



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 PM UTC

PDB ID : 1MC8 / pdb\_00001mc8  
Title : Crystal Structure of Flap Endonuclease-1 R42E mutant from *Pyrococcus horikoshii*  
Authors : Matsui, E.; Musti, K.V.; Abe, J.; Yamazaki, K.; Matsui, I.; Harata, K.  
Deposited on : 2002-08-06  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

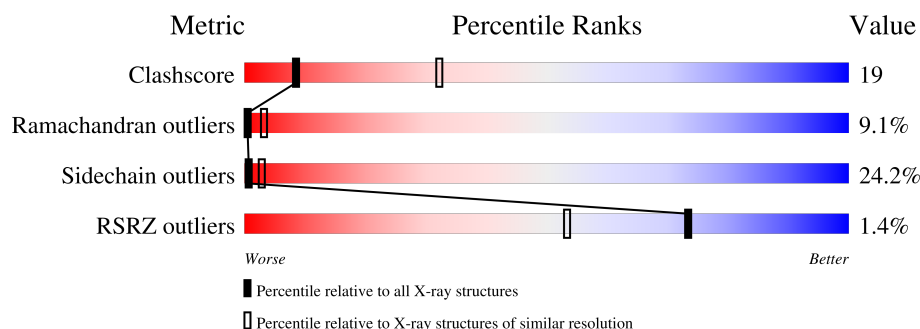
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1539 (3.10-3.10)                                      |
| Ramachandran outliers | 187476                      | 1467 (3.10-3.10)                                      |
| Sidechain outliers    | 187428                      | 1467 (3.10-3.10)                                      |
| RSRZ outliers         | 180081                      | 1456 (3.10-3.10)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 343    | <div> <div>29%</div> <div>39%</div> <div>21%</div> <div>8%</div> <div>•</div> </div> |
| 1   | B     | 343    | <div> <div>31%</div> <div>44%</div> <div>17%</div> <div>5%</div> <div>•</div> </div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5274 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.

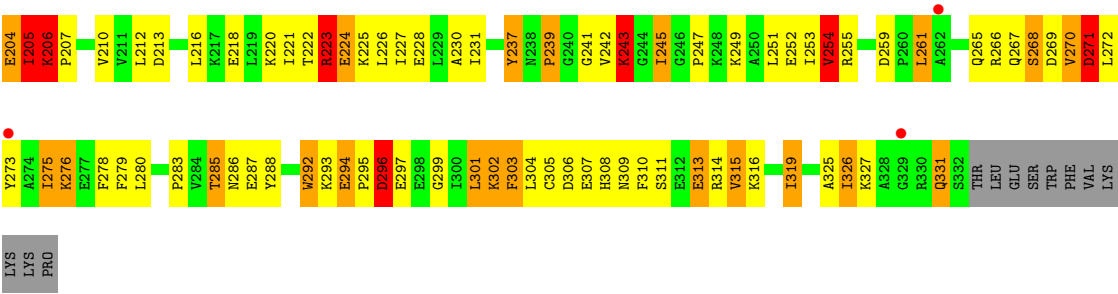
- Molecule 1 is a protein called Flap Endonuclease-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 331      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2637  | 1683 | 453 | 494 | 7 |         |         |       |
| 1   | B     | 331      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2637  | 1683 | 453 | 494 | 7 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 42      | GLU      | ARG    | engineered mutation | UNP O50123 |
| B     | 42      | GLU      | ARG    | engineered mutation | UNP O50123 |





## 4 Data and refinement statistics

| Property                                                                | Value                                                          | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------|------------------|
| Space group                                                             | P 31                                                           | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 62.67Å 62.67Å 180.69Å<br>90.00° 90.00° 120.00°                 | Depositor        |
| Resolution (Å)                                                          | 8.00 – 3.10<br>8.00 – 3.10                                     | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (8.00-3.10)<br>100.0 (8.00-3.10)               | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                           | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.55 (at 3.00Å)                                                | Xtriage          |
| Refinement program                                                      | X-PLOR                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.190 , 0.279<br>0.194 , (Not available)                       | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                         | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 76.7                                                           | Xtriage          |
| Anisotropy                                                              | 0.112                                                          | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 70.2                                                    | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$    | Xtriage          |
| Estimated twinning fraction                                             | 0.021 for -h,-k,l<br>0.469 for h,-h-k,-l<br>0.025 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.98                                                           | EDS              |
| Total number of atoms                                                   | 5274                                                           | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 41.0                                                           | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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     | 1.24         | 8/2682 (0.3%)  | 2.41        | 168/3606 (4.7%) |
| 1   | B     | 1.16         | 4/2682 (0.1%)  | 2.31        | 147/3606 (4.1%) |
| All | All   | 1.20         | 12/5364 (0.2%) | 2.36        | 315/7212 (4.4%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 4                   |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 326 | ILE  | CA-CB   | 8.87  | 1.65        | 1.54     |
| 1   | B     | 73  | ILE  | CA-CB   | 8.45  | 1.65        | 1.54     |
| 1   | A     | 54  | ILE  | CA-CB   | 8.35  | 1.63        | 1.54     |
| 1   | A     | 57  | HIS  | CD2-NE2 | -6.73 | 1.30        | 1.37     |
| 1   | A     | 105 | TRP  | CA-CB   | 6.43  | 1.61        | 1.52     |
| 1   | A     | 146 | ILE  | CA-CB   | 6.34  | 1.60        | 1.53     |
| 1   | A     | 308 | HIS  | CD2-NE2 | -6.31 | 1.30        | 1.37     |
| 1   | B     | 57  | HIS  | CD2-NE2 | -5.89 | 1.31        | 1.37     |
| 1   | B     | 308 | HIS  | CD2-NE2 | -5.80 | 1.31        | 1.37     |
| 1   | A     | 9   | VAL  | CA-CB   | 5.72  | 1.59        | 1.53     |
| 1   | B     | 254 | VAL  | CA-CB   | 5.22  | 1.61        | 1.54     |
| 1   | A     | 203 | VAL  | CA-CB   | 5.01  | 1.61        | 1.54     |

All (315) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | A     | 118 | ARG  | N-CA-C   | -14.19 | 93.81       | 112.68   |
| 1   | A     | 213 | ASP  | CA-CB-CG | 13.01  | 125.61      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 1   | A     | 156 | GLN  | N-CA-C     | -12.45 | 96.38       | 111.69   |
| 1   | B     | 84  | PRO  | N-CA-C     | 11.64  | 128.99      | 113.40   |
| 1   | A     | 86  | PHE  | N-CA-C     | 11.45  | 126.81      | 113.19   |
| 1   | A     | 200 | ASP  | N-CA-C     | -11.26 | 90.06       | 108.41   |
| 1   | A     | 271 | ASP  | CA-CB-CG   | 11.15  | 123.75      | 112.60   |
| 1   | A     | 8   | LEU  | CA-C-N     | -11.02 | 114.66      | 122.59   |
| 1   | A     | 8   | LEU  | C-N-CA     | -11.02 | 114.66      | 122.59   |
| 1   | B     | 9   | VAL  | N-CA-CB    | -10.99 | 95.82       | 111.21   |
| 1   | B     | 87  | LYS  | N-CA-C     | 10.74  | 126.38      | 110.48   |
| 1   | B     | 167 | TYR  | N-CA-C     | -10.60 | 99.26       | 111.03   |
| 1   | A     | 86  | PHE  | CA-CB-CG   | -10.52 | 103.28      | 113.80   |
| 1   | B     | 213 | ASP  | CA-CB-CG   | 10.36  | 122.95      | 112.60   |
| 1   | A     | 106 | LYS  | N-CA-C     | -10.34 | 88.78       | 110.80   |
| 1   | A     | 80  | ASP  | CA-CB-CG   | 10.16  | 122.76      | 112.60   |
| 1   | B     | 30  | ASN  | OD1-CG-ND2 | -10.10 | 112.50      | 122.60   |
| 1   | B     | 43  | ASP  | CA-CB-CG   | 9.99   | 122.59      | 112.60   |
| 1   | B     | 49  | ASP  | CA-CB-CG   | 9.96   | 122.56      | 112.60   |
| 1   | A     | 27  | ASP  | CA-CB-CG   | 9.65   | 122.25      | 112.60   |
