



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:43 PM UTC

PDB ID : 5LZL / pdb\_00005lzl  
Title : Pyrobaculum calidifontis 5-aminolaevulinic acid dehydratase  
Authors : Azim, N.; Erskine, P.T.; Guo, J.; Cooper, J.B.  
Deposited on : 2016-09-30  
Resolution : 3.47 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                                                             |

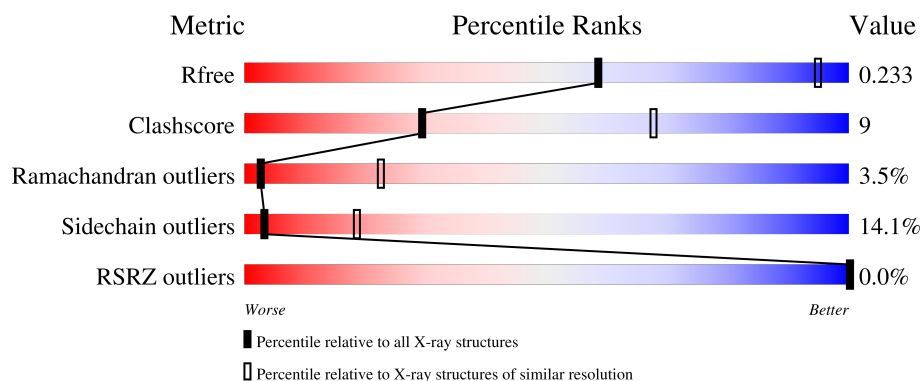
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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                      | 1083 (3.52-3.44)                                      |
| Clashscore            | 190562                      | 1139 (3.52-3.44)                                      |
| Ramachandran outliers | 187476                      | 1111 (3.52-3.44)                                      |
| Sidechain outliers    | 187428                      | 1112 (3.52-3.44)                                      |
| RSRZ outliers         | 180081                      | 1082 (3.52-3.44)                                      |

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     | 338    | <div> <div>65%</div> <div>27%</div> <div>7%</div> <div>..</div> </div> |
| 1   | B     | 338    | <div> <div>64%</div> <div>26%</div> <div>8%</div> <div>..</div> </div> |
| 1   | C     | 338    | <div> <div>66%</div> <div>27%</div> <div>6%</div> <div>.</div> </div>  |
| 1   | D     | 338    | <div> <div>70%</div> <div>25%</div> <div>.</div> <div>..</div> </div>  |
| 1   | E     | 338    | <div> <div>71%</div> <div>22%</div> <div>5%</div> <div>..</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                |
|-----|-------|--------|-----------------------------------------------------------------|
| 1   | F     | 338    | <div><div></div><div>70%25%<div></div><div></div></div></div>   |
| 1   | G     | 338    | <div><div></div><div>65%29%5%<div></div><div></div></div></div> |
| 1   | H     | 338    | <div><div></div><div>68%22%8%<div></div><div></div></div></div> |
| 1   | I     | 338    | <div><div></div><div>70%23%5%<div></div><div></div></div></div> |
| 1   | J     | 338    | <div><div></div><div>73%21%<div></div><div></div></div></div>   |
| 1   | K     | 338    | <div><div></div><div>72%22%5%<div></div><div></div></div></div> |
| 1   | L     | 338    | <div><div></div><div>72%22%<div></div><div></div></div></div>   |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 31739 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 Delta-aminolevulinic acid dehydratase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | B     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | C     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | D     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | E     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | F     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | G     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | H     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | I     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | J     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | K     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |
| 1   | L     | 336      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2640  | 1696 | 453 | 480 | 11 |         |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | C     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | D     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | E     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | F     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | G     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | H     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | I     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | J     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | K     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |
| 2   | L     | 2        | Total<br>2 | Zn<br>2 | 0       | 0       |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 3   | A     | 6        | Total<br>6 | O<br>6 | 0       | 0       |
| 3   | B     | 6        | Total<br>6 | O<br>6 | 0       | 0       |
| 3   | C     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 3   | D     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 3   | E     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 3   | G     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 3   | I     | 3        | Total<br>3 | O<br>3 | 0       | 0       |

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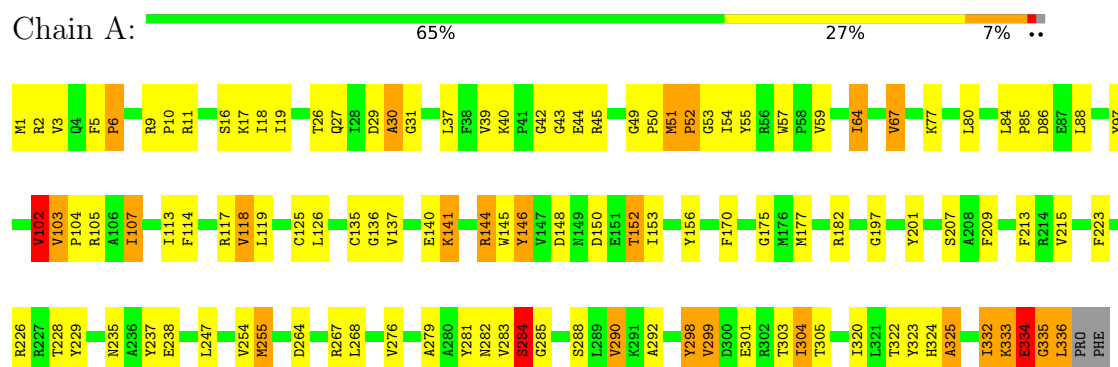
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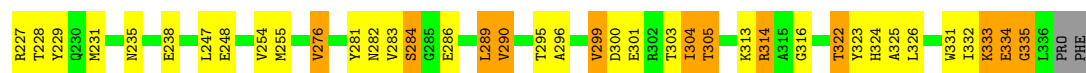
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3   | J     | 3        | Total | O | 0       | 0       |
|     |       |          | 3     | 3 |         |         |

### 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.

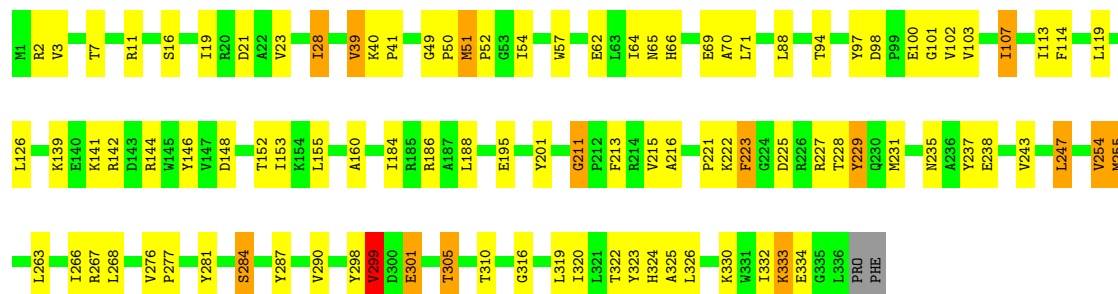
- Molecule 1: Delta-aminolevulinic acid dehydratase





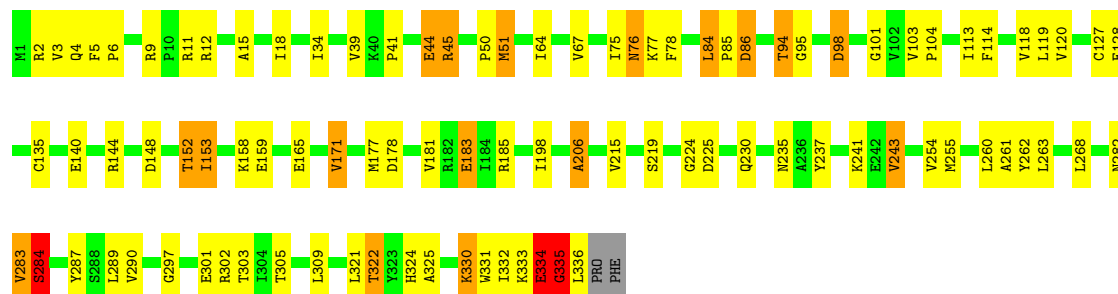
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain D: 70% 25% . .



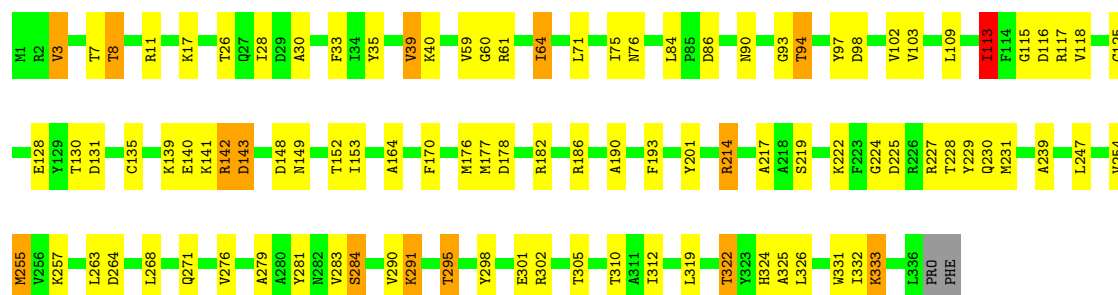
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain E: 71% 22% 5% . .



• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain F: 70% 25% . .

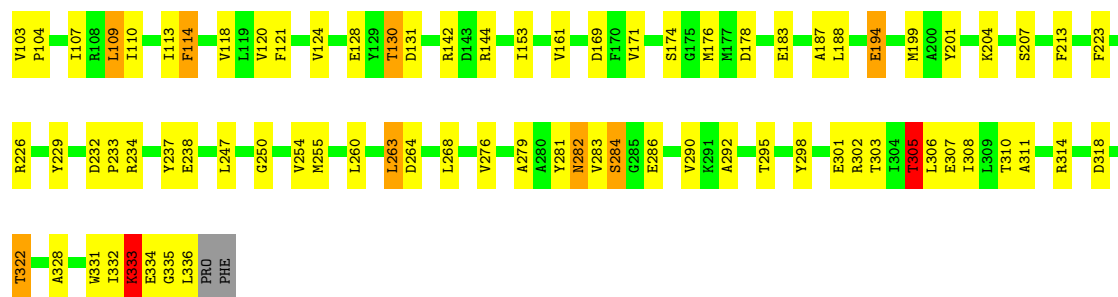


• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain G: 65% 29% 5% . .

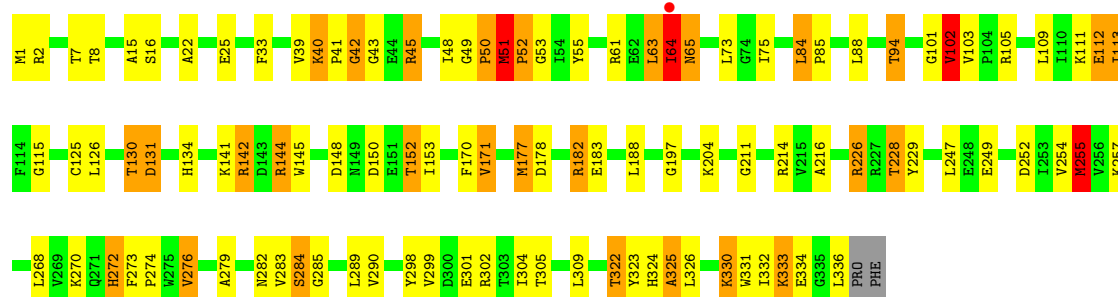






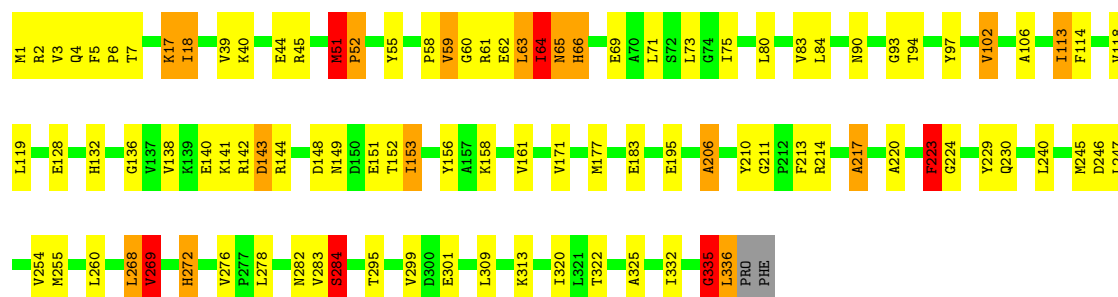
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain H: 68% 22% 8% ..



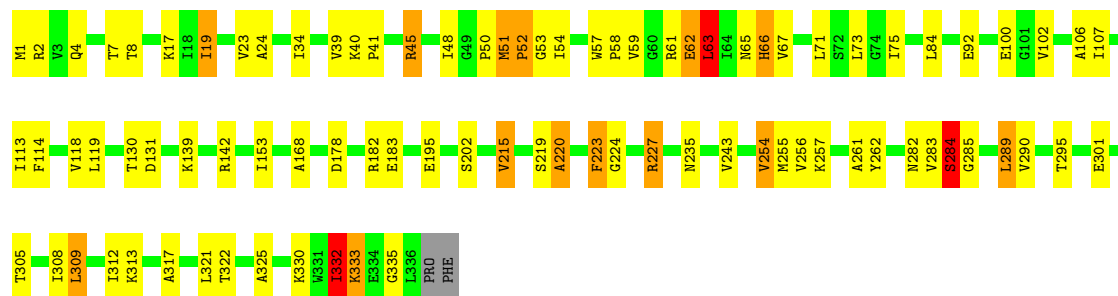
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain I: 70% 23% 5% ..



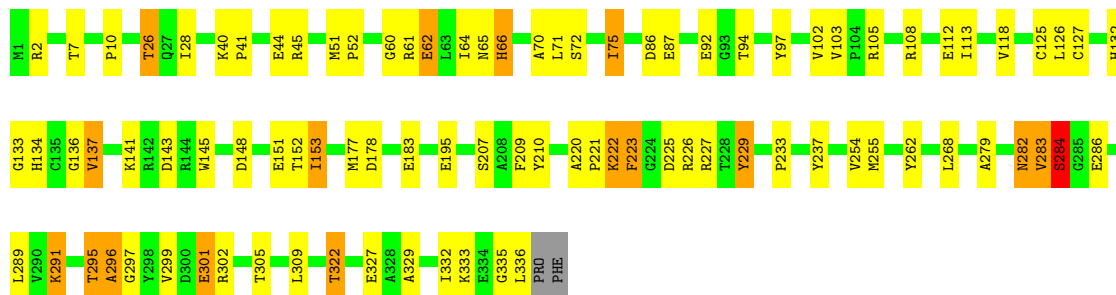
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain J: 73% 21% ..



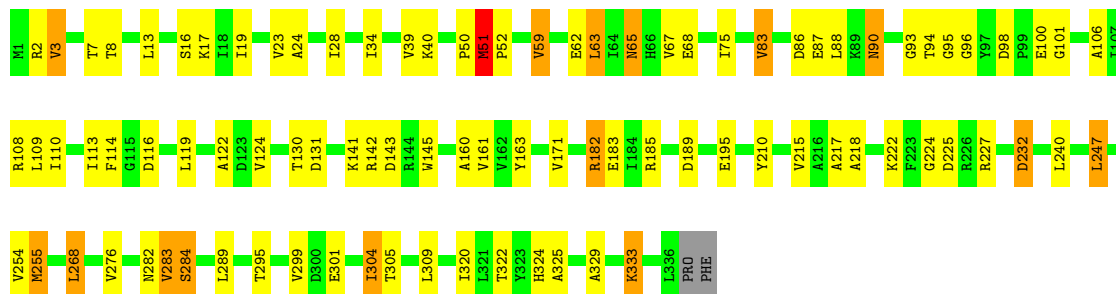
• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain K:  72% 22% 5% .



• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain L:  72% 22% . .



