



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:43 PM UTC

PDB ID : 2INP / pdb\_00002inp  
Title : Structure of the Phenol Hydroxylase-Regulatory Protein Complex  
Authors : Sazinsky, M.S.; Dunten, P.W.; McCormick, M.S.; Lippard, S.J.  
Deposited on : 2006-10-08  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

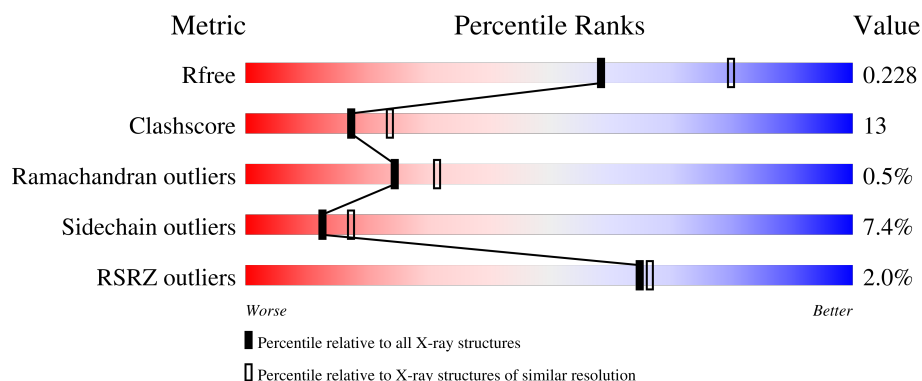
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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                      | 6319 (2.30-2.30)                                      |
| Clashscore            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |
| RSRZ outliers         | 180081                      | 6325 (2.30-2.30)                                      |

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     | 494    | <div> <div></div> <div>73%22%.</div> </div>    |
| 1   | B     | 494    | <div> <div>%</div> <div>68%26%5%.</div> </div> |
| 2   | C     | 328    | <div> <div></div> <div>69%23%5%.</div> </div>  |
| 2   | D     | 328    | <div> <div>%</div> <div>75%22%..</div> </div>  |
| 3   | E     | 118    | <div> <div></div> <div>70%25%5%</div> </div>   |

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| Mol | Chain | Length | Quality of chain                                                                                                 |
|-----|-------|--------|------------------------------------------------------------------------------------------------------------------|
| 3   | F     | 118    | <div><div>%</div><div><div></div><div>64%</div><div>35%</div><div></div></div><div></div></div>                  |
| 4   | L     | 89     | <div><div>31%</div><div><div></div><div>63%</div><div>25%</div><div>6%</div><div>7%</div></div><div></div></div> |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17022 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 Phenol hydroxylase component phN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 494      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4119  | 2649 | 692 | 754 | 24 |         |         |       |
| 1   | B     | 493      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 4153  | 2675 | 694 | 760 | 24 |         |         |       |

- Molecule 2 is a protein called Phenol hydroxylase component phL.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | C     | 318      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2589  | 1630 | 449 | 492 | 18 |         |         |       |
| 2   | D     | 328      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2659  | 1673 | 461 | 507 | 18 |         |         |       |

- Molecule 3 is a protein called Phenol hydroxylase component phO.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | E     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 925   | 602 | 145 | 173 | 5 |         |         |       |
| 3   | F     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 925   | 602 | 145 | 173 | 5 |         |         |       |

- Molecule 4 is a protein called Phenol hydroxylase component phM.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | L     | 83       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 624   | 389 | 105 | 125 | 5 |         |         |       |

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | A     | 2        | Total | Fe | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 5   | B     | 2        | Total<br>2 | Fe<br>2 | 0       | 0       |

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 6   | A     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 6   | B     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

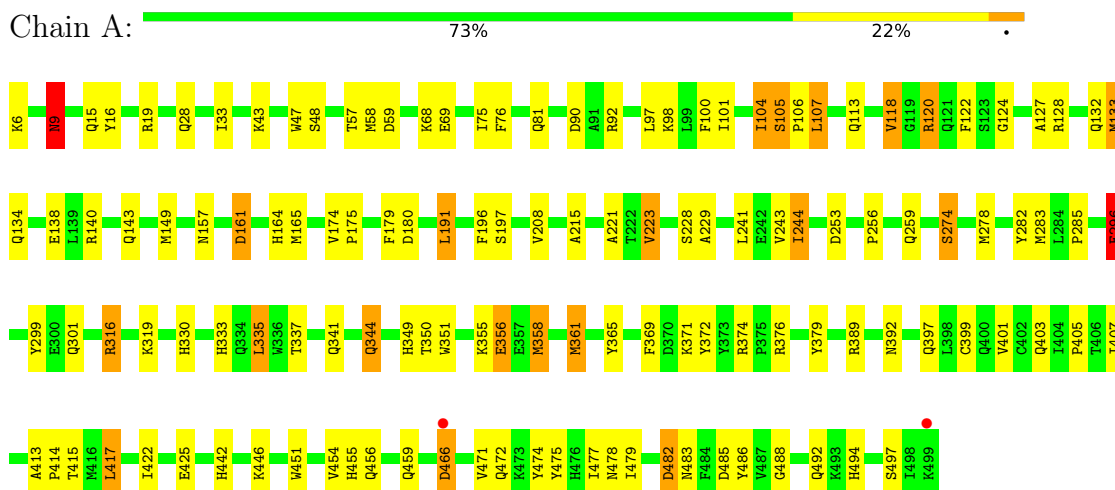
- Molecule 7 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7   | A     | 253      | Total<br>253 | O<br>253 | 0       | 0       |
| 7   | B     | 245      | Total<br>245 | O<br>245 | 0       | 0       |
| 7   | C     | 177      | Total<br>177 | O<br>177 | 0       | 0       |
| 7   | D     | 219      | Total<br>219 | O<br>219 | 0       | 0       |
| 7   | E     | 76       | Total<br>76  | O<br>76  | 0       | 0       |
| 7   | F     | 49       | Total<br>49  | O<br>49  | 0       | 0       |
| 7   | L     | 3        | Total<br>3   | O<br>3   | 0       | 0       |