| 1   | A     | 69  | MET  | N-CA-C     | -9.59  | 100.90      | 111.36   |
| 1   | B     | 66  | ILE  | N-CA-C     | -9.59  | 102.54      | 111.45   |
| 1   | A     | 319 | ILE  | CB-CA-C    | -9.50  | 99.31       | 112.14   |
| 1   | B     | 205 | ILE  | N-CA-C     | 9.50   | 129.10      | 109.34   |
| 1   | B     | 269 | ASP  | CA-CB-CG   | 9.02   | 121.62      | 112.60   |
| 1   | B     | 113 | ASN  | OD1-CG-ND2 | -9.00  | 113.60      | 122.60   |
| 1   | A     | 325 | ALA  | N-CA-C     | 8.94   | 121.11      | 111.36   |
| 1   | B     | 113 | ASN  | CA-CB-CG   | 8.91   | 121.51      | 112.60   |
| 1   | A     | 331 | GLN  | N-CA-C     | -8.88  | 91.89       | 110.80   |
| 1   | A     | 92  | GLU  | CB-CG-CD   | 8.72   | 127.43      | 112.60   |
| 1   | B     | 13  | GLU  | CA-CB-CG   | 8.65   | 131.40      | 114.10   |
| 1   | A     | 53  | ARG  | N-CA-C     | 8.59   | 122.03      | 110.35   |
| 1   | B     | 67  | ASN  | OD1-CG-ND2 | -8.58  | 114.02      | 122.60   |
| 1   | A     | 284 | VAL  | N-CA-C     | 8.53   | 120.40      | 108.12   |
| 1   | B     | 239 | PRO  | N-CA-C     | 8.52   | 124.97      | 113.98   |
| 1   | B     | 303 | PHE  | CA-CB-CG   | 8.51   | 122.31      | 113.80   |
| 1   | B     | 144 | ILE  | N-CA-CB    | -8.48  | 102.53      | 111.61   |
| 1   | A     | 82  | LYS  | N-CA-C     | -8.37  | 97.03       | 109.42   |
| 1   | A     | 328 | ALA  | N-CA-C     | 8.37   | 123.53      | 113.16   |
| 1   | B     | 57  | HIS  | CA-CB-CG   | 8.35   | 122.15      | 113.80   |
| 1   | A     | 31  | ALA  | N-CA-C     | -8.30  | 101.15      | 111.11   |
| 1   | B     | 326 | ILE  | N-CA-C     | 8.21   | 119.95      | 111.00   |
| 1   | A     | 49  | ASP  | CA-CB-CG   | 8.21   | 120.81      | 112.60   |
| 1   | A     | 291 | SER  | CA-C-O     | -8.17  | 111.74      | 121.05   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 105 | TRP  | N-CA-C     | -8.13 | 93.48       | 110.80   |
| 1   | A     | 296 | ASP  | CA-CB-CG   | 8.11  | 120.71      | 112.60   |
| 1   | A     | 199 | LYS  | N-CA-C     | -8.11 | 93.54       | 110.80   |
| 1   | A     | 330 | ARG  | N-CA-C     | 8.02  | 127.87      | 110.80   |
| 1   | B     | 83  | PRO  | N-CA-C     | 7.99  | 120.45      | 110.70   |
| 1   | B     | 30  | ASN  | CB-CG-ND2  | 7.99  | 128.38      | 116.40   |
| 1   | A     | 316 | LYS  | N-CA-C     | -7.85 | 102.66      | 111.14   |
| 1   | B     | 93  | LYS  | N-CA-C     | 7.83  | 121.88      | 110.28   |
| 1   | A     | 104 | LYS  | N-CA-C     | -7.81 | 94.16       | 110.80   |
| 1   | A     | 188 | LEU  | N-CA-C     | 7.81  | 119.79      | 111.28   |
| 1   | A     | 113 | ASN  | OD1-CG-ND2 | -7.77 | 114.83      | 122.60   |
| 1   | A     | 111 | LYS  | N-CA-C     | -7.71 | 102.87      | 111.82   |
| 1   | B     | 114 | LEU  | N-CA-C     | 7.70  | 120.97      | 108.41   |
| 1   | B     | 163 | LYS  | N-CA-C     | -7.63 | 98.16       | 109.15   |
| 1   | B     | 18  | ASN  | OD1-CG-ND2 | -7.60 | 115.00      | 122.60   |
| 1   | A     | 31  | ALA  | CA-C-O     | -7.46 | 112.92      | 120.90   |
| 1   | B     | 3   | VAL  | N-CA-CB    | -7.46 | 100.77      | 111.21   |
| 1   | B     | 116 | GLU  | N-CA-C     | -7.46 | 103.23      | 111.36   |
| 1   | B     | 32  | ILE  | N-CA-C     | -7.41 | 103.11      | 110.30   |
| 1   | A     | 113 | ASN  | N-CA-C     | 7.40  | 120.14      | 108.67   |
| 1   | B     | 271 | ASP  | N-CA-C     | 7.40  | 126.56      | 110.80   |
| 1   | B     | 80  | ASP  | CA-CB-CG   | 7.36  | 119.96      | 112.60   |
| 1   | A     | 106 | LYS  | CA-CB-CG   | -7.33 | 99.43       | 114.10   |
| 1   | A     | 205 | ILE  | O-C-N      | 7.32  | 131.72      | 122.57   |
| 1   | A     | 156 | GLN  | CA-C-O     | -7.29 | 112.14      | 120.24   |
| 1   | A     | 266 | ARG  | N-CA-C     | -7.26 | 103.06      | 110.97   |
| 1   | B     | 21  | GLY  | N-CA-C     | -7.25 | 105.50      | 114.92   |
| 1   | A     | 319 | ILE  | N-CA-CB    | 7.24  | 120.39      | 110.54   |
| 1   | A     | 28  | ALA  | CA-C-O     | -7.24 | 113.40      | 121.00   |
| 1   | A     | 308 | HIS  | CA-CB-CG   | -7.23 | 106.57      | 113.80   |
| 1   | A     | 35  | PHE  | CA-C-O     | -7.23 | 113.21      | 120.80   |
| 1   | A     | 127 | VAL  | O-C-N      | 7.21  | 131.58      | 122.57   |
| 1   | B     | 242 | VAL  | N-CA-C     | -7.19 | 97.23       | 108.23   |
| 1   | A     | 90  | GLU  | N-CA-C     | 7.18  | 126.10      | 110.80   |
| 1   | A     | 250 | ALA  | N-CA-C     | -7.18 | 103.45      | 111.28   |
| 1   | B     | 142 | MET  | CA-CB-CG   | 7.18  | 128.45      | 114.10   |
| 1   | B     | 20  | TYR  | CA-CB-CG   | 7.17  | 126.81      | 113.90   |
| 1   | B     | 135 | ALA  | N-CA-C     | -7.17 | 101.72      | 112.04   |
| 1   | A     | 292 | TRP  | N-CA-C     | 7.14  | 126.01      | 110.80   |
| 1   | B     | 331 | GLN  | CA-C-O     | -7.12 | 114.63      | 119.68   |
| 1   | B     | 131 | LEU  | CA-C-O     | -7.10 | 113.36      | 120.82   |
| 1   | A     | 268 | SER  | N-CA-C     | 7.09  | 125.89      | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 332 | SER  | CA-CB-OG   | -7.08 | 96.93       | 111.10   |
| 1   | B     | 87  | LYS  | N-CA-CB    | -7.05 | 99.58       | 110.29   |
| 1   | A     | 294 | GLU  | CA-C-O     | -6.97 | 114.21      | 120.56   |
| 1   | B     | 315 | VAL  | N-CA-C     | -6.95 | 103.75      | 110.42   |
| 1   | A     | 105 | TRP  | CA-CB-CG   | 6.94  | 126.79      | 113.60   |
| 1   | A     | 238 | ASN  | CA-C-N     | 6.92  | 128.49      | 119.84   |
| 1   | A     | 238 | ASN  | C-N-CA     | 6.92  | 128.49      | 119.84   |
| 1   | A     | 120 | TYR  | N-CA-C     | -6.87 | 96.17       | 110.80   |
| 1   | A     | 66  | ILE  | O-C-N      | -6.85 | 115.20      | 121.91   |
| 1   | B     | 306 | ASP  | CA-CB-CG   | 6.83  | 119.43      | 112.60   |
| 1   | A     | 290 | LEU  | O-C-N      | -6.82 | 113.52      | 122.59   |
| 1   | A     | 110 | ALA  | N-CA-C     | 6.82  | 125.32      | 110.80   |
| 1   | B     | 144 | ILE  | CB-CA-C    | 6.80  | 117.65      | 110.37   |
| 1   | B     | 122 | GLN  | OE1-CD-NE2 | -6.77 | 115.83      | 122.60   |
| 1   | B     | 102 | GLU  | CA-C-O     | 6.77  | 129.58      | 121.66   |
| 1   | A     | 285 | THR  | CA-CB-OG1  | -6.74 | 99.49       | 109.60   |
| 1   | B     | 144 | ILE  | N-CA-C     | -6.74 | 100.55      | 107.89   |
| 1   | A     | 55  | THR  | N-CA-CB    | -6.68 | 100.59      | 111.01   |
| 1   | B     | 33  | TYR  | CA-CB-CG   | -6.63 | 101.96      | 113.90   |
| 1   | B     | 113 | ASN  | O-C-N      | -6.63 | 113.77      | 122.59   |
| 1   | A     | 289 | SER  | N-CA-C     | -6.62 | 98.61       | 109.40   |
| 1   | B     | 140 | GLN  | OE1-CD-NE2 | -6.60 | 116.00      | 122.60   |
| 1   | A     | 172 | GLN  | N-CA-C     | -6.60 | 105.54      | 112.93   |
| 1   | B     | 145 | PRO  | N-CA-C     | 6.60  | 121.44      | 111.14   |
| 1   | A     | 127 | VAL  | CA-C-O     | 6.59  | 129.01      | 120.78   |