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 31 2 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 205.56Å 205.56Å 199.17Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 178.02 – 3.47<br>178.02 – 3.47                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (178.02-3.47)<br>100.0 (178.02-3.47)                  | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.71 (at 3.49Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0107                                             | Depositor        |
| R, $R_{free}$                                                           | 0.148 , 0.250<br>(Not available) , 0.233                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 3154 reflections (4.98%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 89.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.268                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 62.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.023 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 31739                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 93.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.87         | 0/2702          | 1.16        | 5/3664 (0.1%)    |
| 1   | B     | 0.97         | 0/2702          | 1.17        | 5/3664 (0.1%)    |
| 1   | C     | 0.95         | 1/2702 (0.0%)   | 1.19        | 13/3664 (0.4%)   |
| 1   | D     | 0.88         | 0/2702          | 1.13        | 10/3664 (0.3%)   |
| 1   | E     | 0.97         | 1/2702 (0.0%)   | 1.20        | 9/3664 (0.2%)    |
| 1   | F     | 0.96         | 1/2702 (0.0%)   | 1.18        | 12/3664 (0.3%)   |
| 1   | G     | 0.96         | 0/2702          | 1.18        | 5/3664 (0.1%)    |
| 1   | H     | 1.06         | 4/2702 (0.1%)   | 1.30        | 23/3664 (0.6%)   |
| 1   | I     | 0.92         | 2/2702 (0.1%)   | 1.18        | 11/3664 (0.3%)   |
| 1   | J     | 0.88         | 0/2702          | 1.15        | 6/3664 (0.2%)    |
| 1   | K     | 0.86         | 0/2702          | 1.10        | 3/3664 (0.1%)    |
| 1   | L     | 0.86         | 1/2702 (0.0%)   | 1.10        | 4/3664 (0.1%)    |
| All | All   | 0.93         | 10/32424 (0.0%) | 1.17        | 106/43968 (0.2%) |

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   | A     | 0                   | 5                   |
| 1   | B     | 0                   | 4                   |
| 1   | C     | 0                   | 5                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 1                   |
| 1   | F     | 0                   | 2                   |
| 1   | G     | 0                   | 4                   |
| 1   | H     | 0                   | 6                   |
| 1   | I     | 0                   | 3                   |
| 1   | J     | 0                   | 6                   |
| 1   | K     | 0                   | 3                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | L     | 0                   | 1                   |
| All | All   | 0                   | 42                  |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | H     | 331 | TRP  | CA-C  | 6.09  | 1.60        | 1.53     |
| 1   | C     | 331 | TRP  | CA-C  | 5.79  | 1.60        | 1.52     |
| 1   | L     | 40  | LYS  | CA-C  | 5.62  | 1.57        | 1.52     |
| 1   | H     | 255 | MET  | N-CA  | 5.60  | 1.53        | 1.45     |
| 1   | I     | 66  | HIS  | CA-C  | -5.47 | 1.48        | 1.52     |
| 1   | F     | 331 | TRP  | CA-C  | 5.43  | 1.59        | 1.53     |
| 1   | E     | 103 | VAL  | CA-CB | 5.42  | 1.57        | 1.53     |
| 1   | H     | 270 | LYS  | CA-C  | -5.35 | 1.45        | 1.52     |
| 1   | H     | 273 | PHE  | N-CA  | -5.19 | 1.41        | 1.46     |
| 1   | I     | 64  | ILE  | CA-CB | 5.17  | 1.61        | 1.54     |

All (106) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | H     | 84  | LEU  | N-CA-C  | 10.52 | 117.59      | 108.13   |
| 1   | C     | 334 | GLU  | N-CA-C  | 9.23  | 123.38      | 109.25   |
| 1   | I     | 156 | TYR  | N-CA-C  | -9.12 | 100.90      | 111.03   |
| 1   | E     | 334 | GLU  | N-CA-C  | 8.97  | 122.55      | 110.35   |
| 1   | J     | 257 | LYS  | N-CA-C  | -8.79 | 98.73       | 109.72   |
| 1   | J     | 255 | MET  | N-CA-C  | 8.41  | 119.74      | 108.38   |
| 1   | H     | 171 | VAL  | N-CA-C  | -8.28 | 96.12       | 108.46   |
| 1   | I     | 102 | VAL  | CB-CA-C | -8.08 | 101.53      | 111.88   |
| 1   | G     | 334 | GLU  | N-CA-C  | 7.97  | 122.55      | 109.24   |
| 1   | E     | 241 | LYS  | N-CA-C  | -7.80 | 102.72      | 111.07   |
| 1   | B     | 334 | GLU  | N-CA-C  | 7.77  | 120.79      | 110.53   |
| 1   | C     | 27  | GLN  | N-CA-C  | 6.83  | 119.45      | 109.07   |
| 1   | J     | 19  | ILE  | N-CA-CB | 6.69  | 118.21      | 110.65   |
| 1   | J     | 333 | LYS  | N-CA-C  | 6.69  | 125.04      | 110.80   |
| 1   | A     | 102 | VAL  | CB-CA-C | -6.68 | 106.03      | 111.71   |
| 1   | D     | 64  | ILE  | N-CA-C  | -6.68 | 103.82      | 110.30   |
| 1   | H     | 334 | GLU  | N-CA-C  | 6.59  | 119.57      | 108.23   |
| 1   | A     | 235 | ASN  | N-CA-C  | 6.57  | 119.23      | 108.52   |
| 1   | C     | 276 | VAL  | CB-CA-C | -6.55 | 103.70      | 110.71   |
| 1   | H     | 285 | GLY  | N-CA-C  | 6.45  | 121.03      | 112.77   |
| 1   | D     | 211 | GLY  | CA-C-N  | 6.43  | 125.66      | 118.97   |
| 1   | D     | 211 | GLY  | C-N-CA  | 6.43  | 125.66      | 118.97   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 255 | MET  | N-CA-C    | 6.33  | 118.57      | 109.14   |
| 1   | C     | 322 | THR  | CB-CA-C   | -6.23 | 96.73       | 109.38   |
| 1   | D     | 223 | PHE  | N-CA-CB   | 6.19  | 118.92      | 110.57   |
| 1   | I     | 102 | VAL  | N-CA-C    | 6.16  | 116.83      | 110.36   |
| 1   | H     | 84  | LEU  | CA-C-N    | 6.13  | 126.08      | 119.76   |
| 1   | H     | 84  | LEU  | C-N-CA    | 6.13  | 126.08      | 119.76   |
| 1   | F     | 298 | TYR  | N-CA-C    | 6.12  | 119.21      | 111.69   |
| 1   | H     | 322 | THR  | CB-CA-C   | -6.04 | 99.10       | 110.16   |
| 1   | E     | 235 | ASN  | N-CA-C    | 6.02  | 118.33      | 108.52   |
| 1   | D     | 235 | ASN  | N-CA-C    | 6.00  | 118.52      | 108.73   |
| 1   | G     | 51  | MET  | CB-CA-C   | 5.99  | 121.97      | 110.17   |
| 1   | F     | 103 | VAL  | CA-C-N    | -5.97 | 112.76      | 118.97   |
| 1   | F     | 103 | VAL  | C-N-CA    | -5.97 | 112.76      | 118.97   |
| 1   | H     | 331 | TRP  | CB-CA-C   | 5.96  | 121.27      | 111.50   |
| 1   | H     | 53  | GLY  | N-CA-C    | -5.95 | 107.11      | 115.32   |
| 1   | H     | 188 | LEU  | N-CA-C    | 5.94  | 117.43      | 111.07   |
| 1   | K     | 207 | SER  | N-CA-C    | 5.93  | 118.43      | 109.23   |
| 1   | A     | 255 | MET  | N-CA-C    | 5.84  | 117.67      | 108.96   |
| 1   | D     | 57  | TRP  | N-CA-C    | 5.84  | 117.01      | 109.65   |
| 1   | F     | 113 | ILE  | N-CA-C    | 5.82  | 117.34      | 111.00   |
| 1   | B     | 331 | TRP  | CB-CA-C   | 5.70  | 120.00      | 110.88   |
| 1   | I     | 153 | ILE  | N-CA-C    | 5.66  | 117.07      | 110.62   |
| 1   | F     | 90  | ASN  | N-CA-C    | 5.65  | 113.31      | 108.22   |
| 1   | C     | 331 | TRP  | CB-CA-C   | 5.64  | 120.59      | 111.05   |
| 1   | D     | 153 | ILE  | CB-CA-C   | -5.64 | 104.66      | 111.88   |
| 1   | E     | 224 | GLY  | N-CA-C    | 5.63  | 118.59      | 112.29   |
| 1   | A     | 86  | ASP  | N-CA-C    | 5.62  | 118.34      | 111.82   |
| 1   | H     | 144 | ARG  | N-CA-C    | 5.62  | 117.16      | 109.18   |
| 1   | C     | 235 | ASN  | N-CA-C    | 5.62  | 117.88      | 108.73   |
| 1   | D     | 281 | TYR  | CA-CB-CG  | 5.62  | 124.01      | 113.90   |
| 1   | H     | 15  | ALA  | N-CA-C    | 5.62  | 118.33      | 111.82   |
| 1   | B     | 154 | LYS  | N-CA-C    | -5.60 | 105.94      | 112.89   |
| 1   | J     | 224 | GLY  | N-CA-C    | 5.60  | 126.44      | 113.18   |
| 1   | H     | 171 | VAL  | CB-CA-C   | 5.58  | 119.09      | 110.50   |
| 1   | B     | 255 | MET  | N-CA-C    | 5.57  | 117.43      | 109.14   |
| 1   | H     | 130 | THR  | N-CA-C    | 5.53  | 117.91      | 108.90   |
| 1   | F     | 322 | THR  | CA-CB-CG2 | 5.52  | 119.89      | 110.50   |
| 1   | C     | 286 | GLU  | N-CA-C    | -5.51 | 106.56      | 113.28   |
| 1   | K     | 26  | THR  | N-CA-C    | 5.50  | 118.15      | 108.75   |
| 1   | E     | 243 | VAL  | CB-CA-C   | -5.48 | 104.84      | 112.02   |
| 1   | F     | 93  | GLY  | N-CA-C    | 5.46  | 121.19      | 114.69   |
| 1   | C     | 63  | LEU  | N-CA-C    | -5.46 | 99.17       | 110.80   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 51  | MET  | CB-CG-SD   | 5.45  | 129.04      | 112.70   |
| 1   | I     | 255 | MET  | N-CA-C     | 5.41  | 117.41      | 109.24   |
| 1   | H     | 298 | TYR  | N-CA-C     | 5.40  | 118.08      | 111.82   |
| 1   | G     | 263 | LEU  | N-CA-C     | -5.37 | 105.60      | 111.82   |
| 1   | J     | 235 | ASN  | N-CA-C     | 5.37  | 117.49      | 107.99   |
| 1   | F     | 322 | THR  | OG1-CB-CG2 | 5.35  | 120.00      | 109.30   |
| 1   | F     | 190 | ALA  | N-CA-C     | 5.34  | 116.91      | 111.14   |
| 1   | I     | 335 | GLY  | N-CA-C     | -5.33 | 104.90      | 112.37   |
| 1   | I     | 269 | VAL  | CB-CA-C    | -5.33 | 105.06      | 112.04   |
| 1   | C     | 42  | GLY  | N-CA-C     | 5.30  | 117.74      | 110.69   |
| 1   | F     | 255 | MET  | N-CA-C     | 5.30  | 116.33      | 108.86   |
| 1   | A     | 298 | TYR  | N-CA-C     | 5.30  | 117.05      | 111.28   |
| 1   | I     | 217 | ALA  | N-CA-C     | 5.29  | 119.84      | 113.17   |
| 1   | F     | 331 | TRP  | CB-CA-C    | 5.25  | 120.45      | 112.00   |
| 1   | I     | 335 | GLY  | CA-C-N     | 5.24  | 131.14      | 121.70   |
| 1   | I     | 335 | GLY  | C-N-CA     | 5.24  | 131.14      | 121.70   |
| 1   | L     | 247 | LEU  | N-CA-C     | 5.21  | 116.77      | 111.14   |
| 1   | E     | 181 | VAL  | N-CA-C     | -5.20 | 105.47      | 110.72   |
| 1   | G     | 305 | THR  | N-CA-CB    | 5.19  | 117.70      | 110.07   |
| 1   | C     | 211 | GLY  | CA-C-N     | 5.18  | 124.36      | 118.97   |
| 1   | C     | 211 | GLY  | C-N-CA     | 5.18  | 124.36      | 118.97   |
| 1   | G     | 7   | THR  | N-CA-C     | -5.16 | 105.73      | 111.36   |
| 1   | H     | 255 | MET  | N-CA-C     | 5.15  | 117.51      | 109.52   |
| 1   | L     | 255 | MET  | N-CA-C     | 5.15  | 117.56      | 108.75   |
| 1   | D     | 299 | VAL  | N-CA-C     | 5.13  | 114.97      | 107.88   |
| 1   | B     | 298 | TYR  | N-CA-C     | 5.13  | 119.59      | 113.23   |
| 1   | K     | 86  | ASP  | N-CA-C     | 5.12  | 117.60      | 111.71   |
| 1   | E     | 171 | VAL  | N-CA-C     | -5.11 | 100.76      | 108.12   |
| 1   | L     | 110 | ILE  | N-CA-C     | -5.10 | 105.52      | 110.42   |
| 1   | H     | 211 | GLY  | CA-C-N     | 5.10  | 125.13      | 119.32   |
| 1   | H     | 211 | GLY  | C-N-CA     | 5.10  | 125.13      | 119.32   |
| 1   | L     | 130 | THR  | N-CA-C     | 5.09  | 117.36      | 108.76   |
| 1   | H     | 134 | HIS  | N-CA-C     | 5.07  | 117.08      | 110.43   |
| 1   | E     | 98  | ASP  | CA-C-N     | 5.07  | 125.52      | 120.04   |
| 1   | E     | 98  | ASP  | C-N-CA     | 5.07  | 125.52      | 120.04   |
| 1   | C     | 187 | ALA  | N-CA-C     | -5.06 | 105.45      | 110.97   |
| 1   | H     | 64  | ILE  | N-CA-C     | -5.04 | 107.56      | 112.29   |
| 1   | H     | 42  | GLY  | N-CA-C     | 5.04  | 125.12      | 113.18   |
| 1   | H     | 102 | VAL  | CB-CA-C    | -5.04 | 105.37      | 111.87   |
| 1   | F     | 94  | THR  | N-CA-C     | 5.02  | 121.49      | 110.80   |
| 1   | I     | 220 | ALA  | N-CA-C     | 5.01  | 115.36      | 109.60   |
| 1   | C     | 305 | THR  | N-CA-CB    | 5.00  | 118.03      | 110.28   |

There are no chirality outliers.

