



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:26 AM UTC

PDB ID : 8AFF / pdb\_00008aff  
Title : Wild type oxalyl-CoA synthetase Pcs60p  
Authors : Burgi, J.; Chojnowski, G.; Giannopoulou, E.A.; Wilmanns, M.  
Deposited on : 2022-07-17  
Resolution : 2.87 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                                                             |

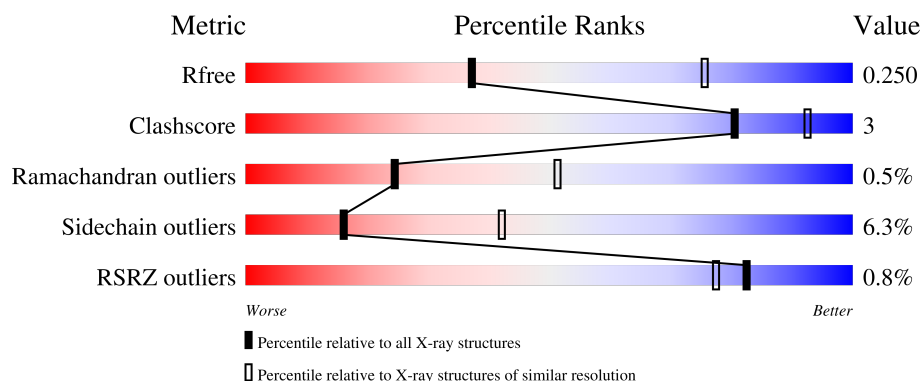
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3557 (2.90-2.86)                                      |
| Clashscore            | 190562                      | 3801 (2.90-2.86)                                      |
| Ramachandran outliers | 187476                      | 3699 (2.90-2.86)                                      |
| Sidechain outliers    | 187428                      | 3702 (2.90-2.86)                                      |
| RSRZ outliers         | 180081                      | 3558 (2.90-2.86)                                      |

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     | 543    | <div> <div>82%</div> <div>12%</div> <div>.</div> <div>.</div> </div>               |
| 1   | B     | 543    | <div> <div>68%</div> <div>9%</div> <div>.</div> <div>21%</div> </div>              |
| 1   | C     | 543    | <div> <div>67%</div> <div>10%</div> <div>.</div> <div>21%</div> </div>             |
| 1   | D     | 543    | <div> <div>%</div> <div>81%</div> <div>11%</div> <div>.</div> <div>6%</div> </div> |
| 1   | E     | 543    | <div> <div>69%</div> <div>8%</div> <div>.</div> <div>22%</div> </div>              |

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| Mol | Chain | Length | Quality of chain                            |
|-----|-------|--------|---------------------------------------------|
| 1   | F     | 543    | <div><div></div><div>68%10%21%</div></div>  |
| 1   | G     | 543    | <div><div></div><div>%67%9%22%</div></div>  |
| 1   | H     | 543    | <div><div></div><div>%68%9%21%</div></div>  |
| 1   | I     | 543    | <div><div></div><div>%82%12%5%</div></div>  |
| 1   | J     | 543    | <div><div></div><div>69%8%21%</div></div>   |
| 1   | K     | 543    | <div><div></div><div>%69%8%22%</div></div>  |
| 1   | L     | 543    | <div><div></div><div>2%68%9%22%</div></div> |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 42783 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 Oxalate–CoA ligase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 525      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4134  | 2660 | 698 | 758 | 18 |         |         |       |
| 1   | B     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3370  | 2163 | 571 | 621 | 15 |         |         |       |
| 1   | C     | 430      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3386  | 2173 | 574 | 624 | 15 |         |         |       |
| 1   | D     | 511      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4023  | 2590 | 676 | 739 | 18 |         |         |       |
| 1   | E     | 426      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3353  | 2152 | 569 | 617 | 15 |         |         |       |
| 1   | F     | 429      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3378  | 2169 | 572 | 622 | 15 |         |         |       |
| 1   | G     | 423      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3325  | 2134 | 562 | 614 | 15 |         |         |       |
| 1   | H     | 427      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3362  | 2157 | 570 | 620 | 15 |         |         |       |
| 1   | I     | 518      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4076  | 2622 | 691 | 746 | 17 |         |         |       |
| 1   | J     | 427      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3362  | 2157 | 570 | 620 | 15 |         |         |       |
| 1   | K     | 425      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3344  | 2146 | 567 | 616 | 15 |         |         |       |
| 1   | L     | 426      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3353  | 2152 | 569 | 617 | 15 |         |         |       |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 2   | B     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |

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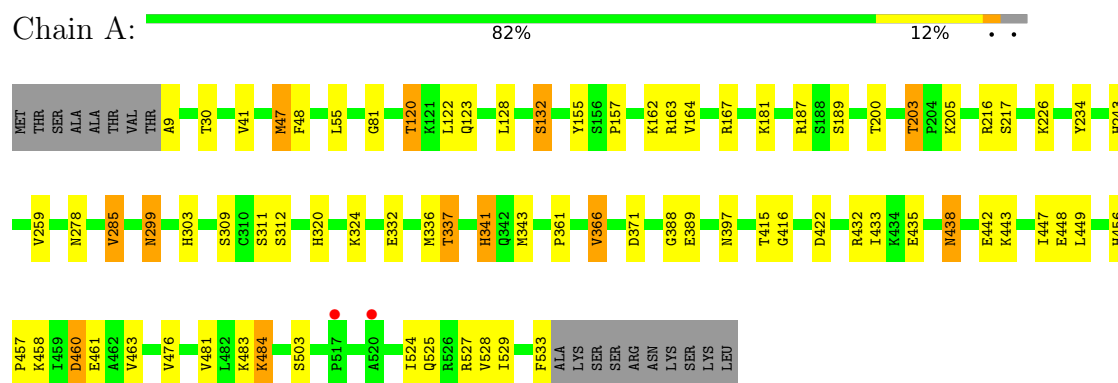
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 2   | C     | 58       | Total<br>58 | O<br>58 | 0       | 0       |
| 2   | D     | 58       | Total<br>58 | O<br>58 | 0       | 0       |
| 2   | E     | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 2   | F     | 33       | Total<br>33 | O<br>33 | 0       | 0       |
| 2   | G     | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 2   | H     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 2   | I     | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 2   | J     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 2   | K     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 2   | L     | 2        | Total<br>2  | O<br>2  | 0       | 0       |

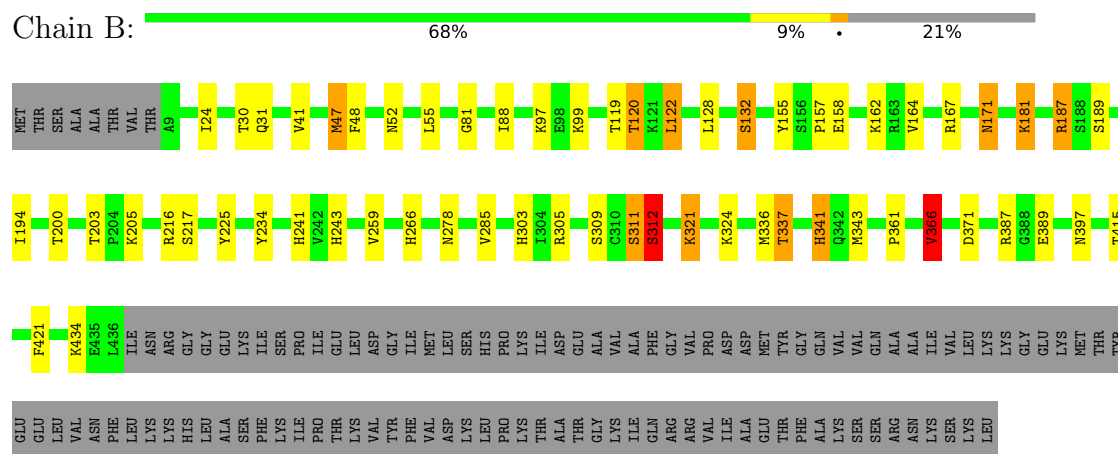
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

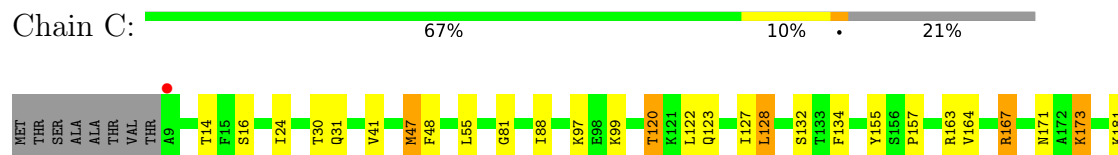
#### • Molecule 1: Oxalate–CoA ligase

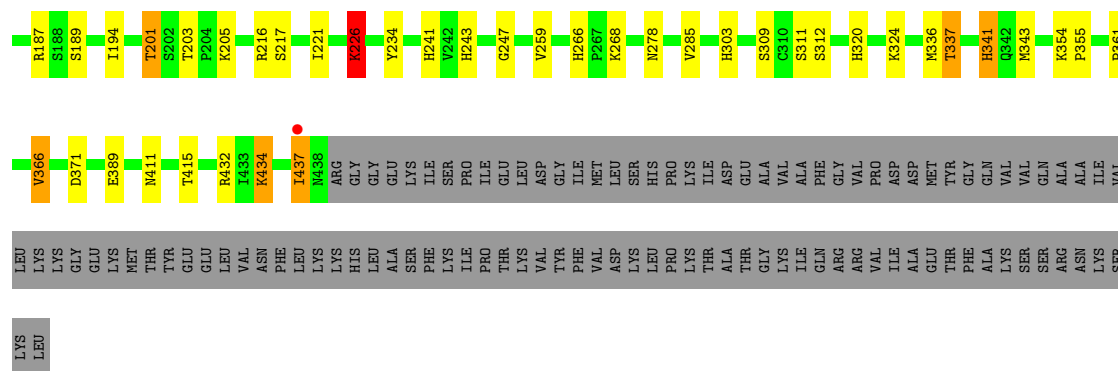


#### • Molecule 1: Oxalate–CoA ligase

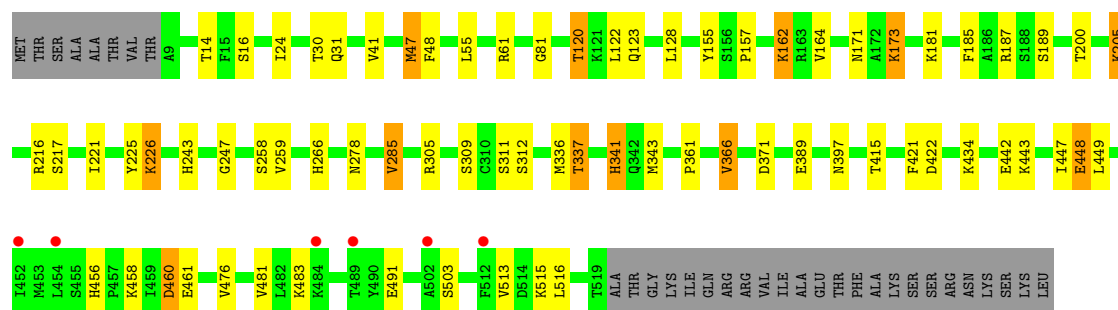
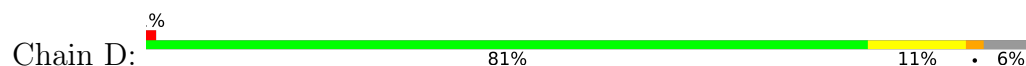