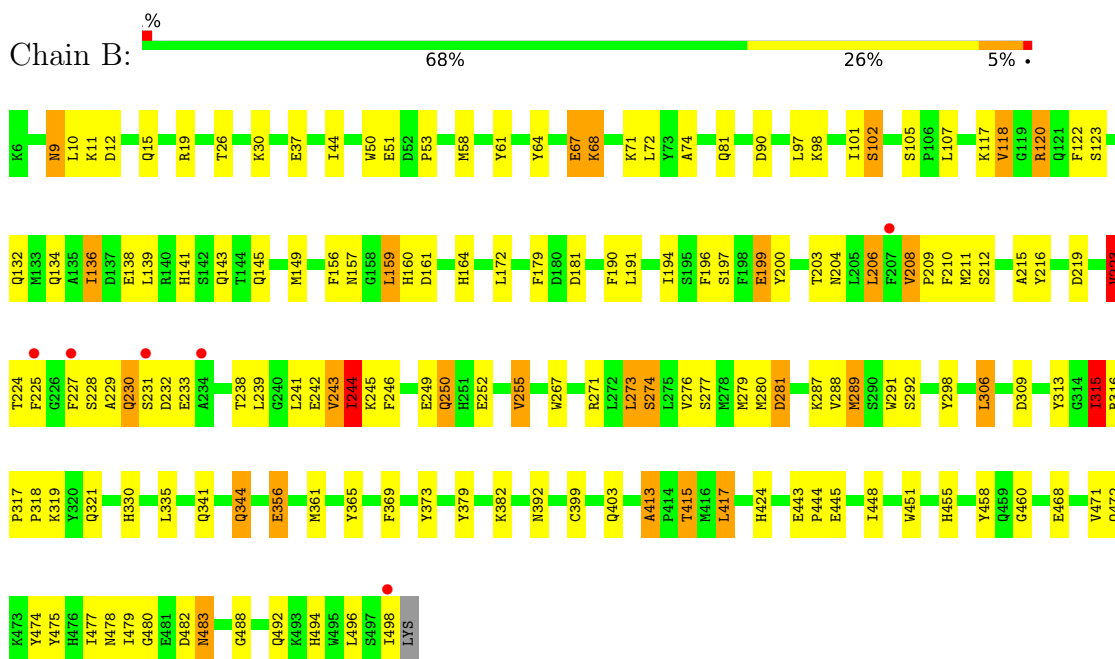
### 3 Residue-property plots

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

- Molecule 1: Phenol hydroxylase component pHN

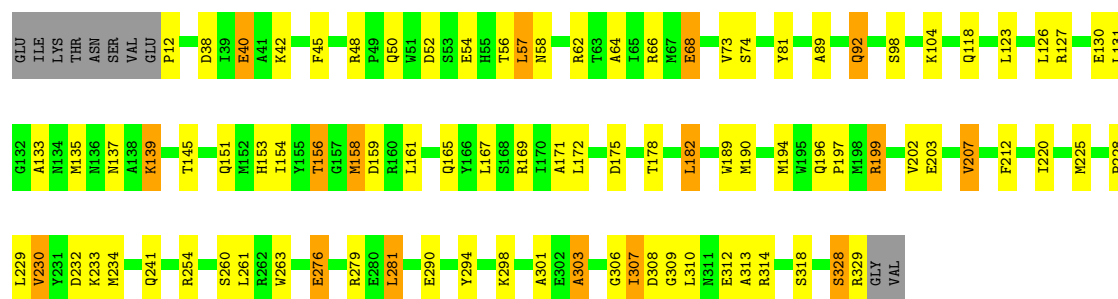


- Molecule 1: Phenol hydroxylase component pHN



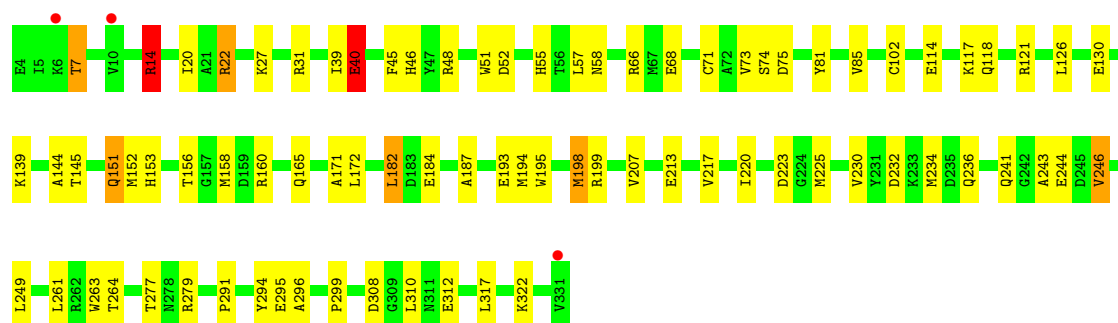
- Molecule 2: Phenol hydroxylase component pHL