All (42) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 136 | GLY  | Peptide |
| 1   | A     | 144 | ARG  | Peptide |
| 1   | A     | 282 | ASN  | Peptide |
| 1   | A     | 332 | ILE  | Peptide |
| 1   | A     | 335 | GLY  | Peptide |
| 1   | B     | 2   | ARG  | Peptide |
| 1   | B     | 223 | PHE  | Peptide |
| 1   | B     | 296 | ALA  | Peptide |
| 1   | B     | 62  | GLU  | Peptide |
| 1   | C     | 282 | ASN  | Peptide |
| 1   | C     | 335 | GLY  | Peptide |
| 1   | C     | 62  | GLU  | Peptide |
| 1   | C     | 65  | ASN  | Peptide |
| 1   | C     | 84  | LEU  | Peptide |
| 1   | D     | 3   | VAL  | Peptide |
| 1   | D     | 62  | GLU  | Peptide |
| 1   | E     | 335 | GLY  | Peptide |
| 1   | F     | 130 | THR  | Peptide |
| 1   | F     | 224 | GLY  | Peptide |
| 1   | G     | 130 | THR  | Peptide |
| 1   | G     | 282 | ASN  | Peptide |
| 1   | G     | 335 | GLY  | Peptide |
| 1   | G     | 62  | GLU  | Peptide |
| 1   | H     | 112 | GLU  | Peptide |
| 1   | H     | 130 | THR  | Peptide |
| 1   | H     | 51  | MET  | Peptide |
| 1   | H     | 61  | ARG  | Peptide |
| 1   | H     | 64  | ILE  | Peptide |
| 1   | H     | 65  | ASN  | Peptide |
| 1   | I     | 223 | PHE  | Peptide |
| 1   | I     | 335 | GLY  | Peptide |
| 1   | I     | 62  | GLU  | Peptide |
| 1   | J     | 130 | THR  | Peptide |
| 1   | J     | 223 | PHE  | Peptide |
| 1   | J     | 332 | ILE  | Peptide |
| 1   | J     | 335 | GLY  | Peptide |
| 1   | J     | 51  | MET  | Peptide |
| 1   | J     | 61  | ARG  | Peptide |
| 1   | K     | 282 | ASN  | Peptide |
| 1   | K     | 296 | ALA  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | K     | 335 | GLY  | Peptide |
| 1   | L     | 116 | ASP  | 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     | 2640  | 0        | 2638     | 60      | 0            |
| 1   | B     | 2640  | 0        | 2640     | 67      | 0            |
| 1   | C     | 2640  | 0        | 2638     | 64      | 0            |
| 1   | D     | 2640  | 0        | 2638     | 39      | 0            |
| 1   | E     | 2640  | 0        | 2638     | 52      | 0            |
| 1   | F     | 2640  | 0        | 2639     | 39      | 0            |
| 1   | G     | 2640  | 0        | 2638     | 51      | 0            |
| 1   | H     | 2640  | 0        | 2639     | 56      | 0            |
| 1   | I     | 2640  | 0        | 2638     | 45      | 0            |
| 1   | J     | 2640  | 0        | 2639     | 31      | 0            |
| 1   | K     | 2640  | 0        | 2636     | 41      | 0            |
| 1   | L     | 2640  | 0        | 2638     | 36      | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 1       | 0            |
| 2   | C     | 2     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | E     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 2     | 0        | 0        | 0       | 0            |
| 2   | G     | 2     | 0        | 0        | 0       | 0            |
| 2   | H     | 2     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | J     | 2     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |
| 2   | L     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 6     | 0        | 0        | 0       | 0            |
| 3   | B     | 6     | 0        | 0        | 0       | 0            |
| 3   | C     | 3     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 4     | 0        | 0        | 0       | 0            |
| 3   | F     | 3     | 0        | 0        | 1       | 0            |
| 3   | G     | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 3     | 0        | 0        | 0       | 0            |
| 3   | J     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 31739 | 0        | 31659    | 546     | 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 9.