#### • Molecule 1: Oxalate–CoA ligase

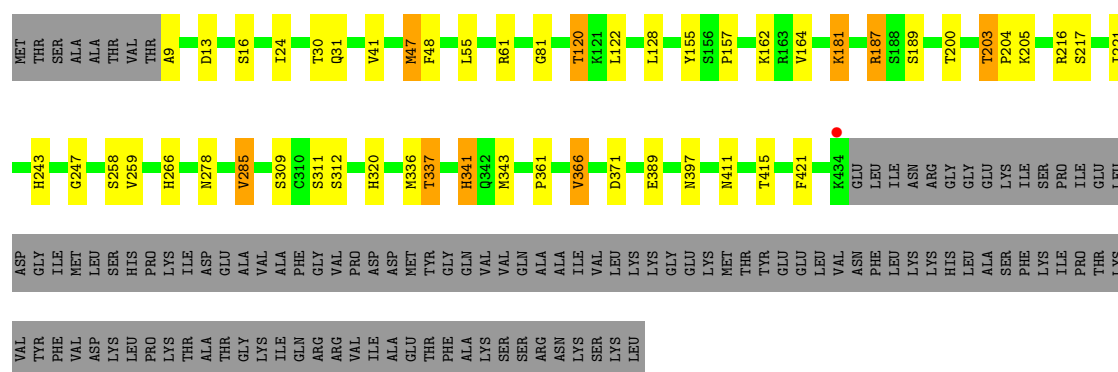




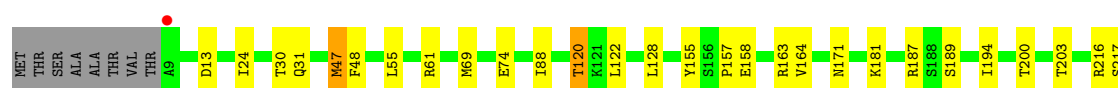
• Molecule 1: Oxalate–CoA ligase



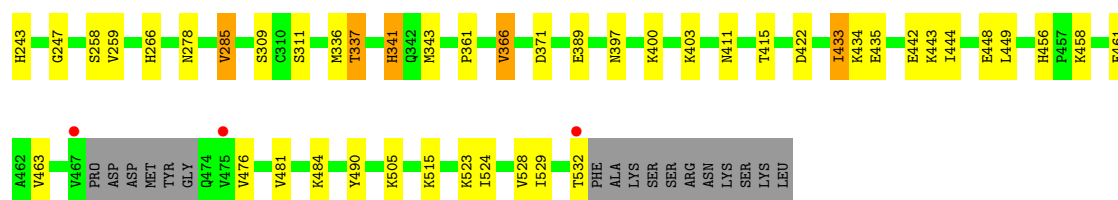
• Molecule 1: Oxalate–CoA ligase



• Molecule 1: Oxalate–CoA ligase

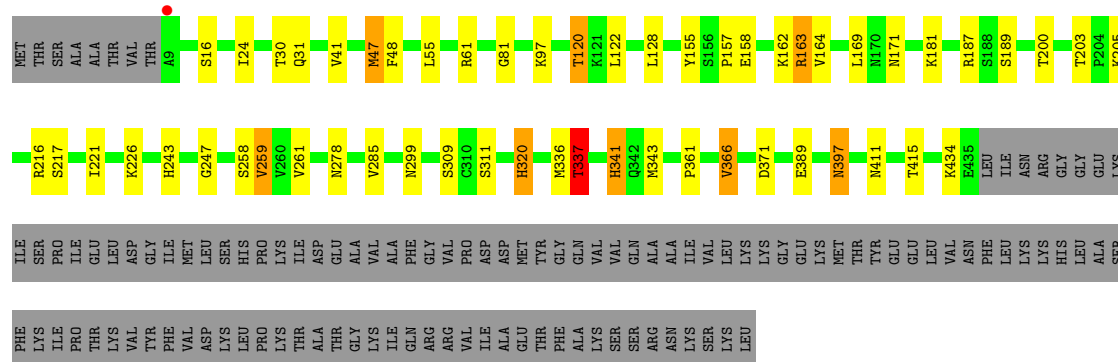






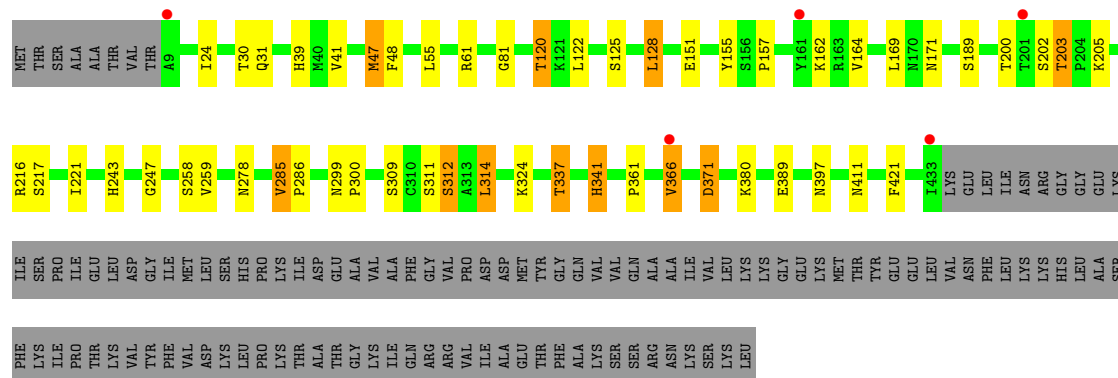
• Molecule 1: Oxalate–CoA ligase

Chain J: 69% 8% 21%



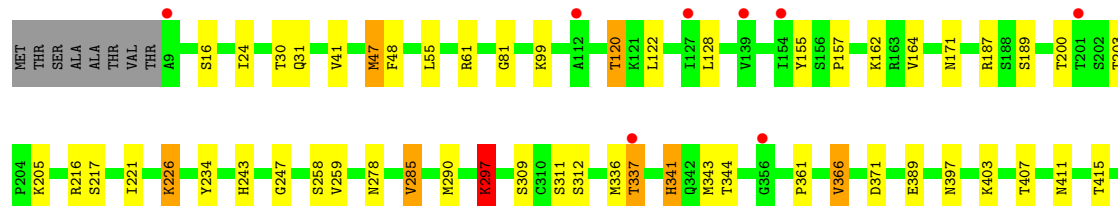
• Molecule 1: Oxalate–CoA ligase

Chain K: 69% 8% 22%



• Molecule 1: Oxalate–CoA ligase

Chain L: 68% 9% 22%



[illegible]

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 109.03Å 93.72Å 356.49Å<br>90.00° 93.81° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 29.98 – 2.87<br>29.98 – 2.87                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (29.98-2.87)<br>99.0 (29.98-2.87)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.67 (at 2.85Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0267                                             | Depositor        |
| R, $R_{free}$                                                           | 0.227 , 0.250<br>0.227 , 0.250                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 8269 reflections (5.02%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 60.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.531                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 51.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.93                                                        | EDS              |
| Total number of atoms                                                   | 42783                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 80.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$      |
| 1   | A     | 0.70         | 3/4237 (0.1%)   | 1.37        | 20/5753 (0.3%)   |
| 1   | B     | 0.71         | 3/3458 (0.1%)   | 1.34        | 16/4704 (0.3%)   |
| 1   | C     | 0.72         | 2/3474 (0.1%)   | 1.35        | 20/4726 (0.4%)   |
| 1   | D     | 0.71         | 0/4125          | 1.37        | 23/5603 (0.4%)   |
| 1   | E     | 0.68         | 2/3441 (0.1%)   | 1.31        | 11/4681 (0.2%)   |
| 1   | F     | 0.68         | 0/3466          | 1.32        | 11/4715 (0.2%)   |
| 1   | G     | 0.62         | 0/3413          | 1.33        | 17/4645 (0.4%)   |
| 1   | H     | 0.60         | 0/3450          | 1.30        | 13/4693 (0.3%)   |
| 1   | I     | 0.67         | 1/4175 (0.0%)   | 1.36        | 17/5667 (0.3%)   |
| 1   | J     | 0.67         | 1/3450 (0.0%)   | 1.30        | 14/4693 (0.3%)   |
| 1   | K     | 0.64         | 1/3432 (0.0%)   | 1.31        | 12/4670 (0.3%)   |
| 1   | L     | 0.60         | 0/3441          | 1.30        | 16/4681 (0.3%)   |
| All | All   | 0.67         | 13/43562 (0.0%) | 1.33        | 190/59231 (0.3%) |

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   | H     | 0                   | 1                   |

All (13) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | B     | 266 | HIS  | CE1-NE2 | 7.82 | 1.40        | 1.32     |
| 1   | A     | 303 | HIS  | CE1-NE2 | 7.29 | 1.39        | 1.32     |
| 1   | C     | 241 | HIS  | CE1-NE2 | 6.91 | 1.39        | 1.32     |
| 1   | K     | 39  | HIS  | CE1-NE2 | 6.57 | 1.39        | 1.32     |
| 1   | E     | 9   | ALA  | N-CA    | 6.16 | 1.57        | 1.46     |
| 1   | C     | 303 | HIS  | CE1-NE2 | 5.80 | 1.38        | 1.32     |
| 1   | E     | 266 | HIS  | CE1-NE2 | 5.75 | 1.38        | 1.32     |
| 1   | B     | 303 | HIS  | CE1-NE2 | 5.73 | 1.38        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | A     | 320 | HIS  | CE1-NE2 | 5.64 | 1.38        | 1.32     |
| 1   | J     | 320 | HIS  | CE1-NE2 | 5.63 | 1.38        | 1.32     |
| 1   | B     | 241 | HIS  | CE1-NE2 | 5.58 | 1.38        | 1.32     |
| 1   | I     | 266 | HIS  | CE1-NE2 | 5.23 | 1.37        | 1.32     |
| 1   | A     | 9   | ALA  | N-CA    | 5.09 | 1.55        | 1.46     |