Chain C: 



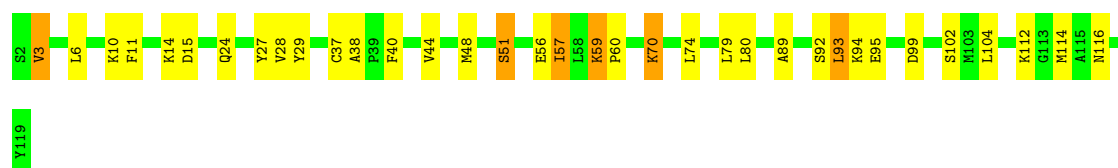
• Molecule 2: Phenol hydroxylase component phL

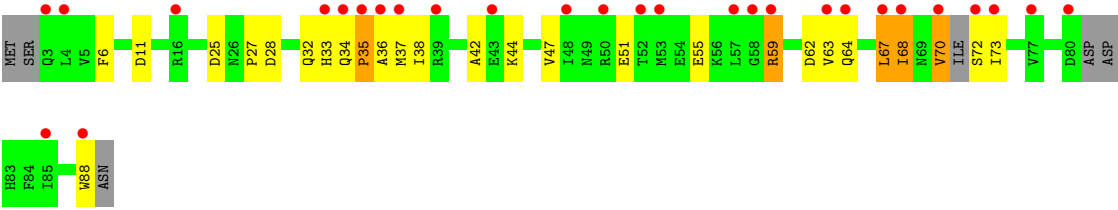
Chain D: 



• Molecule 3: Phenol hydroxylase component phO

Chain E: 





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 87.75Å 146.31Å 190.02Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 30.00 – 2.30<br>30.00 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (30.00-2.30)<br>99.8 (30.00-2.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.09                                                        | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 4.21 (at 2.31Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0005                                             | Depositor        |
| R, $R_{free}$                                                           | 0.192 , 0.236<br>0.172 , 0.228                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 5424 reflections (4.98%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 37.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.508                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 50.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 17022                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 40.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: FE, 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     | 1.38         | 15/4253 (0.4%)  | 1.30        | 20/5762 (0.3%)  |
| 1   | B     | 1.40         | 13/4290 (0.3%)  | 1.27        | 28/5813 (0.5%)  |
| 2   | C     | 1.43         | 5/2648 (0.2%)   | 1.38        | 17/3580 (0.5%)  |
| 2   | D     | 1.39         | 7/2718 (0.3%)   | 1.28        | 12/3676 (0.3%)  |
| 3   | E     | 1.44         | 7/953 (0.7%)    | 1.26        | 2/1297 (0.2%)   |
| 3   | F     | 1.20         | 1/953 (0.1%)    | 1.28        | 8/1297 (0.6%)   |
| 4   | L     | 0.83         | 0/632           | 1.11        | 3/857 (0.4%)    |
| All | All   | 1.37         | 48/16447 (0.3%) | 1.29        | 90/22282 (0.4%) |

