



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:36 am BST

PDB ID : 3R6Y  
Title : Crystal structure of chymotrypsin-treated aspartase from Bacillus sp. YM55-1  
Authors : Fibriansah, G.; Puthan Veetil, V.; Poelarends, G.J.; Thunnissen, A.-M.W.H.  
Deposited on : 2011-03-22  
Resolution : 3.00 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   |

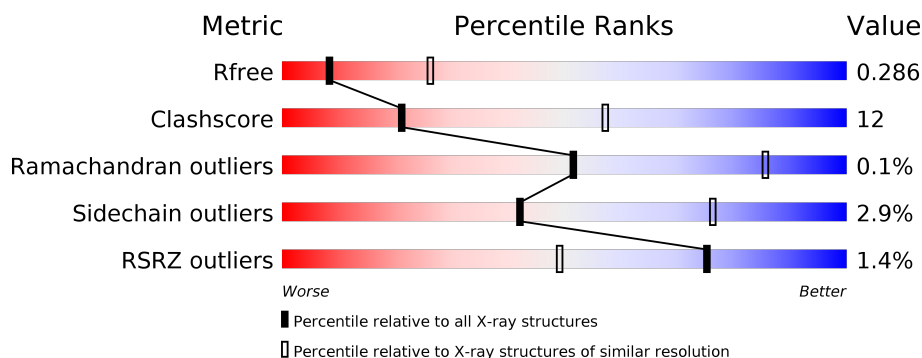
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 2092 (3.00-3.00)                                      |
| Clashscore            | 141614                      | 2416 (3.00-3.00)                                      |
| Ramachandran outliers | 138981                      | 2333 (3.00-3.00)                                      |
| Sidechain outliers    | 138945                      | 2336 (3.00-3.00)                                      |
| RSRZ outliers         | 127900                      | 1990 (3.00-3.00)                                      |

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     | 401    | <div> <div>%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>• •</div> </div> </div>  |
| 1   | B     | 401    | <div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>• •</div> </div> </div> |
| 1   | C     | 401    | <div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>•</div> </div> </div>   |
| 1   | D     | 401    | <div> <div>%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>•</div> </div> </div>    |
| 1   | E     | 401    | <div> <div>%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>•</div> </div> </div>    |
| 1   | F     | 401    | <div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>•</div> </div> </div>   |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 401    | <div><div></div><div>70%</div><div>25%</div><div>• •</div></div> |
| 1   | H     | 401    | <div><div></div><div>72%</div><div>24%</div><div>• •</div></div> |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23984 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 Aspartase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 390      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3000  | 1892 | 511 | 578 | 19 |         |         |       |
| 1   | B     | 390      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3000  | 1892 | 511 | 578 | 19 |         |         |       |
| 1   | C     | 383      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2952  | 1862 | 503 | 569 | 18 |         |         |       |
| 1   | D     | 390      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3000  | 1892 | 511 | 578 | 19 |         |         |       |
| 1   | E     | 391      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3009  | 1897 | 512 | 581 | 19 |         |         |       |
| 1   | F     | 390      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3000  | 1892 | 511 | 578 | 19 |         |         |       |
| 1   | G     | 384      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2961  | 1867 | 504 | 572 | 18 |         |         |       |
| 1   | H     | 390      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3000  | 1892 | 511 | 578 | 19 |         |         |       |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | F     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | A     | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |
| 3   | B     | 8        | Total | O | 0       | 0       |
|     |       |          | 8     | 8 |         |         |

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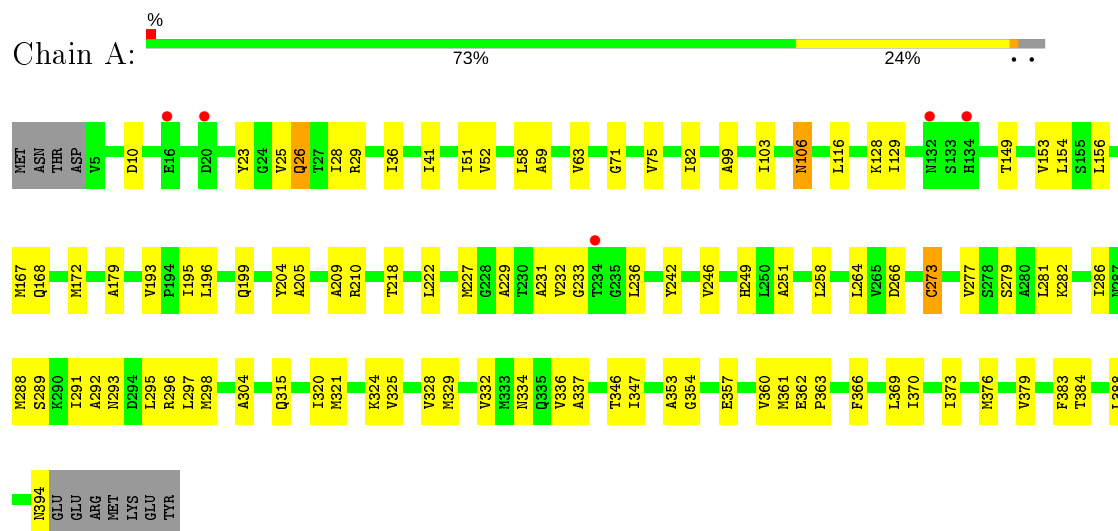
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | C     | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 3   | D     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 3   | E     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | F     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 3   | G     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 3   | H     | 6        | Total<br>6  | O<br>6  | 0       | 0       |

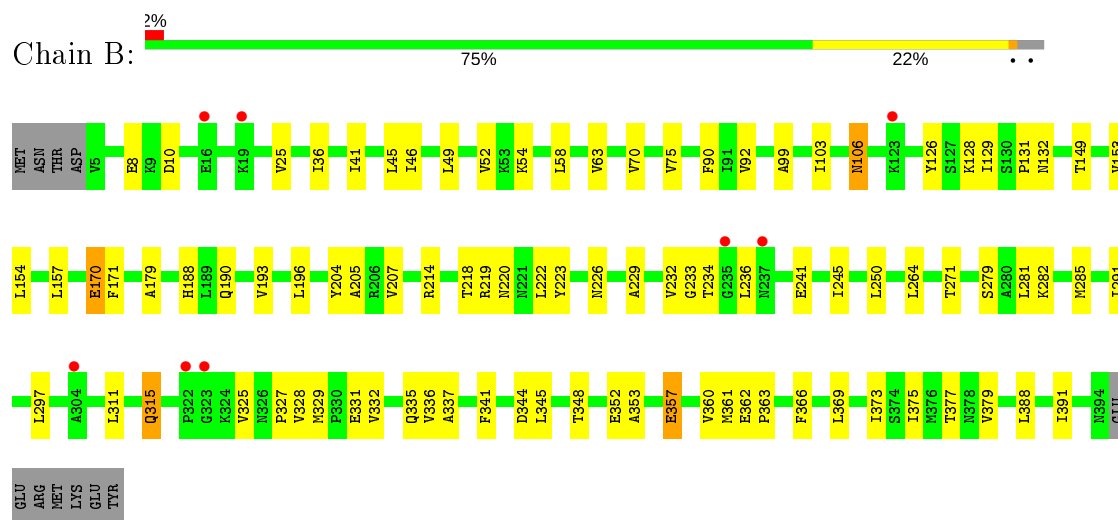
### 3 Residue-property plots [i](#)

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.

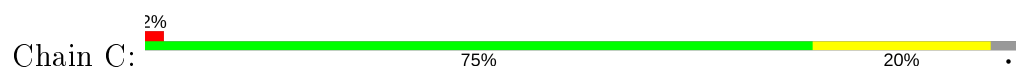
#### • Molecule 1: Aspartase

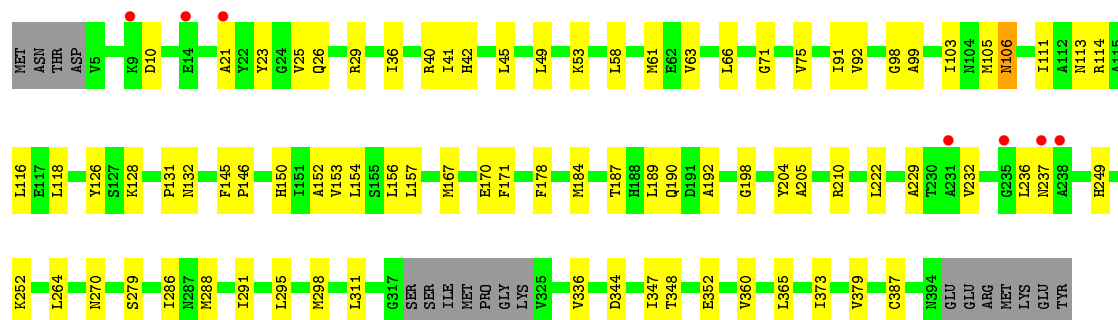


#### • Molecule 1: Aspartase

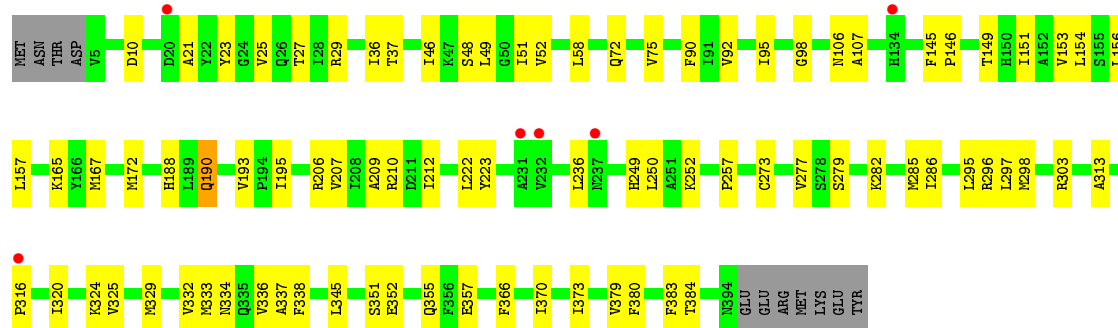
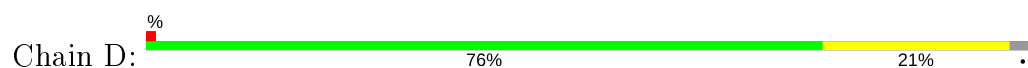


#### • Molecule 1: Aspartase

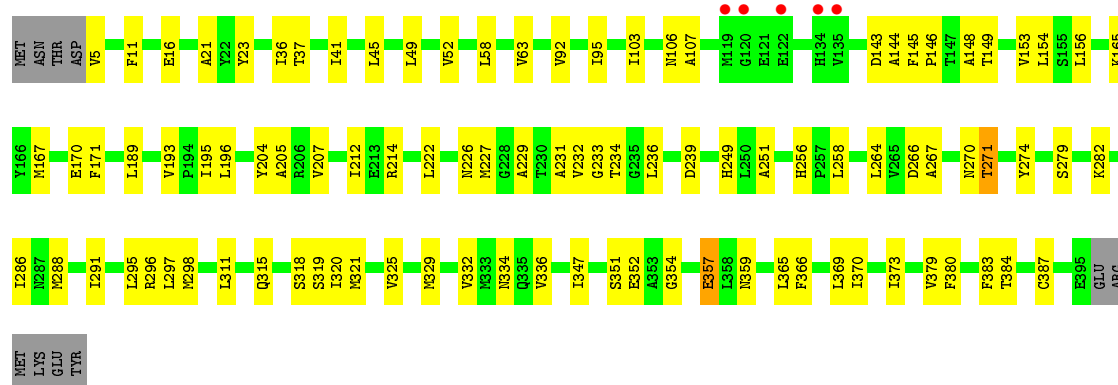
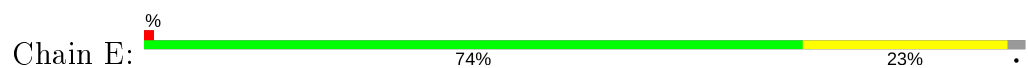