All (190) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | B     | 167 | ARG  | CG-CD-NE | 9.71  | 133.37      | 112.00   |
| 1   | D     | 187 | ARG  | CB-CG-CD | -9.32 | 89.86       | 111.30   |
| 1   | B     | 187 | ARG  | CB-CG-CD | -8.75 | 91.17       | 111.30   |
| 1   | E     | 285 | VAL  | N-CA-CB  | -8.38 | 106.05      | 111.83   |
| 1   | I     | 285 | VAL  | N-CA-CB  | -8.33 | 106.08      | 111.83   |
| 1   | D     | 173 | LYS  | CG-CD-CE | 8.24  | 130.25      | 111.30   |
| 1   | A     | 285 | VAL  | N-CA-CB  | -8.21 | 106.16      | 111.83   |
| 1   | F     | 285 | VAL  | N-CA-CB  | -8.18 | 106.19      | 111.83   |
| 1   | G     | 226 | LYS  | CB-CG-CD | 8.01  | 129.72      | 111.30   |
| 1   | H     | 337 | THR  | CB-CA-C  | 7.92  | 125.28      | 110.63   |
| 1   | I     | 337 | THR  | CB-CA-C  | 7.89  | 125.82      | 110.67   |
| 1   | J     | 187 | ARG  | CB-CG-CD | -7.85 | 93.25       | 111.30   |
| 1   | J     | 337 | THR  | CB-CA-C  | 7.80  | 125.65      | 110.67   |
| 1   | C     | 437 | ILE  | CB-CA-C  | 7.78  | 121.41      | 110.84   |
| 1   | G     | 285 | VAL  | N-CA-CB  | -7.75 | 106.48      | 111.83   |
| 1   | D     | 285 | VAL  | N-CA-CB  | -7.68 | 106.53      | 111.83   |
| 1   | L     | 285 | VAL  | N-CA-CB  | -7.68 | 106.53      | 111.83   |
| 1   | G     | 337 | THR  | CB-CA-C  | 7.64  | 125.35      | 110.67   |
| 1   | C     | 167 | ARG  | CB-CG-CD | 7.62  | 128.82      | 111.30   |
| 1   | A     | 278 | ASN  | CB-CA-C  | -7.61 | 100.38      | 112.09   |
| 1   | I     | 278 | ASN  | CB-CA-C  | -7.60 | 100.39      | 112.09   |
| 1   | L     | 337 | THR  | CB-CA-C  | 7.53  | 125.14      | 110.67   |
| 1   | K     | 285 | VAL  | N-CA-CB  | -7.50 | 106.65      | 111.83   |
| 1   | E     | 337 | THR  | CB-CA-C  | 7.50  | 125.06      | 110.67   |
| 1   | B     | 337 | THR  | CB-CA-C  | 7.49  | 125.05      | 110.67   |
| 1   | C     | 203 | THR  | CB-CA-C  | 7.44  | 121.10      | 109.42   |
| 1   | J     | 278 | ASN  | CB-CA-C  | -7.42 | 100.66      | 112.09   |
| 1   | E     | 278 | ASN  | CB-CA-C  | -7.37 | 100.73      | 112.09   |
| 1   | D     | 278 | ASN  | CB-CA-C  | -7.37 | 100.74      | 112.09   |
| 1   | F     | 187 | ARG  | CB-CG-CD | -7.26 | 94.60       | 111.30   |
| 1   | C     | 337 | THR  | CB-CA-C  | 7.24  | 124.57      | 110.67   |
| 1   | K     | 337 | THR  | CB-CA-C  | 7.23  | 124.55      | 110.67   |
| 1   | B     | 203 | THR  | CB-CA-C  | 7.19  | 120.71      | 109.42   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | D     | 337 | THR  | CB-CA-C  | 7.19  | 124.48      | 110.67   |
| 1   | K     | 278 | ASN  | CB-CA-C  | -7.19 | 101.02      | 112.09   |
| 1   | C     | 278 | ASN  | CB-CA-C  | -7.13 | 101.11      | 112.09   |
| 1   | F     | 278 | ASN  | CB-CA-C  | -7.12 | 101.12      | 112.09   |
| 1   | L     | 203 | THR  | CB-CA-C  | 7.09  | 120.56      | 109.42   |
| 1   | G     | 278 | ASN  | CB-CA-C  | -7.08 | 101.19      | 112.09   |
| 1   | B     | 278 | ASN  | CB-CA-C  | -7.08 | 101.19      | 112.09   |
| 1   | I     | 203 | THR  | CB-CA-C  | 7.07  | 120.51      | 109.42   |
| 1   | A     | 203 | THR  | CB-CA-C  | 7.05  | 120.49      | 109.42   |
| 1   | J     | 181 | LYS  | CB-CG-CD | 7.01  | 127.42      | 111.30   |
| 1   | E     | 181 | LYS  | CB-CG-CD | 6.99  | 127.38      | 111.30   |
| 1   | I     | 30  | THR  | CB-CA-C  | 6.98  | 121.25      | 109.80   |
| 1   | F     | 337 | THR  | CB-CA-C  | 6.96  | 124.04      | 110.67   |
| 1   | H     | 30  | THR  | CB-CA-C  | 6.96  | 121.21      | 109.80   |
| 1   | G     | 30  | THR  | CB-CA-C  | 6.94  | 121.19      | 109.80   |
| 1   | E     | 30  | THR  | CB-CA-C  | 6.94  | 121.18      | 109.80   |
| 1   | A     | 337 | THR  | CB-CA-C  | 6.90  | 123.92      | 110.67   |
| 1   | A     | 187 | ARG  | CB-CG-CD | -6.89 | 95.46       | 111.30   |
| 1   | J     | 30  | THR  | CB-CA-C  | 6.87  | 121.07      | 109.80   |
| 1   | B     | 30  | THR  | CB-CA-C  | 6.85  | 121.03      | 109.80   |
| 1   | J     | 163 | ARG  | CB-CG-CD | 6.84  | 127.03      | 111.30   |
| 1   | L     | 278 | ASN  | CB-CA-C  | -6.82 | 101.58      | 112.09   |
| 1   | J     | 203 | THR  | CB-CA-C  | 6.78  | 120.07      | 109.42   |
| 1   | H     | 278 | ASN  | CB-CA-C  | -6.77 | 101.67      | 112.09   |
| 1   | D     | 30  | THR  | CB-CA-C  | 6.74  | 120.86      | 109.80   |
| 1   | G     | 181 | LYS  | CB-CG-CD | 6.73  | 126.77      | 111.30   |
| 1   | L     | 30  | THR  | CB-CA-C  | 6.73  | 120.83      | 109.80   |
| 1   | K     | 30  | THR  | CB-CA-C  | 6.72  | 120.82      | 109.80   |
| 1   | C     | 163 | ARG  | CB-CG-CD | 6.72  | 126.75      | 111.30   |
| 1   | E     | 203 | THR  | CB-CA-C  | 6.71  | 119.95      | 109.42   |
| 1   | G     | 198 | SER  | N-CA-C   | 6.70  | 125.06      | 110.80   |
| 1   | F     | 181 | LYS  | CB-CG-CD | 6.65  | 126.59      | 111.30   |
| 1   | F     | 203 | THR  | CB-CA-C  | 6.63  | 119.83      | 109.42   |
| 1   | G     | 203 | THR  | CB-CA-C  | 6.60  | 119.78      | 109.42   |
| 1   | K     | 203 | THR  | CB-CA-C  | 6.59  | 119.77      | 109.42   |
| 1   | H     | 203 | THR  | CB-CA-C  | 6.59  | 119.76      | 109.42   |
| 1   | F     | 30  | THR  | CB-CA-C  | 6.56  | 120.57      | 109.80   |
| 1   | H     | 371 | ASP  | CA-CB-CG | 6.49  | 119.09      | 112.60   |
| 1   | A     | 484 | LYS  | CB-CA-C  | 6.48  | 119.50      | 110.16   |
| 1   | C     | 226 | LYS  | CB-CG-CD | 6.47  | 126.19      | 111.30   |
| 1   | C     | 30  | THR  | CB-CA-C  | 6.46  | 120.40      | 109.80   |
| 1   | A     | 30  | THR  | CB-CA-C  | 6.45  | 120.37      | 109.80   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 132 | SER  | CA-CB-OG  | 6.42  | 123.93      | 111.10   |
| 1   | C     | 173 | LYS  | CG-CD-CE  | 6.36  | 125.93      | 111.30   |
| 1   | A     | 132 | SER  | CA-CB-OG  | 6.32  | 123.75      | 111.10   |
| 1   | A     | 324 | LYS  | CG-CD-CE  | 6.32  | 125.83      | 111.30   |
| 1   | D     | 181 | LYS  | CB-CG-CD  | 6.23  | 125.64      | 111.30   |
| 1   | C     | 123 | GLN  | CB-CA-C   | 6.18  | 120.54      | 110.95   |
| 1   | K     | 157 | PRO  | CA-C-N    | 6.17  | 128.83      | 120.38   |
| 1   | K     | 157 | PRO  | C-N-CA    | 6.17  | 128.83      | 120.38   |
| 1   | H     | 187 | ARG  | CB-CG-CD  | -6.16 | 97.12       | 111.30   |
| 1   | I     | 157 | PRO  | CA-C-N    | 6.16  | 128.82      | 120.38   |
| 1   | I     | 157 | PRO  | C-N-CA    | 6.16  | 128.82      | 120.38   |
| 1   | I     | 433 | ILE  | CA-CB-CG1 | 6.14  | 120.84      | 110.40   |
| 1   | A     | 157 | PRO  | CA-C-N    | 6.12  | 128.76      | 120.38   |
| 1   | A     | 157 | PRO  | C-N-CA    | 6.12  | 128.76      | 120.38   |
| 1   | B     | 157 | PRO  | CA-C-N    | 6.11  | 128.75      | 120.38   |
| 1   | B     | 157 | PRO  | C-N-CA    | 6.11  | 128.75      | 120.38   |
| 1   | E     | 157 | PRO  | CA-C-N    | 6.07  | 128.70      | 120.38   |
| 1   | E     | 157 | PRO  | C-N-CA    | 6.07  | 128.70      | 120.38   |
| 1   | C     | 157 | PRO  | CA-C-N    | 6.06  | 128.68      | 120.38   |
| 1   | C     | 157 | PRO  | C-N-CA    | 6.06  | 128.68      | 120.38   |
| 1   | B     | 321 | LYS  | CB-CG-CD  | 6.05  | 125.22      | 111.30   |
| 1   | G     | 200 | THR  | CB-CA-C   | 6.04  | 120.83      | 110.86   |
| 1   | L     | 157 | PRO  | CA-C-N    | 6.01  | 128.61      | 120.38   |
| 1   | L     | 157 | PRO  | C-N-CA    | 6.01  | 128.61      | 120.38   |
| 1   | F     | 157 | PRO  | CA-C-N    | 5.99  | 128.59      | 120.38   |
| 1   | F     | 157 | PRO  | C-N-CA    | 5.99  | 128.59      | 120.38   |
| 1   | I     | 226 | LYS  | CB-CG-CD  | 5.99  | 125.06      | 111.30   |
| 1   | H     | 157 | PRO  | CA-C-N    | 5.94  | 128.51      | 120.38   |
| 1   | H     | 157 | PRO  | C-N-CA    | 5.94  | 128.51      | 120.38   |
| 1   | H     | 285 | VAL  | CA-CB-CG2 | 5.93  | 120.47      | 110.40   |
| 1   | C     | 171 | ASN  | CB-CA-C   | 5.92  | 119.57      | 109.80   |
| 1   | J     | 157 | PRO  | CA-C-N    | 5.92  | 128.49      | 120.38   |
| 1   | J     | 157 | PRO  | C-N-CA    | 5.92  | 128.49      | 120.38   |
| 1   | C     | 163 | ARG  | CG-CD-NE  | 5.91  | 124.99      | 112.00   |
| 1   | A     | 442 | GLU  | CB-CG-CD  | 5.89  | 122.61      | 112.60   |
| 1   | G     | 157 | PRO  | CA-C-N    | 5.88  | 128.44      | 120.38   |
| 1   | G     | 157 | PRO  | C-N-CA    | 5.88  | 128.44      | 120.38   |
| 1   | K     | 200 | THR  | CB-CA-C   | 5.84  | 120.50      | 110.86   |
| 1   | A     | 181 | LYS  | CB-CG-CD  | 5.84  | 124.73      | 111.30   |
| 1   | D     | 157 | PRO  | CA-C-N    | 5.81  | 128.34      | 120.38   |
| 1   | D     | 157 | PRO  | C-N-CA    | 5.81  | 128.34      | 120.38   |
| 1   | H     | 200 | THR  | CB-CA-C   | 5.80  | 120.42      | 110.86   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | F     | 200 | THR  | CB-CA-C  | 5.75  | 120.35      | 110.86   |
| 1   | E     | 200 | THR  | CB-CA-C  | 5.68  | 120.23      | 110.86   |
| 1   | L     | 200 | THR  | CB-CA-C  | 5.67  | 120.21      | 110.86   |
| 1   | I     | 200 | THR  | CB-CA-C  | 5.65  | 120.18      | 110.86   |
| 1   | C     | 226 | LYS  | CG-CD-CE | 5.64  | 124.28      | 111.30   |
| 1   | D     | 171 | ASN  | CB-CA-C  | 5.63  | 119.09      | 109.80   |
| 1   | A     | 200 | THR  | CB-CA-C  | 5.62  | 120.13      | 110.86   |
| 1   | K     | 371 | ASP  | CA-CB-CG | 5.60  | 118.20      | 112.60   |
| 1   | D     | 187 | ARG  | CG-CD-NE | 5.60  | 124.32      | 112.00   |
| 1   | B     | 200 | THR  | CB-CA-C  | 5.58  | 120.08      | 110.86   |
| 1   | D     | 226 | LYS  | CB-CG-CD | 5.53  | 124.01      | 111.30   |
| 1   | D     | 460 | ASP  | CA-CB-CG | 5.52  | 118.12      | 112.60   |
| 1   | L     | 403 | LYS  | CB-CG-CD | 5.46  | 123.85      | 111.30   |
| 1   | A     | 533 | PHE  | CA-CB-CG | 5.45  | 119.25      | 113.80   |
| 1   | D     | 442 | GLU  | CB-CG-CD | 5.44  | 121.85      | 112.60   |
| 1   | D     | 200 | THR  | CB-CA-C  | 5.44  | 119.83      | 110.86   |
| 1   | J     | 226 | LYS  | CB-CG-CD | 5.41  | 123.73      | 111.30   |
| 1   | I     | 162 | LYS  | CB-CA-C  | 5.41  | 120.45      | 110.88   |
| 1   | A     | 435 | GLU  | CB-CG-CD | 5.40  | 121.78      | 112.60   |
| 1   | G     | 400 | LYS  | CA-CB-CG | 5.39  | 124.87      | 114.10   |
| 1   | L     | 226 | LYS  | CB-CG-CD | 5.39  | 123.69      | 111.30   |
| 1   | H     | 162 | LYS  | CB-CA-C  | 5.38  | 120.40      | 110.88   |
| 1   | L     | 187 | ARG  | CB-CG-CD | -5.37 | 98.96       | 111.30   |
| 1   | D     | 422 | ASP  | CA-CB-CG | 5.36  | 117.96      | 112.60   |
| 1   | G     | 171 | ASN  | CB-CA-C  | 5.33  | 119.67      | 110.45   |
| 1   | I     | 434 | LYS  | CB-CA-C  | 5.33  | 119.87      | 111.72   |
| 1   | A     | 422 | ASP  | CA-CB-CG | 5.31  | 117.91      | 112.60   |
| 1   | E     | 187 | ARG  | CB-CG-CD | -5.31 | 99.08       | 111.30   |
| 1   | E     | 162 | LYS  | CB-CA-C  | 5.30  | 120.26      | 110.88   |
| 1   | K     | 162 | LYS  | CB-CA-C  | 5.30  | 120.25      | 110.88   |
| 1   | J     | 397 | ASN  | CB-CA-C  | -5.29 | 103.75      | 112.06   |
| 1   | D     | 513 | VAL  | CA-C-N   | 5.28  | 127.63      | 120.44   |
| 1   | D     | 513 | VAL  | C-N-CA   | 5.28  | 127.63      | 120.44   |
| 1   | J     | 162 | LYS  | CB-CA-C  | 5.28  | 120.23      | 110.88   |
| 1   | J     | 200 | THR  | CB-CA-C  | 5.27  | 119.55      | 110.86   |
| 1   | J     | 171 | ASN  | CB-CA-C  | 5.25  | 119.53      | 110.45   |
| 1   | G     | 234 | TYR  | CB-CA-C  | 5.20  | 118.90      | 110.22   |
| 1   | H     | 234 | TYR  | CB-CA-C  | 5.20  | 118.90      | 110.22   |
| 1   | B     | 266 | HIS  | CB-CA-C  | 5.19  | 115.63      | 110.33   |
| 1   | C     | 201 | THR  | N-CA-CB  | 5.18  | 117.45      | 110.10   |
| 1   | L     | 422 | ASP  | CA-CB-CG | 5.18  | 117.78      | 112.60   |
| 1   | B     | 162 | LYS  | CB-CA-C  | 5.17  | 120.04      | 110.88   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | F     | 171 | ASN  | CB-CA-C   | 5.16  | 119.38      | 110.45   |
| 1   | G     | 198 | SER  | CA-C-O    | -5.16 | 113.14      | 120.51   |
| 1   | I     | 442 | GLU  | CB-CG-CD  | 5.16  | 121.36      | 112.60   |
| 1   | A     | 162 | LYS  | CB-CA-C   | 5.13  | 119.97      | 110.88   |
| 1   | K     | 151 | GLU  | CB-CG-CD  | 5.13  | 121.32      | 112.60   |
| 1   | L     | 171 | ASN  | CB-CA-C   | 5.13  | 119.32      | 110.45   |
| 1   | C     | 266 | HIS  | CB-CA-C   | 5.12  | 115.56      | 110.33   |
| 1   | I     | 435 | GLU  | CB-CG-CD  | 5.12  | 121.31      | 112.60   |
| 1   | D     | 14  | THR  | CA-CB-OG1 | -5.12 | 101.92      | 109.60   |
| 1   | A     | 460 | ASP  | CA-CB-CG  | 5.11  | 117.71      | 112.60   |
| 1   | C     | 234 | TYR  | CB-CA-C   | 5.11  | 118.75      | 110.22   |
| 1   | I     | 490 | TYR  | CA-C-N    | 5.11  | 127.12      | 120.28   |
| 1   | I     | 490 | TYR  | C-N-CA    | 5.11  | 127.12      | 120.28   |
| 1   | G     | 299 | ASN  | CA-CB-CG  | -5.10 | 107.50      | 112.60   |
| 1   | L     | 234 | TYR  | CB-CA-C   | 5.09  | 118.72      | 110.22   |
| 1   | B     | 234 | TYR  | CB-CA-C   | 5.08  | 118.70      | 110.22   |
| 1   | L     | 162 | LYS  | CB-CA-C   | 5.07  | 119.86      | 110.88   |
| 1   | B     | 366 | VAL  | CB-CA-C   | 5.05  | 117.24      | 110.42   |
| 1   | D     | 491 | GLU  | CA-C-N    | 5.04  | 127.04      | 120.28   |
| 1   | D     | 491 | GLU  | C-N-CA    | 5.04  | 127.04      | 120.28   |
| 1   | I     | 422 | ASP  | CA-CB-CG  | 5.04  | 117.64      | 112.60   |
| 1   | C     | 14  | THR  | CA-CB-OG1 | -5.02 | 102.07      | 109.60   |
| 1   | A     | 234 | TYR  | CB-CA-C   | 5.02  | 118.61      | 110.22   |
| 1   | C     | 134 | PHE  | CB-CA-C   | 5.02  | 118.38      | 109.65   |
| 1   | D     | 266 | HIS  | CB-CA-C   | 5.02  | 115.45      | 110.33   |
| 1   | L     | 297 | LYS  | CA-CB-CG  | 5.02  | 124.13      | 114.10   |
| 1   | G     | 226 | LYS  | CA-CB-CG  | 5.01  | 124.13      | 114.10   |
| 1   | H     | 151 | GLU  | CB-CG-CD  | 5.01  | 121.12      | 112.60   |
| 1   | B     | 171 | ASN  | CB-CA-C   | 5.01  | 119.12      | 110.45   |
| 1   | D     | 162 | LYS  | CB-CA-C   | 5.01  | 119.74      | 110.88   |
| 1   | K     | 171 | ASN  | CB-CA-C   | 5.00  | 119.10      | 110.45   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | H     | 299 | ASN  | 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     | 4134  | 0        | 4152     | 21      | 0            |
| 1   | B     | 3370  | 0        | 3348     | 20      | 0            |
| 1   | C     | 3386  | 0        | 3365     | 23      | 0            |
| 1   | D     | 4023  | 0        | 4032     | 21      | 0            |
| 1   | E     | 3353  | 0        | 3331     | 18      | 0            |
| 1   | F     | 3378  | 0        | 3359     | 21      | 0            |
| 1   | G     | 3325  | 0        | 3294     | 18      | 0            |
| 1   | H     | 3362  | 0        | 3337     | 17      | 0            |
| 1   | I     | 4076  | 0        | 4106     | 19      | 0            |
| 1   | J     | 3362  | 0        | 3337     | 16      | 0            |
| 1   | K     | 3344  | 0        | 3318     | 17      | 0            |
| 1   | L     | 3353  | 0        | 3331     | 17      | 0            |
| 2   | A     | 31    | 0        | 0        | 0       | 0            |
| 2   | B     | 36    | 0        | 0        | 2       | 0            |
| 2   | C     | 58    | 0        | 0        | 6       | 0            |
| 2   | D     | 58    | 0        | 0        | 3       | 0            |
| 2   | E     | 18    | 0        | 0        | 2       | 0            |
| 2   | F     | 33    | 0        | 0        | 3       | 0            |
| 2   | G     | 13    | 0        | 0        | 2       | 0            |
| 2   | H     | 14    | 0        | 0        | 1       | 0            |
| 2   | I     | 25    | 0        | 0        | 0       | 0            |
| 2   | J     | 20    | 0        | 0        | 2       | 0            |
| 2   | K     | 9     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 1       | 0            |
| All | All   | 42783 | 0        | 42310    | 217     | 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 3.