All (48) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 255 | VAL  | CA-CB | 10.01 | 1.59        | 1.54     |
| 1   | A     | 75  | ILE  | C-O   | 7.98  | 1.33        | 1.24     |
| 1   | B     | 315 | ILE  | CA-CB | 7.24  | 1.63        | 1.54     |
| 1   | A     | 208 | VAL  | CA-CB | 7.02  | 1.58        | 1.53     |
| 2   | D     | 85  | VAL  | C-O   | -6.88 | 1.15        | 1.24     |
| 2   | D     | 198 | MET  | N-CA  | 6.66  | 1.54        | 1.46     |
| 1   | A     | 76  | PHE  | C-O   | -6.52 | 1.16        | 1.24     |
| 1   | A     | 221 | ALA  | C-O   | -6.46 | 1.16        | 1.24     |
| 3   | E     | 59  | LYS  | N-CA  | -6.46 | 1.40        | 1.46     |
| 1   | B     | 243 | VAL  | CA-CB | 6.32  | 1.62        | 1.54     |
| 3   | F     | 86  | THR  | CA-CB | 6.31  | 1.60        | 1.53     |
| 1   | B     | 229 | ALA  | CA-C  | 6.28  | 1.61        | 1.52     |
| 2   | D     | 39  | ILE  | CA-CB | 6.16  | 1.63        | 1.54     |
| 2   | C     | 73  | VAL  | CA-CB | 6.14  | 1.61        | 1.54     |
| 1   | A     | 127 | ALA  | CA-CB | -6.13 | 1.43        | 1.53     |
| 2   | C     | 303 | ALA  | CA-CB | -6.12 | 1.42        | 1.53     |
| 1   | B     | 67  | GLU  | CA-C  | 6.05  | 1.60        | 1.52     |
| 1   | B     | 194 | ILE  | CA-CB | 5.98  | 1.62        | 1.54     |
| 2   | C     | 133 | ALA  | CA-CB | -5.96 | 1.44        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 479 | ILE  | CA-CB | 5.95  | 1.61        | 1.54     |
| 2   | C     | 202 | VAL  | CA-CB | 5.93  | 1.60        | 1.54     |
| 3   | E     | 38  | ALA  | C-O   | 5.83  | 1.29        | 1.24     |
| 1   | A     | 296 | GLU  | N-CA  | -5.75 | 1.39        | 1.46     |
| 3   | E     | 57  | ILE  | CA-CB | 5.73  | 1.60        | 1.55     |
| 3   | E     | 51  | SER  | N-CA  | -5.68 | 1.39        | 1.46     |
| 1   | B     | 210 | PHE  | CA-C  | 5.62  | 1.59        | 1.52     |
| 2   | D     | 20  | ILE  | CA-CB | 5.62  | 1.61        | 1.54     |
| 2   | C     | 220 | ILE  | CA-CB | 5.60  | 1.60        | 1.55     |
| 1   | B     | 208 | VAL  | CA-CB | 5.53  | 1.61        | 1.54     |
| 1   | A     | 229 | ALA  | CA-CB | 5.52  | 1.63        | 1.53     |
| 3   | E     | 94  | LYS  | CA-C  | 5.48  | 1.59        | 1.52     |
| 1   | A     | 454 | VAL  | CA-CB | 5.47  | 1.61        | 1.54     |
| 1   | A     | 401 | VAL  | CA-C  | 5.43  | 1.59        | 1.52     |
| 1   | B     | 317 | PRO  | CA-C  | 5.36  | 1.57        | 1.52     |
| 1   | A     | 483 | ASN  | CA-CB | 5.35  | 1.62        | 1.53     |
| 1   | B     | 120 | ARG  | CA-C  | 5.35  | 1.59        | 1.52     |
| 1   | A     | 208 | VAL  | CA-C  | 5.34  | 1.57        | 1.52     |
| 3   | E     | 44  | VAL  | N-CA  | 5.32  | 1.51        | 1.46     |
| 2   | D     | 187 | ALA  | CA-CB | 5.27  | 1.61        | 1.53     |
| 1   | A     | 100 | PHE  | C-O   | 5.24  | 1.30        | 1.24     |
| 2   | D     | 317 | LEU  | CA-C  | 5.23  | 1.59        | 1.52     |
| 2   | D     | 144 | ALA  | CA-C  | -5.20 | 1.46        | 1.52     |
| 1   | A     | 9   | ASN  | CB-CG | -5.16 | 1.39        | 1.52     |
| 1   | A     | 316 | ARG  | CA-C  | 5.16  | 1.60        | 1.52     |
| 1   | A     | 180 | ASP  | C-O   | -5.15 | 1.18        | 1.24     |
| 1   | B     | 190 | PHE  | N-CA  | 5.12  | 1.52        | 1.46     |
| 1   | B     | 74  | ALA  | C-O   | -5.03 | 1.18        | 1.24     |
| 3   | E     | 3   | VAL  | CA-CB | 5.02  | 1.59        | 1.54     |