• Molecule 1: Aspartase

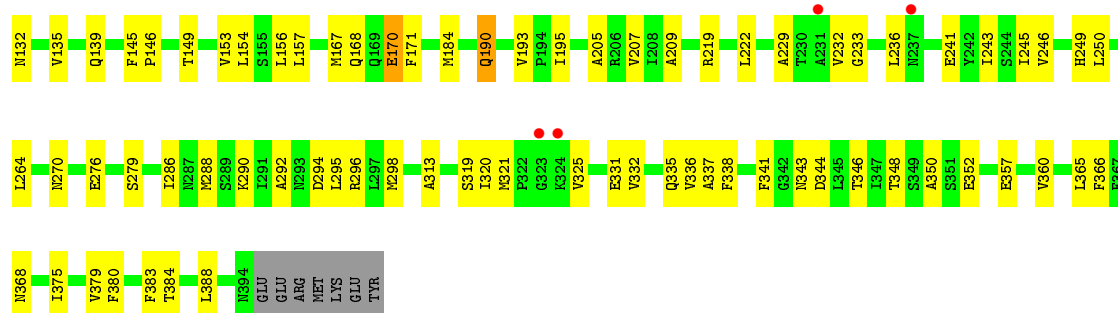


• Molecule 1: Aspartase



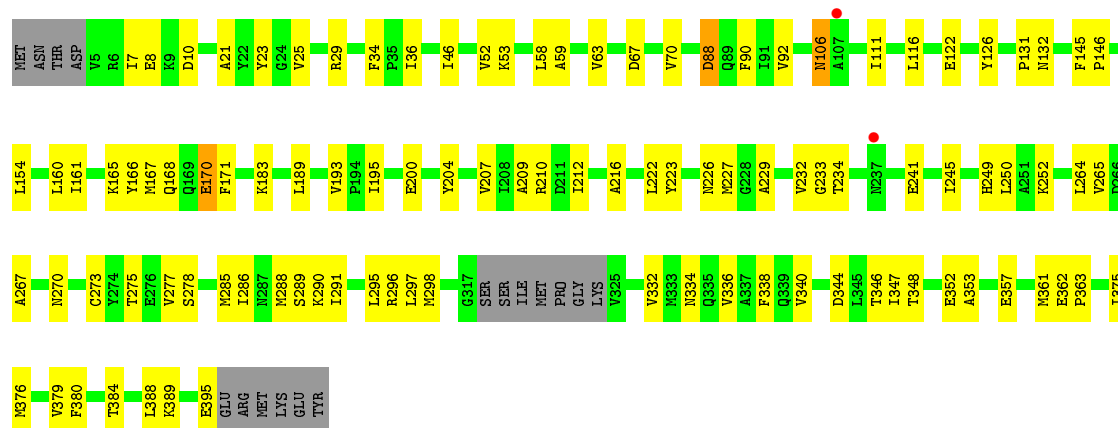
• Molecule 1: Aspartase





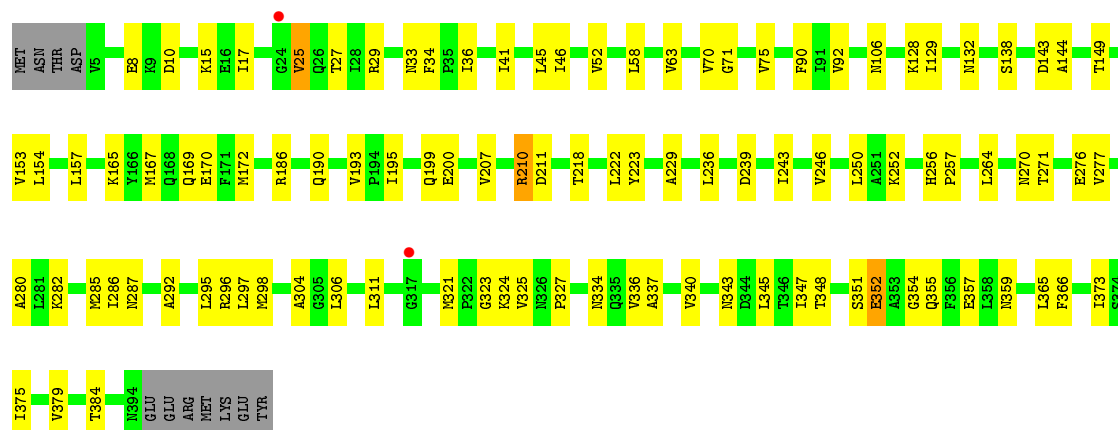
• Molecule 1: Aspartase

Chain G: 70% 25%



• Molecule 1: Aspartase

Chain H: 72% 24%





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 70.31Å 168.94Å 149.08Å<br>90.00° 92.23° 90.00°              | Depositor        |
| Resolution (Å)  | 40.00 – 3.00<br>38.26 – 3.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.6 (40.00-3.00)<br>88.0 (38.26-3.00)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.09  | Depositor        |
| $R_{sym}$   | 0.09  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.84 (at 3.01Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0109   | Depositor        |
| R, $R_{free}$   | 0.240 , 0.297<br>0.238 , 0.286                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3466 reflections (5.06%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 69.5  | Xtriage          |
| Anisotropy  | 0.119   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 15.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction   | 0.126 for h,-k,-l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.92  | EDS              |
| Total number of atoms   | 23984   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 67.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.37% 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 [i](#)

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

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

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     | 0.38         | 0/3049  | 0.50        | 0/4126  |
| 1   | B     | 0.38         | 0/3049  | 0.49        | 0/4126  |
| 1   | C     | 0.37         | 0/2999  | 0.50        | 0/4058  |
| 1   | D     | 0.38         | 0/3049  | 0.50        | 0/4126  |
| 1   | E     | 0.39         | 0/3058  | 0.51        | 0/4138  |
| 1   | F     | 0.39         | 0/3049  | 0.50        | 0/4126  |
| 1   | G     | 0.38         | 0/3008  | 0.50        | 0/4070  |
| 1   | H     | 0.39         | 0/3049  | 0.51        | 0/4126  |
| All | All   | 0.38         | 0/24310 | 0.50        | 0/32896 |

There are no bond length outliers.

There are no bond angle outliers.

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     | 3000  | 0        | 3015     | 88      | 0            |
| 1   | B     | 3000  | 0        | 3015     | 95      | 0            |
| 1   | C     | 2952  | 0        | 2961     | 68      | 0            |
| 1   | D     | 3000  | 0        | 3015     | 74      | 0            |
| 1   | E     | 3009  | 0        | 3021     | 98      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | F     | 3000  | 0        | 3015     | 86      | 0            |
| 1   | G     | 2961  | 0        | 2967     | 100     | 0            |
| 1   | H     | 3000  | 0        | 3015     | 105     | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 7     | 0        | 0        | 0       | 0            |
| 3   | B     | 8     | 0        | 0        | 1       | 0            |
| 3   | C     | 8     | 0        | 0        | 1       | 0            |
| 3   | D     | 12    | 0        | 0        | 0       | 0            |
| 3   | E     | 10    | 0        | 0        | 0       | 0            |
| 3   | F     | 4     | 0        | 0        | 0       | 0            |
| 3   | G     | 5     | 0        | 0        | 0       | 0            |
| 3   | H     | 6     | 0        | 0        | 0       | 0            |
| All | All   | 23984 | 0        | 24024    | 582     | 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 12.