All (217) 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:L:336:MET:HE1 | 1:L:415:THR:HB  | 1.45                     | 0.97              |
| 1:H:336:MET:HE1 | 1:H:415:THR:HB  | 1.46                     | 0.95              |
| 1:K:125:SER:OG  | 1:K:128:LEU:HB2 | 1.73                     | 0.89              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:205:LYS:HE2  | 2:D:655:HOH:O    | 1.77                     | 0.84              |
| 1:A:438:ASN:HD21 | 1:A:443:LYS:HE2  | 1.45                     | 0.81              |
| 1:B:336:MET:HE1  | 1:B:415:THR:HG22 | 1.63                     | 0.80              |
| 1:A:336:MET:HE1  | 1:A:415:THR:HG22 | 1.66                     | 0.78              |
| 1:C:336:MET:HE1  | 1:C:415:THR:HG22 | 1.65                     | 0.78              |
| 1:J:336:MET:HE1  | 1:J:415:THR:HG22 | 1.66                     | 0.78              |
| 1:G:147:ARG:HB2  | 2:G:601:HOH:O    | 1.84                     | 0.77              |
| 1:G:336:MET:HE1  | 1:G:415:THR:HG22 | 1.66                     | 0.77              |
| 1:I:336:MET:HE1  | 1:I:415:THR:HG22 | 1.65                     | 0.77              |
| 1:D:336:MET:HE1  | 1:D:415:THR:HG22 | 1.65                     | 0.77              |
| 1:E:336:MET:HE1  | 1:E:415:THR:HG22 | 1.67                     | 0.76              |
| 1:F:336:MET:HE1  | 1:F:415:THR:HG22 | 1.68                     | 0.76              |
| 1:E:13:ASP:OD1   | 1:E:181:LYS:NZ   | 2.17                     | 0.74              |
| 1:E:320:HIS:HD2  | 2:E:604:HOH:O    | 1.73                     | 0.69              |
| 1:H:424:GLU:HG2  | 2:H:604:HOH:O    | 1.92                     | 0.69              |
| 1:J:320:HIS:HE1  | 2:J:620:HOH:O    | 1.75                     | 0.69              |
| 1:A:299:ASN:C    | 1:A:299:ASN:HD22 | 2.02                     | 0.67              |
| 1:C:320:HIS:HD2  | 2:C:608:HOH:O    | 1.78                     | 0.66              |
| 1:C:127:ILE:HG22 | 2:C:642:HOH:O    | 1.98                     | 0.63              |
| 1:L:336:MET:HE3  | 1:L:343:MET:HE1  | 1.81                     | 0.62              |
| 1:B:52:ASN:HD21  | 1:B:171:ASN:HD21 | 1.48                     | 0.62              |
| 1:H:336:MET:HE3  | 1:H:343:MET:HE1  | 1.80                     | 0.61              |
| 1:A:361:PRO:HG3  | 1:A:366:VAL:HG22 | 1.83                     | 0.60              |
| 1:A:416:GLY:C    | 1:A:433:ILE:HD12 | 2.26                     | 0.60              |
| 1:F:336:MET:HE2  | 1:F:343:MET:SD   | 2.42                     | 0.60              |
| 1:A:309:SER:OG   | 1:A:332:GLU:HG2  | 2.02                     | 0.60              |
| 1:E:411:ASN:HB2  | 1:F:61:ARG:HD3   | 1.84                     | 0.59              |
| 1:E:336:MET:HE2  | 1:E:343:MET:SD   | 2.43                     | 0.59              |
| 1:J:336:MET:HE2  | 1:J:343:MET:SD   | 2.43                     | 0.58              |
| 1:C:47:MET:HE2   | 1:C:48:PHE:CZ    | 2.39                     | 0.58              |
| 1:D:47:MET:HE2   | 1:D:48:PHE:CZ    | 2.39                     | 0.58              |
| 1:A:463:VAL:HG11 | 1:A:529:ILE:HD13 | 1.85                     | 0.57              |
| 1:D:448:GLU:HG3  | 2:D:645:HOH:O    | 2.04                     | 0.57              |
| 1:I:463:VAL:HG11 | 1:I:529:ILE:HD13 | 1.86                     | 0.57              |
| 1:F:47:MET:HE2   | 1:F:48:PHE:CZ    | 2.39                     | 0.57              |
| 1:L:47:MET:HE2   | 1:L:48:PHE:CZ    | 2.40                     | 0.57              |
| 1:F:320:HIS:HD2  | 2:F:627:HOH:O    | 1.87                     | 0.57              |
| 1:A:47:MET:HE2   | 1:A:48:PHE:CZ    | 2.40                     | 0.57              |
| 1:H:47:MET:HE2   | 1:H:48:PHE:CZ    | 2.40                     | 0.57              |
| 1:J:47:MET:HE2   | 1:J:48:PHE:CZ    | 2.40                     | 0.56              |
| 1:G:47:MET:HE2   | 1:G:48:PHE:CZ    | 2.40                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:47:MET:HE2   | 1:K:48:PHE:CZ    | 2.40                     | 0.56              |
| 1:L:407:THR:HA   | 2:L:601:HOH:O    | 2.05                     | 0.56              |
| 1:G:336:MET:HE2  | 1:G:343:MET:SD   | 2.45                     | 0.56              |
| 1:E:47:MET:HE2   | 1:E:48:PHE:CZ    | 2.41                     | 0.56              |
| 1:A:336:MET:HE2  | 1:A:343:MET:SD   | 2.45                     | 0.56              |
| 1:I:47:MET:HE2   | 1:I:48:PHE:CZ    | 2.40                     | 0.56              |
| 1:E:320:HIS:CD2  | 2:E:604:HOH:O    | 2.53                     | 0.56              |
| 1:C:336:MET:HE2  | 1:C:343:MET:SD   | 2.46                     | 0.55              |
| 1:I:336:MET:HE2  | 1:I:343:MET:SD   | 2.46                     | 0.55              |
| 1:B:311:SER:O    | 1:B:312:SER:HB3  | 2.06                     | 0.55              |
| 1:B:47:MET:HE2   | 1:B:48:PHE:CZ    | 2.41                     | 0.55              |
| 1:B:336:MET:HE2  | 1:B:343:MET:SD   | 2.47                     | 0.55              |
| 1:D:336:MET:HE2  | 1:D:343:MET:SD   | 2.47                     | 0.54              |
| 1:B:158:GLU:HA   | 2:B:634:HOH:O    | 2.07                     | 0.53              |
| 1:J:361:PRO:HG3  | 1:J:366:VAL:HG13 | 1.91                     | 0.53              |
| 1:K:411:ASN:HB2  | 1:L:61:ARG:HD3   | 1.91                     | 0.53              |
| 1:D:216:ARG:HG2  | 1:D:389:GLU:HB2  | 1.90                     | 0.53              |
| 1:I:24:ILE:HG12  | 1:I:31:GLN:HG2   | 1.90                     | 0.53              |
| 1:B:24:ILE:HG12  | 1:B:31:GLN:HG2   | 1.91                     | 0.52              |
| 1:C:201:THR:OG1  | 1:C:434:LYS:HD2  | 2.09                     | 0.52              |
| 1:F:361:PRO:HG3  | 1:F:366:VAL:HG13 | 1.91                     | 0.52              |
| 1:G:226:LYS:HG2  | 1:G:348:LEU:HD23 | 1.91                     | 0.51              |
| 1:I:411:ASN:HB2  | 1:J:61:ARG:HD3   | 1.92                     | 0.51              |
| 1:F:294:ASN:HB2  | 2:F:618:HOH:O    | 2.10                     | 0.51              |
| 1:J:337:THR:HB   | 2:J:612:HOH:O    | 2.09                     | 0.51              |
| 1:D:361:PRO:HG3  | 1:D:366:VAL:HG13 | 1.94                     | 0.50              |
| 1:G:361:PRO:HG3  | 1:G:366:VAL:HG13 | 1.93                     | 0.50              |
| 1:G:411:ASN:HB2  | 1:H:61:ARG:HD3   | 1.93                     | 0.50              |
| 1:C:361:PRO:HG3  | 1:C:366:VAL:HG13 | 1.93                     | 0.50              |
| 1:H:24:ILE:HG12  | 1:H:31:GLN:HG2   | 1.93                     | 0.50              |
| 1:D:24:ILE:HG12  | 1:D:31:GLN:HG2   | 1.92                     | 0.50              |
| 1:G:185:PHE:HB2  | 2:G:610:HOH:O    | 2.11                     | 0.49              |
| 1:H:361:PRO:HG3  | 1:H:366:VAL:HG13 | 1.94                     | 0.49              |
| 1:B:387:ARG:HA   | 2:B:629:HOH:O    | 2.11                     | 0.49              |
| 1:E:216:ARG:HG2  | 1:E:389:GLU:HB2  | 1.94                     | 0.49              |
| 1:E:243:HIS:HA   | 1:E:341:HIS:CE1  | 2.48                     | 0.49              |
| 1:E:361:PRO:HG3  | 1:E:366:VAL:HG13 | 1.95                     | 0.49              |
| 1:I:361:PRO:HG3  | 1:I:366:VAL:HG13 | 1.94                     | 0.49              |
| 1:A:388:GLY:O    | 1:B:187:ARG:NH2  | 2.46                     | 0.48              |
| 1:L:216:ARG:HG2  | 1:L:389:GLU:HB2  | 1.95                     | 0.48              |
| 1:I:449:LEU:HD11 | 1:I:476:VAL:HG11 | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:243:HIS:HA   | 1:H:341:HIS:CE1  | 2.49                     | 0.48              |
| 1:J:216:ARG:HG2  | 1:J:389:GLU:HB2  | 1.96                     | 0.48              |
| 1:A:243:HIS:HA   | 1:A:341:HIS:CE1  | 2.49                     | 0.48              |
| 1:B:243:HIS:HA   | 1:B:341:HIS:CE1  | 2.49                     | 0.48              |
| 1:F:243:HIS:HA   | 1:F:341:HIS:CE1  | 2.49                     | 0.48              |
| 1:G:243:HIS:HA   | 1:G:341:HIS:CE1  | 2.48                     | 0.48              |
| 1:K:24:ILE:HG12  | 1:K:31:GLN:HG2   | 1.95                     | 0.48              |
| 1:K:243:HIS:HA   | 1:K:341:HIS:CE1  | 2.48                     | 0.48              |
| 1:C:24:ILE:HG12  | 1:C:31:GLN:HG2   | 1.96                     | 0.47              |
| 1:I:216:ARG:HG2  | 1:I:389:GLU:HB2  | 1.95                     | 0.47              |
| 1:K:61:ARG:HD3   | 1:L:411:ASN:HB2  | 1.95                     | 0.47              |
| 1:C:216:ARG:HG2  | 1:C:389:GLU:HB2  | 1.95                     | 0.47              |
| 1:J:24:ILE:HG12  | 1:J:31:GLN:HG2   | 1.95                     | 0.47              |
| 1:A:456:HIS:HE1  | 1:A:458:LYS:HE3  | 1.79                     | 0.47              |
| 1:K:47:MET:HG2   | 1:K:55:LEU:HD12  | 1.96                     | 0.47              |
| 1:E:24:ILE:HG12  | 1:E:31:GLN:HG2   | 1.96                     | 0.47              |
| 1:I:61:ARG:HD3   | 1:J:411:ASN:HB2  | 1.96                     | 0.47              |
| 1:C:226:LYS:HE2  | 2:C:656:HOH:O    | 2.14                     | 0.47              |
| 1:I:243:HIS:HA   | 1:I:341:HIS:CE1  | 2.50                     | 0.47              |
| 1:C:411:ASN:HB2  | 1:D:61:ARG:HD3   | 1.96                     | 0.47              |
| 1:D:243:HIS:HA   | 1:D:341:HIS:CE1  | 2.50                     | 0.47              |
| 1:L:47:MET:HG2   | 1:L:55:LEU:HD12  | 1.97                     | 0.47              |
| 1:G:61:ARG:HD3   | 1:H:411:ASN:HB2  | 1.97                     | 0.47              |
| 1:C:432:ARG:HH21 | 1:C:434:LYS:HZ3  | 1.62                     | 0.46              |
| 1:K:216:ARG:HG2  | 1:K:389:GLU:HB2  | 1.97                     | 0.46              |
| 1:L:243:HIS:HA   | 1:L:341:HIS:CE1  | 2.50                     | 0.46              |
| 1:J:243:HIS:HA   | 1:J:341:HIS:CE1  | 2.51                     | 0.46              |
| 1:A:47:MET:HG2   | 1:A:55:LEU:HD12  | 1.98                     | 0.46              |
| 1:A:216:ARG:HG2  | 1:A:389:GLU:HB2  | 1.97                     | 0.46              |
| 1:G:187:ARG:HH11 | 1:H:389:GLU:HA   | 1.80                     | 0.46              |
| 1:B:47:MET:HG2   | 1:B:55:LEU:HD12  | 1.98                     | 0.46              |
| 1:H:216:ARG:HG2  | 1:H:389:GLU:HB2  | 1.97                     | 0.46              |
| 1:A:449:LEU:HD11 | 1:A:476:VAL:HG11 | 1.98                     | 0.46              |
| 1:B:119:THR:HA   | 1:B:122:LEU:HD12 | 1.96                     | 0.46              |