All (546) 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:E:330:LYS:O    | 1:E:332:ILE:CD1  | 1.73                     | 1.32              |
| 1:E:330:LYS:O    | 1:E:332:ILE:HD12 | 1.32                     | 1.22              |
| 1:H:322:THR:HG22 | 1:H:324:HIS:H    | 1.04                     | 1.13              |
| 1:E:330:LYS:O    | 1:E:332:ILE:HD13 | 1.57                     | 1.04              |
| 1:C:322:THR:HG22 | 1:C:324:HIS:H    | 1.16                     | 1.04              |
| 1:E:302:ARG:NH2  | 1:E:333:LYS:O    | 1.89                     | 1.03              |
| 1:J:63:LEU:HD21  | 1:J:113:ILE:HG21 | 1.39                     | 1.03              |
| 1:H:322:THR:HG22 | 1:H:324:HIS:N    | 1.76                     | 0.99              |
| 1:C:322:THR:HG22 | 1:C:324:HIS:N    | 1.81                     | 0.95              |
| 1:E:148:ASP:O    | 1:E:152:THR:HG22 | 1.70                     | 0.91              |
| 1:E:330:LYS:C    | 1:E:332:ILE:HD12 | 1.96                     | 0.89              |
| 1:B:75:ILE:HD13  | 1:B:326:LEU:HD12 | 1.56                     | 0.88              |
| 1:K:226:ARG:HG2  | 1:K:229:TYR:OH   | 1.74                     | 0.87              |
| 1:J:52:PRO:O     | 1:J:54:ILE:N     | 2.10                     | 0.84              |
| 1:H:322:THR:CG2  | 1:H:324:HIS:H    | 1.89                     | 0.81              |
| 1:K:302:ARG:NH2  | 1:K:333:LYS:O    | 2.14                     | 0.81              |
| 1:K:134:HIS:CD2  | 1:K:223:PHE:HE1  | 2.00                     | 0.80              |
| 1:A:64:ILE:HG13  | 1:A:113:ILE:HG21 | 1.64                     | 0.80              |
| 1:C:322:THR:CG2  | 1:C:324:HIS:H    | 1.93                     | 0.79              |
| 1:K:134:HIS:HD2  | 1:K:223:PHE:HE1  | 1.30                     | 0.78              |
| 1:A:299:VAL:HG11 | 1:A:304:ILE:HD12 | 1.67                     | 0.76              |
| 1:C:332:ILE:HG22 | 1:C:332:ILE:O    | 1.86                     | 0.75              |
| 1:G:290:VAL:HG11 | 1:G:305:THR:HG22 | 1.66                     | 0.74              |
| 1:H:148:ASP:O    | 1:H:152:THR:CG2  | 2.36                     | 0.74              |
| 1:K:133:GLY:O    | 1:K:226:ARG:NH2  | 2.21                     | 0.74              |
| 1:A:207:SER:OG   | 1:G:307:GLU:OE1  | 2.06                     | 0.72              |
| 1:E:206:ALA:HB2  | 1:E:230:GLN:HB2  | 1.71                     | 0.72              |
| 1:C:332:ILE:C    | 1:C:333:LYS:HD3  | 2.13                     | 0.72              |
| 1:L:282:ASN:HB3  | 1:L:322:THR:HG22 | 1.72                     | 0.71              |
| 1:I:141:LYS:O    | 1:I:143:ASP:N    | 2.25                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:255:MET:HB3  | 1:K:279:ALA:HB3  | 1.74                     | 0.69              |
| 1:C:63:LEU:HG    | 1:C:64:ILE:HG23  | 1.75                     | 0.68              |
| 1:G:124:VAL:HG21 | 1:G:171:VAL:HG13 | 1.76                     | 0.68              |
| 1:K:127:CYS:HB2  | 1:K:226:ARG:HH22 | 1.58                     | 0.67              |
| 1:K:134:HIS:CD2  | 1:K:223:PHE:CE1  | 2.83                     | 0.67              |
| 1:H:322:THR:HG22 | 1:H:323:TYR:N    | 2.08                     | 0.67              |
| 1:F:247:LEU:HD11 | 1:F:276:VAL:HG21 | 1.75                     | 0.67              |
| 1:F:128:GLU:HG2  | 1:F:217:ALA:HB1  | 1.75                     | 0.66              |
| 1:C:58:PRO:O     | 1:C:60:GLY:N     | 2.28                     | 0.66              |
| 1:F:231:MET:HE1  | 1:F:239:ALA:HB2  | 1.77                     | 0.66              |
| 1:E:332:ILE:HD12 | 1:E:332:ILE:N    | 2.11                     | 0.66              |
| 1:J:332:ILE:HG22 | 1:J:332:ILE:O    | 1.96                     | 0.66              |
| 1:J:285:GLY:O    | 1:J:289:LEU:HB2  | 1.96                     | 0.65              |
| 1:C:322:THR:HG21 | 1:C:324:HIS:HB2  | 1.76                     | 0.65              |
| 1:A:301:GLU:O    | 1:A:305:THR:HG23 | 1.97                     | 0.64              |
| 1:F:148:ASP:O    | 1:F:152:THR:HG22 | 1.97                     | 0.64              |
| 1:B:70:ALA:HB2   | 1:B:326:LEU:HD11 | 1.80                     | 0.64              |
| 1:K:62:GLU:HA    | 1:K:65:ASN:HB2   | 1.82                     | 0.62              |
| 1:J:39:VAL:HG12  | 1:J:102:VAL:HG12 | 1.80                     | 0.62              |
| 1:I:282:ASN:HB3  | 1:I:322:THR:HG22 | 1.81                     | 0.62              |
| 1:B:22:ALA:HB1   | 1:F:319:LEU:HD21 | 1.80                     | 0.62              |
| 1:B:127:CYS:SG   | 2:B:401:ZN:ZN    | 1.89                     | 0.62              |
| 1:E:75:ILE:HD12  | 1:E:325:ALA:HB1  | 1.82                     | 0.62              |
| 1:B:124:VAL:HG21 | 1:B:171:VAL:HG13 | 1.82                     | 0.62              |
| 1:F:141:LYS:O    | 1:F:143:ASP:N    | 2.33                     | 0.61              |
| 1:C:322:THR:HG22 | 1:C:323:TYR:N    | 2.15                     | 0.61              |
| 1:G:63:LEU:HD11  | 1:G:113:ILE:HG23 | 1.81                     | 0.61              |
| 1:G:255:MET:HB3  | 1:G:279:ALA:HB3  | 1.81                     | 0.61              |
| 1:C:63:LEU:HG    | 1:C:64:ILE:N     | 2.16                     | 0.61              |
| 1:B:247:LEU:HD21 | 1:B:276:VAL:HG21 | 1.82                     | 0.60              |
| 1:L:247:LEU:HD11 | 1:L:276:VAL:HG11 | 1.83                     | 0.60              |
| 1:E:334:GLU:HA   | 1:E:334:GLU:OE1  | 2.00                     | 0.60              |
| 1:K:134:HIS:HD2  | 1:K:223:PHE:CE1  | 2.14                     | 0.60              |
| 1:D:324:HIS:O    | 1:D:326:LEU:N    | 2.35                     | 0.60              |
| 1:B:40:LYS:HD2   | 1:B:46:GLU:OE2   | 2.03                     | 0.59              |
| 1:K:309:LEU:HD21 | 1:K:322:THR:HG21 | 1.84                     | 0.59              |
| 1:A:177:MET:HE3  | 1:A:177:MET:HA   | 1.85                     | 0.59              |
| 1:G:28:ILE:HD11  | 1:G:310:THR:OG1  | 2.03                     | 0.58              |
| 1:H:48:ILE:HG21  | 1:H:216:ALA:HB2  | 1.85                     | 0.58              |
| 1:I:45:ARG:HD3   | 1:I:55:TYR:CD2   | 2.38                     | 0.58              |
| 1:I:17:LYS:O     | 1:I:18:ILE:C     | 2.44                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:75:ILE:HD13  | 1:I:325:ALA:HB1  | 1.84                     | 0.58              |
| 1:J:312:ILE:HG22 | 1:J:317:ALA:HB3  | 1.85                     | 0.58              |
| 1:H:101:GLY:O    | 1:H:105:ARG:HG3  | 2.03                     | 0.58              |
| 1:H:226:ARG:NH1  | 1:H:229:TYR:OH   | 2.36                     | 0.58              |
| 1:A:209:PHE:O    | 1:A:285:GLY:HA3  | 2.04                     | 0.58              |
| 1:A:85:PRO:HD2   | 1:A:88:LEU:HD12  | 1.85                     | 0.58              |
| 1:H:301:GLU:O    | 1:H:305:THR:HG23 | 2.02                     | 0.58              |
| 1:K:132:HIS:O    | 1:K:222:LYS:HG2  | 2.03                     | 0.58              |
| 1:E:76:ASN:O     | 1:E:76:ASN:ND2   | 2.37                     | 0.58              |
| 1:K:223:PHE:O    | 1:K:223:PHE:HD1  | 1.86                     | 0.58              |
| 1:E:330:LYS:O    | 1:E:332:ILE:N    | 2.36                     | 0.58              |
| 1:H:142:ARG:HD2  | 1:H:142:ARG:N    | 2.19                     | 0.58              |
| 1:H:150:ASP:HA   | 1:H:153:ILE:HD12 | 1.86                     | 0.57              |
| 1:K:226:ARG:HG2  | 1:K:229:TYR:CZ   | 2.39                     | 0.57              |
| 1:E:283:VAL:HG12 | 1:E:284:SER:OG   | 2.04                     | 0.57              |
| 1:H:282:ASN:OD1  | 1:H:322:THR:HG23 | 2.03                     | 0.57              |
| 1:A:213:PHE:HB2  | 1:A:284:SER:HB3  | 1.87                     | 0.57              |
| 1:B:233:PRO:HG2  | 1:H:336:LEU:HD22 | 1.86                     | 0.57              |
| 1:G:333:LYS:O    | 1:G:333:LYS:HG2  | 2.05                     | 0.57              |
| 1:H:322:THR:CG2  | 1:H:323:TYR:N    | 2.68                     | 0.57              |
| 1:A:64:ILE:CG1   | 1:A:113:ILE:HG21 | 2.34                     | 0.57              |
| 1:A:125:CYS:SG   | 1:A:126:LEU:N    | 2.78                     | 0.57              |
| 1:L:63:LEU:HD13  | 1:L:109:LEU:CD2  | 2.35                     | 0.57              |
| 1:B:56:ARG:HD3   | 1:B:83:VAL:HG11  | 1.86                     | 0.56              |
| 1:C:182:ARG:HG2  | 1:C:186:ARG:HD3  | 1.85                     | 0.56              |
| 1:A:51:MET:HB3   | 1:A:52:PRO:O     | 2.06                     | 0.56              |
| 1:B:55:TYR:HB2   | 1:B:57:TRP:CZ2   | 2.40                     | 0.56              |
| 1:G:39:VAL:HG12  | 1:G:102:VAL:HG12 | 1.87                     | 0.56              |
| 1:I:206:ALA:HA   | 1:I:230:GLN:HE21 | 1.69                     | 0.56              |
| 1:B:11:ARG:NH1   | 1:H:177:MET:CE   | 2.69                     | 0.56              |
| 1:I:90:ASN:ND2   | 1:I:94:THR:OG1   | 2.39                     | 0.56              |
| 1:D:332:ILE:O    | 1:D:332:ILE:HG22 | 2.06                     | 0.56              |
| 1:G:302:ARG:NH2  | 1:G:333:LYS:O    | 2.35                     | 0.56              |
| 1:L:160:ALA:HB1  | 1:L:171:VAL:HG21 | 1.88                     | 0.56              |
| 1:I:63:LEU:HD23  | 1:I:64:ILE:N     | 2.20                     | 0.56              |
| 1:I:51:MET:CB    | 1:I:52:PRO:HA    | 2.35                     | 0.56              |
| 1:J:153:ILE:HD11 | 1:J:178:ASP:O    | 2.06                     | 0.56              |
| 1:K:177:MET:HE3  | 1:K:177:MET:HA   | 1.88                     | 0.56              |
| 1:B:225:ASP:OD1  | 1:B:227:ARG:HG3  | 2.06                     | 0.56              |
| 1:F:39:VAL:HG12  | 1:F:102:VAL:HG12 | 1.88                     | 0.55              |
| 1:G:255:MET:HE1  | 1:G:281:TYR:HB2  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:33:PHE:CE1   | 1:B:309:LEU:HD13 | 2.42                     | 0.55              |
| 1:I:240:LEU:HD21 | 1:I:268:LEU:HD22 | 1.89                     | 0.55              |
| 1:B:84:LEU:HD21  | 1:B:102:VAL:HG21 | 1.88                     | 0.55              |
| 1:C:149:ASN:HA   | 1:C:177:MET:HE2  | 1.88                     | 0.55              |
| 1:E:335:GLY:HA3  | 1:E:336:LEU:HG   | 1.89                     | 0.55              |
| 1:H:330:LYS:O    | 1:H:332:ILE:HG22 | 2.06                     | 0.55              |
| 1:H:204:LYS:HA   | 1:H:257:LYS:O    | 2.07                     | 0.54              |
| 1:C:174:SER:HB3  | 1:C:201:TYR:CE1  | 2.42                     | 0.54              |
| 1:A:320:ILE:HG22 | 1:A:322:THR:HG23 | 1.89                     | 0.54              |
| 1:E:86:ASP:OD1   | 1:E:86:ASP:N     | 2.37                     | 0.54              |
| 1:K:127:CYS:CB   | 1:K:226:ARG:HH22 | 2.21                     | 0.54              |
| 1:D:201:TYR:HA   | 1:D:255:MET:HG3  | 1.89                     | 0.54              |
| 1:L:63:LEU:HD11  | 1:L:113:ILE:CG2  | 2.38                     | 0.54              |
| 1:H:111:LYS:O    | 1:H:115:GLY:HA2  | 2.09                     | 0.53              |
| 1:A:201:TYR:HA   | 1:A:255:MET:HG3  | 1.89                     | 0.53              |
| 1:B:84:LEU:CD2   | 1:B:102:VAL:HG21 | 2.38                     | 0.53              |
| 1:H:332:ILE:HG23 | 1:H:332:ILE:O    | 2.08                     | 0.53              |
| 1:C:177:MET:HE1  | 1:E:11:ARG:NH1   | 2.24                     | 0.53              |
| 1:H:255:MET:HB2  | 1:H:279:ALA:HB3  | 1.90                     | 0.53              |
| 1:E:290:VAL:HG11 | 1:E:305:THR:CG2  | 2.39                     | 0.53              |
| 1:H:322:THR:HG21 | 1:H:324:HIS:HB2  | 1.91                     | 0.53              |
| 1:I:128:GLU:HG2  | 1:I:217:ALA:HB1  | 1.91                     | 0.53              |
| 1:I:158:LYS:O    | 1:I:161:VAL:HG12 | 2.08                     | 0.53              |
| 1:H:148:ASP:O    | 1:H:152:THR:HG23 | 2.09                     | 0.53              |
| 1:H:63:LEU:HD11  | 1:H:113:ILE:HG12 | 1.89                     | 0.52              |
| 1:C:35:TYR:CE2   | 1:C:326:LEU:HD13 | 2.44                     | 0.52              |
| 1:E:332:ILE:CD1  | 1:E:332:ILE:N    | 2.72                     | 0.52              |
| 1:A:267:ARG:NH1  | 1:G:264:ASP:OD2  | 2.43                     | 0.52              |
| 1:B:281:TYR:HA   | 1:B:321:LEU:HB2  | 1.90                     | 0.52              |
| 1:D:290:VAL:HG11 | 1:D:305:THR:HG23 | 1.91                     | 0.52              |
| 1:A:150:ASP:HA   | 1:A:153:ILE:HD12 | 1.91                     | 0.52              |
| 1:C:136:GLY:HA2  | 1:C:152:THR:OG1  | 2.09                     | 0.52              |
| 1:G:213:PHE:HB2  | 1:G:284:SER:HB3  | 1.90                     | 0.52              |
| 1:H:226:ARG:C    | 1:H:228:THR:H    | 2.18                     | 0.52              |
| 1:K:233:PRO:HB3  | 1:K:262:TYR:OH   | 2.09                     | 0.52              |
| 1:A:324:HIS:O    | 1:A:325:ALA:C    | 2.52                     | 0.52              |
| 1:B:63:LEU:HD11  | 1:B:113:ILE:HD11 | 1.91                     | 0.52              |
| 1:A:213:PHE:HB2  | 1:A:284:SER:CB   | 2.40                     | 0.52              |
| 1:A:255:MET:HE1  | 1:A:281:TYR:HB2  | 1.91                     | 0.52              |
| 1:A:298:TYR:CE2  | 1:G:292:ALA:HB2  | 2.45                     | 0.52              |
| 1:C:289:LEU:HD22 | 1:E:289:LEU:HB3  | 1.92                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:282:ASN:HB3  | 1:G:322:THR:HG23 | 1.92                     | 0.51              |
| 1:L:282:ASN:CB   | 1:L:322:THR:HG22 | 2.38                     | 0.51              |
| 1:B:149:ASN:O    | 1:B:152:THR:HG22 | 2.10                     | 0.51              |
| 1:C:77:LYS:HE2   | 1:H:22:ALA:HB2   | 1.92                     | 0.51              |
| 1:C:132:HIS:CD2  | 1:C:134:HIS:HB2  | 2.46                     | 0.51              |
| 1:H:153:ILE:HD11 | 1:H:178:ASP:O    | 2.11                     | 0.51              |
| 1:D:301:GLU:O    | 1:D:305:THR:OG1  | 2.24                     | 0.51              |
| 1:F:64:ILE:HG13  | 1:F:113:ILE:HG21 | 1.92                     | 0.51              |
| 1:A:59:VAL:HG23  | 1:A:59:VAL:O     | 2.10                     | 0.51              |
| 1:B:39:VAL:HG12  | 1:B:102:VAL:HG12 | 1.93                     | 0.51              |
| 1:I:113:ILE:HG22 | 1:I:114:PHE:CD1  | 2.45                     | 0.51              |
| 1:A:237:TYR:O    | 1:A:238:GLU:C    | 2.54                     | 0.51              |
| 1:G:63:LEU:HD23  | 1:G:64:ILE:N     | 2.25                     | 0.51              |
| 1:L:299:VAL:HG11 | 1:L:304:ILE:HD13 | 1.92                     | 0.51              |
| 1:C:332:ILE:O    | 1:C:332:ILE:CG2  | 2.58                     | 0.51              |
| 1:G:104:PRO:HA   | 1:G:107:ILE:HG12 | 1.92                     | 0.51              |
| 1:I:39:VAL:HG21  | 1:I:80:LEU:HD22  | 1.92                     | 0.51              |
| 1:J:290:VAL:HG11 | 1:J:305:THR:CG2  | 2.40                     | 0.51              |
| 1:L:39:VAL:HG11  | 1:L:106:ALA:HB2  | 1.92                     | 0.51              |
| 1:J:113:ILE:HG23 | 1:J:114:PHE:CD2  | 2.46                     | 0.51              |
| 1:I:313:LYS:HG2  | 1:I:320:ILE:HD11 | 1.92                     | 0.50              |
| 1:B:282:ASN:OD1  | 1:B:322:THR:HG22 | 2.12                     | 0.50              |
| 1:A:67:VAL:CG2   | 1:A:114:PHE:CE2  | 2.94                     | 0.50              |
| 1:F:61:ARG:HA    | 1:F:64:ILE:HG22  | 1.94                     | 0.50              |
| 1:K:94:THR:HA    | 1:K:97:TYR:CZ    | 2.47                     | 0.50              |
| 1:K:125:CYS:SG   | 1:K:126:LEU:N    | 2.84                     | 0.50              |
| 1:B:306:LEU:HD11 | 1:B:331:TRP:HB3  | 1.94                     | 0.50              |
| 1:C:12:ARG:HD2   | 1:H:252:ASP:OD1  | 2.12                     | 0.50              |
| 1:A:145:TRP:O    | 1:A:146:TYR:HB3  | 2.12                     | 0.50              |
| 1:D:28:ILE:HD11  | 1:D:310:THR:HB   | 1.94                     | 0.50              |
| 1:D:113:ILE:HG23 | 1:D:114:PHE:CD1  | 2.46                     | 0.50              |
| 1:C:231:MET:HE3  | 1:C:238:GLU:HG2  | 1.93                     | 0.50              |
| 1:D:231:MET:HE3  | 1:D:238:GLU:HG2  | 1.93                     | 0.50              |
| 1:D:319:LEU:HD21 | 1:G:22:ALA:HB1   | 1.92                     | 0.50              |
| 1:L:240:LEU:HD21 | 1:L:268:LEU:HD22 | 1.94                     | 0.50              |
| 1:B:233:PRO:CG   | 1:H:336:LEU:HD22 | 2.42                     | 0.50              |
| 1:I:213:PHE:HB2  | 1:I:284:SER:OG   | 2.11                     | 0.50              |
| 1:F:3:VAL:HG13   | 1:F:8:THR:HG21   | 1.93                     | 0.49              |
| 1:I:132:HIS:HE1  | 1:I:136:GLY:O    | 1.94                     | 0.49              |
| 1:A:290:VAL:HG11 | 1:A:305:THR:HG22 | 1.94                     | 0.49              |
| 1:F:255:MET:HE1  | 1:F:281:TYR:HB2  | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:63:LEU:HD11  | 1:G:113:ILE:CG2  | 2.42                     | 0.49              |
| 1:B:332:ILE:C    | 1:B:333:LYS:CG   | 2.85                     | 0.49              |
| 1:C:94:THR:O     | 1:C:94:THR:HG22  | 2.12                     | 0.49              |
| 1:I:269:VAL:HG12 | 1:I:278:LEU:HD22 | 1.94                     | 0.49              |
| 1:B:332:ILE:CG2  | 1:B:332:ILE:O    | 2.60                     | 0.49              |
| 1:C:14:ARG:O     | 1:C:20:ARG:NH1   | 2.45                     | 0.49              |
| 1:B:19:ILE:HD11  | 1:F:170:PHE:CE1  | 2.48                     | 0.49              |
| 1:B:187:ALA:O    | 1:B:188:LEU:C    | 2.55                     | 0.49              |
| 1:C:182:ARG:HA   | 1:C:185:ARG:HB3  | 1.95                     | 0.49              |
| 1:F:201:TYR:HA   | 1:F:255:MET:HG3  | 1.94                     | 0.49              |
| 1:K:148:ASP:O    | 1:K:152:THR:HG22 | 2.13                     | 0.49              |
| 1:D:16:SER:OG    | 1:D:19:ILE:HG22  | 2.13                     | 0.49              |
| 1:H:290:VAL:HG11 | 1:H:305:THR:HG22 | 1.93                     | 0.49              |
| 1:K:210:TYR:HD1  | 1:K:283:VAL:HG11 | 1.78                     | 0.49              |
| 1:B:324:HIS:O    | 1:B:325:ALA:C    | 2.55                     | 0.49              |
| 1:G:290:VAL:CG1  | 1:G:305:THR:HG22 | 2.38                     | 0.49              |
| 1:K:282:ASN:ND2  | 1:K:286:GLU:OE1  | 2.46                     | 0.49              |
| 1:C:63:LEU:HD13  | 1:C:109:LEU:HD22 | 1.95                     | 0.49              |
| 1:E:282:ASN:HB3  | 1:E:322:THR:HG23 | 1.94                     | 0.49              |
| 1:A:148:ASP:O    | 1:A:152:THR:CG2  | 2.61                     | 0.48              |
| 1:B:16:SER:HB2   | 1:B:18:ILE:HD12  | 1.94                     | 0.48              |
| 1:J:57:TRP:CZ2   | 1:J:66:HIS:CD2   | 3.00                     | 0.48              |
| 1:K:283:VAL:HG12 | 1:K:284:SER:N    | 2.28                     | 0.48              |
| 1:E:206:ALA:HA   | 1:E:230:GLN:NE2  | 2.28                     | 0.48              |
| 1:I:5:PHE:CG     | 1:I:6:PRO:HA     | 2.48                     | 0.48              |
| 1:I:149:ASN:O    | 1:I:152:THR:HG22 | 2.14                     | 0.48              |
| 1:J:202:SER:OG   | 1:J:254:VAL:HG22 | 2.12                     | 0.48              |
| 1:F:263:LEU:HD21 | 1:F:312:ILE:HD13 | 1.95                     | 0.48              |
| 1:E:148:ASP:O    | 1:E:152:THR:CG2  | 2.52                     | 0.48              |
| 1:I:5:PHE:CD2    | 1:I:6:PRO:HA     | 2.48                     | 0.48              |
| 1:F:214:ARG:NH1  | 3:F:501:HOH:O    | 2.46                     | 0.48              |
| 1:H:204:LYS:HD2  | 1:H:257:LYS:HD3  | 1.94                     | 0.48              |
| 1:B:201:TYR:HA   | 1:B:255:MET:HG3  | 1.96                     | 0.48              |
| 1:C:148:ASP:O    | 1:C:152:THR:HG22 | 2.14                     | 0.48              |
| 1:K:60:GLY:C     | 1:K:62:GLU:H     | 2.22                     | 0.48              |
| 1:L:232:ASP:OD1  | 1:L:232:ASP:C    | 2.57                     | 0.48              |
| 1:B:217:ALA:O    | 1:B:218:ALA:HB3  | 2.13                     | 0.48              |
| 1:C:231:MET:HE3  | 1:C:238:GLU:CG   | 2.43                     | 0.48              |
| 1:D:103:VAL:O    | 1:D:107:ILE:HG13 | 2.14                     | 0.48              |
| 1:L:283:VAL:HG12 | 1:L:284:SER:H    | 1.77                     | 0.48              |
| 1:A:45:ARG:NH2   | 1:A:55:TYR:CE2   | 2.82                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:324:HIS:O    | 1:C:326:LEU:N    | 2.46                     | 0.48              |
| 1:E:330:LYS:C    | 1:E:332:ILE:CD1  | 2.65                     | 0.48              |
| 1:H:302:ARG:NH2  | 1:H:333:LYS:O    | 2.47                     | 0.48              |
| 1:I:282:ASN:CB   | 1:I:322:THR:HG22 | 2.44                     | 0.48              |
| 1:J:57:TRP:CH2   | 1:J:66:HIS:CD2   | 3.02                     | 0.48              |
| 1:D:69:GLU:O     | 1:D:70:ALA:C     | 2.57                     | 0.48              |
| 1:D:97:TYR:CZ    | 1:D:155:LEU:HD22 | 2.49                     | 0.48              |
| 1:D:139:LYS:HG3  | 1:D:148:ASP:HB2  | 1.95                     | 0.48              |
| 1:B:90:ASN:OD1   | 1:B:90:ASN:N     | 2.46                     | 0.48              |
| 1:C:247:LEU:HD11 | 1:C:276:VAL:HG21 | 1.96                     | 0.48              |
| 1:F:290:VAL:HG11 | 1:F:305:THR:HG22 | 1.95                     | 0.48              |
| 1:H:177:MET:HE3  | 1:H:177:MET:HA   | 1.94                     | 0.48              |
| 1:H:247:LEU:HD21 | 1:H:276:VAL:HG11 | 1.95                     | 0.48              |
| 1:K:71:LEU:HD12  | 1:K:118:VAL:CG1  | 2.44                     | 0.48              |
| 1:A:49:GLY:N     | 1:A:50:PRO:CD    | 2.76                     | 0.47              |
| 1:A:144:ARG:HA   | 1:A:144:ARG:NE   | 2.28                     | 0.47              |
| 1:B:63:LEU:C     | 1:B:63:LEU:HD23  | 2.39                     | 0.47              |
| 1:F:153:ILE:HD11 | 1:F:178:ASP:O    | 2.14                     | 0.47              |
| 1:C:322:THR:CG2  | 1:C:323:TYR:N    | 2.76                     | 0.47              |
| 1:I:149:ASN:HA   | 1:I:177:MET:HE2  | 1.94                     | 0.47              |
| 1:E:332:ILE:CD1  | 1:E:332:ILE:H    | 2.27                     | 0.47              |
| 1:L:3:VAL:HG13   | 1:L:8:THR:HB     | 1.94                     | 0.47              |
| 1:G:237:TYR:O    | 1:G:238:GLU:C    | 2.56                     | 0.47              |
| 1:I:213:PHE:HB2  | 1:I:284:SER:CB   | 2.45                     | 0.47              |
| 1:K:66:HIS:O     | 1:K:70:ALA:N     | 2.43                     | 0.47              |
| 1:C:150:ASP:O    | 1:C:153:ILE:HG22 | 2.15                     | 0.47              |
| 1:L:75:ILE:HD11  | 1:L:329:ALA:HB2  | 1.97                     | 0.47              |
| 1:B:259:ALA:O    | 1:B:262:TYR:N    | 2.38                     | 0.47              |
| 1:F:64:ILE:CG1   | 1:F:113:ILE:HG21 | 2.44                     | 0.47              |
| 1:A:18:ILE:HG21  | 1:E:119:LEU:HB2  | 1.97                     | 0.47              |
| 1:D:39:VAL:HG12  | 1:D:102:VAL:HG12 | 1.96                     | 0.47              |
| 1:G:59:VAL:HG23  | 1:G:109:LEU:HD12 | 1.97                     | 0.47              |
| 1:B:5:PHE:CD1    | 1:B:6:PRO:HA     | 2.49                     | 0.47              |
| 1:I:51:MET:HB3   | 1:I:52:PRO:HA    | 1.95                     | 0.47              |
| 1:B:255:MET:HB3  | 1:B:279:ALA:HB3  | 1.96                     | 0.47              |
| 1:C:128:GLU:HG2  | 1:C:217:ALA:HB1  | 1.95                     | 0.47              |
| 1:D:148:ASP:O    | 1:D:152:THR:HG22 | 2.14                     | 0.47              |
| 1:G:107:ILE:HG23 | 1:G:120:VAL:HG11 | 1.96                     | 0.47              |
| 1:A:135:CYS:SG   | 1:A:226:ARG:NH1  | 2.88                     | 0.47              |
| 1:B:327:GLU:HA   | 1:B:330:LYS:HE3  | 1.96                     | 0.47              |
| 1:C:37:LEU:HD11  | 1:C:67:VAL:HG22  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:110:ILE:O    | 1:G:114:PHE:HB2  | 2.15                     | 0.47              |
| 1:J:283:VAL:HG12 | 1:J:284:SER:N    | 2.30                     | 0.47              |
| 1:A:39:VAL:HA    | 1:A:57:TRP:O     | 2.15                     | 0.46              |
| 1:B:70:ALA:CB    | 1:B:326:LEU:HD11 | 2.43                     | 0.46              |
| 1:C:177:MET:HE1  | 1:E:11:ARG:CZ    | 2.44                     | 0.46              |
| 1:F:39:VAL:HG12  | 1:F:102:VAL:CG1  | 2.45                     | 0.46              |
| 1:L:185:ARG:NE   | 1:L:189:ASP:OD1  | 2.49                     | 0.46              |
| 1:E:260:LEU:O    | 1:E:263:LEU:HG   | 2.15                     | 0.46              |
| 1:H:255:MET:CB   | 1:H:279:ALA:HB3  | 2.45                     | 0.46              |
| 1:L:75:ILE:HD11  | 1:L:329:ALA:CB   | 2.46                     | 0.46              |
| 1:I:71:LEU:HD11  | 1:I:118:VAL:CG1  | 2.46                     | 0.46              |
| 1:E:153:ILE:HG23 | 1:E:183:GLU:HG2  | 1.98                     | 0.46              |
| 1:F:64:ILE:HD11  | 1:F:113:ILE:HG21 | 1.98                     | 0.46              |
| 1:L:63:LEU:HD11  | 1:L:113:ILE:HG23 | 1.97                     | 0.46              |
| 1:B:63:LEU:HD11  | 1:B:113:ILE:CD1  | 2.46                     | 0.46              |
| 1:F:149:ASN:HA   | 1:F:177:MET:HE2  | 1.98                     | 0.46              |
| 1:J:243:VAL:HG13 | 1:J:254:VAL:HG11 | 1.98                     | 0.46              |
| 1:A:255:MET:HB3  | 1:A:279:ALA:HB3  | 1.98                     | 0.46              |
| 1:G:153:ILE:HD11 | 1:G:178:ASP:O    | 2.16                     | 0.46              |
| 1:H:324:HIS:O    | 1:H:325:ALA:C    | 2.59                     | 0.46              |
| 1:J:75:ILE:HD13  | 1:J:325:ALA:HB1  | 1.97                     | 0.46              |
| 1:H:324:HIS:O    | 1:H:326:LEU:N    | 2.49                     | 0.46              |
| 1:I:94:THR:O     | 1:I:97:TYR:N     | 2.49                     | 0.46              |
| 1:J:305:THR:O    | 1:J:309:LEU:HG   | 2.16                     | 0.46              |
| 1:B:62:GLU:N     | 1:B:62:GLU:CD    | 2.74                     | 0.45              |
| 1:E:324:HIS:O    | 1:E:325:ALA:C    | 2.58                     | 0.45              |
| 1:L:67:VAL:HG23  | 1:L:114:PHE:CE2  | 2.51                     | 0.45              |
| 1:A:9:ARG:O      | 1:A:11:ARG:N     | 2.49                     | 0.45              |
| 1:B:63:LEU:HD11  | 1:B:113:ILE:HG12 | 1.98                     | 0.45              |
| 1:D:247:LEU:HD21 | 1:D:276:VAL:HG11 | 1.97                     | 0.45              |
| 1:G:282:ASN:ND2  | 1:G:286:GLU:OE1  | 2.50                     | 0.45              |
| 1:L:98:ASP:O     | 1:L:101:GLY:N    | 2.49                     | 0.45              |
| 1:L:124:VAL:HG21 | 1:L:171:VAL:HG13 | 1.97                     | 0.45              |
| 1:B:153:ILE:CG2  | 1:B:183:GLU:HB3  | 2.47                     | 0.45              |
| 1:C:217:ALA:O    | 1:C:218:ALA:HB3  | 2.16                     | 0.45              |
| 1:I:335:GLY:HA2  | 1:I:336:LEU:C    | 2.42                     | 0.45              |
| 1:K:105:ARG:HA   | 1:K:108:ARG:HD2  | 1.97                     | 0.45              |
| 1:D:263:LEU:HA   | 1:D:266:ILE:HD12 | 1.99                     | 0.45              |
| 1:G:77:LYS:C     | 1:G:78:PHE:CD1   | 2.94                     | 0.45              |
| 1:A:37:LEU:HD12  | 1:A:80:LEU:HD21  | 1.99                     | 0.45              |
| 1:D:287:TYR:CD2  | 1:D:324:HIS:CE1  | 3.05                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:101:GLY:C    | 1:E:104:PRO:HD2  | 2.41                     | 0.45              |
| 1:G:332:ILE:HG23 | 1:G:332:ILE:O    | 2.16                     | 0.45              |
| 1:L:305:THR:HG22 | 1:L:324:HIS:CE1  | 2.52                     | 0.45              |
| 1:F:291:LYS:O    | 1:F:295:THR:HB   | 2.16                     | 0.45              |
| 1:H:49:GLY:O     | 1:H:51:MET:N     | 2.50                     | 0.45              |
| 1:J:40:LYS:HG3   | 1:J:58:PRO:HA    | 1.99                     | 0.45              |
| 1:D:243:VAL:HG13 | 1:D:254:VAL:HG21 | 1.98                     | 0.45              |
| 1:H:41:PRO:O     | 1:H:43:GLY:N     | 2.50                     | 0.45              |
| 1:I:58:PRO:O     | 1:I:60:GLY:N     | 2.50                     | 0.45              |
| 1:B:83:VAL:HG13  | 1:B:217:ALA:C    | 2.42                     | 0.45              |
| 1:J:282:ASN:HB3  | 1:J:322:THR:HG22 | 1.99                     | 0.45              |
| 1:D:119:LEU:HB2  | 1:G:18:ILE:HG21  | 1.97                     | 0.45              |
| 1:J:153:ILE:HG22 | 1:J:183:GLU:HG2  | 1.98                     | 0.45              |
| 1:E:261:ALA:C    | 1:E:262:TYR:CD1  | 2.95                     | 0.45              |
| 1:E:287:TYR:CD2  | 1:E:324:HIS:CE1  | 3.05                     | 0.45              |
| 1:L:51:MET:HB3   | 1:L:52:PRO:CA    | 2.47                     | 0.45              |
| 1:L:59:VAL:HG13  | 1:L:59:VAL:O     | 2.17                     | 0.45              |
| 1:A:333:LYS:O    | 1:A:334:GLU:HG2  | 2.17                     | 0.44              |
| 1:A:336:LEU:HD22 | 1:G:233:PRO:HG2  | 1.99                     | 0.44              |
| 1:B:143:ASP:N    | 1:B:143:ASP:OD1  | 2.49                     | 0.44              |
| 1:C:59:VAL:HG13  | 1:C:59:VAL:O     | 2.16                     | 0.44              |
| 1:F:71:LEU:HA    | 1:F:75:ILE:O     | 2.17                     | 0.44              |
| 1:K:136:GLY:O    | 1:K:137:VAL:C    | 2.61                     | 0.44              |
| 1:E:127:CYS:HB3  | 1:E:135:CYS:SG   | 2.56                     | 0.44              |
| 1:K:62:GLU:HA    | 1:K:65:ASN:CB    | 2.46                     | 0.44              |
| 1:A:283:VAL:HG12 | 1:A:284:SER:N    | 2.32                     | 0.44              |
| 1:B:14:ARG:O     | 1:H:228:THR:HA   | 2.17                     | 0.44              |
| 1:C:313:LYS:O    | 1:C:314:ARG:C    | 2.60                     | 0.44              |
| 1:G:328:ALA:HA   | 1:G:331:TRP:CE3  | 2.51                     | 0.44              |
| 1:H:33:PHE:CE1   | 1:H:309:LEU:HD13 | 2.53                     | 0.44              |
| 1:B:299:VAL:CG1  | 1:B:304:ILE:HG21 | 2.48                     | 0.44              |
| 1:E:34:ILE:HG12  | 1:E:77:LYS:HG3   | 1.99                     | 0.44              |
| 1:I:59:VAL:HG13  | 1:I:59:VAL:O     | 2.18                     | 0.44              |
| 1:I:148:ASP:OD2  | 1:I:151:GLU:HB2  | 2.17                     | 0.44              |
| 1:C:125:CYS:SG   | 1:C:135:CYS:HB3  | 2.56                     | 0.44              |
| 1:C:300:ASP:OD1  | 1:C:300:ASP:C    | 2.60                     | 0.44              |
| 1:E:50:PRO:CG    | 1:E:215:VAL:HG11 | 2.48                     | 0.44              |
| 1:E:243:VAL:HG13 | 1:E:254:VAL:HG11 | 2.00                     | 0.44              |
| 1:I:39:VAL:HG11  | 1:I:106:ALA:HB2  | 1.99                     | 0.44              |
| 1:G:44:GLU:O     | 1:G:46:GLU:N     | 2.51                     | 0.44              |
| 1:G:51:MET:HB3   | 1:G:52:PRO:O     | 2.18                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:71:LEU:HA    | 1:G:75:ILE:O     | 2.18                     | 0.44              |
| 1:A:84:LEU:HD11  | 1:A:102:VAL:HG21 | 1.99                     | 0.44              |
| 1:B:109:LEU:O    | 1:B:110:ILE:C    | 2.61                     | 0.44              |
| 1:D:141:LYS:HB2  | 1:D:146:TYR:CE1  | 2.52                     | 0.44              |
| 1:G:70:ALA:HA    | 1:G:73:LEU:HD12  | 1.98                     | 0.44              |
| 1:K:75:ILE:HD11  | 1:K:329:ALA:HB2  | 1.99                     | 0.44              |
| 1:K:225:ASP:HB2  | 1:K:227:ARG:HG2  | 2.00                     | 0.44              |
| 1:A:50:PRO:CB    | 1:A:215:VAL:HG11 | 2.48                     | 0.44              |
| 1:B:35:TYR:O     | 1:B:78:PHE:HA    | 2.18                     | 0.44              |
| 1:B:161:VAL:HG11 | 1:B:191:HIS:CD2  | 2.53                     | 0.44              |
| 1:I:132:HIS:CE1  | 1:I:138:VAL:HG23 | 2.53                     | 0.44              |
| 1:I:223:PHE:CD1  | 1:I:223:PHE:N    | 2.85                     | 0.44              |
| 1:B:298:TYR:CE1  | 1:H:50:PRO:HA    | 2.53                     | 0.44              |
| 1:D:229:TYR:HB3  | 1:F:11:ARG:HE    | 1.83                     | 0.44              |
| 1:D:320:ILE:HG22 | 1:D:322:THR:HG23 | 1.99                     | 0.44              |
| 1:B:153:ILE:HD11 | 1:B:178:ASP:O    | 2.17                     | 0.43              |
| 1:C:125:CYS:SG   | 1:C:135:CYS:CB   | 3.06                     | 0.43              |
| 1:F:164:ALA:HB1  | 1:F:193:PHE:CD2  | 2.53                     | 0.43              |
| 1:H:170:PHE:CE2  | 1:H:197:GLY:HA3  | 2.53                     | 0.43              |
| 1:C:324:HIS:O    | 1:C:325:ALA:C    | 2.61                     | 0.43              |
| 1:H:148:ASP:O    | 1:H:152:THR:HG22 | 2.16                     | 0.43              |
| 1:I:245:MET:O    | 1:I:246:ASP:C    | 2.60                     | 0.43              |
| 1:J:39:VAL:HG11  | 1:J:106:ALA:HB2  | 2.00                     | 0.43              |
| 1:C:11:ARG:NH1   | 1:E:177:MET:HE1  | 2.33                     | 0.43              |
| 1:C:63:LEU:CG    | 1:C:64:ILE:HG23  | 2.45                     | 0.43              |
| 1:E:67:VAL:HG23  | 1:E:78:PHE:CZ    | 2.53                     | 0.43              |
| 1:F:97:TYR:N     | 1:F:97:TYR:CD1   | 2.86                     | 0.43              |
| 1:I:64:ILE:CG2   | 1:I:65:ASN:N     | 2.80                     | 0.43              |
| 1:L:62:GLU:HA    | 1:L:65:ASN:HB3   | 2.00                     | 0.43              |
| 1:L:225:ASP:OD1  | 1:L:227:ARG:HG3  | 2.19                     | 0.43              |
| 1:F:176:MET:HG3  | 1:F:230:GLN:HA   | 2.01                     | 0.43              |
| 1:G:187:ALA:O    | 1:G:188:LEU:C    | 2.59                     | 0.43              |
| 1:D:298:TYR:O    | 1:D:299:VAL:HG13 | 2.18                     | 0.43              |
| 1:H:63:LEU:HD13  | 1:H:109:LEU:CD2  | 2.47                     | 0.43              |
| 1:A:119:LEU:HB2  | 1:E:18:ILE:HG21  | 2.01                     | 0.43              |
| 1:A:141:LYS:O    | 1:A:144:ARG:N    | 2.52                     | 0.43              |
| 1:D:277:PRO:HG3  | 1:G:23:VAL:HG13  | 2.01                     | 0.43              |
| 1:L:83:VAL:HG12  | 1:L:217:ALA:HA   | 2.00                     | 0.43              |
| 1:C:132:HIS:HB2  | 1:C:223:PHE:CE1  | 2.54                     | 0.43              |
| 1:K:295:THR:O    | 1:K:297:GLY:N    | 2.51                     | 0.43              |
| 1:A:42:GLY:O     | 1:A:44:GLU:N     | 2.52                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:324:HIS:O    | 1:B:326:LEU:N    | 2.52                     | 0.43              |
| 1:G:247:LEU:HD11 | 1:G:276:VAL:HG11 | 2.01                     | 0.43              |
| 1:H:45:ARG:HD3   | 1:H:55:TYR:HB3   | 2.01                     | 0.43              |
| 1:H:51:MET:CB    | 1:H:52:PRO:HA    | 2.49                     | 0.43              |
| 1:B:247:LEU:HD21 | 1:B:276:VAL:CG2  | 2.48                     | 0.43              |
| 1:E:321:LEU:N    | 1:E:321:LEU:HD12 | 2.34                     | 0.43              |
| 1:I:213:PHE:HB2  | 1:I:284:SER:HB3  | 2.01                     | 0.43              |
| 1:A:5:PHE:CD1    | 1:A:6:PRO:HA     | 2.53                     | 0.43              |
| 1:B:98:ASP:O     | 1:B:101:GLY:N    | 2.52                     | 0.43              |
| 1:C:51:MET:HE1   | 1:C:323:TYR:CD2  | 2.53                     | 0.43              |
| 1:B:290:VAL:HG11 | 1:B:305:THR:CG2  | 2.49                     | 0.42              |
| 1:C:63:LEU:HD11  | 1:C:113:ILE:HG21 | 2.00                     | 0.42              |
| 1:H:125:CYS:SG   | 1:H:126:LEU:N    | 2.92                     | 0.42              |
| 1:J:66:HIS:O     | 1:J:67:VAL:C     | 2.62                     | 0.42              |
| 1:A:264:ASP:HB3  | 1:G:263:LEU:HB3  | 2.00                     | 0.42              |
| 1:C:149:ASN:O    | 1:C:153:ILE:HB   | 2.20                     | 0.42              |
| 1:A:292:ALA:HB2  | 1:G:298:TYR:CE2  | 2.54                     | 0.42              |
| 1:C:90:ASN:HB2   | 1:C:91:PRO:HD2   | 2.00                     | 0.42              |
| 1:L:309:LEU:HD21 | 1:L:322:THR:HG21 | 2.00                     | 0.42              |
| 1:E:333:LYS:CE   | 1:J:65:ASN:HD21  | 2.32                     | 0.42              |
| 1:I:69:GLU:O     | 1:I:73:LEU:HD12  | 2.18                     | 0.42              |
| 1:J:107:ILE:HD13 | 1:J:168:ALA:HB2  | 2.01                     | 0.42              |
| 1:A:156:TYR:OH   | 1:A:175:GLY:HA3  | 2.19                     | 0.42              |
| 1:B:48:ILE:HG21  | 1:B:216:ALA:HB2  | 2.02                     | 0.42              |
| 1:B:236:ALA:N    | 1:H:25:GLU:OE2   | 2.51                     | 0.42              |
| 1:C:77:LYS:HE2   | 1:H:22:ALA:CB    | 2.50                     | 0.42              |
| 1:C:334:GLU:O    | 1:C:335:GLY:C    | 2.61                     | 0.42              |
| 1:D:160:ALA:HB1  | 1:D:188:LEU:HD11 | 2.01                     | 0.42              |
| 1:H:51:MET:HB3   | 1:H:52:PRO:HA    | 2.02                     | 0.42              |
| 1:J:41:PRO:HG3   | 1:J:102:VAL:HG22 | 2.01                     | 0.42              |
| 1:B:18:ILE:HG23  | 1:F:76:ASN:ND2   | 2.35                     | 0.42              |
| 1:D:333:LYS:HD3  | 1:D:333:LYS:N    | 2.35                     | 0.42              |
| 1:G:232:ASP:OD1  | 1:G:234:ARG:HB2  | 2.20                     | 0.42              |
| 1:G:260:LEU:HD13 | 1:G:308:ILE:HG23 | 2.02                     | 0.42              |
| 1:H:182:ARG:HB2  | 1:H:249:GLU:HG2  | 2.01                     | 0.42              |
| 1:K:282:ASN:HB3  | 1:K:322:THR:HG23 | 2.01                     | 0.42              |
| 1:L:90:ASN:OD1   | 1:L:90:ASN:N     | 2.52                     | 0.42              |
| 1:C:289:LEU:HD21 | 1:E:290:VAL:HA   | 2.00                     | 0.42              |
| 1:C:39:VAL:HG12  | 1:C:102:VAL:HG12 | 2.01                     | 0.42              |
| 1:E:335:GLY:HA3  | 1:E:336:LEU:CB   | 2.50                     | 0.42              |
| 1:K:153:ILE:HD11 | 1:K:178:ASP:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:210:TYR:CD1  | 1:K:283:VAL:HG11 | 2.55                     | 0.42              |
| 1:L:247:LEU:HD11 | 1:L:276:VAL:CG1  | 2.48                     | 0.42              |
| 1:A:170:PHE:CE1  | 1:A:197:GLY:HA3  | 2.55                     | 0.42              |
| 1:F:149:ASN:OD1  | 1:F:177:MET:HE3  | 2.19                     | 0.42              |
| 1:I:309:LEU:HD21 | 1:I:322:THR:HG21 | 2.01                     | 0.42              |
| 1:L:100:GLU:OE2  | 1:L:108:ARG:NH2  | 2.53                     | 0.42              |
| 1:A:29:ASP:O     | 1:A:31:GLY:N     | 2.53                     | 0.42              |
| 1:B:57:TRP:CZ2   | 1:B:66:HIS:CD2   | 3.08                     | 0.42              |
| 1:E:9:ARG:HD2    | 1:E:12:ARG:NH2   | 2.35                     | 0.42              |
| 1:F:60:GLY:O     | 1:F:61:ARG:C     | 2.63                     | 0.42              |
| 1:G:199:MET:HE3  | 1:G:255:MET:SD   | 2.60                     | 0.42              |
| 1:I:18:ILE:HD12  | 1:I:18:ILE:H     | 1.84                     | 0.42              |
| 1:K:153:ILE:HG23 | 1:K:183:GLU:HG2  | 2.02                     | 0.42              |
| 1:A:50:PRO:HG2   | 1:A:215:VAL:HG11 | 2.02                     | 0.41              |
| 1:B:63:LEU:HD11  | 1:B:113:ILE:CG1  | 2.49                     | 0.41              |
| 1:B:79:ILE:HA    | 1:B:121:PHE:O    | 2.20                     | 0.41              |
| 1:C:11:ARG:CZ    | 1:E:177:MET:HE1  | 2.50                     | 0.41              |
| 1:D:213:PHE:HA   | 1:D:216:ALA:HB3  | 2.02                     | 0.41              |
| 1:F:255:MET:CE   | 1:F:257:LYS:HB2  | 2.50                     | 0.41              |
| 1:A:117:ARG:O    | 1:A:118:VAL:HG23 | 2.19                     | 0.41              |
| 1:B:275:TRP:HA   | 1:D:237:TYR:HB3  | 2.02                     | 0.41              |
| 1:D:19:ILE:O     | 1:D:23:VAL:HG22  | 2.21                     | 0.41              |
| 1:E:94:THR:O     | 1:E:95:GLY:C     | 2.62                     | 0.41              |
| 1:G:301:GLU:O    | 1:G:302:ARG:C    | 2.62                     | 0.41              |
| 1:H:40:LYS:HA    | 1:H:102:VAL:HG11 | 2.02                     | 0.41              |
| 1:H:109:LEU:O    | 1:H:113:ILE:HG22 | 2.20                     | 0.41              |
| 1:J:57:TRP:CD1   | 1:J:62:GLU:HB2   | 2.55                     | 0.41              |
| 1:A:148:ASP:O    | 1:A:152:THR:HG22 | 2.19                     | 0.41              |
| 1:D:49:GLY:N     | 1:D:50:PRO:HD2   | 2.34                     | 0.41              |
| 1:F:324:HIS:O    | 1:F:325:ALA:C    | 2.63                     | 0.41              |
| 1:G:13:LEU:HD22  | 1:G:23:VAL:HG21  | 2.03                     | 0.41              |
| 1:G:201:TYR:HA   | 1:G:255:MET:HG3  | 2.02                     | 0.41              |
| 1:K:291:LYS:NZ   | 1:K:327:GLU:OE2  | 2.52                     | 0.41              |
| 1:A:29:ASP:O     | 1:A:30:ALA:C     | 2.62                     | 0.41              |
| 1:A:247:LEU:HD21 | 1:A:276:VAL:HG11 | 2.02                     | 0.41              |
| 1:I:83:VAL:HG13  | 1:I:217:ALA:HA   | 2.00                     | 0.41              |
| 1:J:219:SER:O    | 1:J:220:ALA:C    | 2.64                     | 0.41              |
| 1:D:184:ILE:O    | 1:D:188:LEU:HD13 | 2.20                     | 0.41              |
| 1:G:79:ILE:HA    | 1:G:121:PHE:O    | 2.19                     | 0.41              |
| 1:I:210:TYR:O    | 1:I:211:GLY:C    | 2.62                     | 0.41              |
| 1:K:301:GLU:O    | 1:K:305:THR:HG23 | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:LEU:HD12  | 1:A:107:ILE:CD1  | 2.51                     | 0.41              |
| 1:B:328:ALA:HA   | 1:B:331:TRP:CE3  | 2.56                     | 0.41              |
| 1:D:320:ILE:HG22 | 1:D:322:THR:CG2  | 2.50                     | 0.41              |
| 1:F:30:ALA:HA    | 1:F:33:PHE:CD2   | 2.55                     | 0.41              |
| 1:G:92:GLU:O     | 1:G:93:GLY:C     | 2.64                     | 0.41              |
| 1:B:63:LEU:HD21  | 1:B:113:ILE:HD11 | 2.03                     | 0.41              |
| 1:C:56:ARG:HD3   | 1:C:83:VAL:HG11  | 2.02                     | 0.41              |
| 1:E:158:LYS:O    | 1:E:159:GLU:C    | 2.63                     | 0.41              |
| 1:G:79:ILE:HG23  | 1:G:81:PHE:HE1   | 1.85                     | 0.41              |
| 1:H:299:VAL:HG11 | 1:H:304:ILE:HG21 | 2.02                     | 0.41              |
| 1:I:247:LEU:HD21 | 1:I:276:VAL:HG11 | 2.03                     | 0.41              |
| 1:C:63:LEU:HG    | 1:C:64:ILE:CG2   | 2.48                     | 0.41              |
| 1:D:267:ARG:NH1  | 1:F:264:ASP:HB2  | 2.36                     | 0.41              |
| 1:D:287:TYR:CD2  | 1:D:323:TYR:HB2  | 2.56                     | 0.41              |
| 1:F:35:TYR:CE2   | 1:F:326:LEU:HD11 | 2.56                     | 0.41              |
| 1:F:125:CYS:SG   | 1:F:135:CYS:HB3  | 2.60                     | 0.41              |
| 1:G:311:ALA:HA   | 1:G:314:ARG:NH1  | 2.36                     | 0.41              |
| 1:L:13:LEU:HD22  | 1:L:23:VAL:HG21  | 2.02                     | 0.41              |
| 1:A:284:SER:N    | 1:A:323:TYR:HE2  | 2.19                     | 0.41              |
| 1:B:98:ASP:O     | 1:B:99:PRO:C     | 2.64                     | 0.41              |
| 1:B:184:ILE:O    | 1:B:185:ARG:C    | 2.63                     | 0.41              |
| 1:B:231:MET:HE3  | 1:B:238:GLU:HG2  | 2.03                     | 0.41              |
| 1:C:144:ARG:O    | 1:C:145:TRP:C    | 2.63                     | 0.41              |
| 1:C:144:ARG:HD3  | 1:C:144:ARG:N    | 2.35                     | 0.41              |
| 1:C:299:VAL:HG11 | 1:C:304:ILE:HD13 | 2.02                     | 0.41              |
| 1:D:98:ASP:O     | 1:D:101:GLY:N    | 2.51                     | 0.41              |
| 1:E:237:TYR:CD2  | 1:H:274:PRO:HB2  | 2.55                     | 0.41              |
| 1:L:50:PRO:CD    | 1:L:215:VAL:HG11 | 2.51                     | 0.41              |
| 1:L:51:MET:HB3   | 1:L:52:PRO:HA    | 2.03                     | 0.41              |
| 1:L:182:ARG:HB3  | 1:L:182:ARG:NH1  | 2.35                     | 0.41              |
| 1:C:39:VAL:HG11  | 1:C:106:ALA:HB2  | 2.03                     | 0.41              |
| 1:C:255:MET:HE2  | 1:C:281:TYR:HB2  | 2.02                     | 0.41              |
| 1:H:85:PRO:O     | 1:H:88:LEU:HD23  | 2.21                     | 0.41              |
| 1:J:34:ILE:HD12  | 1:J:321:LEU:HD11 | 2.03                     | 0.41              |
| 1:J:261:ALA:C    | 1:J:262:TYR:CD1  | 2.99                     | 0.41              |
| 1:L:124:VAL:CG2  | 1:L:171:VAL:HG13 | 2.51                     | 0.41              |
| 1:A:5:PHE:CG     | 1:A:6:PRO:HA     | 2.56                     | 0.40              |
| 1:A:26:THR:HG22  | 1:A:27:GLN:N     | 2.35                     | 0.40              |
| 1:E:84:LEU:HB2   | 1:E:85:PRO:CD    | 2.51                     | 0.40              |
| 1:E:153:ILE:CD1  | 1:E:178:ASP:O    | 2.69                     | 0.40              |
| 1:F:301:GLU:O    | 1:F:305:THR:HG23 | 2.20                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:103:VAL:CG1  | 1:G:104:PRO:HD3  | 2.51                     | 0.40              |
| 1:L:122:ALA:HB1  | 1:L:163:TYR:CD2  | 2.56                     | 0.40              |
| 1:A:59:VAL:HG21  | 1:A:105:ARG:CZ   | 2.50                     | 0.40              |
| 1:I:153:ILE:HG22 | 1:I:183:GLU:HG2  | 2.02                     | 0.40              |
| 1:K:220:ALA:HB1  | 1:K:221:PRO:HD2  | 2.03                     | 0.40              |
| 1:D:126:LEU:HD11 | 1:D:155:LEU:HD12 | 2.04                     | 0.40              |
| 1:J:50:PRO:HG3   | 1:J:215:VAL:HG11 | 2.04                     | 0.40              |
| 1:J:54:ILE:N     | 1:J:54:ILE:HD13  | 2.37                     | 0.40              |
| 1:K:237:TYR:CD1  | 1:K:268:LEU:HD21 | 2.55                     | 0.40              |
| 1:A:103:VAL:HG22 | 1:A:104:PRO:HD3  | 2.03                     | 0.40              |
| 1:G:176:MET:CG   | 1:G:204:LYS:HB3  | 2.51                     | 0.40              |
| 1:I:64:ILE:HG22  | 1:I:65:ASN:H     | 1.87                     | 0.40              |
| 1:J:332:ILE:HD13 | 1:J:332:ILE:HG21 | 1.93                     | 0.40              |
| 1:A:209:PHE:O    | 1:A:285:GLY:CA   | 2.69                     | 0.40              |
| 1:B:40:LYS:CD    | 1:B:46:GLU:OE2   | 2.68                     | 0.40              |
| 1:C:177:MET:HE3  | 1:C:177:MET:HA   | 2.04                     | 0.40              |
| 1:C:290:VAL:HG11 | 1:C:305:THR:HG22 | 2.02                     | 0.40              |
| 1:C:313:LYS:O    | 1:C:316:GLY:N    | 2.54                     | 0.40              |
| 1:D:11:ARG:NH1   | 1:F:177:MET:HE1  | 2.37                     | 0.40              |
| 1:E:5:PHE:CG     | 1:E:6:PRO:HA     | 2.56                     | 0.40              |
| 1:E:309:LEU:HD21 | 1:E:322:THR:HG21 | 2.03                     | 0.40              |
| 1:F:255:MET:HB3  | 1:F:279:ALA:HB3  | 2.03                     | 0.40              |
| 1:K:102:VAL:HG23 | 1:K:103:VAL:N    | 2.37                     | 0.40              |
| 1:L:94:THR:O     | 1:L:96:GLY:N     | 2.54                     | 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     | 334/338 (99%) | 286 (86%) | 36 (11%) | 12 (4%)  | <b>2</b> <b>21</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | B     | 334/338 (99%)   | 284 (85%)  | 38 (11%)  | 12 (4%)  | 2           | 21 |
| 1   | C     | 334/338 (99%)   | 289 (86%)  | 38 (11%)  | 7 (2%)   | 5           | 31 |
| 1   | D     | 334/338 (99%)   | 287 (86%)  | 36 (11%)  | 11 (3%)  | 3           | 23 |
| 1   | E     | 334/338 (99%)   | 286 (86%)  | 35 (10%)  | 13 (4%)  | 2           | 20 |
| 1   | F     | 334/338 (99%)   | 284 (85%)  | 42 (13%)  | 8 (2%)   | 4           | 29 |
| 1   | G     | 334/338 (99%)   | 283 (85%)  | 36 (11%)  | 15 (4%)  | 2           | 17 |
| 1   | H     | 334/338 (99%)   | 282 (84%)  | 40 (12%)  | 12 (4%)  | 2           | 21 |
| 1   | I     | 334/338 (99%)   | 286 (86%)  | 37 (11%)  | 11 (3%)  | 3           | 23 |
| 1   | J     | 334/338 (99%)   | 287 (86%)  | 32 (10%)  | 15 (4%)  | 2           | 17 |
| 1   | K     | 334/338 (99%)   | 280 (84%)  | 44 (13%)  | 10 (3%)  | 3           | 25 |
| 1   | L     | 334/338 (99%)   | 280 (84%)  | 41 (12%)  | 13 (4%)  | 2           | 20 |
| All | All   | 4008/4056 (99%) | 3414 (85%) | 455 (11%) | 139 (4%) | 3           | 22 |