All (90) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 223 | VAL  | CB-CA-C   | -9.17 | 99.76       | 112.14   |
| 1   | A     | 466 | ASP  | CA-CB-CG  | -8.73 | 103.87      | 112.60   |
| 3   | F     | 108 | THR  | CA-C-N    | -8.68 | 110.94      | 120.14   |
| 3   | F     | 108 | THR  | C-N-CA    | -8.68 | 110.94      | 120.14   |
| 2   | D     | 14  | ARG  | NE-CZ-NH2 | -8.45 | 111.60      | 119.20   |
| 1   | B     | 289 | MET  | N-CA-C    | -8.01 | 96.10       | 108.76   |
| 2   | C     | 207 | VAL  | CB-CA-C   | 7.56  | 119.24      | 110.93   |
| 1   | B     | 208 | VAL  | CA-C-N    | -7.26 | 111.42      | 118.97   |
| 1   | B     | 208 | VAL  | C-N-CA    | -7.26 | 111.42      | 118.97   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 128 | ARG  | N-CA-C    | 7.18  | 118.80      | 110.97   |
| 1   | B     | 232 | ASP  | N-CA-C    | -7.08 | 102.99      | 111.69   |
| 1   | B     | 37  | GLU  | N-CA-C    | 6.98  | 121.62      | 113.18   |
| 2   | C     | 313 | ALA  | N-CA-C    | -6.96 | 105.32      | 113.88   |
| 4   | L     | 59  | ARG  | CB-CA-C   | 6.87  | 121.97      | 110.43   |
| 2   | C     | 309 | GLY  | N-CA-C    | -6.73 | 104.35      | 112.49   |
| 2   | C     | 158 | MET  | N-CA-C    | -6.68 | 104.06      | 111.82   |
| 3   | F     | 73  | PHE  | N-CA-C    | -6.68 | 101.68      | 110.43   |
| 2   | C     | 167 | LEU  | N-CA-C    | -6.63 | 104.14      | 111.36   |
| 1   | A     | 76  | PHE  | N-CA-C    | -6.52 | 104.17      | 111.28   |
| 2   | C     | 230 | VAL  | N-CA-C    | 6.44  | 116.58      | 110.53   |
| 1   | A     | 374 | ARG  | CA-C-N    | -6.37 | 113.06      | 119.56   |
| 1   | A     | 374 | ARG  | C-N-CA    | -6.37 | 113.06      | 119.56   |
| 1   | A     | 282 | TYR  | N-CA-C    | 6.32  | 121.66      | 113.88   |
| 1   | B     | 101 | ILE  | N-CA-C    | 6.32  | 118.99      | 111.09   |
| 1   | A     | 413 | ALA  | CA-C-N    | 6.32  | 127.13      | 120.12   |
| 1   | A     | 413 | ALA  | C-N-CA    | 6.32  | 127.13      | 120.12   |
| 1   | B     | 102 | SER  | CB-CA-C   | -6.15 | 99.45       | 110.70   |
| 1   | A     | 483 | ASN  | N-CA-C    | 6.12  | 118.81      | 110.55   |
| 1   | B     | 181 | ASP  | N-CA-C    | -6.08 | 104.57      | 111.07   |
| 1   | A     | 208 | VAL  | CA-C-N    | -6.07 | 112.31      | 119.05   |
| 1   | A     | 208 | VAL  | C-N-CA    | -6.07 | 112.31      | 119.05   |
| 3   | F     | 58  | LEU  | N-CA-C    | 6.03  | 117.52      | 111.07   |
| 2   | D     | 14  | ARG  | CD-NE-CZ  | 6.01  | 132.82      | 124.40   |
| 2   | D     | 22  | ARG  | CG-CD-NE  | -5.99 | 98.81       | 112.00   |
| 2   | D     | 40  | GLU  | CA-CB-CG  | 5.95  | 126.00      | 114.10   |
| 3   | F     | 118 | GLY  | N-CA-C    | -5.95 | 99.09       | 113.18   |
| 2   | D     | 31  | ARG  | N-CA-C    | -5.93 | 104.82      | 111.28   |
| 1   | A     | 113 | GLN  | CA-C-N    | 5.87  | 126.45      | 119.94   |
| 1   | A     | 113 | GLN  | C-N-CA    | 5.87  | 126.45      | 119.94   |
| 2   | C     | 263 | TRP  | N-CA-C    | 5.81  | 119.55      | 112.23   |
| 1   | A     | 482 | ASP  | N-CA-C    | -5.75 | 106.10      | 113.23   |
| 1   | A     | 197 | SER  | N-CA-C    | 5.73  | 117.20      | 111.07   |
| 2   | D     | 14  | ARG  | CG-CD-NE  | -5.70 | 99.45       | 112.00   |
| 1   | B     | 255 | VAL  | CA-C-N    | -5.68 | 113.17      | 119.19   |
| 1   | B     | 255 | VAL  | C-N-CA    | -5.68 | 113.17      | 119.19   |
| 2   | D     | 27  | LYS  | CA-C-N    | -5.65 | 113.94      | 119.76   |
| 2   | D     | 27  | LYS  | C-N-CA    | -5.65 | 113.94      | 119.76   |
| 2   | D     | 22  | ARG  | NE-CZ-NH2 | -5.64 | 114.12      | 119.20   |
| 4   | L     | 47  | VAL  | N-CA-C    | 5.62  | 116.77      | 108.45   |
| 1   | B     | 197 | SER  | N-CA-C    | 5.52  | 117.38      | 111.36   |
| 3   | F     | 50  | PHE  | N-CA-C    | 5.52  | 117.73      | 111.11   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | F     | 117 | ALA  | N-CA-C    | -5.48 | 99.12       | 110.80   |
| 1   | B     | 105 | SER  | CA-C-N    | -5.44 | 114.01      | 119.56   |