| 1:F:216:ARG:HG2  | 1:F:389:GLU:HB2  | 1.98                     | 0.46              |
| 1:L:361:PRO:HG3  | 1:L:366:VAL:HG13 | 1.96                     | 0.46              |
| 1:C:243:HIS:HA   | 1:C:341:HIS:CE1  | 2.51                     | 0.45              |
| 1:G:47:MET:HG2   | 1:G:55:LEU:HD12  | 1.98                     | 0.45              |
| 1:H:47:MET:HG2   | 1:H:55:LEU:HD12  | 1.97                     | 0.45              |
| 1:B:216:ARG:HG2  | 1:B:389:GLU:HB2  | 1.98                     | 0.45              |
| 1:B:361:PRO:HG3  | 1:B:366:VAL:HG13 | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:361:PRO:HG3  | 1:K:366:VAL:HG13 | 1.96                     | 0.45              |
| 1:E:47:MET:HG2   | 1:E:55:LEU:HD12  | 1.99                     | 0.45              |
| 1:A:461:GLU:HB2  | 1:A:481:VAL:HB   | 1.99                     | 0.45              |
| 1:G:216:ARG:HG2  | 1:G:389:GLU:HB2  | 1.97                     | 0.45              |
| 1:I:444:ILE:CG1  | 1:I:505:LYS:HG2  | 2.46                     | 0.45              |
| 1:I:461:GLU:HB2  | 1:I:481:VAL:HB   | 1.99                     | 0.45              |
| 1:D:460:ASP:HB2  | 1:D:483:LYS:HG3  | 1.99                     | 0.45              |
| 1:D:461:GLU:HB2  | 1:D:481:VAL:HB   | 1.99                     | 0.44              |
| 1:F:47:MET:HG2   | 1:F:55:LEU:HD12  | 1.99                     | 0.44              |
| 1:L:336:MET:HE1  | 1:L:415:THR:CB   | 2.32                     | 0.44              |
| 1:I:444:ILE:HG12 | 1:I:505:LYS:HG2  | 1.98                     | 0.44              |
| 1:C:47:MET:HG2   | 1:C:55:LEU:HD12  | 2.00                     | 0.44              |
| 1:C:226:LYS:CE   | 2:C:656:HOH:O    | 2.66                     | 0.43              |
| 1:D:47:MET:HG2   | 1:D:55:LEU:HD12  | 1.99                     | 0.43              |
| 1:D:185:PHE:HB2  | 2:D:644:HOH:O    | 2.17                     | 0.43              |
| 1:K:286:PRO:HG3  | 1:K:314:LEU:HD23 | 2.00                     | 0.43              |
| 1:F:436:LEU:O    | 1:F:437:ILE:HG13 | 2.19                     | 0.43              |
| 1:D:120:THR:HG21 | 1:D:155:TYR:CZ   | 2.54                     | 0.43              |
| 1:J:120:THR:HG21 | 1:J:155:TYR:CZ   | 2.54                     | 0.43              |
| 1:K:299:ASN:HA   | 1:K:300:PRO:C    | 2.44                     | 0.43              |
| 1:L:297:LYS:HE2  | 1:L:297:LYS:HB3  | 1.76                     | 0.43              |
| 1:A:120:THR:HG21 | 1:A:155:TYR:CZ   | 2.54                     | 0.43              |
| 1:C:434:LYS:HD3  | 2:C:625:HOH:O    | 2.18                     | 0.43              |
| 1:E:41:VAL:HG13  | 1:E:81:GLY:HA2   | 2.00                     | 0.43              |
| 1:E:120:THR:HG21 | 1:E:155:TYR:CZ   | 2.54                     | 0.43              |
| 1:J:47:MET:HG2   | 1:J:55:LEU:HD12  | 2.01                     | 0.43              |
| 1:L:221:ILE:HD13 | 1:L:247:GLY:HA2  | 2.01                     | 0.43              |
| 1:F:290:MET:HB2  | 2:F:608:HOH:O    | 2.19                     | 0.43              |
| 1:C:41:VAL:HG13  | 1:C:81:GLY:HA2   | 2.01                     | 0.42              |
| 1:K:286:PRO:HG2  | 1:K:312:SER:OG   | 2.19                     | 0.42              |
| 1:E:366:VAL:HG22 | 1:E:421:PHE:HZ   | 1.84                     | 0.42              |
| 1:K:41:VAL:HG13  | 1:K:81:GLY:HA2   | 2.00                     | 0.42              |
| 1:F:120:THR:HG21 | 1:F:155:TYR:CZ   | 2.54                     | 0.42              |
| 1:J:221:ILE:HD13 | 1:J:247:GLY:HA2  | 2.02                     | 0.42              |
| 1:G:41:VAL:HG13  | 1:G:81:GLY:HA2   | 2.02                     | 0.42              |
| 1:G:226:LYS:HG2  | 1:G:348:LEU:CD2  | 2.49                     | 0.42              |
| 1:I:47:MET:HG2   | 1:I:55:LEU:HD12  | 2.00                     | 0.42              |
| 1:C:120:THR:HG21 | 1:C:155:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:221:ILE:HD13 | 1:C:247:GLY:HA2  | 2.01                     | 0.42              |
| 1:G:120:THR:HG21 | 1:G:155:TYR:CZ   | 2.54                     | 0.42              |
| 1:I:41:VAL:HG13  | 1:I:81:GLY:HA2   | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:24:ILE:HG12  | 1:L:31:GLN:HG2   | 2.01                     | 0.42              |
| 1:E:61:ARG:HD3   | 1:F:411:ASN:HB2  | 2.01                     | 0.42              |
| 1:H:299:ASN:HA   | 1:H:300:PRO:C    | 2.44                     | 0.42              |
| 1:K:120:THR:HG21 | 1:K:155:TYR:CZ   | 2.54                     | 0.42              |
| 1:K:221:ILE:HD13 | 1:K:247:GLY:HA2  | 2.01                     | 0.42              |
| 1:B:88:ILE:HG21  | 1:B:194:ILE:HD12 | 2.02                     | 0.42              |
| 1:B:120:THR:HG21 | 1:B:155:TYR:CZ   | 2.55                     | 0.42              |
| 1:C:354:LYS:HA   | 1:C:355:PRO:HD3  | 1.96                     | 0.42              |
| 1:D:456:HIS:HE1  | 1:D:458:LYS:HE3  | 1.84                     | 0.42              |
| 1:F:293:LEU:HD22 | 1:F:321:LYS:HE2  | 2.02                     | 0.42              |
| 1:H:221:ILE:HD13 | 1:H:247:GLY:HA2  | 2.02                     | 0.42              |
| 1:B:225:TYR:O    | 1:B:305:ARG:NH2  | 2.39                     | 0.42              |
| 1:F:88:ILE:HG21  | 1:F:194:ILE:HD12 | 2.02                     | 0.42              |
| 1:H:120:THR:HG21 | 1:H:155:TYR:CZ   | 2.55                     | 0.41              |
| 1:J:41:VAL:HG13  | 1:J:81:GLY:HA2   | 2.01                     | 0.41              |
| 1:A:449:LEU:CD1  | 1:A:476:VAL:HG11 | 2.50                     | 0.41              |
| 1:F:221:ILE:HD13 | 1:F:247:GLY:HA2  | 2.02                     | 0.41              |
| 1:D:221:ILE:HD13 | 1:D:247:GLY:HA2  | 2.03                     | 0.41              |
| 1:G:221:ILE:HD13 | 1:G:247:GLY:HA2  | 2.02                     | 0.41              |
| 1:D:225:TYR:O    | 1:D:305:ARG:NH2  | 2.39                     | 0.41              |
| 1:D:449:LEU:HD11 | 1:D:476:VAL:HG11 | 2.03                     | 0.41              |
| 1:F:259:VAL:HG13 | 1:F:261:VAL:HG22 | 2.02                     | 0.41              |
| 1:I:221:ILE:HD13 | 1:I:247:GLY:HA2  | 2.02                     | 0.41              |
| 1:A:299:ASN:C    | 1:A:299:ASN:ND2  | 2.72                     | 0.41              |
| 1:F:69:MET:HE1   | 1:F:74:GLU:HB3   | 2.03                     | 0.41              |
| 1:H:41:VAL:HG13  | 1:H:81:GLY:HA2   | 2.01                     | 0.41              |
| 1:I:456:HIS:HE1  | 1:I:458:LYS:HE3  | 1.85                     | 0.41              |
| 1:L:120:THR:HG21 | 1:L:155:TYR:CZ   | 2.55                     | 0.41              |
| 1:I:120:THR:HG21 | 1:I:155:TYR:CZ   | 2.55                     | 0.41              |
| 1:L:41:VAL:HG13  | 1:L:81:GLY:HA2   | 2.02                     | 0.41              |
| 1:A:460:ASP:HB2  | 1:A:483:LYS:HG3  | 2.02                     | 0.41              |
| 1:C:268:LYS:HB2  | 2:C:658:HOH:O    | 2.20                     | 0.41              |
| 1:D:41:VAL:HG13  | 1:D:81:GLY:HA2   | 2.02                     | 0.41              |
| 1:E:221:ILE:HD13 | 1:E:247:GLY:HA2  | 2.03                     | 0.41              |
| 1:F:24:ILE:HG12  | 1:F:31:GLN:HG2   | 2.03                     | 0.41              |
| 1:H:88:ILE:HG21  | 1:H:194:ILE:HD12 | 2.03                     | 0.41              |
| 1:C:88:ILE:HG21  | 1:C:194:ILE:HD12 | 2.03                     | 0.40              |
| 1:E:203:THR:HA   | 1:E:204:PRO:HD3  | 1.99                     | 0.40              |
| 1:L:344:THR:HG22 | 1:L:361:PRO:HA   | 2.03                     | 0.40              |
| 1:B:181:LYS:HE3  | 1:B:181:LYS:HB3  | 1.77                     | 0.40              |
| 1:G:299:ASN:HA   | 1:G:300:PRO:C    | 2.46                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:259:VAL:HG13 | 1:J:261:VAL:HG22 | 2.03                     | 0.40              |
| 1:B:41:VAL:HG13  | 1:B:81:GLY:HA2   | 2.02                     | 0.40              |
| 1:F:366:VAL:HG22 | 1:F:421:PHE:HZ   | 1.87                     | 0.40              |
| 1:A:41:VAL:HG13  | 1:A:81:GLY:HA2   | 2.02                     | 0.40              |
| 1:B:366:VAL:HG22 | 1:B:421:PHE:HZ   | 1.86                     | 0.40              |
| 1:D:366:VAL:HG22 | 1:D:421:PHE:HZ   | 1.86                     | 0.40              |
| 1:K:128:LEU:HD22 | 1:K:128:LEU:HA   | 1.96                     | 0.40              |
| 1:C:128:LEU:HD22 | 1:C:128:LEU:HA   | 1.96                     | 0.40              |
| 1:K:366:VAL:HG22 | 1:K:421:PHE:HZ   | 1.86                     | 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     | 523/543 (96%)   | 505 (97%)  | 16 (3%)  | 2 (0%)   | 30          | 56 |
| 1   | B     | 426/543 (78%)   | 414 (97%)  | 10 (2%)  | 2 (0%)   | 24          | 51 |
| 1   | C     | 428/543 (79%)   | 418 (98%)  | 8 (2%)   | 2 (0%)   | 24          | 51 |
| 1   | D     | 509/543 (94%)   | 493 (97%)  | 14 (3%)  | 2 (0%)   | 30          | 56 |
| 1   | E     | 424/543 (78%)   | 412 (97%)  | 10 (2%)  | 2 (0%)   | 24          | 51 |
| 1   | F     | 427/543 (79%)   | 415 (97%)  | 10 (2%)  | 2 (0%)   | 24          | 51 |
| 1   | G     | 421/543 (78%)   | 407 (97%)  | 11 (3%)  | 3 (1%)   | 18          | 44 |
| 1   | H     | 425/543 (78%)   | 412 (97%)  | 11 (3%)  | 2 (0%)   | 24          | 51 |
| 1   | I     | 514/543 (95%)   | 496 (96%)  | 16 (3%)  | 2 (0%)   | 30          | 56 |
| 1   | J     | 425/543 (78%)   | 413 (97%)  | 10 (2%)  | 2 (0%)   | 24          | 51 |
| 1   | K     | 423/543 (78%)   | 410 (97%)  | 11 (3%)  | 2 (0%)   | 24          | 51 |
| 1   | L     | 424/543 (78%)   | 413 (97%)  | 9 (2%)   | 2 (0%)   | 24          | 51 |
| All | All   | 5369/6516 (82%) | 5208 (97%) | 136 (2%) | 25 (0%)  | 24          | 51 |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 312 | SER  |
| 1   | A     | 341 | HIS  |
| 1   | B     | 341 | HIS  |
| 1   | C     | 311 | SER  |
| 1   | C     | 341 | HIS  |
| 1   | D     | 341 | HIS  |
| 1   | E     | 341 | HIS  |
| 1   | F     | 311 | SER  |
| 1   | F     | 341 | HIS  |
| 1   | G     | 341 | HIS  |
| 1   | H     | 341 | HIS  |
| 1   | I     | 341 | HIS  |
| 1   | J     | 341 | HIS  |
| 1   | K     | 341 | HIS  |
| 1   | L     | 341 | HIS  |
| 1   | A     | 311 | SER  |
| 1   | D     | 311 | SER  |
| 1   | E     | 311 | SER  |
| 1   | G     | 311 | SER  |
| 1   | H     | 311 | SER  |
| 1   | I     | 311 | SER  |
| 1   | J     | 311 | SER  |
| 1   | K     | 311 | SER  |
| 1   | L     | 311 | SER  |
| 1   | G     | 198 | SER  |