All (139) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | GLY  |
| 1   | A     | 52  | PRO  |
| 1   | A     | 284 | SER  |
| 1   | B     | 131 | ASP  |
| 1   | B     | 187 | ALA  |
| 1   | B     | 188 | LEU  |
| 1   | C     | 143 | ASP  |
| 1   | D     | 52  | PRO  |
| 1   | D     | 325 | ALA  |
| 1   | E     | 15  | ALA  |
| 1   | E     | 94  | THR  |
| 1   | E     | 297 | GLY  |
| 1   | F     | 94  | THR  |
| 1   | F     | 131 | ASP  |
| 1   | F     | 142 | ARG  |
| 1   | F     | 143 | ASP  |
| 1   | F     | 333 | LYS  |
| 1   | G     | 45  | ARG  |
| 1   | G     | 51  | MET  |
| 1   | G     | 52  | PRO  |
| 1   | G     | 131 | ASP  |
| 1   | G     | 142 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 194 | GLU  |
| 1   | G     | 284 | SER  |
| 1   | G     | 333 | LYS  |
| 1   | H     | 42  | GLY  |
| 1   | H     | 51  | MET  |
| 1   | H     | 52  | PRO  |
| 1   | H     | 63  | LEU  |
| 1   | H     | 131 | ASP  |
| 1   | H     | 325 | ALA  |
| 1   | I     | 51  | MET  |
| 1   | I     | 52  | PRO  |
| 1   | I     | 93  | GLY  |
| 1   | I     | 142 | ARG  |
| 1   | J     | 51  | MET  |
| 1   | J     | 52  | PRO  |
| 1   | J     | 53  | GLY  |
| 1   | J     | 131 | ASP  |
| 1   | K     | 137 | VAL  |
| 1   | L     | 95  | GLY  |
| 1   | L     | 333 | LYS  |
| 1   | A     | 30  | ALA  |
| 1   | A     | 53  | GLY  |
| 1   | A     | 146 | TYR  |
| 1   | A     | 325 | ALA  |
| 1   | A     | 335 | GLY  |
| 1   | B     | 93  | GLY  |
| 1   | B     | 137 | VAL  |
| 1   | B     | 140 | GLU  |
| 1   | B     | 142 | ARG  |
| 1   | B     | 325 | ALA  |
| 1   | C     | 59  | VAL  |
| 1   | C     | 284 | SER  |
| 1   | C     | 296 | ALA  |
| 1   | D     | 41  | PRO  |
| 1   | D     | 225 | ASP  |
| 1   | D     | 284 | SER  |
| 1   | E     | 225 | ASP  |
| 1   | E     | 284 | SER  |
| 1   | F     | 115 | GLY  |
| 1   | F     | 284 | SER  |
| 1   | G     | 87  | GLU  |
| 1   | G     | 93  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 113 | ILE  |
| 1   | I     | 18  | ILE  |
| 1   | I     | 143 | ASP  |
| 1   | I     | 206 | ALA  |
| 1   | I     | 272 | HIS  |
| 1   | I     | 284 | SER  |
| 1   | J     | 45  | ARG  |
| 1   | J     | 59  | VAL  |
| 1   | J     | 62  | GLU  |
| 1   | J     | 142 | ARG  |
| 1   | J     | 332 | ILE  |
| 1   | K     | 143 | ASP  |
| 1   | K     | 209 | PHE  |
| 1   | K     | 284 | SER  |
| 1   | K     | 295 | THR  |
| 1   | L     | 63  | LEU  |
| 1   | L     | 93  | GLY  |
| 1   | L     | 131 | ASP  |
| 1   | L     | 143 | ASP  |
| 1   | L     | 224 | GLY  |
| 1   | L     | 325 | ALA  |
| 1   | A     | 51  | MET  |
| 1   | C     | 314 | ARG  |
| 1   | E     | 41  | PRO  |
| 1   | E     | 45  | ARG  |
| 1   | E     | 51  | MET  |
| 1   | E     | 331 | TRP  |
| 1   | F     | 86  | ASP  |
| 1   | G     | 250 | GLY  |
| 1   | H     | 284 | SER  |
| 1   | J     | 24  | ALA  |
| 1   | K     | 145 | TRP  |
| 1   | K     | 296 | ALA  |
| 1   | L     | 59  | VAL  |
| 1   | L     | 218 | ALA  |
| 1   | A     | 10  | PRO  |
| 1   | A     | 137 | VAL  |
| 1   | A     | 334 | GLU  |
| 1   | B     | 333 | LYS  |
| 1   | C     | 63  | LEU  |
| 1   | C     | 201 | TYR  |
| 1   | D     | 51  | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 114 | PHE  |
| 1   | E     | 206 | ALA  |
| 1   | G     | 63  | LEU  |
| 1   | H     | 142 | ARG  |
| 1   | H     | 272 | HIS  |
| 1   | I     | 59  | VAL  |
| 1   | J     | 63  | LEU  |
| 1   | L     | 51  | MET  |
| 1   | B     | 3   | VAL  |
| 1   | B     | 284 | SER  |
| 1   | D     | 142 | ARG  |
| 1   | E     | 44  | GLU  |
| 1   | G     | 10  | PRO  |
| 1   | I     | 224 | GLY  |
| 1   | J     | 220 | ALA  |
| 1   | J     | 227 | ARG  |
| 1   | J     | 284 | SER  |
| 1   | K     | 41  | PRO  |
| 1   | L     | 24  | ALA  |
| 1   | D     | 65  | ASN  |
| 1   | D     | 221 | PRO  |
| 1   | G     | 57  | TRP  |
| 1   | G     | 114 | PHE  |
| 1   | H     | 94  | THR  |
| 1   | J     | 333 | LYS  |
| 1   | K     | 51  | MET  |
| 1   | L     | 141 | LYS  |
| 1   | E     | 335 | GLY  |
| 1   | H     | 50  | PRO  |
| 1   | D     | 211 | GLY  |
| 1   | D     | 316 | GLY  |
| 1   | B     | 220 | ALA  |
| 1   | K     | 52  | PRO  |