| 1   | A     | 15  | ASP  | CA-CB-CG   | -6.58 | 106.02      | 112.60   |
| 1   | B     | 93  | LYS  | CA-C-O     | 6.56  | 128.50      | 121.16   |
| 1   | A     | 278 | PHE  | N-CA-CB    | -6.54 | 100.58      | 110.07   |
| 1   | B     | 113 | ASN  | CB-CG-ND2  | 6.54  | 126.21      | 116.40   |
| 1   | A     | 201 | VAL  | CB-CA-C    | -6.54 | 102.80      | 110.91   |
| 1   | B     | 83  | PRO  | CA-C-N     | 6.53  | 125.97      | 118.85   |
| 1   | B     | 83  | PRO  | C-N-CA     | 6.53  | 125.97      | 118.85   |
| 1   | A     | 7   | ASP  | CA-CB-CG   | 6.52  | 119.12      | 112.60   |
| 1   | B     | 80  | ASP  | O-C-N      | 6.49  | 130.19      | 122.79   |
| 1   | B     | 91  | LEU  | N-CA-C     | -6.49 | 96.98       | 110.80   |
| 1   | B     | 33  | TYR  | N-CA-C     | 6.48  | 118.35      | 111.28   |
| 1   | A     | 201 | VAL  | N-CA-CB    | 6.48  | 117.78      | 110.72   |
| 1   | A     | 270 | VAL  | CB-CA-C    | 6.43  | 118.66      | 111.45   |
| 1   | A     | 292 | TRP  | CG-CD2-CE3 | 6.42  | 140.32      | 133.90   |
| 1   | B     | 3   | VAL  | CA-C-N     | 6.39  | 127.82      | 119.84   |
| 1   | B     | 3   | VAL  | C-N-CA     | 6.39  | 127.82      | 119.84   |
| 1   | A     | 123 | ARG  | CA-CB-CG   | 6.37  | 126.83      | 114.10   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 184 | LEU  | N-CA-C     | -6.36 | 97.19       | 108.13   |
| 1   | A     | 181 | ALA  | CA-C-N     | 6.35  | 125.84      | 119.24   |
| 1   | A     | 181 | ALA  | C-N-CA     | 6.35  | 125.84      | 119.24   |
| 1   | A     | 297 | GLU  | CA-C-O     | -6.32 | 113.84      | 120.92   |
| 1   | B     | 193 | LYS  | N-CA-C     | 6.31  | 119.85      | 108.17   |
| 1   | A     | 155 | ALA  | N-CA-C     | 6.30  | 118.95      | 111.71   |
| 1   | B     | 148 | GLN  | N-CA-C     | -6.29 | 102.41      | 110.53   |
| 1   | A     | 205 | ILE  | CA-CB-CG2  | -6.29 | 99.81       | 110.50   |
| 1   | B     | 267 | GLN  | N-CA-C     | -6.22 | 100.84      | 110.10   |
| 1   | B     | 331 | GLN  | N-CA-C     | 6.21  | 118.72      | 108.48   |
| 1   | A     | 42  | GLU  | CA-CB-CG   | 6.18  | 126.47      | 114.10   |
| 1   | B     | 28  | ALA  | CB-CA-C    | -6.17 | 101.16      | 110.90   |
| 1   | B     | 267 | GLN  | O-C-N      | 6.15  | 130.58      | 122.95   |
| 1   | A     | 308 | HIS  | CB-CG-CD2  | -6.15 | 123.21      | 131.20   |
| 1   | A     | 45  | THR  | N-CA-C     | -6.14 | 102.69      | 108.22   |
| 1   | B     | 218 | GLU  | CA-CB-CG   | -6.13 | 101.84      | 114.10   |
| 1   | A     | 105 | TRP  | CB-CG-CD1  | -6.12 | 117.71      | 126.90   |
| 1   | B     | 9   | VAL  | CA-C-N     | 6.11  | 126.07      | 119.78   |
| 1   | B     | 9   | VAL  | C-N-CA     | 6.11  | 126.07      | 119.78   |
| 1   | B     | 20  | TYR  | O-C-N      | 6.10  | 130.18      | 123.04   |
| 1   | A     | 300 | ILE  | CA-C-O     | -6.08 | 113.18      | 120.78   |
| 1   | B     | 26  | ILE  | O-C-N      | -6.05 | 116.10      | 122.81   |
| 1   | B     | 306 | ASP  | N-CA-C     | -6.04 | 104.32      | 111.03   |
| 1   | B     | 325 | ALA  | O-C-N      | -6.04 | 115.16      | 122.22   |
| 1   | B     | 99  | GLU  | N-CA-C     | -6.03 | 100.97      | 109.96   |
| 1   | B     | 72  | GLY  | CA-C-O     | -6.03 | 112.59      | 118.98   |
| 1   | A     | 106 | LYS  | N-CA-CB    | 6.02  | 120.66      | 110.49   |
| 1   | A     | 321 | ARG  | NE-CZ-NH1  | 6.02  | 127.52      | 121.50   |
| 1   | B     | 114 | LEU  | O-C-N      | -6.01 | 116.30      | 123.27   |
| 1   | B     | 147 | ILE  | N-CA-C     | -6.00 | 97.15       | 107.24   |
| 1   | B     | 102 | GLU  | CB-CG-CD   | 5.99  | 122.78      | 112.60   |
| 1   | B     | 120 | TYR  | CA-CB-CG   | 5.99  | 124.68      | 113.90   |
| 1   | A     | 290 | LEU  | CA-C-O     | -5.99 | 111.95      | 120.51   |
| 1   | A     | 65  | THR  | N-CA-C     | -5.97 | 104.85      | 111.36   |
| 1   | B     | 128 | ASN  | OD1-CG-ND2 | -5.96 | 116.64      | 122.60   |
| 1   | A     | 270 | VAL  | N-CA-C     | -5.95 | 103.49      | 110.21   |
| 1   | A     | 76  | ALA  | O-C-N      | -5.94 | 116.32      | 123.27   |
| 1   | B     | 56  | SER  | N-CA-C     | -5.93 | 104.81      | 111.28   |
| 1   | B     | 111 | LYS  | N-CA-C     | -5.92 | 104.82      | 111.28   |
| 1   | A     | 147 | ILE  | O-C-N      | -5.91 | 116.36      | 122.63   |
| 1   | A     | 156 | GLN  | OE1-CD-NE2 | -5.91 | 116.69      | 122.60   |
| 1   | B     | 259 | ASP  | CA-CB-CG   | 5.91  | 118.51      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 105 | TRP  | CG-CD2-CE3 | 5.90  | 139.80      | 133.90   |
| 1   | A     | 82  | LYS  | CA-C-N     | 5.89  | 123.96      | 119.66   |
| 1   | A     | 82  | LYS  | C-N-CA     | 5.89  | 123.96      | 119.66   |
| 1   | A     | 22  | LYS  | N-CA-C     | 5.88  | 119.21      | 109.46   |
| 1   | A     | 309 | ASN  | N-CA-C     | 5.87  | 123.30      | 110.80   |
| 1   | B     | 223 | ARG  | N-CA-C     | 5.87  | 123.29      | 110.80   |
| 1   | B     | 27  | ASP  | N-CA-C     | -5.85 | 100.99      | 109.59   |
| 1   | A     | 18  | ASN  | OD1-CG-ND2 | -5.85 | 116.75      | 122.60   |
| 1   | A     | 156 | GLN  | CG-CD-NE2  | 5.83  | 125.15      | 116.40   |
| 1   | B     | 73  | ILE  | O-C-N      | -5.83 | 115.32      | 122.61   |
| 1   | B     | 99  | GLU  | CB-CG-CD   | 5.82  | 122.50      | 112.60   |
| 1   | B     | 249 | LYS  | N-CA-C     | -5.81 | 104.86      | 111.14   |
| 1   | A     | 113 | ASN  | CA-C-O     | 5.81  | 127.16      | 120.60   |
| 1   | B     | 309 | ASN  | N-CA-C     | 5.80  | 119.67      | 112.24   |
| 1   | A     | 79  | PHE  | CA-CB-CG   | -5.80 | 108.00      | 113.80   |
| 1   | B     | 313 | GLU  | CB-CG-CD   | 5.79  | 122.45      | 112.60   |
| 1   | B     | 206 | LYS  | O-C-N      | -5.79 | 116.05      | 121.72   |
| 1   | A     | 294 | GLU  | N-CA-C     | 5.76  | 113.20      | 108.07   |
| 1   | B     | 24  | ILE  | O-C-N      | -5.76 | 115.37      | 122.57   |
| 1   | B     | 237 | TYR  | CA-C-O     | 5.75  | 126.39      | 119.43   |
| 1   | B     | 308 | HIS  | CB-CG-CD2  | -5.74 | 123.73      | 131.20   |
| 1   | A     | 265 | GLN  | OE1-CD-NE2 | -5.73 | 116.87      | 122.60   |
| 1   | B     | 230 | ALA  | CA-C-O     | -5.73 | 113.62      | 120.10   |
| 1   | B     | 169 | SER  | O-C-N      | -5.72 | 116.05      | 122.75   |
| 1   | A     | 112 | GLY  | N-CA-C     | -5.72 | 99.62       | 113.18   |
| 1   | A     | 242 | VAL  | N-CA-C     | -5.71 | 100.09      | 108.54   |
| 1   | B     | 9   | VAL  | CB-CA-C    | 5.69  | 121.72      | 111.36   |
| 1   | A     | 202 | TYR  | N-CA-C     | -5.69 | 97.29       | 107.98   |
| 1   | A     | 246 | GLY  | CA-C-O     | -5.68 | 113.39      | 121.52   |
| 1   | A     | 205 | ILE  | CA-CB-CG1  | 5.67  | 120.05      | 110.40   |
| 1   | A     | 232 | LEU  | CA-C-O     | -5.66 | 114.87      | 120.70   |
| 1   | B     | 268 | SER  | N-CA-C     | -5.63 | 98.80       | 110.80   |
| 1   | A     | 149 | ALA  | CA-C-O     | -5.63 | 115.06      | 120.64   |