### 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     | 461/476 (97%) | 428 (93%) | 33 (7%)  | 13          | 36 |
| 1   | B     | 378/476 (79%) | 354 (94%) | 24 (6%)  | 16          | 42 |
| 1   | C     | 380/476 (80%) | 353 (93%) | 27 (7%)  | 13          | 37 |
| 1   | D     | 450/476 (94%) | 421 (94%) | 29 (6%)  | 16          | 42 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | E     | 376/476 (79%)   | 357 (95%)  | 19 (5%)  | 21          | 50 |
| 1   | F     | 379/476 (80%)   | 359 (95%)  | 20 (5%)  | 20          | 49 |
| 1   | G     | 373/476 (78%)   | 347 (93%)  | 26 (7%)  | 14          | 37 |
| 1   | H     | 377/476 (79%)   | 354 (94%)  | 23 (6%)  | 17          | 43 |
| 1   | I     | 455/476 (96%)   | 423 (93%)  | 32 (7%)  | 14          | 37 |
| 1   | J     | 377/476 (79%)   | 354 (94%)  | 23 (6%)  | 17          | 43 |
| 1   | K     | 375/476 (79%)   | 352 (94%)  | 23 (6%)  | 17          | 43 |
| 1   | L     | 376/476 (79%)   | 354 (94%)  | 22 (6%)  | 18          | 45 |
| All | All   | 4757/5712 (83%) | 4456 (94%) | 301 (6%) | 16          | 42 |