### 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     | 268/270 (99%)   | 232 (87%)  | 36 (13%)  | 4           | 20 |
| 1   | B     | 268/270 (99%)   | 226 (84%)  | 42 (16%)  | 2           | 15 |
| 1   | C     | 268/270 (99%)   | 227 (85%)  | 41 (15%)  | 3           | 16 |
| 1   | D     | 268/270 (99%)   | 235 (88%)  | 33 (12%)  | 4           | 22 |
| 1   | E     | 268/270 (99%)   | 233 (87%)  | 35 (13%)  | 4           | 20 |
| 1   | F     | 268/270 (99%)   | 227 (85%)  | 41 (15%)  | 3           | 16 |
| 1   | G     | 268/270 (99%)   | 227 (85%)  | 41 (15%)  | 3           | 16 |
| 1   | H     | 268/270 (99%)   | 228 (85%)  | 40 (15%)  | 3           | 17 |
| 1   | I     | 268/270 (99%)   | 231 (86%)  | 37 (14%)  | 3           | 19 |
| 1   | J     | 268/270 (99%)   | 233 (87%)  | 35 (13%)  | 4           | 20 |
| 1   | K     | 268/270 (99%)   | 233 (87%)  | 35 (13%)  | 4           | 20 |
| 1   | L     | 268/270 (99%)   | 231 (86%)  | 37 (14%)  | 3           | 19 |
| All | All   | 3216/3240 (99%) | 2763 (86%) | 453 (14%) | 3           | 18 |