All (582) 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:36:ILE:HD12  | 1:D:379:VAL:HG12 | 1.27                     | 1.12              |
| 1:E:320:ILE:HD13 | 1:H:236:LEU:HD23 | 1.28                     | 1.12              |
| 1:F:336:VAL:HG21 | 1:F:379:VAL:HG11 | 1.29                     | 1.12              |
| 1:E:36:ILE:HD12  | 1:H:379:VAL:HG12 | 1.31                     | 1.10              |
| 1:D:336:VAL:HG21 | 1:D:379:VAL:HG11 | 1.23                     | 1.10              |
| 1:G:348:THR:HG23 | 1:H:286:ILE:HD11 | 1.26                     | 1.10              |
| 1:A:336:VAL:HG21 | 1:A:379:VAL:HG11 | 1.22                     | 1.09              |
| 1:B:336:VAL:HG21 | 1:B:379:VAL:HG11 | 1.15                     | 1.09              |
| 1:C:336:VAL:HG21 | 1:C:379:VAL:HG11 | 1.36                     | 1.04              |
| 1:E:320:ILE:CD1  | 1:H:236:LEU:HD23 | 1.90                     | 1.02              |
| 1:G:336:VAL:HG21 | 1:G:379:VAL:HG11 | 1.41                     | 1.02              |
| 1:F:379:VAL:HG12 | 1:G:36:ILE:HD12  | 1.43                     | 1.00              |
| 1:A:336:VAL:HG21 | 1:A:379:VAL:CG1  | 1.92                     | 0.99              |
| 1:B:379:VAL:HG12 | 1:C:36:ILE:HD12  | 1.45                     | 0.99              |
| 1:E:336:VAL:HG21 | 1:E:379:VAL:HG11 | 1.44                     | 0.98              |
| 1:B:41:ILE:HD12  | 1:B:45:LEU:HD22  | 1.45                     | 0.95              |
| 1:A:286:ILE:HD11 | 1:B:348:THR:HG23 | 1.50                     | 0.94              |
| 1:C:348:THR:HG23 | 1:D:286:ILE:HD11 | 1.48                     | 0.94              |
| 1:E:379:VAL:HG12 | 1:H:36:ILE:HD12  | 1.50                     | 0.91              |
| 1:G:229:ALA:HB2  | 1:G:264:LEU:HD22 | 1.54                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:336:VAL:CG2  | 1:A:379:VAL:HG11 | 2.04                     | 0.87              |
| 1:E:36:ILE:HD12  | 1:H:379:VAL:CG1  | 2.05                     | 0.87              |
| 1:B:379:VAL:CG1  | 1:C:36:ILE:HD12  | 2.05                     | 0.86              |
| 1:B:36:ILE:HD12  | 1:C:379:VAL:HG12 | 1.57                     | 0.85              |
| 1:A:379:VAL:HG12 | 1:D:36:ILE:HD12  | 1.56                     | 0.85              |
| 1:E:320:ILE:HD13 | 1:H:236:LEU:CD2  | 2.05                     | 0.84              |
| 1:F:332:VAL:HG21 | 1:G:34:PHE:CD2   | 2.12                     | 0.84              |
| 1:G:232:VAL:HG21 | 1:H:193:VAL:HG22 | 1.59                     | 0.83              |
| 1:F:380:PHE:O    | 1:F:384:THR:HG23 | 1.80                     | 0.82              |
| 1:G:380:PHE:O    | 1:G:384:THR:HG23 | 1.81                     | 0.81              |
| 1:G:348:THR:HG23 | 1:H:286:ILE:CD1  | 2.09                     | 0.81              |
| 1:C:229:ALA:HB2  | 1:C:264:LEU:HD22 | 1.63                     | 0.81              |
| 1:E:286:ILE:HD11 | 1:F:348:THR:HG23 | 1.64                     | 0.80              |
| 1:B:10:ASP:HB2   | 1:B:25:VAL:HG11  | 1.64                     | 0.79              |
| 1:G:234:THR:HG22 | 1:H:199:GLN:HE22 | 1.48                     | 0.79              |
| 1:F:350:ALA:HB3  | 1:F:365:LEU:HD12 | 1.64                     | 0.79              |
| 1:F:379:VAL:CG1  | 1:G:36:ILE:HD12  | 2.12                     | 0.79              |
| 1:B:336:VAL:CG2  | 1:B:379:VAL:HG11 | 2.07                     | 0.79              |
| 1:G:10:ASP:HB2   | 1:G:25:VAL:HG11  | 1.66                     | 0.78              |
| 1:H:336:VAL:HG21 | 1:H:379:VAL:HG11 | 1.64                     | 0.77              |
| 1:H:336:VAL:HG13 | 1:H:375:ILE:HD12 | 1.67                     | 0.77              |
| 1:F:336:VAL:HG21 | 1:F:379:VAL:CG1  | 2.14                     | 0.77              |
| 1:E:380:PHE:O    | 1:E:384:THR:HG23 | 1.86                     | 0.76              |
| 1:B:336:VAL:HG21 | 1:B:379:VAL:CG1  | 2.06                     | 0.75              |
| 1:B:154:LEU:HG   | 1:B:222:LEU:HD23 | 1.69                     | 0.74              |
| 1:A:167:MET:HA   | 1:A:384:THR:HG21 | 1.69                     | 0.74              |
| 1:E:311:LEU:HD22 | 1:E:387:CYS:SG   | 2.26                     | 0.74              |
| 1:C:10:ASP:HB2   | 1:C:25:VAL:HG11  | 1.67                     | 0.74              |
| 1:G:170:GLU:HB3  | 1:G:388:LEU:HD23 | 1.69                     | 0.74              |
| 1:H:153:VAL:CG1  | 1:H:222:LEU:HD21 | 2.17                     | 0.74              |
| 1:A:36:ILE:HD12  | 1:D:379:VAL:CG1  | 2.13                     | 0.72              |
| 1:F:379:VAL:HG12 | 1:G:36:ILE:CD1   | 2.18                     | 0.72              |
| 1:E:195:ILE:HD11 | 1:F:232:VAL:HG11 | 1.71                     | 0.72              |
| 1:A:36:ILE:CD1   | 1:D:379:VAL:HG12 | 2.13                     | 0.72              |
| 1:E:36:ILE:CD1   | 1:H:379:VAL:HG12 | 2.16                     | 0.72              |
| 1:A:195:ILE:CD1  | 1:B:232:VAL:HG11 | 2.20                     | 0.71              |
| 1:B:157:LEU:HD13 | 1:B:373:ILE:CD1  | 2.20                     | 0.71              |
| 1:E:149:THR:HG21 | 1:E:366:PHE:CG   | 2.24                     | 0.71              |
| 1:B:153:VAL:CG1  | 1:B:222:LEU:HD21 | 2.21                     | 0.71              |
| 1:E:195:ILE:HD11 | 1:F:232:VAL:CG1  | 2.21                     | 0.71              |
| 1:G:154:LEU:HG   | 1:G:222:LEU:HD23 | 1.73                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:270:ASN:CG   | 1:H:207:VAL:HG21 | 2.11                     | 0.70              |
| 1:E:21:ALA:HB1   | 1:E:23:TYR:CE1   | 2.26                     | 0.70              |
| 1:A:153:VAL:CG1  | 1:A:222:LEU:HD21 | 2.22                     | 0.70              |
| 1:E:229:ALA:HB2  | 1:E:264:LEU:HD22 | 1.73                     | 0.70              |
| 1:F:99:ALA:HB2   | 1:F:360:VAL:HA   | 1.73                     | 0.70              |
| 1:G:286:ILE:HD11 | 1:H:348:THR:HG23 | 1.74                     | 0.69              |
| 1:H:229:ALA:HB2  | 1:H:264:LEU:HD22 | 1.73                     | 0.69              |
| 1:B:379:VAL:HG12 | 1:C:36:ILE:CD1   | 2.23                     | 0.69              |
| 1:B:171:PHE:HB3  | 1:B:205:ALA:HB2  | 1.74                     | 0.68              |
| 1:G:167:MET:HE2  | 1:G:288:MET:CE   | 2.24                     | 0.68              |
| 1:C:41:ILE:HB    | 1:C:45:LEU:HD23  | 1.76                     | 0.68              |
| 1:E:320:ILE:HG21 | 1:H:236:LEU:HD21 | 1.76                     | 0.67              |
| 1:D:336:VAL:HG21 | 1:D:379:VAL:CG1  | 2.12                     | 0.67              |
| 1:E:297:LEU:HD23 | 1:G:189:LEU:HD13 | 1.77                     | 0.67              |
| 1:C:153:VAL:CG1  | 1:C:222:LEU:HD21 | 2.26                     | 0.66              |
| 1:F:171:PHE:HB3  | 1:F:205:ALA:HB2  | 1.77                     | 0.66              |
| 1:F:332:VAL:HG21 | 1:G:34:PHE:CE2   | 2.31                     | 0.66              |
| 1:E:320:ILE:HG21 | 1:H:236:LEU:CD2  | 2.25                     | 0.66              |
| 1:A:324:LYS:NZ   | 1:C:187:THR:OG1  | 2.28                     | 0.66              |
| 1:H:41:ILE:HB    | 1:H:45:LEU:HD23  | 1.77                     | 0.66              |
| 1:C:348:THR:HG23 | 1:D:286:ILE:CD1  | 2.23                     | 0.65              |
| 1:A:71:GLY:O     | 1:A:75:VAL:HG23  | 1.97                     | 0.65              |
| 1:D:156:LEU:CD1  | 1:D:370:ILE:HG23 | 2.27                     | 0.65              |
| 1:F:154:LEU:HG   | 1:F:222:LEU:HD23 | 1.77                     | 0.65              |
| 1:F:350:ALA:CB   | 1:F:365:LEU:HD12 | 2.26                     | 0.65              |
| 1:H:10:ASP:HB2   | 1:H:25:VAL:HG11  | 1.79                     | 0.65              |
| 1:A:195:ILE:HD12 | 1:B:232:VAL:HG11 | 1.79                     | 0.65              |
| 1:B:157:LEU:HD13 | 1:B:373:ILE:HD13 | 1.79                     | 0.64              |
| 1:B:388:LEU:HA   | 1:B:391:ILE:HD12 | 1.78                     | 0.64              |
| 1:B:41:ILE:HB    | 1:B:45:LEU:HD13  | 1.78                     | 0.64              |
| 1:E:37:THR:CG2   | 1:E:95:ILE:HD12  | 2.26                     | 0.64              |
| 1:G:270:ASN:OD1  | 1:H:207:VAL:HG21 | 1.99                     | 0.63              |
| 1:G:189:LEU:HD11 | 1:H:355:GLN:HE22 | 1.61                     | 0.63              |
| 1:A:321:MET:HE1  | 1:C:192:ALA:HB1  | 1.81                     | 0.63              |
| 1:C:150:HIS:ND1  | 1:C:222:LEU:O    | 2.30                     | 0.63              |
| 1:C:236:LEU:HD22 | 1:D:193:VAL:HG21 | 1.80                     | 0.63              |
| 1:G:167:MET:HE2  | 1:G:288:MET:HE1  | 1.81                     | 0.63              |
| 1:G:234:THR:HG22 | 1:H:199:GLN:NE2  | 2.14                     | 0.63              |
| 1:B:345:LEU:HD11 | 1:D:345:LEU:HD11 | 1.81                     | 0.62              |
| 1:A:282:LYS:NZ   | 1:B:344:ASP:OD1  | 2.32                     | 0.62              |
| 1:B:325:VAL:O    | 1:D:190:GLN:NE2  | 2.31                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:273:CYS:O    | 1:D:277:VAL:HG23 | 1.99                     | 0.62              |
| 1:D:157:LEU:HD13 | 1:D:373:ILE:CD1  | 2.28                     | 0.62              |
| 1:E:251:ALA:HB2  | 1:E:258:LEU:HB2  | 1.81                     | 0.62              |
| 1:D:380:PHE:O    | 1:D:384:THR:HG23 | 1.99                     | 0.62              |
| 1:F:112:ALA:HB2  | 1:F:135:VAL:HG21 | 1.82                     | 0.62              |
| 1:F:153:VAL:CG1  | 1:F:222:LEU:HD21 | 2.29                     | 0.62              |
| 1:A:154:LEU:HD21 | 1:A:222:LEU:HB3  | 1.82                     | 0.61              |
| 1:A:295:LEU:HD23 | 1:A:298:MET:CE   | 2.29                     | 0.61              |
| 1:C:204:TYR:CD1  | 1:C:291:ILE:HG12 | 2.36                     | 0.61              |
| 1:F:295:LEU:HA   | 1:F:298:MET:HE3  | 1.82                     | 0.61              |
| 1:G:232:VAL:HG11 | 1:H:195:ILE:HG21 | 1.81                     | 0.61              |
| 1:G:285:MET:HG3  | 1:G:340:VAL:HG21 | 1.83                     | 0.61              |
| 1:A:23:TYR:CE2   | 1:A:28:ILE:HD11  | 2.36                     | 0.60              |
| 1:A:286:ILE:CD1  | 1:B:348:THR:HG23 | 2.29                     | 0.60              |
| 1:G:52:VAL:HA    | 1:G:250:LEU:HD21 | 1.83                     | 0.60              |
| 1:B:229:ALA:HB2  | 1:B:264:LEU:HD22 | 1.82                     | 0.60              |
| 1:A:193:VAL:HG11 | 1:B:236:LEU:HD22 | 1.82                     | 0.60              |
| 1:B:297:LEU:HD21 | 1:D:297:LEU:HD21 | 1.82                     | 0.60              |
| 1:C:295:LEU:HD23 | 1:C:298:MET:CE   | 2.31                     | 0.60              |
| 1:E:193:VAL:HG11 | 1:F:236:LEU:HD13 | 1.84                     | 0.60              |
| 1:F:46:ILE:HG23  | 1:F:90:PHE:CE1   | 2.36                     | 0.60              |
| 1:A:251:ALA:HB2  | 1:A:258:LEU:HB2  | 1.84                     | 0.60              |
| 1:A:321:MET:CE   | 1:C:192:ALA:HB1  | 2.31                     | 0.60              |
| 1:F:153:VAL:O    | 1:F:157:LEU:HB2  | 2.01                     | 0.60              |
| 1:E:347:ILE:HG23 | 1:E:365:LEU:HD21 | 1.83                     | 0.60              |
| 1:A:384:THR:HG22 | 1:A:388:LEU:HD23 | 1.83                     | 0.59              |
| 1:H:153:VAL:HG12 | 1:H:222:LEU:HD21 | 1.83                     | 0.59              |
| 1:D:149:THR:HG21 | 1:D:366:PHE:CG   | 2.37                     | 0.59              |
| 1:E:286:ILE:CD1  | 1:F:348:THR:HG23 | 2.32                     | 0.59              |
| 1:H:58:LEU:CD1   | 1:H:75:VAL:CG2   | 2.80                     | 0.59              |
| 1:B:271:THR:HG23 | 3:B:410:HOH:O    | 2.01                     | 0.59              |
| 1:A:353:ALA:CB   | 1:A:361:MET:HG3  | 2.33                     | 0.59              |
| 1:A:167:MET:HE3  | 1:A:383:PHE:CD1  | 2.38                     | 0.59              |
| 1:E:229:ALA:HB1  | 1:E:233:GLY:HA2  | 1.84                     | 0.59              |
| 1:E:282:LYS:NZ   | 1:F:344:ASP:OD1  | 2.35                     | 0.59              |
| 1:F:41:ILE:HB    | 1:F:45:LEU:HD23  | 1.85                     | 0.59              |
| 1:F:149:THR:HG21 | 1:F:366:PHE:CD2  | 2.37                     | 0.59              |
| 1:G:154:LEU:HD21 | 1:G:222:LEU:HB3  | 1.82                     | 0.59              |
| 1:H:167:MET:HA   | 1:H:384:THR:HG21 | 1.85                     | 0.58              |
| 1:G:336:VAL:HG21 | 1:G:379:VAL:CG1  | 2.24                     | 0.58              |
| 1:E:320:ILE:HD12 | 1:H:236:LEU:HD23 | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:295:LEU:HD23 | 1:H:298:MET:HE3  | 1.85                     | 0.58              |
| 1:B:353:ALA:CB   | 1:B:361:MET:HG3  | 2.33                     | 0.57              |
| 1:C:336:VAL:HG21 | 1:C:379:VAL:CG1  | 2.23                     | 0.57              |
| 1:B:214:ARG:O    | 1:B:218:THR:HG23 | 2.03                     | 0.57              |