All (301) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | MET  |
| 1   | A     | 120 | THR  |
| 1   | A     | 122 | LEU  |
| 1   | A     | 123 | GLN  |
| 1   | A     | 128 | LEU  |
| 1   | A     | 132 | SER  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 164 | VAL  |
| 1   | A     | 167 | ARG  |
| 1   | A     | 189 | SER  |
| 1   | A     | 203 | THR  |
| 1   | A     | 205 | LYS  |
| 1   | A     | 217 | SER  |
| 1   | A     | 226 | LYS  |
| 1   | A     | 259 | VAL  |
| 1   | A     | 285 | VAL  |
| 1   | A     | 299 | ASN  |
| 1   | A     | 312 | SER  |
| 1   | A     | 337 | THR  |
| 1   | A     | 366 | VAL  |
| 1   | A     | 371 | ASP  |
| 1   | A     | 397 | ASN  |
| 1   | A     | 432 | ARG  |
| 1   | A     | 438 | ASN  |
| 1   | A     | 447 | ILE  |
| 1   | A     | 448 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 457 | PRO  |
| 1   | A     | 484 | LYS  |
| 1   | A     | 503 | SER  |
| 1   | A     | 524 | ILE  |
| 1   | A     | 525 | GLN  |
| 1   | A     | 527 | ARG  |
| 1   | A     | 528 | VAL  |
| 1   | B     | 47  | MET  |
| 1   | B     | 97  | LYS  |
| 1   | B     | 99  | LYS  |
| 1   | B     | 120 | THR  |
| 1   | B     | 122 | LEU  |
| 1   | B     | 128 | LEU  |
| 1   | B     | 132 | SER  |
| 1   | B     | 164 | VAL  |
| 1   | B     | 181 | LYS  |
| 1   | B     | 189 | SER  |
| 1   | B     | 205 | LYS  |
| 1   | B     | 217 | SER  |
| 1   | B     | 259 | VAL  |
| 1   | B     | 285 | VAL  |
| 1   | B     | 309 | SER  |
| 1   | B     | 311 | SER  |
| 1   | B     | 312 | SER  |
| 1   | B     | 321 | LYS  |
| 1   | B     | 324 | LYS  |
| 1   | B     | 337 | THR  |
| 1   | B     | 366 | VAL  |
| 1   | B     | 371 | ASP  |
| 1   | B     | 397 | ASN  |
| 1   | B     | 434 | LYS  |
| 1   | C     | 16  | SER  |
| 1   | C     | 47  | MET  |
| 1   | C     | 97  | LYS  |
| 1   | C     | 99  | LYS  |
| 1   | C     | 120 | THR  |
| 1   | C     | 122 | LEU  |
| 1   | C     | 128 | LEU  |
| 1   | C     | 132 | SER  |
| 1   | C     | 164 | VAL  |
| 1   | C     | 167 | ARG  |
| 1   | C     | 173 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 181 | LYS  |
| 1   | C     | 187 | ARG  |
| 1   | C     | 189 | SER  |
| 1   | C     | 205 | LYS  |
| 1   | C     | 217 | SER  |
| 1   | C     | 226 | LYS  |
| 1   | C     | 259 | VAL  |
| 1   | C     | 285 | VAL  |
| 1   | C     | 309 | SER  |
| 1   | C     | 312 | SER  |
| 1   | C     | 324 | LYS  |
| 1   | C     | 337 | THR  |
| 1   | C     | 366 | VAL  |
| 1   | C     | 371 | ASP  |
| 1   | C     | 434 | LYS  |
| 1   | C     | 437 | ILE  |
| 1   | D     | 16  | SER  |
| 1   | D     | 47  | MET  |
| 1   | D     | 120 | THR  |
| 1   | D     | 122 | LEU  |
| 1   | D     | 123 | GLN  |
| 1   | D     | 128 | LEU  |
| 1   | D     | 162 | LYS  |
| 1   | D     | 164 | VAL  |
| 1   | D     | 173 | LYS  |
| 1   | D     | 189 | SER  |
| 1   | D     | 205 | LYS  |
| 1   | D     | 217 | SER  |
| 1   | D     | 226 | LYS  |
| 1   | D     | 258 | SER  |
| 1   | D     | 259 | VAL  |
| 1   | D     | 285 | VAL  |
| 1   | D     | 309 | SER  |
| 1   | D     | 312 | SER  |
| 1   | D     | 337 | THR  |
| 1   | D     | 366 | VAL  |
| 1   | D     | 371 | ASP  |
| 1   | D     | 397 | ASN  |
| 1   | D     | 434 | LYS  |
| 1   | D     | 443 | LYS  |
| 1   | D     | 447 | ILE  |
| 1   | D     | 448 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 503 | SER  |
| 1   | D     | 515 | LYS  |
| 1   | D     | 516 | LEU  |
| 1   | E     | 16  | SER  |
| 1   | E     | 47  | MET  |
| 1   | E     | 120 | THR  |
| 1   | E     | 122 | LEU  |
| 1   | E     | 128 | LEU  |
| 1   | E     | 164 | VAL  |
| 1   | E     | 187 | ARG  |
| 1   | E     | 189 | SER  |
| 1   | E     | 205 | LYS  |
| 1   | E     | 217 | SER  |
| 1   | E     | 258 | SER  |
| 1   | E     | 259 | VAL  |
| 1   | E     | 285 | VAL  |
| 1   | E     | 309 | SER  |
| 1   | E     | 312 | SER  |
| 1   | E     | 337 | THR  |
| 1   | E     | 366 | VAL  |
| 1   | E     | 371 | ASP  |
| 1   | E     | 397 | ASN  |
| 1   | F     | 13  | ASP  |
| 1   | F     | 47  | MET  |
| 1   | F     | 120 | THR  |
| 1   | F     | 122 | LEU  |
| 1   | F     | 128 | LEU  |
| 1   | F     | 158 | GLU  |
| 1   | F     | 163 | ARG  |
| 1   | F     | 164 | VAL  |
| 1   | F     | 189 | SER  |
| 1   | F     | 217 | SER  |
| 1   | F     | 258 | SER  |
| 1   | F     | 259 | VAL  |
| 1   | F     | 285 | VAL  |
| 1   | F     | 309 | SER  |
| 1   | F     | 312 | SER  |
| 1   | F     | 337 | THR  |
| 1   | F     | 366 | VAL  |
| 1   | F     | 371 | ASP  |
| 1   | F     | 397 | ASN  |
| 1   | F     | 435 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 13  | ASP  |
| 1   | G     | 16  | SER  |
| 1   | G     | 47  | MET  |
| 1   | G     | 120 | THR  |
| 1   | G     | 122 | LEU  |
| 1   | G     | 128 | LEU  |
| 1   | G     | 162 | LYS  |
| 1   | G     | 164 | VAL  |
| 1   | G     | 169 | LEU  |
| 1   | G     | 189 | SER  |
| 1   | G     | 198 | SER  |
| 1   | G     | 205 | LYS  |
| 1   | G     | 217 | SER  |
| 1   | G     | 226 | LYS  |
| 1   | G     | 258 | SER  |
| 1   | G     | 259 | VAL  |
| 1   | G     | 268 | LYS  |
| 1   | G     | 285 | VAL  |
| 1   | G     | 309 | SER  |
| 1   | G     | 312 | SER  |
| 1   | G     | 337 | THR  |
| 1   | G     | 366 | VAL  |
| 1   | G     | 371 | ASP  |
| 1   | G     | 397 | ASN  |
| 1   | G     | 400 | LYS  |
| 1   | G     | 408 | LYS  |
| 1   | H     | 16  | SER  |
| 1   | H     | 47  | MET  |
| 1   | H     | 97  | LYS  |
| 1   | H     | 99  | LYS  |
| 1   | H     | 120 | THR  |
| 1   | H     | 122 | LEU  |
| 1   | H     | 128 | LEU  |
| 1   | H     | 162 | LYS  |
| 1   | H     | 164 | VAL  |
| 1   | H     | 169 | LEU  |
| 1   | H     | 189 | SER  |
| 1   | H     | 205 | LYS  |
| 1   | H     | 217 | SER  |
| 1   | H     | 226 | LYS  |
| 1   | H     | 259 | VAL  |
| 1   | H     | 297 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 309 | SER  |
| 1   | H     | 312 | SER  |
| 1   | H     | 337 | THR  |
| 1   | H     | 366 | VAL  |
| 1   | H     | 371 | ASP  |
| 1   | H     | 397 | ASN  |
| 1   | H     | 403 | LYS  |
| 1   | I     | 16  | SER  |
| 1   | I     | 47  | MET  |
| 1   | I     | 99  | LYS  |
| 1   | I     | 120 | THR  |
| 1   | I     | 122 | LEU  |
| 1   | I     | 128 | LEU  |
| 1   | I     | 158 | GLU  |
| 1   | I     | 164 | VAL  |
| 1   | I     | 189 | SER  |
| 1   | I     | 203 | THR  |
| 1   | I     | 205 | LYS  |
| 1   | I     | 217 | SER  |
| 1   | I     | 226 | LYS  |
| 1   | I     | 258 | SER  |
| 1   | I     | 259 | VAL  |
| 1   | I     | 285 | VAL  |
| 1   | I     | 309 | SER  |
| 1   | I     | 337 | THR  |
| 1   | I     | 366 | VAL  |
| 1   | I     | 371 | ASP  |
| 1   | I     | 397 | ASN  |
| 1   | I     | 400 | LYS  |
| 1   | I     | 403 | LYS  |
| 1   | I     | 433 | ILE  |
| 1   | I     | 443 | LYS  |
| 1   | I     | 448 | GLU  |
| 1   | I     | 484 | LYS  |
| 1   | I     | 515 | LYS  |
| 1   | I     | 523 | LYS  |
| 1   | I     | 524 | ILE  |
| 1   | I     | 528 | VAL  |
| 1   | I     | 532 | THR  |
| 1   | J     | 16  | SER  |
| 1   | J     | 47  | MET  |
| 1   | J     | 97  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 120 | THR  |
| 1   | J     | 122 | LEU  |
| 1   | J     | 128 | LEU  |
| 1   | J     | 158 | GLU  |
| 1   | J     | 163 | ARG  |
| 1   | J     | 164 | VAL  |
| 1   | J     | 169 | LEU  |
| 1   | J     | 189 | SER  |
| 1   | J     | 205 | LYS  |
| 1   | J     | 217 | SER  |
| 1   | J     | 258 | SER  |
| 1   | J     | 259 | VAL  |
| 1   | J     | 285 | VAL  |
| 1   | J     | 299 | ASN  |
| 1   | J     | 309 | SER  |
| 1   | J     | 337 | THR  |
| 1   | J     | 366 | VAL  |
| 1   | J     | 371 | ASP  |
| 1   | J     | 397 | ASN  |
| 1   | J     | 434 | LYS  |
| 1   | K     | 47  | MET  |
| 1   | K     | 120 | THR  |
| 1   | K     | 122 | LEU  |
| 1   | K     | 128 | LEU  |
| 1   | K     | 164 | VAL  |
| 1   | K     | 169 | LEU  |
| 1   | K     | 189 | SER  |
| 1   | K     | 202 | SER  |
| 1   | K     | 203 | THR  |
| 1   | K     | 205 | LYS  |
| 1   | K     | 217 | SER  |
| 1   | K     | 258 | SER  |
| 1   | K     | 259 | VAL  |
| 1   | K     | 285 | VAL  |
| 1   | K     | 309 | SER  |
| 1   | K     | 312 | SER  |
| 1   | K     | 314 | LEU  |
| 1   | K     | 324 | LYS  |
| 1   | K     | 337 | THR  |
| 1   | K     | 366 | VAL  |
| 1   | K     | 371 | ASP  |
| 1   | K     | 380 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 397 | ASN  |
| 1   | L     | 16  | SER  |
| 1   | L     | 47  | MET  |
| 1   | L     | 99  | LYS  |
| 1   | L     | 120 | THR  |
| 1   | L     | 122 | LEU  |
| 1   | L     | 128 | LEU  |
| 1   | L     | 164 | VAL  |
| 1   | L     | 189 | SER  |
| 1   | L     | 205 | LYS  |
| 1   | L     | 217 | SER  |
| 1   | L     | 226 | LYS  |
| 1   | L     | 258 | SER  |
| 1   | L     | 259 | VAL  |
| 1   | L     | 285 | VAL  |
| 1   | L     | 290 | MET  |
| 1   | L     | 297 | LYS  |
| 1   | L     | 309 | SER  |
| 1   | L     | 312 | SER  |
| 1   | L     | 337 | THR  |
| 1   | L     | 366 | VAL  |
| 1   | L     | 371 | ASP  |
| 1   | L     | 397 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 106 | ASN  |
| 1   | A     | 171 | ASN  |
| 1   | A     | 266 | HIS  |
| 1   | A     | 299 | ASN  |
| 1   | A     | 303 | HIS  |
| 1   | A     | 374 | ASN  |
| 1   | A     | 438 | ASN  |
| 1   | B     | 106 | ASN  |
| 1   | B     | 171 | ASN  |
| 1   | B     | 266 | HIS  |
| 1   | B     | 374 | ASN  |
| 1   | C     | 171 | ASN  |
| 1   | C     | 266 | HIS  |
| 1   | C     | 320 | HIS  |
| 1   | C     | 374 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 31  | GLN  |
| 1   | D     | 171 | ASN  |
| 1   | D     | 266 | HIS  |
| 1   | D     | 374 | ASN  |
| 1   | E     | 171 | ASN  |
| 1   | E     | 266 | HIS  |
| 1   | E     | 374 | ASN  |
| 1   | F     | 171 | ASN  |
| 1   | F     | 266 | HIS  |
| 1   | F     | 374 | ASN  |
| 1   | G     | 171 | ASN  |
| 1   | G     | 266 | HIS  |
| 1   | G     | 299 | ASN  |
| 1   | G     | 374 | ASN  |
| 1   | H     | 31  | GLN  |
| 1   | H     | 106 | ASN  |
| 1   | H     | 171 | ASN  |
| 1   | H     | 266 | HIS  |
| 1   | H     | 299 | ASN  |
| 1   | H     | 374 | ASN  |
| 1   | I     | 171 | ASN  |
| 1   | I     | 266 | HIS  |
| 1   | I     | 374 | ASN  |
| 1   | J     | 171 | ASN  |
| 1   | J     | 266 | HIS  |
| 1   | J     | 374 | ASN  |
| 1   | K     | 123 | GLN  |
| 1   | K     | 171 | ASN  |
| 1   | K     | 266 | HIS  |
| 1   | K     | 327 | ASN  |
| 1   | K     | 374 | ASN  |
| 1   | L     | 171 | ASN  |
| 1   | L     | 266 | HIS  |
| 1   | L     | 299 | ASN  |
| 1   | L     | 374 | ASN  |

