| 1   | B     | 257 | GLY  |
| 1   | C     | 257 | GLY  |
| 1   | B     | 169 | GLU  |
| 1   | B     | 243 | ASP  |
| 1   | A     | 29  | PRO  |
| 1   | A     | 136 | PRO  |
| 1   | A     | 93  | VAL  |
| 1   | C     | 93  | VAL  |
| 1   | C     | 136 | PRO  |

### 5.3.2 Protein sidechains [i](#)

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     | 399/409 (98%)   | 367 (92%)  | 32 (8%)  | 12          | 31 |
| 1   | B     | 398/409 (97%)   | 367 (92%)  | 31 (8%)  | 12          | 32 |
| 1   | C     | 398/409 (97%)   | 368 (92%)  | 30 (8%)  | 13          | 34 |
| All | All   | 1195/1227 (97%) | 1102 (92%) | 93 (8%)  | 12          | 32 |

All (93) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | GLU  |
| 1   | A     | 30  | HIS  |
| 1   | A     | 46  | ASP  |
| 1   | A     | 54  | THR  |
| 1   | A     | 56  | HIS  |
| 1   | A     | 88  | VAL  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 107 | ARG  |
| 1   | A     | 108 | ARG  |
| 1   | A     | 128 | LYS  |
| 1   | A     | 134 | MET  |
| 1   | A     | 155 | VAL  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 209 | ASP  |
| 1   | A     | 236 | GLU  |
| 1   | A     | 256 | SER  |
| 1   | A     | 263 | ASP  |
| 1   | A     | 294 | LEU  |
| 1   | A     | 301 | LEU  |
| 1   | A     | 318 | LEU  |
| 1   | A     | 319 | ARG  |
| 1   | A     | 330 | GLU  |
| 1   | A     | 341 | VAL  |
| 1   | A     | 347 | LEU  |
| 1   | A     | 370 | ASP  |
| 1   | A     | 377 | MET  |
| 1   | A     | 397 | ASP  |
| 1   | A     | 398 | SER  |
| 1   | A     | 408 | THR  |
| 1   | A     | 421 | GLU  |
| 1   | A     | 432 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 437 | VAL  |
| 1   | B     | 20  | GLU  |
| 1   | B     | 54  | THR  |
| 1   | B     | 62  | MET  |
| 1   | B     | 68  | SER  |
| 1   | B     | 93  | VAL  |
| 1   | B     | 97  | THR  |
| 1   | B     | 107 | ARG  |
| 1   | B     | 108 | ARG  |
| 1   | B     | 113 | LYS  |
| 1   | B     | 119 | THR  |
| 1   | B     | 155 | VAL  |
| 1   | B     | 171 | VAL  |
| 1   | B     | 208 | LEU  |
| 1   | B     | 236 | GLU  |
| 1   | B     | 243 | ASP  |
| 1   | B     | 256 | SER  |
| 1   | B     | 294 | LEU  |
| 1   | B     | 301 | LEU  |
| 1   | B     | 318 | LEU  |
| 1   | B     | 319 | ARG  |
| 1   | B     | 330 | GLU  |
| 1   | B     | 341 | VAL  |
| 1   | B     | 347 | LEU  |
| 1   | B     | 370 | ASP  |
| 1   | B     | 376 | GLU  |
| 1   | B     | 377 | MET  |
| 1   | B     | 394 | MET  |
| 1   | B     | 397 | ASP  |
| 1   | B     | 398 | SER  |
| 1   | B     | 399 | ARG  |
| 1   | B     | 432 | GLU  |
| 1   | C     | 20  | GLU  |
| 1   | C     | 54  | THR  |
| 1   | C     | 56  | HIS  |
| 1   | C     | 93  | VAL  |
| 1   | C     | 107 | ARG  |
| 1   | C     | 108 | ARG  |
| 1   | C     | 119 | THR  |
| 1   | C     | 134 | MET  |
| 1   | C     | 155 | VAL  |
| 1   | C     | 171 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 178 | ARG  |
| 1   | C     | 185 | VAL  |
| 1   | C     | 208 | LEU  |
| 1   | C     | 236 | GLU  |
| 1   | C     | 246 | ARG  |
| 1   | C     | 256 | SER  |
| 1   | C     | 281 | GLN  |
| 1   | C     | 294 | LEU  |
| 1   | C     | 296 | ASP  |
| 1   | C     | 301 | LEU  |
| 1   | C     | 318 | LEU  |
| 1   | C     | 319 | ARG  |
| 1   | C     | 330 | GLU  |
| 1   | C     | 341 | VAL  |
| 1   | C     | 347 | LEU  |
| 1   | C     | 377 | MET  |
| 1   | C     | 394 | MET  |
| 1   | C     | 397 | ASP  |
| 1   | C     | 398 | SER  |
| 1   | C     | 437 | VAL  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 56  | HIS  |
| 1   | A     | 221 | HIS  |
| 1   | A     | 280 | ASN  |
| 1   | A     | 288 | GLN  |
| 1   | A     | 439 | HIS  |
| 1   | B     | 45  | ASN  |
| 1   | B     | 221 | HIS  |
| 1   | B     | 288 | GLN  |
| 1   | C     | 56  | HIS  |
| 1   | C     | 213 | ASN  |
| 1   | C     | 219 | HIS  |
| 1   | C     | 221 | HIS  |
| 1   | C     | 232 | HIS  |
| 1   | C     | 251 | HIS  |
| 1   | C     | 288 | GLN  |
| 1   | C     | 290 | HIS  |
| 1   | C     | 439 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 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     | 451/463 (97%)   | -0.03  | 18 (3%) | 38 32 | 8, 28, 84, 122        | 18 (3%) |
| 1   | B     | 450/463 (97%)   | -0.02  | 24 (5%) | 26 22 | 4, 27, 83, 122        | 19 (4%) |
| 1   | C     | 450/463 (97%)   | -0.02  | 23 (5%) | 28 23 | 8, 28, 83, 122        | 19 (4%) |
| All | All   | 1351/1389 (97%) | -0.03  | 65 (4%) | 30 26 | 4, 28, 84, 122        | 56 (4%) |