| 1   | B     | 58  | LEU  | CA-C-O     | -5.62 | 114.91      | 120.70   |
| 1   | A     | 297 | GLU  | CA-CB-CG   | 5.62  | 125.33      | 114.10   |
| 1   | B     | 172 | GLN  | N-CA-C     | -5.61 | 106.11      | 113.12   |
| 1   | B     | 331 | GLN  | OE1-CD-NE2 | -5.60 | 117.00      | 122.60   |
| 1   | A     | 99  | GLU  | CA-CB-CG   | 5.59  | 125.29      | 114.10   |
| 1   | A     | 242 | VAL  | N-CA-CB    | 5.57  | 117.19      | 110.95   |
| 1   | B     | 271 | ASP  | CA-C-O     | 5.57  | 128.47      | 120.51   |
| 1   | B     | 199 | LYS  | CA-C-N     | 5.56  | 132.16      | 121.54   |
| 1   | B     | 199 | LYS  | C-N-CA     | 5.56  | 132.16      | 121.54   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 302 | LYS  | CA-C-O     | -5.55 | 115.18      | 120.90   |
| 1   | B     | 213 | ASP  | CB-CA-C    | -5.55 | 102.09      | 110.92   |
| 1   | B     | 99  | GLU  | CA-CB-CG   | 5.55  | 125.20      | 114.10   |
| 1   | B     | 107 | GLU  | CA-CB-CG   | 5.55  | 125.20      | 114.10   |
| 1   | A     | 205 | ILE  | CA-C-N     | 5.54  | 136.09      | 122.13   |
| 1   | A     | 205 | ILE  | C-N-CA     | 5.54  | 136.09      | 122.13   |
| 1   | B     | 288 | TYR  | N-CA-C     | -5.54 | 100.65      | 109.07   |
| 1   | B     | 149 | ALA  | CA-C-N     | 5.53  | 125.63      | 119.32   |
| 1   | B     | 149 | ALA  | C-N-CA     | 5.53  | 125.63      | 119.32   |
| 1   | B     | 18  | ASN  | CA-CB-CG   | 5.53  | 118.13      | 112.60   |
| 1   | A     | 35  | PHE  | N-CA-C     | -5.52 | 104.11      | 111.24   |
| 1   | A     | 282 | PRO  | CB-CA-C    | 5.52  | 117.66      | 110.92   |
| 1   | A     | 255 | ARG  | CA-C-N     | -5.52 | 114.28      | 122.56   |
| 1   | A     | 255 | ARG  | C-N-CA     | -5.52 | 114.28      | 122.56   |
| 1   | A     | 246 | GLY  | CA-C-N     | 5.51  | 126.73      | 119.84   |
| 1   | A     | 246 | GLY  | C-N-CA     | 5.51  | 126.73      | 119.84   |
| 1   | A     | 43  | ASP  | N-CA-CB    | -5.48 | 103.00      | 110.56   |
| 1   | A     | 100 | GLU  | CA-CB-CG   | -5.48 | 103.15      | 114.10   |
| 1   | A     | 43  | ASP  | CA-CB-CG   | 5.47  | 118.07      | 112.60   |
| 1   | A     | 291 | SER  | N-CA-C     | 5.47  | 118.85      | 110.20   |
| 1   | B     | 109 | LEU  | N-CA-C     | 5.46  | 119.66      | 111.96   |
| 1   | A     | 292 | TRP  | CB-CG-CD1  | -5.46 | 118.72      | 126.90   |
| 1   | A     | 144 | ILE  | N-CA-C     | 5.45  | 120.64      | 108.88   |
| 1   | A     | 215 | VAL  | CG1-CB-CG2 | -5.44 | 98.82       | 110.80   |
| 1   | A     | 251 | LEU  | CB-CA-C    | -5.43 | 99.92       | 110.46   |
| 1   | A     | 251 | LEU  | N-CA-CB    | 5.43  | 118.72      | 110.14   |
| 1   | B     | 18  | ASN  | CB-CG-ND2  | 5.42  | 124.53      | 116.40   |
| 1   | B     | 100 | GLU  | N-CA-C     | -5.41 | 102.29      | 110.24   |
| 1   | B     | 331 | GLN  | CG-CD-NE2  | 5.41  | 124.51      | 116.40   |
| 1   | B     | 196 | MET  | CA-C-N     | 5.40  | 126.59      | 119.84   |
| 1   | B     | 196 | MET  | C-N-CA     | 5.40  | 126.59      | 119.84   |
| 1   | A     | 3   | VAL  | CA-C-N     | 5.38  | 126.57      | 119.84   |
| 1   | A     | 3   | VAL  | C-N-CA     | 5.38  | 126.57      | 119.84   |
| 1   | B     | 108 | ALA  | CA-C-N     | -5.38 | 114.08      | 122.42   |
| 1   | B     | 108 | ALA  | C-N-CA     | -5.38 | 114.08      | 122.42   |
| 1   | A     | 244 | GLY  | O-C-N      | -5.37 | 115.36      | 122.28   |
| 1   | B     | 25  | ALA  | O-C-N      | -5.37 | 115.38      | 122.57   |
| 1   | A     | 111 | LYS  | CA-C-O     | -5.36 | 113.81      | 119.97   |
| 1   | B     | 200 | ASP  | N-CA-C     | -5.35 | 99.40       | 110.80   |
| 1   | A     | 303 | PHE  | CA-CB-CG   | 5.35  | 119.15      | 113.80   |
| 1   | A     | 74  | LYS  | CB-CG-CD   | 5.35  | 123.60      | 111.30   |
| 1   | B     | 243 | LYS  | N-CA-C     | 5.33  | 117.76      | 110.24   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 188 | LEU  | O-C-N      | -5.33 | 116.47      | 122.12   |
| 1   | A     | 242 | VAL  | CB-CA-C    | -5.33 | 104.85      | 111.08   |
| 1   | A     | 169 | SER  | N-CA-C     | -5.32 | 101.89      | 110.14   |
| 1   | A     | 196 | MET  | N-CA-C     | 5.31  | 121.55      | 109.81   |
| 1   | A     | 9   | VAL  | CA-C-O     | 5.30  | 122.28      | 119.15   |
| 1   | A     | 95  | ARG  | O-C-N      | 5.30  | 129.02      | 123.03   |
| 1   | B     | 14  | ILE  | CB-CG1-CD1 | -5.30 | 102.67      | 113.80   |
| 1   | B     | 111 | LYS  | N-CA-CB    | 5.30  | 117.91      | 110.12   |
| 1   | A     | 230 | ALA  | CA-C-O     | -5.30 | 114.26      | 120.20   |
| 1   | B     | 101 | ALA  | N-CA-C     | -5.29 | 99.52       | 110.80   |
| 1   | A     | 270 | VAL  | CA-C-O     | -5.29 | 116.26      | 122.13   |
| 1   | B     | 325 | ALA  | N-CA-C     | 5.28  | 117.78      | 111.71   |
| 1   | B     | 87  | LYS  | CA-C-O     | 5.27  | 127.53      | 121.47   |
| 1   | A     | 99  | GLU  | CB-CG-CD   | 5.26  | 121.55      | 112.60   |
| 1   | A     | 292 | TRP  | CE2-CD2-CG | -5.26 | 100.89      | 107.20   |
| 1   | A     | 285 | THR  | CA-CB-CG2  | 5.24  | 119.41      | 110.50   |
| 1   | A     | 256 | TYR  | CA-CB-CG   | 5.24  | 123.33      | 113.90   |
| 1   | B     | 89  | LYS  | CA-C-O     | 5.24  | 128.00      | 120.51   |
| 1   | B     | 170 | ALA  | N-CA-C     | -5.23 | 101.13      | 109.23   |
| 1   | B     | 129 | GLU  | O-C-N      | 5.23  | 128.70      | 122.27   |
| 1   | B     | 224 | GLU  | CA-CB-CG   | 5.22  | 124.54      | 114.10   |
| 1   | A     | 195 | LYS  | N-CA-C     | 5.21  | 121.91      | 110.80   |
| 1   | B     | 270 | VAL  | CG1-CB-CG2 | -5.20 | 99.35       | 110.80   |
| 1   | B     | 22  | LYS  | N-CA-C     | 5.18  | 117.17      | 109.25   |
| 1   | B     | 31  | ALA  | N-CA-C     | -5.18 | 105.71      | 112.23   |
| 1   | B     | 183 | ARG  | CA-CB-CG   | -5.17 | 103.75      | 114.10   |
| 1   | B     | 200 | ASP  | CA-CB-CG   | 5.17  | 117.77      | 112.60   |
| 1   | A     | 297 | GLU  | CB-CA-C    | -5.15 | 102.19      | 110.74   |
| 1   | A     | 297 | GLU  | N-CA-CB    | 5.15  | 118.17      | 109.78   |
| 1   | A     | 9   | VAL  | CA-C-N     | 5.15  | 126.27      | 119.84   |
| 1   | A     | 9   | VAL  | C-N-CA     | 5.15  | 126.27      | 119.84   |
| 1   | A     | 306 | ASP  | CA-CB-CG   | 5.14  | 117.74      | 112.60   |
| 1   | A     | 205 | ILE  | N-CA-C     | -5.14 | 98.65       | 109.34   |
| 1   | B     | 108 | ALA  | CA-C-O     | -5.13 | 114.30      | 120.10   |
| 1   | A     | 94  | ARG  | CA-CB-CG   | 5.12  | 124.35      | 114.10   |
| 1   | B     | 286 | ASN  | CA-C-N     | -5.12 | 113.31      | 122.32   |
| 1   | B     | 286 | ASN  | C-N-CA     | -5.12 | 113.31      | 122.32   |
| 1   | A     | 267 | GLN  | O-C-N      | 5.12  | 129.39      | 122.59   |
| 1   | A     | 68  | LEU  | CA-C-O     | 5.11  | 125.97      | 120.70   |
| 1   | B     | 86  | PHE  | CA-CB-CG   | 5.11  | 118.91      | 113.80   |