### 5.3.3 RNA ⓘ

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 ⓘ

### 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     | 525/543 (96%)   | -0.05  | 2 (0%) 88 86  | 52, 63, 114, 174      | 0     |
| 1   | B     | 428/543 (78%)   | -0.24  | 0 100 100     | 50, 58, 81, 109       | 0     |
| 1   | C     | 430/543 (79%)   | -0.22  | 2 (0%) 87 83  | 49, 56, 66, 115       | 0     |
| 1   | D     | 511/543 (94%)   | -0.04  | 6 (1%) 76 70  | 48, 57, 149, 206      | 0     |
| 1   | E     | 426/543 (78%)   | -0.13  | 1 (0%) 91 89  | 53, 66, 113, 136      | 0     |
| 1   | F     | 429/543 (79%)   | -0.04  | 2 (0%) 87 83  | 53, 79, 118, 151      | 0     |
| 1   | G     | 423/543 (77%)   | 0.38   | 6 (1%) 73 66  | 66, 105, 143, 174     | 0     |
| 1   | H     | 427/543 (78%)   | 0.29   | 3 (0%) 84 80  | 62, 103, 133, 143     | 0     |
| 1   | I     | 518/543 (95%)   | -0.03  | 4 (0%) 82 77  | 51, 64, 145, 174      | 0     |
| 1   | J     | 427/543 (78%)   | -0.15  | 1 (0%) 91 89  | 52, 62, 92, 131       | 0     |
| 1   | K     | 425/543 (78%)   | 0.28   | 5 (1%) 76 70  | 54, 91, 121, 156      | 0     |
| 1   | L     | 426/543 (78%)   | 0.49   | 9 (2%) 63 55  | 65, 106, 151, 188     | 0     |
| All | All   | 5395/6516 (82%) | 0.04   | 41 (0%) 82 77 | 48, 72, 132, 206      | 0     |

All (41) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 337 | THR  | 3.9  |
| 1   | G     | 9   | ALA  | 3.4  |
| 1   | L     | 139 | VAL  | 3.3  |
| 1   | D     | 484 | LYS  | 3.2  |
| 1   | K     | 9   | ALA  | 3.1  |
| 1   | D     | 502 | ALA  | 3.1  |
| 1   | K     | 433 | ILE  | 3.1  |
| 1   | G     | 172 | ALA  | 3.0  |
| 1   | J     | 9   | ALA  | 3.0  |
| 1   | L     | 9   | ALA  | 2.9  |
| 1   | L     | 112 | ALA  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 9   | ALA  | 2.7  |
| 1   | C     | 437 | ILE  | 2.6  |
| 1   | D     | 454 | LEU  | 2.5  |
| 1   | I     | 467 | VAL  | 2.5  |
| 1   | E     | 434 | LYS  | 2.5  |
| 1   | D     | 452 | ILE  | 2.5  |
| 1   | L     | 356 | GLY  | 2.5  |
| 1   | I     | 532 | THR  | 2.5  |
| 1   | F     | 437 | ILE  | 2.4  |
| 1   | K     | 366 | VAL  | 2.4  |
| 1   | H     | 9   | ALA  | 2.4  |
| 1   | K     | 201 | THR  | 2.3  |
| 1   | G     | 162 | LYS  | 2.3  |
| 1   | L     | 127 | ILE  | 2.3  |
| 1   | G     | 418 | GLN  | 2.2  |
| 1   | L     | 154 | ILE  | 2.2  |
| 1   | F     | 9   | ALA  | 2.2  |
| 1   | I     | 9   | ALA  | 2.2  |
| 1   | G     | 203 | THR  | 2.1  |
| 1   | H     | 282 | PHE  | 2.1  |
| 1   | A     | 520 | ALA  | 2.1  |
| 1   | I     | 475 | VAL  | 2.1  |
| 1   | A     | 517 | PRO  | 2.1  |
| 1   | G     | 431 | GLY  | 2.1  |
| 1   | H     | 381 | VAL  | 2.1  |
| 1   | D     | 512 | PHE  | 2.1  |
| 1   | L     | 433 | ILE  | 2.0  |
| 1   | K     | 161 | TYR  | 2.0  |
| 1   | D     | 489 | THR  | 2.0  |
| 1   | L     | 201 | THR  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no 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.