| 1:G:52:VAL:HG13  | 1:G:227:MET:CE   | 2.35                     | 0.57              |
| 1:H:292:ALA:HB3  | 1:H:334:ASN:HD21 | 1.70                     | 0.57              |
| 1:A:195:ILE:HD11 | 1:B:232:VAL:HG11 | 1.86                     | 0.57              |
| 1:D:58:LEU:HD12  | 1:D:75:VAL:HG21  | 1.86                     | 0.57              |
| 1:D:334:ASN:O    | 1:D:337:ALA:HB3  | 2.05                     | 0.57              |
| 1:B:204:TYR:CD1  | 1:B:291:ILE:HG12 | 2.40                     | 0.57              |
| 1:D:223:TYR:CE2  | 1:D:257:PRO:HD2  | 2.40                     | 0.56              |
| 1:D:336:VAL:CG2  | 1:D:379:VAL:HG11 | 2.17                     | 0.56              |
| 1:C:264:LEU:HD12 | 3:C:402:HOH:O    | 2.06                     | 0.56              |
| 1:H:58:LEU:HD12  | 1:H:75:VAL:HG21  | 1.87                     | 0.56              |
| 1:A:297:LEU:HD23 | 1:C:189:LEU:CD1  | 2.35                     | 0.56              |
| 1:G:295:LEU:HD23 | 1:G:298:MET:CE   | 2.36                     | 0.56              |
| 1:F:229:ALA:HB1  | 1:F:233:GLY:HA2  | 1.87                     | 0.56              |
| 1:H:336:VAL:HG13 | 1:H:375:ILE:CD1  | 2.34                     | 0.56              |
| 1:C:153:VAL:HG11 | 1:C:222:LEU:HD21 | 1.86                     | 0.56              |
| 1:G:168:GLN:HE21 | 1:G:209:ALA:HB2  | 1.69                     | 0.56              |
| 1:H:153:VAL:HG11 | 1:H:222:LEU:HD21 | 1.86                     | 0.56              |
| 1:H:58:LEU:HD12  | 1:H:75:VAL:CG2   | 2.35                     | 0.56              |
| 1:G:21:ALA:HB1   | 1:G:23:TYR:CE1   | 2.40                     | 0.56              |
| 1:C:49:LEU:HD21  | 1:C:103:ILE:HG22 | 1.88                     | 0.56              |
| 1:E:231:ALA:HB1  | 1:H:321:MET:HE1  | 1.88                     | 0.56              |
| 1:H:297:LEU:O    | 1:H:306:LEU:HD12 | 2.05                     | 0.56              |
| 1:F:36:ILE:HD12  | 1:G:379:VAL:CG1  | 2.35                     | 0.56              |
| 1:H:347:ILE:HG23 | 1:H:365:LEU:CD2  | 2.36                     | 0.55              |
| 1:C:42:HIS:CE1   | 1:C:156:LEU:HD21 | 2.41                     | 0.55              |
| 1:G:375:ILE:O    | 1:G:379:VAL:HG22 | 2.05                     | 0.55              |
| 1:G:189:LEU:HD11 | 1:H:355:GLN:NE2  | 2.22                     | 0.55              |
| 1:D:295:LEU:HD23 | 1:D:298:MET:CE   | 2.37                     | 0.55              |
| 1:E:153:VAL:HG21 | 1:E:369:LEU:HD23 | 1.88                     | 0.55              |
| 1:E:236:LEU:CD1  | 1:F:193:VAL:HG11 | 2.37                     | 0.55              |
| 1:C:114:ARG:NH2  | 1:C:118:LEU:HD21 | 2.22                     | 0.55              |
| 1:H:58:LEU:CD1   | 1:H:75:VAL:HG21  | 2.37                     | 0.55              |
| 1:C:347:ILE:HG23 | 1:C:365:LEU:HG   | 1.88                     | 0.55              |
| 1:E:52:VAL:HG13  | 1:E:227:MET:HE1  | 1.89                     | 0.55              |
| 1:E:204:TYR:O    | 1:E:207:VAL:HG12 | 2.07                     | 0.54              |
| 1:D:167:MET:HG3  | 1:D:384:THR:HG22 | 1.89                     | 0.54              |
| 1:A:23:TYR:HE2   | 1:A:28:ILE:HD11  | 1.73                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:273:CYS:O    | 1:A:277:VAL:HG23 | 2.06                     | 0.54              |
| 1:G:207:VAL:HG12 | 1:G:210:ARG:NH2  | 2.23                     | 0.54              |
| 1:G:229:ALA:HB1  | 1:G:233:GLY:HA2  | 1.90                     | 0.54              |
| 1:G:273:CYS:O    | 1:G:277:VAL:HG23 | 2.07                     | 0.54              |
| 1:G:204:TYR:CD1  | 1:G:291:ILE:HG12 | 2.43                     | 0.54              |
| 1:A:167:MET:HE1  | 1:A:288:MET:HE2  | 1.90                     | 0.54              |
| 1:B:8:GLU:HB3    | 1:B:25:VAL:HG23  | 1.90                     | 0.54              |
| 1:E:167:MET:HG3  | 1:E:384:THR:HG22 | 1.90                     | 0.54              |
| 1:G:290:LYS:HG2  | 1:H:354:GLY:O    | 2.08                     | 0.54              |
| 1:B:179:ALA:O    | 1:B:196:LEU:HD22 | 2.08                     | 0.54              |
| 1:B:353:ALA:HB3  | 1:B:361:MET:HG3  | 1.89                     | 0.54              |
| 1:B:157:LEU:HD13 | 1:B:373:ILE:HD11 | 1.88                     | 0.54              |
| 1:H:71:GLY:O     | 1:H:75:VAL:HG23  | 2.07                     | 0.54              |
| 1:A:329:MET:O    | 1:A:332:VAL:HG12 | 2.08                     | 0.54              |
| 1:D:10:ASP:HB2   | 1:D:25:VAL:HG21  | 1.90                     | 0.54              |
| 1:G:195:ILE:HD11 | 1:G:200:GLU:HG3  | 1.88                     | 0.54              |
| 1:C:229:ALA:HB2  | 1:C:264:LEU:CD2  | 2.37                     | 0.54              |
| 1:F:36:ILE:HD12  | 1:G:379:VAL:HG13 | 1.91                     | 0.53              |
| 1:C:344:ASP:OD1  | 1:D:282:LYS:NZ   | 2.41                     | 0.53              |
| 1:E:236:LEU:HD11 | 1:F:193:VAL:HG11 | 1.89                     | 0.53              |
| 1:C:61:MET:HG3   | 1:C:66:LEU:HD23  | 1.91                     | 0.53              |
| 1:E:266:ASP:OD1  | 1:E:270:ASN:ND2  | 2.41                     | 0.53              |
| 1:C:171:PHE:HB3  | 1:C:205:ALA:HB2  | 1.91                     | 0.53              |
| 1:C:336:VAL:CG2  | 1:C:379:VAL:HG11 | 2.25                     | 0.53              |
| 1:D:313:ALA:HB2  | 1:D:325:VAL:HG11 | 1.90                     | 0.53              |
| 1:G:167:MET:CE   | 1:G:288:MET:CE   | 2.86                     | 0.53              |
| 1:A:229:ALA:HB2  | 1:A:264:LEU:HB3  | 1.90                     | 0.53              |
| 1:E:347:ILE:HG23 | 1:E:365:LEU:CD2  | 2.38                     | 0.53              |
| 1:A:297:LEU:HD23 | 1:C:189:LEU:HD13 | 1.90                     | 0.53              |
| 1:A:232:VAL:HG21 | 1:B:193:VAL:HG22 | 1.90                     | 0.53              |
| 1:F:295:LEU:HD23 | 1:F:298:MET:CE   | 2.39                     | 0.53              |
| 1:C:295:LEU:HD23 | 1:C:298:MET:HE3  | 1.89                     | 0.53              |
| 1:D:156:LEU:HD13 | 1:D:370:ILE:HG23 | 1.91                     | 0.53              |
| 1:G:10:ASP:CB    | 1:G:25:VAL:HG11  | 2.36                     | 0.53              |
| 1:E:296:ARG:NH2  | 1:H:355:GLN:OE1  | 2.41                     | 0.53              |
| 1:C:145:PHE:HB3  | 1:C:146:PRO:HD3  | 1.91                     | 0.52              |
| 1:F:42:HIS:CE1   | 1:F:156:LEU:HD21 | 2.43                     | 0.52              |
| 1:F:153:VAL:HG12 | 1:F:222:LEU:HD21 | 1.90                     | 0.52              |
| 1:C:154:LEU:HG   | 1:C:222:LEU:HD23 | 1.92                     | 0.52              |
| 1:G:167:MET:CE   | 1:G:288:MET:HE2  | 2.38                     | 0.52              |
| 1:D:157:LEU:HD13 | 1:D:373:ILE:HD13 | 1.90                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:165:LYS:CG   | 1:E:212:ILE:HD13 | 2.40                     | 0.52              |
| 1:E:251:ALA:N    | 1:E:258:LEU:HD12 | 2.24                     | 0.52              |
| 1:G:286:ILE:CD1  | 1:H:348:THR:HG23 | 2.39                     | 0.52              |
| 1:E:49:LEU:HD23  | 1:E:107:ALA:HB2  | 1.90                     | 0.52              |
| 1:F:56:ALA:HB1   | 1:F:139:GLN:HE22 | 1.73                     | 0.52              |
| 1:G:88:ASP:N     | 1:G:88:ASP:OD2   | 2.42                     | 0.52              |
| 1:E:234:THR:HG21 | 1:F:195:ILE:HG22 | 1.92                     | 0.52              |
| 1:H:143:ASP:OD2  | 1:H:144:ALA:N    | 2.42                     | 0.52              |
| 1:E:336:VAL:HG21 | 1:E:379:VAL:CG1  | 2.30                     | 0.52              |
| 1:B:190:GLN:HB3  | 1:D:324:LYS:HE2  | 1.92                     | 0.52              |
| 1:D:167:MET:HB2  | 1:D:384:THR:HG21 | 1.91                     | 0.52              |
| 1:H:347:ILE:HG23 | 1:H:365:LEU:HG   | 1.92                     | 0.52              |
| 1:C:311:LEU:HD22 | 1:C:387:CYS:SG   | 2.51                     | 0.51              |
| 1:G:59:ALA:HB2   | 1:G:245:ILE:HG22 | 1.92                     | 0.51              |
| 1:H:154:LEU:HB3  | 1:H:256:HIS:CE1  | 2.44                     | 0.51              |
| 1:H:334:ASN:O    | 1:H:337:ALA:HB3  | 2.10                     | 0.51              |
| 1:A:204:TYR:CD1  | 1:A:291:ILE:HG12 | 2.45                     | 0.51              |
| 1:B:336:VAL:HG13 | 1:B:375:ILE:HD12 | 1.93                     | 0.51              |
| 1:E:165:LYS:HG3  | 1:E:212:ILE:HD13 | 1.91                     | 0.51              |
| 1:H:295:LEU:HD23 | 1:H:298:MET:CE   | 2.41                     | 0.51              |
| 1:G:344:ASP:OD1  | 1:H:282:LYS:NZ   | 2.43                     | 0.51              |
| 1:B:45:LEU:C     | 1:B:45:LEU:HD23  | 2.31                     | 0.51              |
| 1:G:357:GLU:OE2  | 1:H:200:GLU:OE2  | 2.28                     | 0.51              |
| 1:F:56:ALA:CB    | 1:F:139:GLN:HE22 | 2.24                     | 0.51              |
| 1:A:153:VAL:HG12 | 1:A:222:LEU:HD21 | 1.91                     | 0.51              |
| 1:B:170:GLU:HB3  | 1:B:388:LEU:HD23 | 1.93                     | 0.51              |
| 1:E:154:LEU:HG   | 1:E:222:LEU:HD23 | 1.92                     | 0.51              |
| 1:E:232:VAL:HG13 | 1:E:357:GLU:CB   | 2.41                     | 0.51              |
| 1:A:149:THR:HG21 | 1:A:366:PHE:CG   | 2.46                     | 0.51              |
| 1:D:193:VAL:O    | 1:D:195:ILE:HG23 | 2.11                     | 0.51              |
| 1:H:149:THR:HG21 | 1:H:366:PHE:CG   | 2.45                     | 0.51              |
| 1:C:167:MET:HE2  | 1:C:288:MET:HE1  | 1.92                     | 0.51              |
| 1:G:336:VAL:CG2  | 1:G:379:VAL:HG11 | 2.27                     | 0.51              |
| 1:H:58:LEU:CD1   | 1:H:75:VAL:HG22  | 2.40                     | 0.51              |
| 1:H:27:THR:HG23  | 1:H:92:VAL:HG13  | 1.93                     | 0.51              |
| 1:D:37:THR:CG2   | 1:D:95:ILE:HD12  | 2.41                     | 0.50              |
| 1:E:351:SER:HB3  | 1:F:286:ILE:HG21 | 1.93                     | 0.50              |
| 1:F:10:ASP:HB2   | 1:F:25:VAL:HG11  | 1.93                     | 0.50              |
| 1:F:167:MET:HE2  | 1:F:288:MET:HE1  | 1.93                     | 0.50              |
| 1:G:52:VAL:HG13  | 1:G:227:MET:HE1  | 1.92                     | 0.50              |
| 1:A:167:MET:HE1  | 1:A:288:MET:CE   | 2.41                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:167:MET:HG3  | 1:F:384:THR:HG22 | 1.93                     | 0.50              |
| 1:F:73:TYR:CD2   | 1:F:119:MET:HB3  | 2.47                     | 0.50              |
| 1:A:153:VAL:HG11 | 1:A:222:LEU:HD21 | 1.91                     | 0.50              |
| 1:A:10:ASP:HB2   | 1:A:25:VAL:HG21  | 1.94                     | 0.50              |
| 1:C:270:ASN:CG   | 1:D:207:VAL:HG21 | 2.32                     | 0.50              |
| 1:C:360:VAL:HG11 | 1:D:188:HIS:HA   | 1.94                     | 0.50              |
| 1:E:279:SER:HB3  | 1:F:279:SER:HB3  | 1.93                     | 0.50              |
| 1:H:218:THR:HB   | 1:H:277:VAL:HG22 | 1.94                     | 0.50              |
| 1:H:295:LEU:HA   | 1:H:298:MET:HE3  | 1.94                     | 0.50              |
| 1:H:167:MET:HG3  | 1:H:384:THR:CG2  | 2.41                     | 0.50              |
| 1:F:149:THR:HG21 | 1:F:366:PHE:CG   | 2.47                     | 0.50              |
| 1:H:296:ARG:NH1  | 1:H:334:ASN:OD1  | 2.45                     | 0.50              |
| 1:F:292:ALA:O    | 1:F:296:ARG:HG3  | 2.11                     | 0.50              |
| 1:C:58:LEU:HD23  | 1:C:249:HIS:CE1  | 2.46                     | 0.50              |
| 1:D:313:ALA:CB   | 1:D:325:VAL:HG11 | 2.41                     | 0.50              |
| 1:A:227:MET:HG2  | 1:A:246:VAL:HG11 | 1.93                     | 0.50              |
| 1:C:26:GLN:HG3   | 1:C:105:MET:HE2  | 1.93                     | 0.50              |
| 1:B:36:ILE:HD12  | 1:C:379:VAL:CG1  | 2.36                     | 0.49              |
| 1:D:333:MET:HE1  | 1:D:383:PHE:CG   | 2.47                     | 0.49              |
| 1:E:156:LEU:CD1  | 1:E:370:ILE:HG23 | 2.42                     | 0.49              |
| 1:A:304:ALA:HB3  | 1:C:184:MET:HG2  | 1.94                     | 0.49              |
| 1:H:347:ILE:HG23 | 1:H:365:LEU:HD21 | 1.93                     | 0.49              |
| 1:A:51:ILE:HA    | 1:A:82:ILE:HD11  | 1.94                     | 0.49              |
| 1:B:153:VAL:HG11 | 1:B:222:LEU:HD21 | 1.91                     | 0.49              |
| 1:C:236:LEU:HD22 | 1:D:193:VAL:CG2  | 2.42                     | 0.49              |
| 1:D:21:ALA:HB1   | 1:D:23:TYR:CE1   | 2.47                     | 0.49              |
| 1:E:232:VAL:HG13 | 1:E:357:GLU:HB3  | 1.94                     | 0.49              |
| 1:A:334:ASN:O    | 1:A:337:ALA:HB3  | 2.13                     | 0.49              |
| 1:A:41:ILE:HD13  | 1:A:103:ILE:HG23 | 1.93                     | 0.49              |