| 1   | A     | 141 | LEU  | N-CA-C     | -5.11 | 105.79      | 111.36   |
| 1   | A     | 96  | GLU  | CB-CG-CD   | 5.10  | 121.27      | 112.60   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | A     | 136 | LYS  | N-CA-C     | -5.10 | 105.72      | 111.28   |
| 1   | B     | 59  | SER  | CB-CA-C    | -5.08 | 102.91      | 110.88   |
| 1   | A     | 114 | LEU  | N-CA-C     | -5.07 | 107.13      | 113.72   |
| 1   | A     | 204 | GLU  | CA-CB-CG   | 5.06  | 124.21      | 114.10   |
| 1   | B     | 292 | TRP  | CE2-CD2-CG | -5.05 | 101.14      | 107.20   |
| 1   | B     | 270 | VAL  | O-C-N      | 5.05  | 128.88      | 122.57   |
| 1   | B     | 196 | MET  | CA-C-O     | -5.03 | 114.96      | 119.59   |
| 1   | B     | 133 | GLU  | CA-CB-CG   | -5.03 | 104.05      | 114.10   |
| 1   | A     | 215 | VAL  | N-CA-C     | -5.03 | 104.81      | 111.09   |
| 1   | A     | 267 | GLN  | N-CA-C     | -5.02 | 100.10      | 110.80   |
| 1   | A     | 267 | GLN  | OE1-CD-NE2 | -5.02 | 117.58      | 122.60   |
| 1   | A     | 164 | GLY  | N-CA-C     | 5.02  | 125.08      | 113.18   |
| 1   | B     | 102 | GLU  | CA-CB-CG   | -5.02 | 104.07      | 114.10   |
| 1   | B     | 204 | GLU  | CA-C-N     | 5.01  | 130.99      | 121.97   |
| 1   | B     | 204 | GLU  | C-N-CA     | 5.01  | 130.99      | 121.97   |
| 1   | A     | 151 | SER  | O-C-N      | -5.01 | 117.49      | 121.65   |
| 1   | A     | 254 | VAL  | N-CA-CB    | -5.01 | 102.97      | 111.23   |
| 1   | A     | 53  | ARG  | CA-CB-CG   | 5.00  | 124.10      | 114.10   |
| 1   | A     | 258 | ARG  | O-C-N      | 5.00  | 129.15      | 122.95   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | B     | 196 | MET  | Peptide   |
| 1   | B     | 20  | TYR  | Sidechain |
| 1   | B     | 82  | LYS  | Peptide   |
| 1   | B     | 83  | PRO  | Peptide   |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2637  | 0        | 2719     | 107     | 0            |
| 1   | B     | 2637  | 0        | 2719     | 100     | 0            |
| All | All   | 5274  | 0        | 5438     | 203     | 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 19.

All (203) 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:14:ILE:HD12  | 1:A:209:LEU:HB2  | 1.59                     | 0.85              |
| 1:A:294:GLU:HG3  | 1:A:326:ILE:HD13 | 1.58                     | 0.84              |
| 1:A:104:LYS:HD3  | 1:A:126:LYS:HD2  | 1.69                     | 0.75              |
| 1:A:221:ILE:HD11 | 1:A:255:ARG:HA   | 1.67                     | 0.74              |
| 1:B:11:ARG:HB3   | 1:B:210:VAL:HG22 | 1.70                     | 0.72              |
| 1:B:11:ARG:HB3   | 1:B:210:VAL:CG2  | 2.19                     | 0.72              |
| 1:B:57:HIS:O     | 1:B:61:LEU:HB2   | 1.90                     | 0.72              |
| 1:B:145:PRO:HD2  | 1:B:292:TRP:CD1  | 2.24                     | 0.71              |
| 1:A:3:VAL:HG22   | 1:A:5:ILE:HG23   | 1.72                     | 0.71              |
| 1:B:138:LEU:HD22 | 1:B:142:MET:SD   | 2.29                     | 0.71              |
| 1:A:294:GLU:HG2  | 1:A:295:PRO:HD3  | 1.73                     | 0.70              |
| 1:A:125:THR:H    | 1:A:126:LYS:HZ2  | 1.40                     | 0.70              |
| 1:A:214:GLU:O    | 1:A:218:GLU:HG2  | 1.92                     | 0.70              |
| 1:A:251:LEU:O    | 1:A:255:ARG:HB2  | 1.91                     | 0.69              |
| 1:B:190:ILE:HD11 | 1:B:201:VAL:HG23 | 1.74                     | 0.69              |
| 1:A:125:THR:N    | 1:A:126:LYS:HZ2  | 1.92                     | 0.68              |
| 1:A:187:ASN:HB2  | 1:A:207:PRO:HA   | 1.76                     | 0.67              |
| 1:B:191:THR:HG23 | 1:B:207:PRO:HD3  | 1.75                     | 0.67              |
| 1:A:305:CYS:SG   | 1:A:312:GLU:HA   | 2.35                     | 0.66              |
| 1:B:29:LEU:HD21  | 1:B:122:GLN:HA   | 1.75                     | 0.66              |
| 1:A:315:VAL:O    | 1:A:319:ILE:HG13 | 1.96                     | 0.65              |
| 1:B:20:TYR:HB3   | 1:B:71:ALA:O     | 1.96                     | 0.65              |
| 1:B:227:ILE:O    | 1:B:231:ILE:HG12 | 1.97                     | 0.64              |
| 1:A:91:LEU:HD12  | 1:A:94:ARG:HG2   | 1.81                     | 0.63              |
| 1:A:16:LEU:HD13  | 1:A:207:PRO:HG3  | 1.78                     | 0.63              |
| 1:A:49:ASP:HA    | 1:A:309:ASN:HD21 | 1.64                     | 0.63              |
| 1:A:16:LEU:CD1   | 1:A:207:PRO:HG3  | 2.28                     | 0.63              |
| 1:A:221:ILE:HG12 | 1:A:255:ARG:HD3  | 1.80                     | 0.63              |
| 1:B:203:VAL:HG12 | 1:B:204:GLU:HG2  | 1.81                     | 0.62              |
| 1:B:61:LEU:HD21  | 1:B:135:ALA:HB1  | 1.81                     | 0.62              |
| 1:B:105:TRP:HE3  | 1:B:106:LYS:HG2  | 1.65                     | 0.62              |
| 1:B:212:LEU:HD21 | 1:B:223:ARG:HD2  | 1.81                     | 0.62              |
| 1:A:183:ARG:HG3  | 1:A:209:LEU:HD21 | 1.82                     | 0.62              |
| 1:B:118:ARG:HG3  | 1:B:122:GLN:HB3  | 1.81                     | 0.61              |
| 1:A:235:THR:HG22 | 1:A:238:ASN:OD1  | 2.00                     | 0.61              |
| 1:B:64:ARG:HH22  | 1:B:191:THR:HB   | 1.66                     | 0.61              |
| 1:B:88:ARG:HB3   | 1:B:93:LYS:HB3   | 1.82                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:79:PHE:HB2   | 1:A:148:GLN:HA   | 1.84                     | 0.60              |
| 1:A:125:THR:H    | 1:A:126:LYS:NZ   | 1.99                     | 0.60              |
| 1:A:312:GLU:O    | 1:A:316:LYS:HG3  | 2.02                     | 0.59              |
| 1:B:119:LYS:HB2  | 1:B:120:TYR:CD2  | 2.37                     | 0.59              |
| 1:A:8:LEU:HD11   | 1:A:247:PRO:HB3  | 1.83                     | 0.59              |
| 1:A:219:LEU:HG   | 1:A:251:LEU:HD21 | 1.85                     | 0.59              |
| 1:A:64:ARG:HE    | 1:A:67:ASN:HD22  | 1.50                     | 0.58              |
| 1:A:109:LEU:HD23 | 1:B:243:LYS:HG2  | 1.86                     | 0.58              |
| 1:A:105:TRP:HA   | 1:A:108:ALA:HB2  | 1.86                     | 0.58              |
| 1:B:311:SER:HB3  | 1:B:314:ARG:HG2  | 1.85                     | 0.58              |
| 1:B:36:LEU:HD11  | 1:B:131:LEU:HD21 | 1.85                     | 0.58              |
| 1:A:19:LEU:HD21  | 1:A:185:ILE:HD13 | 1.86                     | 0.57              |
| 1:B:223:ARG:HG2  | 1:B:223:ARG:HH11 | 1.69                     | 0.57              |
| 1:A:86:PHE:HE1   | 1:A:274:ALA:HB1  | 1.69                     | 0.57              |
| 1:B:41:GLN:HG2   | 1:B:47:LEU:HD23  | 1.85                     | 0.57              |
| 1:B:123:ARG:HH22 | 1:B:239:PRO:HB3  | 1.69                     | 0.57              |
| 1:B:101:ALA:O    | 1:B:103:LEU:HD22 | 2.05                     | 0.57              |