All (453) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 1   | MET  |
| 1   | A     | 2   | ARG  |
| 1   | A     | 3   | VAL  |
| 1   | A     | 6   | PRO  |
| 1   | A     | 16  | SER  |
| 1   | A     | 17  | LYS  |
| 1   | A     | 19  | ILE  |
| 1   | A     | 40  | LYS  |
| 1   | A     | 54  | ILE  |
| 1   | A     | 64  | ILE  |
| 1   | A     | 67  | VAL  |
| 1   | A     | 77  | LYS  |
| 1   | A     | 97  | TYR  |
| 1   | A     | 102 | VAL  |
| 1   | A     | 103 | VAL  |
| 1   | A     | 107 | ILE  |
| 1   | A     | 118 | VAL  |
| 1   | A     | 140 | GLU  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 152 | THR  |
| 1   | A     | 182 | ARG  |
| 1   | A     | 223 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 228 | THR  |
| 1   | A     | 229 | TYR  |
| 1   | A     | 254 | VAL  |
| 1   | A     | 268 | LEU  |
| 1   | A     | 284 | SER  |
| 1   | A     | 288 | SER  |
| 1   | A     | 290 | VAL  |
| 1   | A     | 299 | VAL  |
| 1   | A     | 303 | THR  |
| 1   | A     | 304 | ILE  |
| 1   | A     | 332 | ILE  |
| 1   | A     | 333 | LYS  |
| 1   | A     | 334 | GLU  |
| 1   | A     | 336 | LEU  |
| 1   | B     | 1   | MET  |
| 1   | B     | 2   | ARG  |
| 1   | B     | 3   | VAL  |
| 1   | B     | 7   | THR  |
| 1   | B     | 18  | ILE  |
| 1   | B     | 19  | ILE  |
| 1   | B     | 61  | ARG  |
| 1   | B     | 62  | GLU  |
| 1   | B     | 63  | LEU  |
| 1   | B     | 66  | HIS  |
| 1   | B     | 71  | LEU  |
| 1   | B     | 73  | LEU  |
| 1   | B     | 77  | LYS  |
| 1   | B     | 88  | LEU  |
| 1   | B     | 90  | ASN  |
| 1   | B     | 109 | LEU  |
| 1   | B     | 113 | ILE  |
| 1   | B     | 117 | ARG  |
| 1   | B     | 118 | VAL  |
| 1   | B     | 142 | ARG  |
| 1   | B     | 143 | ASP  |
| 1   | B     | 144 | ARG  |
| 1   | B     | 171 | VAL  |
| 1   | B     | 195 | GLU  |
| 1   | B     | 198 | ILE  |
| 1   | B     | 223 | PHE  |
| 1   | B     | 227 | ARG  |
| 1   | B     | 229 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 248 | GLU  |
| 1   | B     | 254 | VAL  |
| 1   | B     | 268 | LEU  |
| 1   | B     | 276 | VAL  |
| 1   | B     | 283 | VAL  |
| 1   | B     | 284 | SER  |
| 1   | B     | 295 | THR  |
| 1   | B     | 299 | VAL  |
| 1   | B     | 304 | ILE  |
| 1   | B     | 322 | THR  |
| 1   | B     | 330 | LYS  |
| 1   | B     | 332 | ILE  |
| 1   | B     | 333 | LYS  |
| 1   | B     | 334 | GLU  |
| 1   | C     | 1   | MET  |
| 1   | C     | 3   | VAL  |
| 1   | C     | 4   | GLN  |
| 1   | C     | 16  | SER  |
| 1   | C     | 18  | ILE  |
| 1   | C     | 19  | ILE  |
| 1   | C     | 28  | ILE  |
| 1   | C     | 44  | GLU  |
| 1   | C     | 69  | GLU  |
| 1   | C     | 88  | LEU  |
| 1   | C     | 97  | TYR  |
| 1   | C     | 102 | VAL  |
| 1   | C     | 109 | LEU  |
| 1   | C     | 112 | GLU  |
| 1   | C     | 113 | ILE  |
| 1   | C     | 117 | ARG  |
| 1   | C     | 118 | VAL  |
| 1   | C     | 119 | LEU  |
| 1   | C     | 139 | LYS  |
| 1   | C     | 142 | ARG  |
| 1   | C     | 144 | ARG  |
| 1   | C     | 145 | TRP  |
| 1   | C     | 146 | TYR  |
| 1   | C     | 161 | VAL  |
| 1   | C     | 176 | MET  |
| 1   | C     | 182 | ARG  |
| 1   | C     | 227 | ARG  |
| 1   | C     | 228 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 229 | TYR  |
| 1   | C     | 248 | GLU  |
| 1   | C     | 254 | VAL  |
| 1   | C     | 283 | VAL  |
| 1   | C     | 284 | SER  |
| 1   | C     | 289 | LEU  |
| 1   | C     | 290 | VAL  |
| 1   | C     | 295 | THR  |
| 1   | C     | 299 | VAL  |
| 1   | C     | 301 | GLU  |
| 1   | C     | 303 | THR  |
| 1   | C     | 304 | ILE  |
| 1   | C     | 333 | LYS  |
| 1   | D     | 2   | ARG  |
| 1   | D     | 7   | THR  |
| 1   | D     | 21  | ASP  |
| 1   | D     | 28  | ILE  |
| 1   | D     | 39  | VAL  |
| 1   | D     | 40  | LYS  |
| 1   | D     | 51  | MET  |
| 1   | D     | 54  | ILE  |
| 1   | D     | 66  | HIS  |
| 1   | D     | 71  | LEU  |
| 1   | D     | 88  | LEU  |
| 1   | D     | 94  | THR  |
| 1   | D     | 100 | GLU  |
| 1   | D     | 107 | ILE  |
| 1   | D     | 144 | ARG  |
| 1   | D     | 186 | ARG  |
| 1   | D     | 195 | GLU  |
| 1   | D     | 215 | VAL  |
| 1   | D     | 222 | LYS  |
| 1   | D     | 223 | PHE  |
| 1   | D     | 227 | ARG  |
| 1   | D     | 228 | THR  |
| 1   | D     | 229 | TYR  |
| 1   | D     | 247 | LEU  |
| 1   | D     | 254 | VAL  |
| 1   | D     | 268 | LEU  |
| 1   | D     | 284 | SER  |
| 1   | D     | 299 | VAL  |
| 1   | D     | 301 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 305 | THR  |
| 1   | D     | 330 | LYS  |
| 1   | D     | 333 | LYS  |
| 1   | D     | 334 | GLU  |
| 1   | E     | 2   | ARG  |
| 1   | E     | 3   | VAL  |
| 1   | E     | 4   | GLN  |
| 1   | E     | 39  | VAL  |
| 1   | E     | 44  | GLU  |
| 1   | E     | 45  | ARG  |
| 1   | E     | 51  | MET  |
| 1   | E     | 64  | ILE  |
| 1   | E     | 76  | ASN  |
| 1   | E     | 84  | LEU  |
| 1   | E     | 86  | ASP  |
| 1   | E     | 98  | ASP  |
| 1   | E     | 113 | ILE  |
| 1   | E     | 118 | VAL  |
| 1   | E     | 120 | VAL  |
| 1   | E     | 128 | GLU  |
| 1   | E     | 140 | GLU  |
| 1   | E     | 144 | ARG  |
| 1   | E     | 152 | THR  |
| 1   | E     | 153 | ILE  |
| 1   | E     | 165 | GLU  |
| 1   | E     | 171 | VAL  |
| 1   | E     | 183 | GLU  |
| 1   | E     | 185 | ARG  |
| 1   | E     | 198 | ILE  |
| 1   | E     | 219 | SER  |
| 1   | E     | 255 | MET  |
| 1   | E     | 268 | LEU  |
| 1   | E     | 283 | VAL  |
| 1   | E     | 284 | SER  |
| 1   | E     | 301 | GLU  |
| 1   | E     | 303 | THR  |
| 1   | E     | 322 | THR  |
| 1   | E     | 330 | LYS  |
| 1   | E     | 334 | GLU  |
| 1   | F     | 3   | VAL  |
| 1   | F     | 7   | THR  |
| 1   | F     | 8   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 17  | LYS  |
| 1   | F     | 26  | THR  |
| 1   | F     | 28  | ILE  |
| 1   | F     | 39  | VAL  |
| 1   | F     | 40  | LYS  |
| 1   | F     | 59  | VAL  |
| 1   | F     | 64  | ILE  |
| 1   | F     | 84  | LEU  |
| 1   | F     | 98  | ASP  |
| 1   | F     | 109 | LEU  |
| 1   | F     | 113 | ILE  |
| 1   | F     | 116 | ASP  |
| 1   | F     | 117 | ARG  |
| 1   | F     | 118 | VAL  |
| 1   | F     | 139 | LYS  |
| 1   | F     | 140 | GLU  |
| 1   | F     | 142 | ARG  |
| 1   | F     | 182 | ARG  |
| 1   | F     | 186 | ARG  |
| 1   | F     | 214 | ARG  |
| 1   | F     | 219 | SER  |
| 1   | F     | 222 | LYS  |
| 1   | F     | 225 | ASP  |
| 1   | F     | 227 | ARG  |
| 1   | F     | 228 | THR  |
| 1   | F     | 229 | TYR  |
| 1   | F     | 254 | VAL  |
| 1   | F     | 268 | LEU  |
| 1   | F     | 271 | GLN  |
| 1   | F     | 283 | VAL  |
| 1   | F     | 284 | SER  |
| 1   | F     | 291 | LYS  |
| 1   | F     | 295 | THR  |
| 1   | F     | 302 | ARG  |
| 1   | F     | 310 | THR  |
| 1   | F     | 322 | THR  |
| 1   | F     | 332 | ILE  |
| 1   | F     | 333 | LYS  |
| 1   | G     | 1   | MET  |
| 1   | G     | 2   | ARG  |
| 1   | G     | 7   | THR  |
| 1   | G     | 17  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 19  | ILE  |
| 1   | G     | 28  | ILE  |
| 1   | G     | 39  | VAL  |
| 1   | G     | 46  | GLU  |
| 1   | G     | 51  | MET  |
| 1   | G     | 61  | ARG  |
| 1   | G     | 71  | LEU  |
| 1   | G     | 72  | SER  |
| 1   | G     | 77  | LYS  |
| 1   | G     | 84  | LEU  |
| 1   | G     | 97  | TYR  |
| 1   | G     | 98  | ASP  |
| 1   | G     | 109 | LEU  |
| 1   | G     | 118 | VAL  |
| 1   | G     | 128 | GLU  |
| 1   | G     | 130 | THR  |
| 1   | G     | 144 | ARG  |
| 1   | G     | 161 | VAL  |
| 1   | G     | 169 | ASP  |
| 1   | G     | 174 | SER  |
| 1   | G     | 183 | GLU  |
| 1   | G     | 194 | GLU  |
| 1   | G     | 207 | SER  |
| 1   | G     | 223 | PHE  |
| 1   | G     | 226 | ARG  |
| 1   | G     | 229 | TYR  |
| 1   | G     | 254 | VAL  |
| 1   | G     | 268 | LEU  |
| 1   | G     | 283 | VAL  |
| 1   | G     | 295 | THR  |
| 1   | G     | 303 | THR  |
| 1   | G     | 305 | THR  |
| 1   | G     | 306 | LEU  |
| 1   | G     | 318 | ASP  |
| 1   | G     | 322 | THR  |
| 1   | G     | 333 | LYS  |
| 1   | G     | 336 | LEU  |
| 1   | H     | 1   | MET  |
| 1   | H     | 2   | ARG  |
| 1   | H     | 7   | THR  |
| 1   | H     | 8   | THR  |
| 1   | H     | 16  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 39  | VAL  |
| 1   | H     | 40  | LYS  |
| 1   | H     | 45  | ARG  |
| 1   | H     | 51  | MET  |
| 1   | H     | 64  | ILE  |
| 1   | H     | 65  | ASN  |
| 1   | H     | 73  | LEU  |
| 1   | H     | 75  | ILE  |
| 1   | H     | 84  | LEU  |
| 1   | H     | 94  | THR  |
| 1   | H     | 102 | VAL  |
| 1   | H     | 103 | VAL  |
| 1   | H     | 112 | GLU  |
| 1   | H     | 131 | ASP  |
| 1   | H     | 141 | LYS  |
| 1   | H     | 144 | ARG  |
| 1   | H     | 145 | TRP  |
| 1   | H     | 152 | THR  |
| 1   | H     | 171 | VAL  |
| 1   | H     | 177 | MET  |
| 1   | H     | 182 | ARG  |
| 1   | H     | 183 | GLU  |
| 1   | H     | 214 | ARG  |
| 1   | H     | 226 | ARG  |
| 1   | H     | 228 | THR  |
| 1   | H     | 254 | VAL  |
| 1   | H     | 255 | MET  |
| 1   | H     | 268 | LEU  |
| 1   | H     | 272 | HIS  |
| 1   | H     | 276 | VAL  |
| 1   | H     | 283 | VAL  |
| 1   | H     | 284 | SER  |
| 1   | H     | 289 | LEU  |
| 1   | H     | 330 | LYS  |
| 1   | H     | 333 | LYS  |
| 1   | I     | 1   | MET  |
| 1   | I     | 2   | ARG  |
| 1   | I     | 3   | VAL  |
| 1   | I     | 4   | GLN  |
| 1   | I     | 7   | THR  |
| 1   | I     | 17  | LYS  |
| 1   | I     | 40  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 44  | GLU  |
| 1   | I     | 51  | MET  |
| 1   | I     | 61  | ARG  |
| 1   | I     | 63  | LEU  |
| 1   | I     | 64  | ILE  |
| 1   | I     | 65  | ASN  |
| 1   | I     | 66  | HIS  |
| 1   | I     | 84  | LEU  |
| 1   | I     | 102 | VAL  |
| 1   | I     | 113 | ILE  |
| 1   | I     | 119 | LEU  |
| 1   | I     | 140 | GLU  |
| 1   | I     | 144 | ARG  |
| 1   | I     | 171 | VAL  |
| 1   | I     | 195 | GLU  |
| 1   | I     | 214 | ARG  |
| 1   | I     | 223 | PHE  |
| 1   | I     | 229 | TYR  |
| 1   | I     | 254 | VAL  |
| 1   | I     | 260 | LEU  |
| 1   | I     | 268 | LEU  |
| 1   | I     | 269 | VAL  |
| 1   | I     | 272 | HIS  |
| 1   | I     | 283 | VAL  |
| 1   | I     | 284 | SER  |
| 1   | I     | 295 | THR  |
| 1   | I     | 299 | VAL  |
| 1   | I     | 301 | GLU  |
| 1   | I     | 332 | ILE  |
| 1   | I     | 336 | LEU  |
| 1   | J     | 1   | MET  |
| 1   | J     | 2   | ARG  |
| 1   | J     | 4   | GLN  |
| 1   | J     | 7   | THR  |
| 1   | J     | 8   | THR  |
| 1   | J     | 17  | LYS  |
| 1   | J     | 19  | ILE  |
| 1   | J     | 23  | VAL  |
| 1   | J     | 45  | ARG  |
| 1   | J     | 48  | ILE  |
| 1   | J     | 63  | LEU  |
| 1   | J     | 66  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 71  | LEU  |
| 1   | J     | 73  | LEU  |
| 1   | J     | 84  | LEU  |
| 1   | J     | 92  | GLU  |
| 1   | J     | 100 | GLU  |
| 1   | J     | 118 | VAL  |
| 1   | J     | 119 | LEU  |
| 1   | J     | 139 | LYS  |
| 1   | J     | 182 | ARG  |
| 1   | J     | 195 | GLU  |
| 1   | J     | 215 | VAL  |
| 1   | J     | 223 | PHE  |
| 1   | J     | 227 | ARG  |
| 1   | J     | 254 | VAL  |
| 1   | J     | 256 | VAL  |
| 1   | J     | 284 | SER  |
| 1   | J     | 289 | LEU  |
| 1   | J     | 295 | THR  |
| 1   | J     | 301 | GLU  |
| 1   | J     | 308 | ILE  |
| 1   | J     | 309 | LEU  |
| 1   | J     | 313 | LYS  |
| 1   | J     | 330 | LYS  |
| 1   | K     | 2   | ARG  |
| 1   | K     | 7   | THR  |
| 1   | K     | 10  | PRO  |
| 1   | K     | 26  | THR  |
| 1   | K     | 28  | ILE  |
| 1   | K     | 40  | LYS  |
| 1   | K     | 44  | GLU  |
| 1   | K     | 45  | ARG  |
| 1   | K     | 61  | ARG  |
| 1   | K     | 62  | GLU  |
| 1   | K     | 64  | ILE  |
| 1   | K     | 66  | HIS  |
| 1   | K     | 72  | SER  |
| 1   | K     | 75  | ILE  |
| 1   | K     | 87  | GLU  |
| 1   | K     | 92  | GLU  |
| 1   | K     | 112 | GLU  |
| 1   | K     | 113 | ILE  |
| 1   | K     | 141 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 151 | GLU  |
| 1   | K     | 153 | ILE  |
| 1   | K     | 195 | GLU  |
| 1   | K     | 222 | LYS  |
| 1   | K     | 223 | PHE  |
| 1   | K     | 229 | TYR  |
| 1   | K     | 254 | VAL  |
| 1   | K     | 283 | VAL  |
| 1   | K     | 284 | SER  |
| 1   | K     | 289 | LEU  |
| 1   | K     | 291 | LYS  |
| 1   | K     | 299 | VAL  |
| 1   | K     | 301 | GLU  |
| 1   | K     | 322 | THR  |
| 1   | K     | 332 | ILE  |
| 1   | K     | 336 | LEU  |
| 1   | L     | 2   | ARG  |
| 1   | L     | 3   | VAL  |
| 1   | L     | 7   | THR  |
| 1   | L     | 16  | SER  |
| 1   | L     | 17  | LYS  |
| 1   | L     | 19  | ILE  |
| 1   | L     | 28  | ILE  |
| 1   | L     | 34  | ILE  |
| 1   | L     | 51  | MET  |
| 1   | L     | 65  | ASN  |
| 1   | L     | 68  | GLU  |
| 1   | L     | 83  | VAL  |
| 1   | L     | 86  | ASP  |
| 1   | L     | 87  | GLU  |
| 1   | L     | 88  | LEU  |
| 1   | L     | 90  | ASN  |
| 1   | L     | 119 | LEU  |
| 1   | L     | 142 | ARG  |
| 1   | L     | 145 | TRP  |
| 1   | L     | 161 | VAL  |
| 1   | L     | 182 | ARG  |
| 1   | L     | 183 | GLU  |
| 1   | L     | 195 | GLU  |
| 1   | L     | 210 | TYR  |
| 1   | L     | 222 | LYS  |
| 1   | L     | 232 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 254 | VAL  |
| 1   | L     | 255 | MET  |
| 1   | L     | 268 | LEU  |
| 1   | L     | 283 | VAL  |
| 1   | L     | 284 | SER  |
| 1   | L     | 289 | LEU  |
| 1   | L     | 295 | THR  |
| 1   | L     | 301 | GLU  |
| 1   | L     | 304 | ILE  |
| 1   | L     | 320 | ILE  |
| 1   | L     | 333 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 90  | ASN  |
| 1   | A     | 180 | GLN  |
| 1   | A     | 271 | GLN  |
| 1   | A     | 272 | HIS  |
| 1   | A     | 324 | HIS  |
| 1   | B     | 191 | HIS  |
| 1   | C     | 324 | HIS  |
| 1   | D     | 65  | ASN  |
| 1   | D     | 271 | GLN  |
| 1   | D     | 282 | ASN  |
| 1   | E     | 76  | ASN  |
| 1   | E     | 180 | GLN  |
| 1   | E     | 191 | HIS  |
| 1   | E     | 230 | GLN  |
| 1   | E     | 324 | HIS  |
| 1   | F     | 27  | GLN  |
| 1   | F     | 65  | ASN  |
| 1   | F     | 180 | GLN  |
| 1   | F     | 191 | HIS  |
| 1   | F     | 282 | ASN  |
| 1   | G     | 4   | GLN  |
| 1   | H     | 65  | ASN  |
| 1   | H     | 180 | GLN  |
| 1   | H     | 191 | HIS  |
| 1   | I     | 90  | ASN  |
| 1   | I     | 132 | HIS  |
| 1   | J     | 27  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 65  | ASN  |
| 1   | J     | 230 | GLN  |
| 1   | J     | 271 | GLN  |
| 1   | K     | 180 | GLN  |
| 1   | K     | 191 | HIS  |
| 1   | L     | 180 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