| 1:H:15:LYS:O     | 1:H:17:ILE:HD12  | 2.12                     | 0.49              |
| 1:A:236:LEU:HD13 | 1:B:193:VAL:HG11 | 1.93                     | 0.49              |
| 1:A:52:VAL:HG13  | 1:A:227:MET:CE   | 2.42                     | 0.49              |
| 1:C:232:VAL:HG11 | 1:D:195:ILE:HG21 | 1.94                     | 0.49              |
| 1:E:143:ASP:OD2  | 1:E:144:ALA:N    | 2.46                     | 0.49              |
| 1:E:319:SER:OG   | 1:E:320:ILE:N    | 2.44                     | 0.49              |
| 1:A:218:THR:HB   | 1:A:277:VAL:HG22 | 1.95                     | 0.49              |
| 1:B:149:THR:HG21 | 1:B:366:PHE:CG   | 2.47                     | 0.49              |
| 1:F:167:MET:HE3  | 1:F:383:PHE:CD1  | 2.47                     | 0.49              |
| 1:E:270:ASN:ND2  | 1:F:207:VAL:HB   | 2.28                     | 0.49              |
| 1:B:232:VAL:HG13 | 1:B:357:GLU:HB2  | 1.96                     | 0.48              |
| 1:C:113:ASN:HA   | 1:C:116:LEU:HD12 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:266:ASP:C    | 1:A:266:ASP:OD1  | 2.51                     | 0.48              |
| 1:C:53:LYS:HG3   | 1:C:111:ILE:HD12 | 1.95                     | 0.48              |
| 1:F:294:ASP:O    | 1:F:298:MET:HG3  | 2.14                     | 0.48              |
| 1:G:160:LEU:HD21 | 1:G:376:MET:HE2  | 1.95                     | 0.48              |
| 1:B:311:LEU:HD12 | 1:B:327:PRO:HB3  | 1.95                     | 0.48              |
| 1:G:58:LEU:HD23  | 1:G:249:HIS:CD2  | 2.48                     | 0.48              |
| 1:G:336:VAL:HG13 | 1:G:375:ILE:HD12 | 1.96                     | 0.48              |
| 1:G:53:LYS:HG3   | 1:G:111:ILE:HD12 | 1.96                     | 0.48              |
| 1:D:153:VAL:HG11 | 1:D:222:LEU:HD21 | 1.94                     | 0.48              |
| 1:F:375:ILE:HG22 | 1:G:36:ILE:O     | 2.14                     | 0.48              |
| 1:G:7:ILE:O      | 1:G:7:ILE:HG23   | 2.13                     | 0.48              |
| 1:A:154:LEU:HG   | 1:A:222:LEU:HD23 | 1.95                     | 0.48              |
| 1:F:170:GLU:HB3  | 1:F:388:LEU:HD23 | 1.95                     | 0.48              |
| 1:F:58:LEU:HD23  | 1:F:249:HIS:CE1  | 2.49                     | 0.48              |
| 1:F:51:ILE:HG22  | 1:F:250:LEU:HD23 | 1.96                     | 0.48              |
| 1:G:165:LYS:HG3  | 1:G:212:ILE:HD13 | 1.94                     | 0.48              |
| 1:E:379:VAL:CG1  | 1:H:36:ILE:HD12  | 2.35                     | 0.48              |
| 1:D:153:VAL:CG1  | 1:D:222:LEU:HD21 | 2.43                     | 0.48              |
| 1:D:58:LEU:HD23  | 1:D:249:HIS:CE1  | 2.49                     | 0.48              |
| 1:A:328:VAL:HG12 | 1:D:98:GLY:CA    | 2.44                     | 0.48              |
| 1:H:218:THR:HA   | 1:H:276:GLU:OE1  | 2.14                     | 0.48              |
| 1:E:271:THR:HG22 | 1:E:274:TYR:CE1  | 2.49                     | 0.47              |
| 1:A:231:ALA:HB2  | 1:D:320:ILE:HG21 | 1.96                     | 0.47              |
| 1:B:41:ILE:HD12  | 1:B:45:LEU:CD2   | 2.30                     | 0.47              |
| 1:D:285:MET:HE2  | 1:D:336:VAL:HG12 | 1.96                     | 0.47              |
| 1:B:329:MET:O    | 1:B:332:VAL:HG12 | 2.14                     | 0.47              |
| 1:C:71:GLY:O     | 1:C:75:VAL:HG23  | 2.15                     | 0.47              |
| 1:G:166:TYR:OH   | 1:G:389:LYS:NZ   | 2.36                     | 0.47              |
| 1:A:167:MET:HG3  | 1:A:384:THR:CG2  | 2.45                     | 0.47              |
| 1:A:63:VAL:HG12  | 1:A:63:VAL:O     | 2.15                     | 0.47              |
| 1:B:8:GLU:CB     | 1:B:25:VAL:HG23  | 2.44                     | 0.47              |
| 1:D:48:SER:HA    | 1:D:51:ILE:HD12  | 1.97                     | 0.47              |
| 1:A:236:LEU:CD1  | 1:B:193:VAL:HG11 | 2.44                     | 0.47              |
| 1:C:286:ILE:HG21 | 1:D:351:SER:HB3  | 1.97                     | 0.47              |
| 1:G:296:ARG:NH1  | 1:G:334:ASN:OD1  | 2.48                     | 0.47              |
| 1:D:154:LEU:HG   | 1:D:222:LEU:HD23 | 1.96                     | 0.47              |
| 1:E:149:THR:HG21 | 1:E:366:PHE:CD2  | 2.50                     | 0.47              |
| 1:B:204:TYR:O    | 1:B:207:VAL:HG12 | 2.15                     | 0.47              |
| 1:D:49:LEU:HD23  | 1:D:107:ALA:HB2  | 1.96                     | 0.47              |
| 1:E:296:ARG:NH1  | 1:E:334:ASN:OD1  | 2.48                     | 0.47              |
| 1:G:207:VAL:HG11 | 1:H:270:ASN:CG   | 2.35                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:292:ALA:O    | 1:H:296:ARG:HG3  | 2.15                     | 0.47              |
| 1:F:190:GLN:NE2  | 1:H:325:VAL:O    | 2.48                     | 0.47              |
| 1:A:106:ASN:HD22 | 1:A:106:ASN:C    | 2.18                     | 0.47              |
| 1:B:154:LEU:HD21 | 1:B:222:LEU:HB3  | 1.96                     | 0.47              |
| 1:E:154:LEU:HB3  | 1:E:256:HIS:CE1  | 2.50                     | 0.47              |
| 1:F:145:PHE:HB3  | 1:F:146:PRO:HD3  | 1.97                     | 0.47              |
| 1:D:27:THR:HG23  | 1:D:92:VAL:HG13  | 1.97                     | 0.46              |
| 1:F:157:LEU:HD23 | 1:F:219:ARG:HG2  | 1.97                     | 0.46              |
| 1:F:78:ALA:HB2   | 1:F:111:ILE:HD13 | 1.96                     | 0.46              |
| 1:G:278:SER:HB2  | 1:G:347:ILE:HD13 | 1.97                     | 0.46              |
| 1:E:195:ILE:CD1  | 1:F:232:VAL:HG11 | 2.41                     | 0.46              |
| 1:B:70:VAL:HG13  | 1:B:129:ILE:CD1  | 2.44                     | 0.46              |
| 1:D:145:PHE:HB3  | 1:D:146:PRO:HD3  | 1.96                     | 0.46              |
| 1:E:320:ILE:HG21 | 1:H:236:LEU:HD23 | 1.98                     | 0.46              |
| 1:F:52:VAL:HA    | 1:F:250:LEU:HD21 | 1.97                     | 0.46              |
| 1:H:292:ALA:HB3  | 1:H:334:ASN:ND2  | 2.31                     | 0.46              |
| 1:H:46:ILE:HD13  | 1:H:90:PHE:CD1   | 2.50                     | 0.46              |
| 1:B:315:GLN:OE1  | 1:B:328:VAL:HG11 | 2.15                     | 0.46              |
| 1:B:153:VAL:HG12 | 1:B:222:LEU:HD21 | 1.97                     | 0.46              |
| 1:H:351:SER:HA   | 1:H:359:ASN:HD21 | 1.81                     | 0.46              |
| 1:E:329:MET:O    | 1:E:332:VAL:HG12 | 2.16                     | 0.46              |
| 1:A:279:SER:HB3  | 1:B:279:SER:HB3  | 1.97                     | 0.46              |
| 1:E:297:LEU:HD23 | 1:G:189:LEU:CD1  | 2.44                     | 0.46              |
| 1:B:99:ALA:HB2   | 1:B:360:VAL:HA   | 1.98                     | 0.46              |
| 1:D:303:ARG:HB3  | 1:H:323:GLY:HA3  | 1.98                     | 0.46              |
| 1:E:58:LEU:HD23  | 1:E:249:HIS:CD2  | 2.50                     | 0.46              |
| 1:D:333:MET:HE1  | 1:D:383:PHE:CD1  | 2.51                     | 0.46              |
| 1:E:145:PHE:HB3  | 1:E:146:PRO:HD3  | 1.98                     | 0.46              |
| 1:E:295:LEU:HA   | 1:E:298:MET:HE3  | 1.97                     | 0.46              |
| 1:G:183:LYS:NZ   | 1:G:200:GLU:OE1  | 2.38                     | 0.46              |
| 1:F:56:ALA:HB1   | 1:F:139:GLN:NE2  | 2.30                     | 0.45              |
| 1:G:270:ASN:CG   | 1:H:207:VAL:CG2  | 2.82                     | 0.45              |
| 1:A:325:VAL:O    | 1:A:325:VAL:HG13 | 2.16                     | 0.45              |
| 1:C:41:ILE:HD13  | 1:C:103:ILE:HG23 | 1.98                     | 0.45              |
| 1:H:157:LEU:HD13 | 1:H:373:ILE:CD1  | 2.46                     | 0.45              |
| 1:B:126:TYR:CD2  | 1:B:131:PRO:HD3  | 2.51                     | 0.45              |
| 1:B:281:LEU:HD11 | 1:B:373:ILE:HG12 | 1.99                     | 0.45              |
| 1:E:167:MET:HE2  | 1:E:288:MET:HE1  | 1.97                     | 0.45              |
| 1:G:232:VAL:HG13 | 1:G:357:GLU:HG3  | 1.98                     | 0.45              |
| 1:H:345:LEU:O    | 1:H:345:LEU:HD12 | 2.16                     | 0.45              |
| 1:A:199:GLN:HE22 | 1:B:234:THR:HG22 | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:360:VAL:HG11 | 1:B:188:HIS:HA   | 1.99                     | 0.45              |
| 1:E:231:ALA:HB1  | 1:H:321:MET:CE   | 2.45                     | 0.45              |
| 1:G:67:ASP:OD2   | 1:G:70:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:168:GLN:HE21 | 1:A:209:ALA:HB2  | 1.82                     | 0.45              |
| 1:D:167:MET:CB   | 1:D:384:THR:HG21 | 2.47                     | 0.45              |
| 1:E:195:ILE:HG22 | 1:E:196:LEU:N    | 2.32                     | 0.45              |
| 1:F:190:GLN:HB3  | 1:H:324:LYS:HE2  | 1.99                     | 0.45              |
| 1:B:63:VAL:HG12  | 1:B:63:VAL:O     | 2.17                     | 0.45              |
| 1:E:271:THR:HG22 | 1:E:274:TYR:HE1  | 1.81                     | 0.45              |
| 1:F:229:ALA:HB2  | 1:F:264:LEU:HB3  | 1.99                     | 0.45              |
| 1:H:311:LEU:HD12 | 1:H:327:PRO:HB3  | 1.99                     | 0.45              |
| 1:C:99:ALA:HB2   | 1:C:360:VAL:HA   | 1.99                     | 0.45              |
| 1:E:354:GLY:O    | 1:F:290:LYS:HG2  | 2.16                     | 0.45              |
| 1:G:63:VAL:HG12  | 1:G:63:VAL:O     | 2.16                     | 0.45              |
| 1:G:275:THR:HG22 | 1:G:347:ILE:HG22 | 1.98                     | 0.45              |
| 1:H:218:THR:HG21 | 1:H:280:ALA:HB2  | 1.98                     | 0.45              |
| 1:B:337:ALA:HB1  | 1:B:341:PHE:CZ   | 2.52                     | 0.44              |
| 1:C:45:LEU:HA    | 1:C:152:ALA:HB2  | 1.99                     | 0.44              |
| 1:H:70:VAL:HG13  | 1:H:129:ILE:HG12 | 1.99                     | 0.44              |
| 1:A:195:ILE:HD11 | 1:B:232:VAL:CG1  | 2.46                     | 0.44              |
| 1:D:206:ARG:O    | 1:D:209:ALA:HB3  | 2.18                     | 0.44              |
| 1:D:296:ARG:NH1  | 1:D:334:ASN:OD1  | 2.50                     | 0.44              |
| 1:E:195:ILE:CG2  | 1:E:196:LEU:N    | 2.80                     | 0.44              |
| 1:F:336:VAL:CG2  | 1:F:379:VAL:HG11 | 2.21                     | 0.44              |
| 1:H:27:THR:HG23  | 1:H:92:VAL:CG1   | 2.48                     | 0.44              |
| 1:H:33:ASN:HB3   | 1:H:34:PHE:CE2   | 2.52                     | 0.44              |
| 1:B:157:LEU:CD1  | 1:B:373:ILE:HD13 | 2.46                     | 0.44              |
| 1:B:58:LEU:HD12  | 1:B:75:VAL:CG2   | 2.47                     | 0.44              |
| 1:C:126:TYR:CD2  | 1:C:131:PRO:HD3  | 2.51                     | 0.44              |
| 1:E:167:MET:HE1  | 1:E:288:MET:HE2  | 1.99                     | 0.44              |
| 1:D:329:MET:O    | 1:D:332:VAL:HG12 | 2.18                     | 0.44              |
| 1:F:126:TYR:CD2  | 1:F:131:PRO:HD3  | 2.53                     | 0.44              |
| 1:G:161:ILE:HD11 | 1:G:216:ALA:HA   | 1.99                     | 0.44              |
| 1:G:295:LEU:HA   | 1:G:298:MET:HE2  | 1.98                     | 0.44              |
| 1:E:52:VAL:HG13  | 1:E:227:MET:CE   | 2.48                     | 0.44              |
| 1:D:48:SER:O     | 1:D:52:VAL:HG23  | 2.18                     | 0.44              |
| 1:E:45:LEU:O     | 1:E:49:LEU:HB2   | 2.18                     | 0.44              |
| 1:G:332:VAL:O    | 1:G:336:VAL:HG23 | 2.18                     | 0.44              |
| 1:A:58:LEU:HD23  | 1:A:249:HIS:CE1  | 2.52                     | 0.44              |
| 1:B:171:PHE:CD2  | 1:B:388:LEU:HD21 | 2.52                     | 0.44              |
| 1:A:324:LYS:HE2  | 1:C:190:GLN:HB3  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:229:ALA:HB2  | 1:B:264:LEU:CD2  | 2.47                     | 0.43              |
| 1:C:63:VAL:HG12  | 1:C:63:VAL:O     | 2.18                     | 0.43              |
| 1:A:379:VAL:CG1  | 1:D:36:ILE:HD12  | 2.39                     | 0.43              |
| 1:G:46:ILE:HG23  | 1:G:90:PHE:CE1   | 2.53                     | 0.43              |
| 1:A:292:ALA:O    | 1:A:296:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:328:VAL:HG12 | 1:C:98:GLY:CA    | 2.48                     | 0.43              |
| 1:E:5:VAL:HG13   | 1:E:16:GLU:HB3   | 2.00                     | 0.43              |
| 1:G:52:VAL:HG13  | 1:G:227:MET:HE2  | 2.00                     | 0.43              |
| 1:G:289:SER:OG   | 1:G:334:ASN:ND2  | 2.50                     | 0.43              |
| 1:H:243:ILE:O    | 1:H:246:VAL:HG12 | 2.18                     | 0.43              |
| 1:H:34:PHE:HA    | 1:H:36:ILE:HD11  | 1.99                     | 0.43              |
| 1:B:58:LEU:HD12  | 1:B:75:VAL:HG22  | 2.00                     | 0.43              |
| 1:H:153:VAL:O    | 1:H:157:LEU:HB2  | 2.18                     | 0.43              |
| 1:G:193:VAL:HG21 | 1:H:236:LEU:CD2  | 2.48                     | 0.43              |