| 1:A:225:LYS:HA   | 1:A:228:GLU:OE1  | 2.06                     | 0.56              |
| 1:B:295:PRO:HD3  | 1:B:326:ILE:HD11 | 1.89                     | 0.55              |
| 1:A:121:ALA:HA   | 1:A:126:LYS:CG   | 2.36                     | 0.55              |
| 1:A:19:LEU:HB3   | 1:A:73:ILE:HG12  | 1.88                     | 0.55              |
| 1:A:235:THR:HG23 | 1:A:237:TYR:H    | 1.72                     | 0.55              |
| 1:B:119:LYS:HB2  | 1:B:120:TYR:HD2  | 1.72                     | 0.55              |
| 1:A:40:ARG:HH22  | 1:A:111:LYS:HG3  | 1.70                     | 0.55              |
| 1:A:121:ALA:HA   | 1:A:126:LYS:HG3  | 1.88                     | 0.55              |
| 1:B:201:VAL:HG22 | 1:B:202:TYR:H    | 1.73                     | 0.54              |
| 1:A:48:MET:HB3   | 1:A:52:GLY:O     | 2.06                     | 0.54              |
| 1:B:23:LYS:HA    | 1:B:74:LYS:O     | 2.08                     | 0.54              |
| 1:A:14:ILE:CD1   | 1:A:209:LEU:HB2  | 2.36                     | 0.54              |
| 1:A:69:MET:HE1   | 1:A:144:ILE:HD11 | 1.90                     | 0.54              |
| 1:B:29:LEU:CD2   | 1:B:122:GLN:HA   | 2.38                     | 0.54              |
| 1:B:237:TYR:CZ   | 1:B:278:PHE:HE2  | 2.25                     | 0.54              |
| 1:B:23:LYS:HD2   | 1:B:165:ASP:O    | 2.09                     | 0.53              |
| 1:B:273:TYR:O    | 1:B:276:LYS:HB2  | 2.08                     | 0.53              |
| 1:B:313:GLU:HA   | 1:B:316:LYS:HB2  | 1.91                     | 0.53              |
| 1:A:249:LYS:O    | 1:A:253:ILE:HG12 | 2.08                     | 0.53              |
| 1:A:141:LEU:O    | 1:A:295:PRO:HA   | 2.08                     | 0.53              |
| 1:A:301:LEU:HD21 | 1:A:316:LYS:HG2  | 1.90                     | 0.52              |
| 1:A:14:ILE:HG22  | 1:A:207:PRO:HG2  | 1.92                     | 0.52              |
| 1:B:39:ILE:HB    | 1:B:56:SER:HB3   | 1.92                     | 0.52              |
| 1:B:150:PRO:HD3  | 1:B:285:THR:HB   | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:211:VAL:HB   | 1:A:214:GLU:HG3  | 1.91                     | 0.52              |
| 1:A:19:LEU:HD22  | 1:A:24:ILE:HD11  | 1.92                     | 0.51              |
| 1:A:41:GLN:HG3   | 1:A:45:THR:O     | 2.09                     | 0.51              |
| 1:A:110:ALA:O    | 1:A:113:ASN:HA   | 2.11                     | 0.51              |
| 1:B:206:LYS:NZ   | 1:B:206:LYS:HB2  | 2.25                     | 0.51              |
| 1:B:123:ARG:NH2  | 1:B:239:PRO:HB3  | 2.26                     | 0.51              |
| 1:B:275:ILE:HG22 | 1:B:279:PHE:CE2  | 2.45                     | 0.51              |
| 1:A:216:LEU:HD21 | 1:A:226:LEU:HD22 | 1.92                     | 0.51              |
| 1:B:225:LYS:HB3  | 1:B:254:VAL:HG13 | 1.92                     | 0.51              |
| 1:B:6:GLY:HA2    | 1:B:174:TYR:CE2  | 2.46                     | 0.51              |
| 1:B:99:GLU:HG3   | 1:B:127:VAL:HG13 | 1.93                     | 0.51              |
| 1:A:126:LYS:N    | 1:A:126:LYS:HD3  | 2.27                     | 0.50              |
| 1:A:221:ILE:HD12 | 1:A:225:LYS:HB3  | 1.93                     | 0.50              |
| 1:A:26:ILE:O     | 1:A:77:TYR:HA    | 2.12                     | 0.50              |
| 1:B:293:LYS:O    | 1:B:326:ILE:HD12 | 2.12                     | 0.50              |
| 1:A:55:THR:HG23  | 1:A:310:PHE:HE1  | 1.76                     | 0.49              |
| 1:B:116:GLU:O    | 1:B:119:LYS:HG3  | 2.13                     | 0.49              |
| 1:B:195:LYS:C    | 1:B:196:MET:SD   | 2.96                     | 0.49              |
| 1:A:114:LEU:HD11 | 1:B:245:ILE:O    | 2.12                     | 0.49              |
| 1:A:123:ARG:CD   | 1:A:126:LYS:HE3  | 2.42                     | 0.49              |
| 1:A:139:LEU:O    | 1:A:142:MET:HB2  | 2.12                     | 0.49              |
| 1:A:258:ARG:HB3  | 1:A:258:ARG:NH1  | 2.28                     | 0.49              |
| 1:A:74:LYS:NZ    | 1:A:291:SER:HB3  | 2.27                     | 0.49              |
| 1:B:194:ARG:HA   | 1:B:205:ILE:HG12 | 1.95                     | 0.49              |
| 1:A:62:PHE:HD2   | 1:A:142:MET:SD   | 2.35                     | 0.49              |
| 1:A:321:ARG:O    | 1:A:324:LYS:HB3  | 2.13                     | 0.48              |
| 1:B:299:GLY:O    | 1:B:302:LYS:HB2  | 2.13                     | 0.48              |
| 1:B:178:LEU:HD23 | 1:B:279:PHE:CE1  | 2.49                     | 0.48              |
| 1:B:194:ARG:HG3  | 1:B:205:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:55:THR:HG22  | 1:B:58:LEU:HD22  | 1.96                     | 0.48              |
| 1:A:18:ASN:O     | 1:A:18:ASN:ND2   | 2.46                     | 0.48              |
| 1:B:231:ILE:HD12 | 1:B:275:ILE:HB   | 1.95                     | 0.48              |
| 1:A:23:LYS:HB3   | 1:A:166:VAL:HG12 | 1.96                     | 0.47              |
| 1:B:301:LEU:O    | 1:B:305:CYS:HB2  | 2.14                     | 0.47              |
| 1:B:109:LEU:HB3  | 1:B:117:ALA:HB2  | 1.95                     | 0.47              |
| 1:A:36:LEU:HB3   | 1:A:111:LYS:HD3  | 1.96                     | 0.47              |
| 1:B:90:GLU:HG3   | 1:B:95:ARG:HB2   | 1.97                     | 0.47              |
| 1:B:105:TRP:CE3  | 1:B:106:LYS:HG2  | 2.48                     | 0.47              |
| 1:A:275:ILE:O    | 1:A:278:PHE:HB3  | 2.15                     | 0.47              |
| 1:B:276:LYS:CE   | 1:B:280:LEU:HD11 | 2.44                     | 0.47              |
| 1:B:296:ASP:O    | 1:B:299:GLY:N    | 2.48                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:114:LEU:HD21 | 1:B:245:ILE:O    | 2.15                     | 0.47              |
| 1:A:225:LYS:HD3  | 1:A:228:GLU:OE1  | 2.15                     | 0.47              |
| 1:A:136:LYS:HB2  | 1:A:146:ILE:HD12 | 1.97                     | 0.46              |
| 1:A:261:LEU:HD12 | 1:A:272:LEU:HB3  | 1.97                     | 0.46              |
| 1:A:124:ALA:H    | 1:A:126:LYS:HZ1  | 1.62                     | 0.46              |
| 1:A:93:LYS:HZ2   | 1:A:95:ARG:HG2   | 1.81                     | 0.46              |
| 1:A:186:ARG:O    | 1:A:187:ASN:HB2  | 2.15                     | 0.46              |
| 1:B:212:LEU:CD2  | 1:B:223:ARG:HD2  | 2.44                     | 0.46              |
| 1:B:201:VAL:HG22 | 1:B:202:TYR:N    | 2.30                     | 0.46              |
| 1:B:314:ARG:HG3  | 1:B:315:VAL:N    | 2.31                     | 0.46              |
| 1:B:63:TYR:HE1   | 1:B:310:PHE:HE2  | 1.65                     | 0.45              |
| 1:A:292:TRP:O    | 1:A:293:LYS:HB2  | 2.15                     | 0.45              |
| 1:A:304:LEU:O    | 1:A:310:PHE:HB2  | 2.17                     | 0.45              |
| 1:B:11:ARG:HB3   | 1:B:210:VAL:HG23 | 1.99                     | 0.45              |
| 1:B:161:ALA:HB3  | 1:B:182:PRO:HD2  | 1.97                     | 0.45              |