| 1   | B     | 105 | SER  | C-N-CA    | -5.44 | 114.01      | 119.56   |
| 1   | B     | 273 | LEU  | N-CA-C    | 5.44  | 119.02      | 112.38   |
| 1   | A     | 9   | ASN  | CB-CA-C   | -5.43 | 99.62       | 110.42   |
| 2   | D     | 81  | TYR  | N-CA-C    | 5.40  | 117.61      | 111.02   |
| 1   | A     | 118 | VAL  | CB-CA-C   | 5.39  | 120.99      | 112.26   |
| 1   | B     | 118 | VAL  | CB-CA-C   | 5.35  | 119.36      | 112.14   |
| 2   | C     | 169 | ARG  | NE-CZ-NH1 | -5.34 | 116.16      | 121.50   |
| 1   | B     | 244 | ILE  | N-CA-CB   | 5.33  | 117.78      | 110.54   |
| 2   | C     | 123 | LEU  | CA-C-N    | 5.27  | 123.56      | 120.24   |
| 2   | C     | 123 | LEU  | C-N-CA    | 5.27  | 123.56      | 120.24   |
| 2   | D     | 40  | GLU  | CB-CG-CD  | 5.26  | 121.55      | 112.60   |
| 2   | C     | 254 | ARG  | N-CA-C    | 5.26  | 116.70      | 111.07   |
| 1   | B     | 298 | TYR  | CA-C-N    | -5.25 | 114.69      | 122.56   |
| 1   | B     | 298 | TYR  | C-N-CA    | -5.25 | 114.69      | 122.56   |
| 1   | B     | 413 | ALA  | CA-C-N    | 5.25  | 126.40      | 119.84   |
| 1   | B     | 413 | ALA  | C-N-CA    | 5.25  | 126.40      | 119.84   |
| 1   | B     | 306 | LEU  | N-CA-C    | 5.24  | 116.68      | 111.07   |
| 1   | B     | 74  | ALA  | N-CA-C    | -5.22 | 105.67      | 111.36   |
| 3   | F     | 24  | GLN  | CB-CA-C   | -5.21 | 100.44      | 110.24   |
| 2   | C     | 104 | LYS  | CB-CA-C   | -5.21 | 102.14      | 110.79   |
| 3   | E     | 94  | LYS  | CA-C-N    | 5.21  | 127.52      | 120.38   |
| 3   | E     | 94  | LYS  | C-N-CA    | 5.21  | 127.52      | 120.38   |
| 1   | B     | 159 | LEU  | N-CA-C    | -5.20 | 105.60      | 112.94   |
| 1   | B     | 243 | VAL  | CA-C-N    | -5.20 | 113.34      | 120.46   |
| 1   | B     | 243 | VAL  | C-N-CA    | -5.20 | 113.34      | 120.46   |
| 1   | A     | 48  | SER  | N-CA-C    | -5.16 | 107.02      | 113.15   |
| 4   | L     | 37  | MET  | N-CA-C    | 5.14  | 116.88      | 108.55   |
| 1   | A     | 299 | TYR  | CA-CB-CG  | -5.13 | 104.67      | 113.90   |
| 2   | C     | 92  | GLN  | N-CA-C    | 5.11  | 116.85      | 111.28   |
| 1   | B     | 281 | ASP  | N-CA-C    | 5.11  | 117.75      | 111.82   |
| 2   | D     | 14  | ARG  | NE-CZ-NH1 | 5.10  | 126.60      | 121.50   |
| 2   | C     | 130 | GLU  | N-CA-C    | -5.05 | 105.77      | 111.28   |
| 2   | C     | 127 | ARG  | NE-CZ-NH2 | -5.04 | 114.66      | 119.20   |
| 2   | C     | 98  | SER  | N-CA-C    | 5.03  | 116.45      | 111.07   |
| 1   | B     | 267 | TRP  | N-CA-C    | -5.02 | 105.89      | 111.36   |
| 1   | A     | 274 | SER  | N-CA-C    | 5.02  | 118.17      | 111.75   |
| 2   | C     | 199 | ARG  | CG-CD-NE  | -5.00 | 101.00      | 112.00   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 4119  | 0        | 3855     | 105     | 0            |
| 1   | B     | 4153  | 0        | 3870     | 150     | 0            |
| 2   | C     | 2589  | 0        | 2501     | 74      | 0            |
| 2   | D     | 2659  | 0        | 2571     | 69      | 0            |
| 3   | E     | 925   | 0        | 898      | 20      | 0            |
| 3   | F     | 925   | 0        | 898      | 23      | 0            |
| 4   | L     | 624   | 0        | 540      | 32      | 0            |
| 5   | A     | 2     | 0        | 0        | 0       | 0            |
| 5   | B     | 2     | 0        | 0        | 0       | 0            |
| 6   | A     | 1     | 0        | 0        | 0       | 0            |
| 6   | B     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 253   | 0        | 0        | 4       | 1            |
| 7   | B     | 245   | 0        | 0        | 9       | 0            |
| 7   | C     | 177   | 0        | 0        | 3       | 0            |
| 7   | D     | 219   | 0        | 0        | 9       | 0            |
| 7   | E     | 76    | 0        | 0        | 1       | 1            |
| 7   | F     | 49    | 0        | 0        | 1       | 0            |
| 7   | L     | 3     | 0        | 0        | 1       | 0            |
| All | All   | 17022 | 0        | 15133    | 390     | 1            |