All (65) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 259 | LYS  | 5.7  |
| 1   | B     | 232 | HIS  | 5.3  |
| 1   | A     | 232 | HIS  | 5.3  |
| 1   | A     | 227 | CYS  | 5.0  |
| 1   | C     | 232 | HIS  | 4.9  |
| 1   | B     | 229 | ALA  | 4.9  |
| 1   | A     | 229 | ALA  | 4.8  |
| 1   | B     | 259 | LYS  | 4.7  |
| 1   | C     | 229 | ALA  | 4.6  |
| 1   | C     | 230 | SER  | 4.4  |
| 1   | A     | 230 | SER  | 4.4  |
| 1   | C     | 204 | ASP  | 4.4  |
| 1   | B     | 230 | SER  | 4.3  |
| 1   | B     | 231 | ASP  | 4.3  |
| 1   | C     | 257 | GLY  | 4.3  |
| 1   | B     | 227 | CYS  | 4.3  |
| 1   | B     | 256 | SER  | 4.2  |
| 1   | C     | 256 | SER  | 3.9  |
| 1   | A     | 228 | VAL  | 3.9  |
| 1   | B     | 204 | ASP  | 3.8  |
| 1   | A     | 231 | ASP  | 3.8  |
| 1   | B     | 233 | ALA  | 3.8  |
| 1   | C     | 227 | CYS  | 3.7  |

*Continued on next page...*

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 257 | GLY  | 3.4  |
| 1   | B     | 1   | MET  | 3.4  |
| 1   | C     | 243 | ASP  | 3.4  |
| 1   | C     | 157 | THR  | 3.3  |
| 1   | B     | 257 | GLY  | 3.3  |
| 1   | C     | 231 | ASP  | 3.2  |
| 1   | A     | 241 | TYR  | 3.1  |
| 1   | C     | 260 | LEU  | 3.0  |
| 1   | A     | 225 | HIS  | 2.9  |
| 1   | A     | 256 | SER  | 2.9  |
| 1   | C     | 1   | MET  | 2.8  |
| 1   | C     | 141 | ARG  | 2.8  |
| 1   | C     | 263 | ASP  | 2.7  |
| 1   | B     | 225 | HIS  | 2.7  |
| 1   | C     | 241 | TYR  | 2.6  |
| 1   | B     | 234 | LEU  | 2.6  |
| 1   | C     | 233 | ALA  | 2.6  |
| 1   | C     | 226 | GLY  | 2.6  |
| 1   | C     | 228 | VAL  | 2.6  |
| 1   | B     | 200 | ARG  | 2.5  |
| 1   | B     | 261 | THR  | 2.5  |
| 1   | B     | 34  | ASP  | 2.4  |
| 1   | A     | 233 | ALA  | 2.4  |
| 1   | C     | 133 | GLU  | 2.4  |
| 1   | B     | 5   | GLU  | 2.4  |
| 1   | B     | 228 | VAL  | 2.3  |
| 1   | A     | 34  | ASP  | 2.3  |
| 1   | B     | 244 | GLU  | 2.3  |
| 1   | B     | 226 | GLY  | 2.3  |
| 1   | B     | 263 | ASP  | 2.2  |
| 1   | A     | 226 | GLY  | 2.2  |
| 1   | A     | 263 | ASP  | 2.2  |
| 1   | A     | 199 | GLU  | 2.2  |
| 1   | B     | 235 | LEU  | 2.2  |
| 1   | C     | 160 | HIS  | 2.2  |
| 1   | A     | 242 | VAL  | 2.2  |
| 1   | C     | 255 | PHE  | 2.1  |
| 1   | B     | 133 | GLU  | 2.0  |
| 1   | A     | 244 | GLU  | 2.0  |
| 1   | A     | 159 | GLU  | 2.0  |
| 1   | B     | 237 | PRO  | 2.0  |
| 1   | C     | 234 | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.