| 1:B:64:ARG:NH2   | 1:B:191:THR:HB   | 2.30                     | 0.45              |
| 1:A:15:ASP:C     | 1:A:17:GLU:H     | 2.25                     | 0.45              |
| 1:A:221:ILE:HG12 | 1:A:255:ARG:CD   | 2.46                     | 0.45              |
| 1:A:276:LYS:HE3  | 1:A:280:LEU:HD11 | 1.99                     | 0.45              |
| 1:A:118:ARG:HH11 | 1:A:119:LYS:HG2  | 1.82                     | 0.44              |
| 1:A:217:LYS:O    | 1:A:220:LYS:HG3  | 2.18                     | 0.44              |
| 1:B:271:ASP:O    | 1:B:275:ILE:HG12 | 2.17                     | 0.44              |
| 1:A:62:PHE:CD2   | 1:A:142:MET:SD   | 3.11                     | 0.44              |
| 1:B:8:LEU:HD11   | 1:B:247:PRO:HB2  | 1.99                     | 0.44              |
| 1:B:160:MET:HB3  | 1:B:166:VAL:CG2  | 2.47                     | 0.44              |
| 1:A:40:ARG:NH2   | 1:A:111:LYS:O    | 2.51                     | 0.44              |
| 1:A:116:GLU:OE2  | 1:A:116:GLU:HA   | 2.18                     | 0.44              |
| 1:B:275:ILE:HG22 | 1:B:279:PHE:HE2  | 1.81                     | 0.44              |
| 1:A:86:PHE:N     | 1:A:87:LYS:NZ    | 2.66                     | 0.44              |
| 1:B:2:GLY:O      | 1:B:3:VAL:HB     | 2.18                     | 0.44              |
| 1:B:36:LEU:HD11  | 1:B:131:LEU:CD2  | 2.47                     | 0.44              |
| 1:A:198:GLY:HA3  | 1:A:201:VAL:HG13 | 2.00                     | 0.44              |
| 1:A:258:ARG:HB3  | 1:A:258:ARG:HH11 | 1.82                     | 0.43              |
| 1:B:64:ARG:HA    | 1:B:64:ARG:HD2   | 1.87                     | 0.43              |
| 1:B:225:LYS:O    | 1:B:228:GLU:N    | 2.51                     | 0.43              |
| 1:B:265:GLN:OE1  | 1:B:272:LEU:N    | 2.52                     | 0.43              |
| 1:B:35:PHE:CZ    | 1:B:189:THR:HG22 | 2.54                     | 0.43              |
| 1:A:221:ILE:HD13 | 1:A:221:ILE:HA   | 1.60                     | 0.43              |
| 1:A:176:SER:HB2  | 1:A:181:ALA:HB2  | 2.00                     | 0.43              |
| 1:B:98:ARG:HH11  | 1:B:98:ARG:HG2   | 1.83                     | 0.43              |
| 1:A:297:GLU:O    | 1:A:301:LEU:HD12 | 2.19                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:221:ILE:HG21 | 1:B:254:VAL:HG12 | 2.00                     | 0.43              |
| 1:A:81:GLY:HA3   | 1:A:150:PRO:O    | 2.19                     | 0.43              |
| 1:B:120:TYR:CD2  | 1:B:120:TYR:N    | 2.86                     | 0.43              |
| 1:A:8:LEU:CD1    | 1:A:247:PRO:HB3  | 2.49                     | 0.43              |
| 1:A:28:ALA:HA    | 1:A:77:TYR:HD2   | 1.84                     | 0.43              |
| 1:B:216:LEU:HD23 | 1:B:216:LEU:HA   | 1.81                     | 0.42              |
| 1:A:125:THR:HB   | 1:A:126:LYS:H    | 1.60                     | 0.42              |
| 1:A:139:LEU:HA   | 1:A:142:MET:HB2  | 2.02                     | 0.42              |
| 1:B:34:GLN:O     | 1:B:37:SER:HB3   | 2.19                     | 0.42              |
| 1:A:117:ALA:HB1  | 1:A:120:TYR:CD1  | 2.54                     | 0.42              |
| 1:A:9:VAL:HA     | 1:A:10:PRO:HD2   | 1.66                     | 0.42              |
| 1:A:185:ILE:HG12 | 1:A:209:LEU:HD23 | 2.01                     | 0.42              |
| 1:B:87:LYS:HE3   | 1:B:87:LYS:HB3   | 1.96                     | 0.42              |
| 1:B:294:GLU:OE1  | 1:B:327:LYS:HG2  | 2.20                     | 0.42              |
| 1:B:315:VAL:HG12 | 1:B:319:ILE:HD13 | 2.00                     | 0.42              |
| 1:A:97:ALA:O     | 1:A:99:GLU:N     | 2.53                     | 0.42              |
| 1:A:105:TRP:O    | 1:A:128:ASN:ND2  | 2.52                     | 0.42              |
| 1:A:114:LEU:HD11 | 1:B:245:ILE:C    | 2.44                     | 0.42              |
| 1:A:121:ALA:HA   | 1:A:126:LYS:HG2  | 2.01                     | 0.42              |
| 1:B:61:LEU:HD21  | 1:B:135:ALA:CB   | 2.47                     | 0.42              |
| 1:A:36:LEU:HD23  | 1:A:111:LYS:CD   | 2.50                     | 0.42              |
| 1:A:205:ILE:HD13 | 1:A:205:ILE:HG21 | 1.84                     | 0.42              |
| 1:A:255:ARG:HH11 | 1:A:255:ARG:HD2  | 1.72                     | 0.42              |
| 1:B:303:PHE:CD2  | 1:B:304:LEU:HD12 | 2.55                     | 0.41              |
| 1:A:264:PHE:O    | 1:A:266:ARG:N    | 2.54                     | 0.41              |
| 1:B:254:VAL:HG12 | 1:B:255:ARG:N    | 2.35                     | 0.41              |
| 1:A:320:GLU:HA   | 1:A:323:LYS:HD3  | 2.02                     | 0.41              |
| 1:B:196:MET:O    | 1:B:198:GLY:N    | 2.53                     | 0.41              |
| 1:B:33:TYR:OH    | 1:B:121:ALA:HB3  | 2.20                     | 0.41              |
| 1:B:261:LEU:O    | 1:B:265:GLN:N    | 2.53                     | 0.41              |
| 1:B:186:ARG:HH22 | 1:B:202:TYR:CB   | 2.34                     | 0.41              |
| 1:B:252:GLU:O    | 1:B:253:ILE:C    | 2.63                     | 0.41              |
| 1:B:276:LYS:HE2  | 1:B:280:LEU:HD11 | 2.02                     | 0.41              |
| 1:B:111:LYS:O    | 1:B:113:ASN:N    | 2.54                     | 0.41              |
| 1:A:124:ALA:O    | 1:A:125:THR:HG23 | 2.21                     | 0.40              |
| 1:B:29:LEU:HD21  | 1:B:121:ALA:O    | 2.21                     | 0.40              |
| 1:B:9:VAL:HA     | 1:B:10:PRO:HD2   | 1.99                     | 0.40              |
| 1:B:191:THR:CG2  | 1:B:207:PRO:HD3  | 2.49                     | 0.40              |
| 1:B:160:MET:HB3  | 1:B:166:VAL:HG21 | 2.03                     | 0.40              |
| 1:A:55:THR:HG23  | 1:A:310:PHE:CE1  | 2.55                     | 0.40              |
| 1:A:60:GLY:O     | 1:A:61:LEU:C     | 2.64                     | 0.40              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:A:300:ILE:O | 1:A:301:LEU:C   | 2.65                     | 0.40              |
| 1:B:138:LEU:O | 1:B:142:MET:HG2 | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed   | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|-----------|----------|-------------|---|
| 1   | A     | 329/343 (96%) | 228 (69%) | 68 (21%)  | 33 (10%) | 0           | 3 |
| 1   | B     | 329/343 (96%) | 243 (74%) | 59 (18%)  | 27 (8%)  | 0           | 4 |
| All | All   | 658/686 (96%) | 471 (72%) | 127 (19%) | 60 (9%)  | 0           | 3 |

All (60) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | ILE  |
| 1   | A     | 90  | GLU  |
| 1   | A     | 98  | ARG  |
| 1   | A     | 126 | LYS  |
| 1   | A     | 194 | ARG  |
| 1   | A     | 197 | PRO  |
| 1   | A     | 272 | LEU  |
| 1   | A     | 293 | LYS  |
| 1   | A     | 330 | ARG  |
| 1   | A     | 331 | GLN  |
| 1   | B     | 85  | GLU  |
| 1   | B     | 91  | LEU  |
| 1   | B     | 107 | GLU  |
| 1   | B     | 124 | ALA  |
| 1   | B     | 200 | ASP  |