| 1:B:226:ASN:ND2  | 1:B:229:ALA:HB3  | 2.33                     | 0.43              |
| 1:A:347:ILE:HD11 | 1:A:369:LEU:N    | 2.33                     | 0.43              |
| 1:B:220:ASN:HA   | 1:B:223:TYR:CD1  | 2.54                     | 0.43              |
| 1:B:285:MET:HE3  | 1:B:337:ALA:HB2  | 2.00                     | 0.43              |
| 1:C:40:ARG:NH1   | 1:C:91:ILE:HG22  | 2.33                     | 0.43              |
| 1:B:153:VAL:HG12 | 1:B:222:LEU:CD2  | 2.49                     | 0.43              |
| 1:B:49:LEU:HD21  | 1:B:103:ILE:HG22 | 2.00                     | 0.43              |
| 1:C:26:GLN:HE21  | 1:C:105:MET:CE   | 2.32                     | 0.43              |
| 1:E:189:LEU:HD13 | 1:G:297:LEU:HA   | 2.01                     | 0.43              |
| 1:F:343:ASN:OD1  | 1:F:368:ASN:OD1  | 2.36                     | 0.43              |
| 1:G:126:TYR:CD2  | 1:G:131:PRO:HD3  | 2.54                     | 0.43              |
| 1:A:154:LEU:CD2  | 1:A:222:LEU:HD23 | 2.49                     | 0.43              |
| 1:A:26:GLN:HE22  | 1:D:316:PRO:HD2  | 1.83                     | 0.43              |
| 1:A:99:ALA:HB2   | 1:A:360:VAL:HA   | 2.01                     | 0.43              |
| 1:F:241:GLU:O    | 1:F:245:ILE:HD13 | 2.19                     | 0.43              |
| 1:H:52:VAL:HA    | 1:H:250:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:193:VAL:HG22 | 1:B:232:VAL:HG21 | 2.01                     | 0.43              |
| 1:C:270:ASN:OD1  | 1:D:207:VAL:HG21 | 2.19                     | 0.43              |
| 1:D:165:LYS:HA   | 1:D:212:ILE:HD11 | 2.01                     | 0.43              |
| 1:E:165:LYS:HA   | 1:E:212:ILE:CD1  | 2.48                     | 0.43              |
| 1:H:165:LYS:O    | 1:H:169:GLN:HG2  | 2.19                     | 0.43              |
| 1:A:116:LEU:HG   | 1:A:129:ILE:HD12 | 2.01                     | 0.42              |
| 1:A:362:GLU:N    | 1:A:363:PRO:CD   | 2.81                     | 0.42              |
| 1:B:92:VAL:HG13  | 1:B:106:ASN:OD1  | 2.18                     | 0.42              |
| 1:C:21:ALA:HB1   | 1:C:23:TYR:CE1   | 2.54                     | 0.42              |
| 1:E:41:ILE:HD13  | 1:E:103:ILE:HG23 | 2.01                     | 0.42              |
| 1:B:157:LEU:HD23 | 1:B:219:ARG:HG2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:153:VAL:O    | 1:C:157:LEU:HB2  | 2.20                     | 0.42              |
| 1:B:46:ILE:HG23  | 1:B:90:PHE:CE1   | 2.55                     | 0.42              |
| 1:B:36:ILE:HG23  | 1:C:379:VAL:HG13 | 2.02                     | 0.42              |
| 1:E:92:VAL:HG21  | 1:E:103:ILE:HA   | 2.01                     | 0.42              |
| 1:F:168:GLN:HE21 | 1:F:209:ALA:HB2  | 1.84                     | 0.42              |
| 1:F:379:VAL:HG23 | 1:F:380:PHE:N    | 2.34                     | 0.42              |
| 1:E:204:TYR:HB3  | 1:E:291:ILE:HD13 | 2.00                     | 0.42              |
| 1:F:243:ILE:O    | 1:F:246:VAL:HG12 | 2.18                     | 0.42              |
| 1:G:92:VAL:HG13  | 1:G:106:ASN:OD1  | 2.18                     | 0.42              |
| 1:B:345:LEU:HD11 | 1:D:345:LEU:CD1  | 2.49                     | 0.42              |
| 1:E:329:MET:HE2  | 1:E:383:PHE:HA   | 2.02                     | 0.42              |
| 1:F:153:VAL:HG11 | 1:F:222:LEU:HD21 | 2.02                     | 0.42              |
| 1:E:195:ILE:CD1  | 1:F:232:VAL:CG1  | 2.95                     | 0.42              |
| 1:F:82:ILE:O     | 1:F:82:ILE:HG22  | 2.20                     | 0.42              |
| 1:H:167:MET:CB   | 1:H:384:THR:HG21 | 2.48                     | 0.42              |
| 1:C:189:LEU:HG   | 1:D:355:GLN:OE1  | 2.19                     | 0.42              |
| 1:D:52:VAL:HA    | 1:D:250:LEU:HD21 | 2.00                     | 0.42              |
| 1:F:48:SER:O     | 1:F:52:VAL:HG23  | 2.20                     | 0.42              |
| 1:G:229:ALA:HB2  | 1:G:264:LEU:CD2  | 2.36                     | 0.42              |
| 1:B:226:ASN:HD22 | 1:B:229:ALA:HB3  | 1.84                     | 0.42              |
| 1:B:241:GLU:O    | 1:B:245:ILE:HD13 | 2.20                     | 0.42              |
| 1:G:295:LEU:HD23 | 1:G:298:MET:HE3  | 2.02                     | 0.42              |
| 1:H:154:LEU:HG   | 1:H:222:LEU:HD23 | 2.02                     | 0.42              |
| 1:G:167:MET:HE1  | 1:G:288:MET:HE2  | 2.01                     | 0.42              |
| 1:H:236:LEU:HA   | 1:H:236:LEU:HD12 | 1.94                     | 0.42              |
| 1:H:347:ILE:HG23 | 1:H:365:LEU:CG   | 2.50                     | 0.42              |
| 1:D:46:ILE:HG23  | 1:D:90:PHE:CE1   | 2.54                     | 0.42              |
| 1:E:325:VAL:O    | 1:E:325:VAL:HG13 | 2.20                     | 0.42              |
| 1:G:21:ALA:HB1   | 1:G:23:TYR:CD1   | 2.55                     | 0.42              |
| 1:A:172:MET:HG2  | 1:A:205:ALA:HB1  | 2.02                     | 0.42              |
| 1:D:48:SER:OG    | 1:D:151:ILE:HG22 | 2.19                     | 0.42              |
| 1:E:379:VAL:CG1  | 1:H:36:ILE:HG23  | 2.49                     | 0.42              |
| 1:H:8:GLU:HB2    | 1:H:25:VAL:HG23  | 2.02                     | 0.42              |
| 1:A:353:ALA:HB3  | 1:A:361:MET:HG3  | 2.01                     | 0.41              |
| 1:B:232:VAL:HG13 | 1:B:357:GLU:CB   | 2.50                     | 0.41              |
| 1:E:167:MET:CE   | 1:E:288:MET:CE   | 2.97                     | 0.41              |
| 1:E:171:PHE:HB3  | 1:E:205:ALA:HB2  | 2.01                     | 0.41              |
| 1:H:186:ARG:NH2  | 1:H:306:LEU:HD22 | 2.34                     | 0.41              |
| 1:A:293:ASN:OD1  | 1:A:296:ARG:NH1  | 2.52                     | 0.41              |
| 1:B:54:LYS:O     | 1:B:58:LEU:HD13  | 2.20                     | 0.41              |
| 1:E:156:LEU:HB3  | 1:E:373:ILE:HG21 | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:36:ILE:O     | 1:H:375:ILE:HG22 | 2.20                     | 0.41              |
| 1:F:338:PHE:C    | 1:G:346:THR:HG23 | 2.40                     | 0.41              |
| 1:G:226:ASN:HB3  | 1:G:267:ALA:HB1  | 2.02                     | 0.41              |
| 1:H:193:VAL:HG23 | 1:H:195:ILE:HG23 | 2.02                     | 0.41              |
| 1:A:289:SER:OG   | 1:B:352:GLU:OE2  | 2.26                     | 0.41              |
| 1:E:63:VAL:HG11  | 1:E:239:ASP:OD1  | 2.21                     | 0.41              |
| 1:G:154:LEU:HD22 | 1:G:223:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:179:ALA:O    | 1:A:196:LEU:HD13 | 2.20                     | 0.41              |
| 1:B:332:VAL:O    | 1:B:336:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:157:LEU:HD13 | 1:C:373:ILE:CD1  | 2.50                     | 0.41              |
| 1:F:184:MET:HG2  | 1:H:304:ALA:HB3  | 2.03                     | 0.41              |
| 1:F:313:ALA:HB2  | 1:F:325:VAL:HG21 | 2.03                     | 0.41              |
| 1:F:36:ILE:HD12  | 1:G:379:VAL:HG12 | 2.01                     | 0.41              |
| 1:D:285:MET:CE   | 1:D:336:VAL:HG12 | 2.51                     | 0.41              |
| 1:F:319:SER:O    | 1:F:320:ILE:HD13 | 2.20                     | 0.41              |
| 1:A:328:VAL:HG12 | 1:D:98:GLY:HA2   | 2.02                     | 0.41              |
| 1:B:70:VAL:HG13  | 1:B:129:ILE:HG12 | 2.03                     | 0.41              |
| 1:D:165:LYS:HG3  | 1:D:212:ILE:HD13 | 2.02                     | 0.41              |
| 1:E:49:LEU:HD12  | 1:E:148:ALA:HB2  | 2.02                     | 0.41              |
| 1:F:337:ALA:HB1  | 1:F:341:PHE:CZ   | 2.56                     | 0.41              |
| 1:G:116:LEU:HD13 | 1:G:122:GLU:O    | 2.21                     | 0.41              |
| 1:G:145:PHE:HB3  | 1:G:146:PRO:HD3  | 2.02                     | 0.41              |
| 1:G:167:MET:HE3  | 1:G:171:PHE:HE2  | 1.86                     | 0.41              |
| 1:H:63:VAL:HG11  | 1:H:239:ASP:OD1  | 2.20                     | 0.41              |
| 1:A:156:LEU:HD13 | 1:A:370:ILE:HG23 | 2.02                     | 0.41              |
| 1:A:59:ALA:CB    | 1:A:246:VAL:HG23 | 2.51                     | 0.41              |
| 1:B:10:ASP:CB    | 1:B:25:VAL:HG11  | 2.43                     | 0.41              |
| 1:F:331:GLU:O    | 1:F:335:GLN:HG3  | 2.21                     | 0.41              |
| 1:G:289:SER:OG   | 1:H:352:GLU:OE2  | 2.24                     | 0.41              |
| 1:B:229:ALA:HB1  | 1:B:233:GLY:HA2  | 2.03                     | 0.41              |
| 1:C:178:PHE:O    | 1:C:198:GLY:N    | 2.54                     | 0.41              |
| 1:G:362:GLU:N    | 1:G:363:PRO:CD   | 2.83                     | 0.41              |
| 1:F:379:VAL:HG13 | 1:G:36:ILE:HG23  | 2.02                     | 0.41              |
| 1:H:207:VAL:HG22 | 1:H:210:ARG:HH22 | 1.85                     | 0.41              |
| 1:A:281:LEU:HD22 | 1:A:376:MET:SD   | 2.61                     | 0.41              |
| 1:B:52:VAL:HA    | 1:B:250:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:362:GLU:N    | 1:B:363:PRO:CD   | 2.85                     | 0.41              |
| 1:A:320:ILE:HG21 | 1:D:236:LEU:HD23 | 2.03                     | 0.41              |
| 1:E:167:MET:HE2  | 1:E:288:MET:CE   | 2.51                     | 0.41              |
| 1:E:226:ASN:HB3  | 1:E:267:ALA:HB1  | 2.02                     | 0.41              |
| 1:E:214:ARG:HD3  | 1:F:276:GLU:OE2  | 2.22                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:156:LEU:HB3  | 1:A:373:ILE:HG21 | 2.02                     | 0.40              |
| 1:B:379:VAL:HG13 | 1:C:36:ILE:HD12  | 1.97                     | 0.40              |
| 1:E:153:VAL:CG2  | 1:E:369:LEU:HD23 | 2.51                     | 0.40              |
| 1:E:379:VAL:HG13 | 1:H:36:ILE:HG23  | 2.04                     | 0.40              |
| 1:E:207:VAL:HB   | 1:F:270:ASN:ND2  | 2.37                     | 0.40              |
| 1:G:8:GLU:CB     | 1:G:25:VAL:HG23  | 2.51                     | 0.40              |
| 1:H:223:TYR:CE2  | 1:H:257:PRO:HD2  | 2.56                     | 0.40              |
| 1:A:229:ALA:HB1  | 1:A:233:GLY:HA2  | 2.02                     | 0.40              |
| 1:B:331:GLU:O    | 1:B:335:GLN:HG3  | 2.21                     | 0.40              |
| 1:C:279:SER:HB3  | 1:D:279:SER:HB3  | 2.03                     | 0.40              |
| 1:D:295:LEU:HA   | 1:D:298:MET:HE3  | 2.02                     | 0.40              |
| 1:H:211:ASP:OD1  | 1:H:287:ASN:ND2  | 2.55                     | 0.40              |
| 1:A:242:TYR:CZ   | 1:A:246:VAL:HG21 | 2.56                     | 0.40              |
| 1:E:229:ALA:HB2  | 1:E:264:LEU:HB3  | 2.02                     | 0.40              |
| 1:E:320:ILE:HG22 | 1:E:321:MET:N    | 2.36                     | 0.40              |
| 1:F:70:VAL:HG13  | 1:F:129:ILE:HG12 | 2.03                     | 0.40              |
| 1:F:168:GLN:NE2  | 1:F:209:ALA:HB2  | 2.37                     | 0.40              |
| 1:G:160:LEU:O    | 1:G:161:ILE:C    | 2.59                     | 0.40              |
| 1:E:149:THR:HG21 | 1:E:366:PHE:CD1  | 2.56                     | 0.40              |
| 1:G:161:ILE:HD13 | 1:G:216:ALA:HB2  | 2.02                     | 0.40              |
| 1:G:353:ALA:HB3  | 1:G:361:MET:HG3  | 2.02                     | 0.40              |
| 1:H:153:VAL:HG12 | 1:H:222:LEU:CD2  | 2.50                     | 0.40              |
| 1:A:346:THR:HG23 | 1:D:338:PHE:O    | 2.20                     | 0.40              |
| 1:B:157:LEU:CD1  | 1:B:373:ILE:CD1  | 2.96                     | 0.40              |
| 1:C:92:VAL:HG13  | 1:C:106:ASN:OD1  | 2.21                     | 0.40              |
| 1:F:346:THR:HG23 | 1:G:338:PHE:C    | 2.42                     | 0.40              |
| 1:G:241:GLU:O    | 1:G:245:ILE:HD13 | 2.22                     | 0.40              |
| 1:H:285:MET:HG3  | 1:H:340:VAL:HG21 | 2.04                     | 0.40              |
| 1:H:343:ASN:N    | 1:H:343:ASN:HD22 | 2.19                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 388/401 (97%)   | 365 (94%)  | 22 (6%)  | 1 (0%)   | 41          | 76  |
| 1   | B     | 388/401 (97%)   | 369 (95%)  | 19 (5%)  | 0        | 100         | 100 |
| 1   | C     | 379/401 (94%)   | 357 (94%)  | 22 (6%)  | 0        | 100         | 100 |
| 1   | D     | 388/401 (97%)   | 364 (94%)  | 24 (6%)  | 0        | 100         | 100 |
| 1   | E     | 389/401 (97%)   | 360 (92%)  | 28 (7%)  | 1 (0%)   | 41          | 76  |
| 1   | F     | 388/401 (97%)   | 359 (92%)  | 29 (8%)  | 0        | 100         | 100 |
| 1   | G     | 380/401 (95%)   | 360 (95%)  | 20 (5%)  | 0        | 100         | 100 |
| 1   | H     | 388/401 (97%)   | 359 (92%)  | 29 (8%)  | 0        | 100         | 100 |
| All | All   | 3088/3208 (96%) | 2893 (94%) | 193 (6%) | 2 (0%)   | 51          | 85  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 318 | SER  |
| 1   | A     | 354 | GLY  |