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 13.

All (390) 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:B:231:SER:HB3 | 4:L:67:LEU:O     | 1.41                     | 1.17              |
| 2:C:12:PRO:HD3  | 7:C:433:HOH:O    | 1.46                     | 1.14              |
| 2:D:75:ASP:CB   | 2:D:152:MET:HE3  | 1.80                     | 1.09              |
| 1:B:274:SER:HB2 | 1:B:335:LEU:HD11 | 1.34                     | 1.06              |
| 2:C:194:MET:CE  | 2:C:303:ALA:CB   | 2.34                     | 1.04              |
| 1:B:361:MET:HE3 | 1:B:369:PHE:CE1  | 1.92                     | 1.03              |
| 1:B:230:GLN:HG3 | 4:L:72:SER:N     | 1.74                     | 1.03              |
| 1:B:97:LEU:HB3  | 1:B:149:MET:HE1  | 1.41                     | 1.00              |
| 1:B:274:SER:HB2 | 1:B:335:LEU:CD1  | 1.92                     | 0.99              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:B:231:SER:CB   | 4:L:67:LEU:O       | 2.12                     | 0.98              |
| 1:B:230:GLN:HB3  | 4:L:70:VAL:O       | 1.64                     | 0.98              |
| 2:C:194:MET:HE1  | 2:C:303:ALA:CB     | 1.93                     | 0.97              |
| 1:A:344:GLN:H    | 1:A:344:GLN:HE21   | 0.99                     | 0.96              |
| 1:A:379:TYR:CD1  | 3:F:114:MET:HE1    | 2.01                     | 0.95              |
| 2:D:75:ASP:HB2   | 2:D:152:MET:HE3    | 1.44                     | 0.94              |
| 2:C:118:GLN:HE22 | 2:C:241:GLN:HE21   | 1.04                     | 0.94              |
| 3:E:70:LYS:H     | 3:E:70:LYS:HD2     | 1.28                     | 0.94              |
| 1:A:397:GLN:HE22 | 3:F:103:MET:HE3    | 1.31                     | 0.93              |
| 2:C:194:MET:CE   | 2:C:303:ALA:HB3    | 1.99                     | 0.92              |
| 1:A:488:GLY:H    | 1:A:492:GLN:NE2    | 1.70                     | 0.90              |
| 1:A:120:ARG:NH2  | 7:A:679:HOH:O      | 2.05                     | 0.89              |
| 1:B:480:GLY:H    | 1:B:483:ASN:HD21   | 1.22                     | 0.87              |
| 2:C:308:ASP:O    | 2:C:312:GLU:HG3    | 1.75                     | 0.87              |
| 2:C:190:MET:HE2  | 2:C:190:MET:HA     | 1.55                     | 0.87              |
| 1:A:466:ASP:OD1  | 7:A:534:HOH:O      | 1.93                     | 0.86              |
| 1:A:58:MET:HE1   | 1:A:133:MET:CE     | 2.06                     | 0.86              |
| 2:C:118:GLN:HE22 | 2:C:241:GLN:NE2    | 1.74                     | 0.86              |
| 1:B:58:MET:H     | 2:D:165:GLN:HE22   | 1.23                     | 0.85              |
| 1:B:216:TYR:CE1  | 4:L:35:PRO:HD3     | 2.11                     | 0.85              |
| 1:A:143:GLN:HE22 | 2:C:151:GLN:HE22   | 1.20                     | 0.85              |
| 3:F:9:TYR:O      | 3:F:10:LYS:HD2     | 1.76                     | 0.85              |
| 1:A:337:THR:HG21 | 1:A:376:ARG:HH11   | 1.42                     | 0.85              |
| 1:B:274:SER:CB   | 1:B:335:LEU:HD11   | 2.07                     | 0.85              |
| 1:B:211:MET:HE1  | 1:B:225[B]:PHE:HE1 | 1.40                     | 0.85              |
| 1:A:344:GLN:H    | 1:A:344:GLN:NE2    | 1.74                     | 0.84              |
| 1:A:397:GLN:NE2  | 3:F:103:MET:HE3    | 1.92                     | 0.84              |
| 2:D:117:LYS:NZ   | 7:D:492:HOH:O      | 2.01                     | 0.83              |
| 2:C:194:MET:HE1  | 2:C:303:ALA:HB3    | 1.54                     | 0.83              |
| 2:D:160:ARG:NH2  | 2:D:223:ASP:OD2    | 2.11                     | 0.83              |
| 1:B:344:GLN:H    | 1:B:344:GLN:HE21   | 1.26                     | 0.82              |
| 2:D:171:ALA:HB3  | 2:D:182:LEU:HD13   | 1.62                     | 0.82              |
| 2:D:225:MET:HE1  | 2:D:294:TYR:HA     | 1.60                     | 0.82              |
| 1:B:341:GLN:HE21 | 1:B:392:ASN:HD22   | 1.27                     | 0.81              |
| 1:B:216:TYR:CE1  | 4:L:35:PRO:CD      | 2.64                     | 0.80              |
| 1:B:361:MET:CE   | 1:B:369:PHE:CE1    | 2.65                     | 0.79              |
| 1:A:58:MET:CE    | 1:A:133:MET:HE1    | 2.13                     | 0.79              |
| 1:A:58:MET:H     | 2:C:165:GLN:HE22   | 1.27                     | 0.79              |
| 1:B:68:LYS:HD3   | 4:L:68:ILE:HA      | 1.65                     | 0.79              |
| 2:C:194:MET:CE   | 2:C:303:ALA:HB2    | 2.14                     | 0.78              |
| 1:A:472:GLN:HB2  | 1:A:479:ILE:HD12   | 1.66                     | 0.78              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:B:26:THR:OG1   | 2:D:199:ARG:NH2    | 2.15                     | 0.78              |
| 2:D:75:ASP:HA    | 2:D:152:MET:HE1    | 1.64                     | 0.77              |
| 2:C:171:ALA:HB3  | 2:C:182:LEU:HD13   | 1.64                     | 0.77              |
| 1:A:344:GLN:HE21 | 1:A:344:GLN:N      | 1.80                     | 0.77              |
| 1:B:64[A]:TYR:OH | 7:B:660:HOH:O      | 2.02                     | 0.77              |
| 2:D:75:ASP:HA    | 2:D:152:MET:CE     | 2.15                     | 0.77              |