| 1   | B     | 205 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 266 | ARG  |
| 1   | B     | 268 | SER  |
| 1   | B     | 270 | VAL  |
| 1   | B     | 296 | ASP  |
| 1   | B     | 297 | GLU  |
| 1   | A     | 102 | GLU  |
| 1   | A     | 119 | LYS  |
| 1   | A     | 125 | THR  |
| 1   | A     | 153 | GLY  |
| 1   | A     | 164 | GLY  |
| 1   | A     | 265 | GLN  |
| 1   | B     | 96  | GLU  |
| 1   | B     | 97  | ALA  |
| 1   | B     | 121 | ALA  |
| 1   | B     | 201 | VAL  |
| 1   | B     | 271 | ASP  |
| 1   | A     | 92  | GLU  |
| 1   | A     | 96  | GLU  |
| 1   | A     | 220 | LYS  |
| 1   | A     | 223 | ARG  |
| 1   | B     | 130 | MET  |
| 1   | B     | 171 | SER  |
| 1   | B     | 283 | PRO  |
| 1   | A     | 36  | LEU  |
| 1   | A     | 121 | ALA  |
| 1   | A     | 255 | ARG  |
| 1   | A     | 309 | ASN  |
| 1   | A     | 313 | GLU  |
| 1   | A     | 163 | LYS  |
| 1   | A     | 290 | LEU  |
| 1   | A     | 292 | TRP  |
| 1   | B     | 4   | PRO  |
| 1   | B     | 106 | LYS  |
| 1   | A     | 203 | VAL  |
| 1   | A     | 239 | PRO  |
| 1   | A     | 240 | GLY  |
| 1   | B     | 164 | GLY  |
| 1   | A     | 5   | ILE  |
| 1   | B     | 5   | ILE  |
| 1   | B     | 14  | ILE  |
| 1   | A     | 329 | GLY  |
| 1   | B     | 127 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 241 | GLY  |
| 1   | B     | 254 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers  | Percentiles |   |
|-----|-------|---------------|-----------|-----------|-------------|---|
| 1   | A     | 281/293 (96%) | 204 (73%) | 77 (27%)  | 0           | 1 |
| 1   | B     | 281/293 (96%) | 222 (79%) | 59 (21%)  | 1           | 5 |
| All | All   | 562/586 (96%) | 426 (76%) | 136 (24%) | 1           | 3 |

All (136) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ASP  |
| 1   | A     | 11  | ARG  |
| 1   | A     | 14  | ILE  |
| 1   | A     | 16  | LEU  |
| 1   | A     | 17  | GLU  |
| 1   | A     | 20  | TYR  |
| 1   | A     | 23  | LYS  |
| 1   | A     | 32  | ILE  |
| 1   | A     | 43  | ASP  |
| 1   | A     | 45  | THR  |
| 1   | A     | 47  | LEU  |
| 1   | A     | 48  | MET  |
| 1   | A     | 49  | ASP  |
| 1   | A     | 55  | THR  |
| 1   | A     | 56  | SER  |
| 1   | A     | 64  | ARG  |
| 1   | A     | 67  | ASN  |
| 1   | A     | 74  | LYS  |
| 1   | A     | 75  | PRO  |
| 1   | A     | 86  | PHE  |
| 1   | A     | 87  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 93  | LYS  |
| 1   | A     | 99  | GLU  |
| 1   | A     | 105 | TRP  |
| 1   | A     | 109 | LEU  |
| 1   | A     | 111 | LYS  |
| 1   | A     | 113 | ASN  |
| 1   | A     | 115 | GLU  |
| 1   | A     | 118 | ARG  |
| 1   | A     | 119 | LYS  |
| 1   | A     | 123 | ARG  |
| 1   | A     | 125 | THR  |
| 1   | A     | 126 | LYS  |
| 1   | A     | 128 | ASN  |
| 1   | A     | 129 | GLU  |
| 1   | A     | 130 | MET  |
| 1   | A     | 133 | GLU  |
| 1   | A     | 136 | LYS  |
| 1   | A     | 176 | SER  |
| 1   | A     | 177 | LEU  |
| 1   | A     | 183 | ARG  |
| 1   | A     | 184 | LEU  |
| 1   | A     | 194 | ARG  |
| 1   | A     | 197 | PRO  |
| 1   | A     | 201 | VAL  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 209 | LEU  |
| 1   | A     | 214 | GLU  |
| 1   | A     | 216 | LEU  |
| 1   | A     | 218 | GLU  |
| 1   | A     | 219 | LEU  |
| 1   | A     | 220 | LYS  |
| 1   | A     | 221 | ILE  |
| 1   | A     | 224 | GLU  |
| 1   | A     | 229 | LEU  |
| 1   | A     | 236 | ASP  |
| 1   | A     | 242 | VAL  |
| 1   | A     | 251 | LEU  |
| 1   | A     | 255 | ARG  |
| 1   | A     | 256 | TYR  |
| 1   | A     | 258 | ARG  |
| 1   | A     | 277 | GLU  |
| 1   | A     | 286 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 287 | GLU  |
| 1   | A     | 290 | LEU  |
| 1   | A     | 292 | TRP  |
| 1   | A     | 296 | ASP  |
| 1   | A     | 297 | GLU  |
| 1   | A     | 305 | CYS  |
| 1   | A     | 307 | GLU  |
| 1   | A     | 312 | GLU  |
| 1   | A     | 314 | ARG  |
| 1   | A     | 319 | ILE  |
| 1   | A     | 320 | GLU  |
| 1   | A     | 322 | LEU  |
| 1   | A     | 323 | LYS  |
| 1   | A     | 332 | SER  |
| 1   | B     | 11  | ARG  |
| 1   | B     | 12  | LYS  |
| 1   | B     | 15  | ASP  |
| 1   | B     | 18  | ASN  |
| 1   | B     | 19  | LEU  |
| 1   | B     | 32  | ILE  |
| 1   | B     | 42  | GLU  |
| 1   | B     | 49  | ASP  |
| 1   | B     | 58  | LEU  |
| 1   | B     | 68  | LEU  |
| 1   | B     | 73  | ILE  |
| 1   | B     | 75  | PRO  |
| 1   | B     | 91  | LEU  |
| 1   | B     | 92  | GLU  |
| 1   | B     | 93  | LYS  |
| 1   | B     | 95  | ARG  |
| 1   | B     | 98  | ARG  |
| 1   | B     | 102 | GLU  |
| 1   | B     | 107 | GLU  |
| 1   | B     | 111 | LYS  |
| 1   | B     | 113 | ASN  |
| 1   | B     | 114 | LEU  |
| 1   | B     | 120 | TYR  |
| 1   | B     | 122 | GLN  |
| 1   | B     | 123 | ARG  |
| 1   | B     | 129 | GLU  |
| 1   | B     | 130 | MET  |
| 1   | B     | 131 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 133 | GLU  |
| 1   | B     | 138 | LEU  |
| 1   | B     | 139 | LEU  |
| 1   | B     | 152 | GLU  |
| 1   | B     | 162 | SER  |
| 1   | B     | 176 | SER  |
| 1   | B     | 177 | LEU  |
| 1   | B     | 189 | THR  |
| 1   | B     | 205 | ILE  |
| 1   | B     | 206 | LYS  |
| 1   | B     | 220 | LYS  |
| 1   | B     | 222 | THR  |
| 1   | B     | 223 | ARG  |
| 1   | B     | 224 | GLU  |
| 1   | B     | 226 | LEU  |
| 1   | B     | 243 | LYS  |
| 1   | B     | 245 | ILE  |
| 1   | B     | 251 | LEU  |
| 1   | B     | 254 | VAL  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 275 | ILE  |
| 1   | B     | 276 | LYS  |
| 1   | B     | 285 | THR  |
| 1   | B     | 287 | GLU  |
| 1   | B     | 294 | GLU  |
| 1   | B     | 296 | ASP  |
| 1   | B     | 301 | LEU  |
| 1   | B     | 302 | LYS  |
| 1   | B     | 307 | GLU  |
| 1   | B     | 319 | ILE  |
| 1   | B     | 331 | GLN  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | HIS  |
| 1   | A     | 67  | ASN  |
| 1   | A     | 113 | ASN  |
| 1   | A     | 331 | GLN  |
| 1   | B     | 34  | GLN  |
| 1   | B     | 57  | HIS  |
| 1   | B     | 140 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 156 | GLN  |
| 1   | B     | 317 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 331/343 (96%) | -0.72  | 3 (0%)    | 81 63 | 13, 37, 74, 83        | 0       |
| 1   | B     | 331/343 (96%) | -0.70  | 6 (1%)    | 67 47 | 10, 37, 70, 84        | 0       |
| All | All   | 662/686 (96%) | -0.71  | 9 (1%)    | 73 53 | 10, 37, 71, 84        | 0       |

All (9) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 329 | GLY  | 5.1  |
| 1   | A     | 199 | LYS  | 3.7  |
| 1   | B     | 200 | ASP  | 3.7  |
| 1   | B     | 121 | ALA  | 2.5  |
| 1   | B     | 114 | LEU  | 2.4  |
| 1   | A     | 162 | SER  | 2.3  |
| 1   | B     | 262 | ALA  | 2.2  |
| 1   | A     | 103 | LEU  | 2.1  |
| 1   | B     | 273 | TYR  | 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 oligosaccharides 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.