### 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     | 328/339 (97%)   | 319 (97%)  | 9 (3%)   | 44          | 77 |
| 1   | B     | 328/339 (97%)   | 319 (97%)  | 9 (3%)   | 44          | 77 |
| 1   | C     | 322/339 (95%)   | 313 (97%)  | 9 (3%)   | 43          | 77 |
| 1   | D     | 328/339 (97%)   | 319 (97%)  | 9 (3%)   | 44          | 77 |
| 1   | E     | 329/339 (97%)   | 321 (98%)  | 8 (2%)   | 49          | 79 |
| 1   | F     | 328/339 (97%)   | 319 (97%)  | 9 (3%)   | 44          | 77 |
| 1   | G     | 323/339 (95%)   | 314 (97%)  | 9 (3%)   | 43          | 77 |
| 1   | H     | 328/339 (97%)   | 314 (96%)  | 14 (4%)  | 29          | 66 |
| All | All   | 2614/2712 (96%) | 2538 (97%) | 76 (3%)  | 42          | 76 |

All (76) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 26  | GLN  |
| 1   | A     | 29  | ARG  |
| 1   | A     | 106 | ASN  |
| 1   | A     | 128 | LYS  |
| 1   | A     | 210 | ARG  |
| 1   | A     | 273 | CYS  |
| 1   | A     | 315 | GLN  |
| 1   | A     | 357 | GLU  |
| 1   | A     | 394 | ASN  |
| 1   | B     | 106 | ASN  |
| 1   | B     | 128 | LYS  |
| 1   | B     | 132 | ASN  |
| 1   | B     | 170 | GLU  |
| 1   | B     | 282 | LYS  |
| 1   | B     | 315 | GLN  |
| 1   | B     | 357 | GLU  |
| 1   | B     | 369 | LEU  |
| 1   | B     | 377 | THR  |
| 1   | C     | 29  | ARG  |
| 1   | C     | 106 | ASN  |
| 1   | C     | 128 | LYS  |
| 1   | C     | 132 | ASN  |
| 1   | C     | 170 | GLU  |
| 1   | C     | 210 | ARG  |
| 1   | C     | 237 | ASN  |
| 1   | C     | 252 | LYS  |
| 1   | C     | 352 | GLU  |
| 1   | D     | 29  | ARG  |
| 1   | D     | 72  | GLN  |
| 1   | D     | 106 | ASN  |
| 1   | D     | 172 | MET  |
| 1   | D     | 190 | GLN  |
| 1   | D     | 210 | ARG  |
| 1   | D     | 252 | LYS  |
| 1   | D     | 352 | GLU  |
| 1   | D     | 357 | GLU  |
| 1   | E     | 11  | PHE  |
| 1   | E     | 106 | ASN  |
| 1   | E     | 170 | GLU  |
| 1   | E     | 271 | THR  |
| 1   | E     | 315 | GLN  |
| 1   | E     | 352 | GLU  |
| 1   | E     | 357 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 359 | ASN  |
| 1   | F     | 29  | ARG  |
| 1   | F     | 106 | ASN  |
| 1   | F     | 128 | LYS  |
| 1   | F     | 132 | ASN  |
| 1   | F     | 170 | GLU  |
| 1   | F     | 190 | GLN  |
| 1   | F     | 321 | MET  |
| 1   | F     | 352 | GLU  |
| 1   | F     | 357 | GLU  |
| 1   | G     | 29  | ARG  |
| 1   | G     | 88  | ASP  |
| 1   | G     | 106 | ASN  |
| 1   | G     | 132 | ASN  |
| 1   | G     | 170 | GLU  |
| 1   | G     | 252 | LYS  |
| 1   | G     | 265 | VAL  |
| 1   | G     | 352 | GLU  |
| 1   | G     | 395 | GLU  |
| 1   | H     | 25  | VAL  |
| 1   | H     | 29  | ARG  |
| 1   | H     | 106 | ASN  |
| 1   | H     | 128 | LYS  |
| 1   | H     | 132 | ASN  |
| 1   | H     | 138 | SER  |
| 1   | H     | 170 | GLU  |
| 1   | H     | 172 | MET  |
| 1   | H     | 190 | GLN  |
| 1   | H     | 210 | ARG  |
| 1   | H     | 252 | LYS  |
| 1   | H     | 271 | THR  |
| 1   | H     | 352 | GLU  |
| 1   | H     | 357 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 26  | GLN  |
| 1   | B     | 226 | ASN  |
| 1   | C     | 26  | GLN  |
| 1   | C     | 132 | ASN  |
| 1   | C     | 249 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 226 | ASN  |
| 1   | G     | 190 | GLN  |
| 1   | G     | 315 | GLN  |
| 1   | H     | 256 | 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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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     | 390/401 (97%)   | -0.05  | 5 (1%)    | 77 51 | 35, 60, 107, 124      | 0       |
| 1   | B     | 390/401 (97%)   | -0.02  | 8 (2%)    | 63 34 | 37, 65, 106, 120      | 0       |
| 1   | C     | 383/401 (95%)   | -0.04  | 7 (1%)    | 68 40 | 40, 63, 105, 119      | 0       |
| 1   | D     | 390/401 (97%)   | -0.06  | 6 (1%)    | 73 46 | 36, 61, 101, 116      | 0       |
| 1   | E     | 391/401 (97%)   | 0.01   | 5 (1%)    | 77 51 | 36, 60, 107, 124      | 0       |
| 1   | F     | 390/401 (97%)   | 0.01   | 8 (2%)    | 63 34 | 37, 64, 106, 120      | 0       |
| 1   | G     | 384/401 (95%)   | -0.04  | 2 (0%)    | 91 75 | 40, 64, 105, 119      | 0       |
| 1   | H     | 390/401 (97%)   | -0.06  | 2 (0%)    | 91 75 | 36, 61, 101, 116      | 0       |
| All | All   | 3108/3208 (96%) | -0.03  | 43 (1%)   | 75 49 | 35, 62, 105, 124      | 0       |