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     | 336/338 (99%)   | -0.83  | 0 100 100      | 60, 89, 115, 163      | 0     |
| 1   | B     | 336/338 (99%)   | -0.75  | 0 100 100      | 56, 86, 121, 165      | 0     |
| 1   | C     | 336/338 (99%)   | -0.85  | 0 100 100      | 51, 83, 116, 160      | 0     |
| 1   | D     | 336/338 (99%)   | -0.79  | 0 100 100      | 61, 98, 133, 165      | 0     |
| 1   | E     | 336/338 (99%)   | -0.88  | 0 100 100      | 50, 78, 109, 149      | 0     |
| 1   | F     | 336/338 (99%)   | -0.78  | 0 100 100      | 60, 89, 124, 163      | 0     |
| 1   | G     | 336/338 (99%)   | -0.90  | 0 100 100      | 58, 88, 120, 163      | 0     |
| 1   | H     | 336/338 (99%)   | -0.85  | 1 (0%) 90 77   | 52, 73, 104, 144      | 0     |
| 1   | I     | 336/338 (99%)   | -0.85  | 0 100 100      | 56, 80, 107, 147      | 0     |
| 1   | J     | 336/338 (99%)   | -0.79  | 0 100 100      | 66, 98, 132, 179      | 0     |
| 1   | K     | 336/338 (99%)   | -0.81  | 0 100 100      | 72, 109, 137, 184     | 0     |
| 1   | L     | 336/338 (99%)   | -0.78  | 0 100 100      | 81, 121, 155, 167     | 0     |
| All | All   | 4032/4056 (99%) | -0.82  | 1 (0%) 100 100 | 50, 90, 135, 184      | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 64  | ILE  | 2.9  |

### 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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | ZN   | C     | 402 | 1/1   | 0.96 | 0.10 | 121,121,121,121            | 0     |
| 2   | ZN   | K     | 402 | 1/1   | 0.96 | 0.12 | 126,126,126,126            | 0     |
| 2   | ZN   | A     | 402 | 1/1   | 0.97 | 0.10 | 132,132,132,132            | 0     |
| 2   | ZN   | B     | 402 | 1/1   | 0.97 | 0.10 | 127,127,127,127            | 0     |
| 2   | ZN   | F     | 402 | 1/1   | 0.98 | 0.11 | 111,111,111,111            | 0     |
| 2   | ZN   | G     | 402 | 1/1   | 0.98 | 0.06 | 109,109,109,109            | 0     |
| 2   | ZN   | D     | 402 | 1/1   | 0.98 | 0.07 | 113,113,113,113            | 0     |
| 2   | ZN   | L     | 402 | 1/1   | 0.98 | 0.05 | 130,130,130,130            | 0     |
| 2   | ZN   | A     | 401 | 1/1   | 0.99 | 0.04 | 97,97,97,97                | 0     |
| 2   | ZN   | H     | 402 | 1/1   | 0.99 | 0.03 | 86,86,86,86                | 0     |
| 2   | ZN   | I     | 402 | 1/1   | 0.99 | 0.04 | 106,106,106,106            | 0     |
| 2   | ZN   | J     | 402 | 1/1   | 0.99 | 0.03 | 122,122,122,122            | 0     |
| 2   | ZN   | K     | 401 | 1/1   | 0.99 | 0.02 | 103,103,103,103            | 0     |
| 2   | ZN   | E     | 402 | 1/1   | 0.99 | 0.03 | 93,93,93,93                | 0     |
| 2   | ZN   | L     | 401 | 1/1   | 0.99 | 0.02 | 128,128,128,128            | 0     |
| 2   | ZN   | B     | 401 | 1/1   | 0.99 | 0.05 | 83,83,83,83                | 0     |
| 2   | ZN   | I     | 401 | 1/1   | 1.00 | 0.02 | 84,84,84,84                | 0     |
| 2   | ZN   | F     | 401 | 1/1   | 1.00 | 0.02 | 93,93,93,93                | 0     |
| 2   | ZN   | J     | 401 | 1/1   | 1.00 | 0.02 | 106,106,106,106            | 0     |
| 2   | ZN   | C     | 401 | 1/1   | 1.00 | 0.03 | 92,92,92,92                | 0     |
| 2   | ZN   | G     | 401 | 1/1   | 1.00 | 0.03 | 78,78,78,78                | 0     |
| 2   | ZN   | E     | 401 | 1/1   | 1.00 | 0.03 | 75,75,75,75                | 0     |
| 2   | ZN   | H     | 401 | 1/1   | 1.00 | 0.03 | 67,67,67,67                | 0     |
| 2   | ZN   | D     | 401 | 1/1   | 1.00 | 0.03 | 116,116,116,116            | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.