All (43) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 237 | ASN  | 9.5  |
| 1   | B     | 237 | ASN  | 6.0  |
| 1   | E     | 134 | HIS  | 5.5  |
| 1   | C     | 237 | ASN  | 5.4  |
| 1   | C     | 21  | ALA  | 4.3  |
| 1   | D     | 20  | ASP  | 4.2  |
| 1   | G     | 237 | ASN  | 3.9  |
| 1   | D     | 134 | HIS  | 3.7  |
| 1   | A     | 16  | GLU  | 3.2  |
| 1   | D     | 231 | ALA  | 3.1  |
| 1   | H     | 317 | GLY  | 3.0  |
| 1   | A     | 20  | ASP  | 2.9  |
| 1   | B     | 323 | GLY  | 2.8  |
| 1   | E     | 122 | GLU  | 2.6  |
| 1   | D     | 316 | PRO  | 2.6  |
| 1   | E     | 135 | VAL  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 324 | LYS  | 2.6  |
| 1   | F     | 66  | LEU  | 2.6  |
| 1   | A     | 132 | ASN  | 2.5  |
| 1   | B     | 235 | GLY  | 2.5  |
| 1   | F     | 54  | LYS  | 2.5  |
| 1   | C     | 14  | GLU  | 2.5  |
| 1   | C     | 238 | ALA  | 2.4  |
| 1   | F     | 231 | ALA  | 2.4  |
| 1   | E     | 120 | GLY  | 2.3  |
| 1   | F     | 19  | LYS  | 2.3  |
| 1   | B     | 123 | LYS  | 2.3  |
| 1   | A     | 234 | THR  | 2.3  |
| 1   | H     | 24  | GLY  | 2.3  |
| 1   | C     | 231 | ALA  | 2.3  |
| 1   | B     | 322 | PRO  | 2.2  |
| 1   | A     | 134 | HIS  | 2.2  |
| 1   | F     | 323 | GLY  | 2.2  |
| 1   | F     | 5   | VAL  | 2.2  |
| 1   | D     | 232 | VAL  | 2.2  |
| 1   | D     | 237 | ASN  | 2.1  |
| 1   | C     | 235 | GLY  | 2.1  |
| 1   | B     | 16  | GLU  | 2.1  |
| 1   | B     | 19  | LYS  | 2.1  |
| 1   | C     | 9   | LYS  | 2.1  |
| 1   | G     | 107 | ALA  | 2.1  |
| 1   | E     | 119 | MET  | 2.1  |
| 1   | B     | 304 | ALA  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | CA   | B     | 402 | 1/1   | 0.93 | 0.23 | 80,80,80,80                 | 0     |
| 2   | CA   | F     | 402 | 1/1   | 0.94 | 0.24 | 87,87,87,87                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.