| 1:B:230:GLN:HG2  | 4:L:70:VAL:C       | 2.09                     | 0.76              |
| 1:B:156:PHE:O    | 2:D:14:ARG:NH2     | 2.18                     | 0.76              |
| 2:D:75:ASP:CG    | 2:D:152:MET:HE3    | 2.09                     | 0.76              |
| 2:C:189:TRP:CD1  | 2:C:190:MET:HE3    | 2.20                     | 0.76              |
| 1:A:397:GLN:HE22 | 3:F:103:MET:CE     | 1.98                     | 0.76              |
| 1:B:211:MET:HE1  | 1:B:225[B]:PHE:CE1 | 2.20                     | 0.76              |
| 1:B:455:HIS:HD2  | 3:E:15:ASP:OD2     | 1.70                     | 0.75              |
| 1:A:356:GLU:CD   | 1:A:356:GLU:H      | 1.94                     | 0.75              |
| 1:B:361:MET:HE3  | 1:B:369:PHE:HE1    | 1.50                     | 0.75              |
| 1:A:341:GLN:NE2  | 1:A:392:ASN:HD22   | 1.85                     | 0.75              |
| 1:B:274:SER:CB   | 1:B:335:LEU:CD1    | 2.63                     | 0.75              |
| 1:B:219:ASP:O    | 1:B:223:VAL:HG23   | 1.89                     | 0.73              |
| 1:B:120:ARG:HG2  | 2:D:139:LYS:HB2    | 1.71                     | 0.73              |
| 1:B:444:PRO:HD2  | 1:B:445[A]:GLU:OE2 | 1.89                     | 0.72              |
| 1:A:341:GLN:HE21 | 1:A:392:ASN:HD22   | 1.35                     | 0.72              |
| 1:A:472:GLN:HE22 | 1:A:478:ASN:HD22   | 1.37                     | 0.72              |
| 2:D:308:ASP:O    | 2:D:312:GLU:HG3    | 1.88                     | 0.72              |
| 1:A:58:MET:HE1   | 1:A:133:MET:HE2    | 1.72                     | 0.72              |
| 1:B:361:MET:CE   | 1:B:369:PHE:CZ     | 2.73                     | 0.71              |
| 1:B:132:GLN:OE1  | 2:D:158:MET:HE1    | 1.89                     | 0.71              |
| 2:C:225:MET:HE2  | 2:C:310:LEU:HD11   | 1.71                     | 0.71              |
| 2:C:189:TRP:HD1  | 2:C:190:MET:HE3    | 1.54                     | 0.71              |
| 1:B:196:PHE:CD1  | 1:B:244:ILE:HG12   | 2.26                     | 0.71              |
| 3:F:88:LYS:H     | 3:F:96:GLN:HE22    | 1.38                     | 0.70              |
| 1:B:341:GLN:NE2  | 1:B:392:ASN:HD22   | 1.90                     | 0.70              |
| 2:D:118:GLN:HE22 | 2:D:241:GLN:HE21   | 1.40                     | 0.70              |
| 1:B:379:TYR:CD1  | 3:E:114:MET:HE1    | 2.27                     | 0.69              |
| 2:D:225:MET:HE3  | 2:D:310:LEU:HD11   | 1.72                     | 0.69              |
| 1:B:200:TYR:HE1  | 1:B:306:LEU:HD13   | 1.57                     | 0.69              |
| 1:A:143:GLN:HE22 | 2:C:151:GLN:NE2    | 1.90                     | 0.69              |
| 2:C:199:ARG:O    | 2:C:203:GLU:HG3    | 1.93                     | 0.69              |
| 2:C:56:THR:HG23  | 2:C:57:LEU:O       | 1.92                     | 0.69              |
| 1:B:71:LYS:NZ    | 4:L:68:ILE:HD11    | 2.08                     | 0.68              |
| 1:A:164:HIS:HD2  | 7:C:440:HOH:O      | 1.75                     | 0.68              |
| 1:B:361:MET:HE2  | 1:B:369:PHE:CZ     | 2.28                     | 0.68              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:C:318:SER:OG   | 2:C:328:SER:CB     | 2.42                     | 0.67              |
| 1:B:122:PHE:CZ   | 1:B:191:LEU:HD22   | 2.28                     | 0.67              |
| 1:B:233:GLU:HG3  | 7:B:742:HOH:O      | 1.95                     | 0.66              |
| 1:A:455:HIS:HD2  | 3:F:15:ASP:OD1     | 1.77                     | 0.66              |
| 1:A:330:HIS:CE1  | 1:A:414:PRO:HB3    | 2.30                     | 0.66              |
| 1:A:81:GLN:NE2   | 1:B:227[B]:PHE:CD1 | 2.63                     | 0.66              |
| 2:D:75:ASP:CA    | 2:D:152:MET:HE3    | 2.25                     | 0.66              |
| 1:A:397:GLN:NE2  | 3:F:103:MET:CE     | 2.57                     | 0.66              |
| 1:B:216:TYR:HE1  | 4:L:35:PRO:HD3     | 1.61                     | 0.66              |
| 2:C:118:GLN:NE2  | 2:C:241:GLN:HE21   | 1.87                     | 0.66              |
| 3:E:59:LYS:HB3   | 3:E:60:PRO:HD3     | 1.76                     | 0.66              |
| 1:A:333:HIS:O    | 1:A:337:THR:HG22   | 1.95                     | 0.65              |
| 2:C:194:MET:HE3  | 2:C:303:ALA:HB2    | 1.77                     | 0.65              |
| 2:C:171:ALA:HB3  | 2:C:182:LEU:CD1    | 2.27                     | 0.65              |
| 1:B:191:LEU:HD23 | 1:B:243:VAL:HG21   | 1.79                     | 0.65              |
| 2:C:225:MET:HE1  | 2:C:294:TYR:HA     | 1.78                     | 0.64              |
| 1:B:160:HIS:HD2  | 7:B:542:HOH:O      | 1.80                     | 0.64              |
| 1:B:271:ARG:O    | 1:B:274:SER:OG     | 2.16                     | 0.64              |
| 1:A:196:PHE:CD1  | 1:A:244:ILE:HG12   | 2.33                     | 0.63              |
| 1:A:259:GLN:HE22 | 1:A:316:ARG:H      | 1.45                     | 0.63              |
| 1:B:212:SER:O    | 1:B:215:ALA:HB3    | 1.97                     | 0.63              |
| 1:B:480:GLY:H    | 1:B:483:ASN:ND2    | 1.96                     | 0.63              |
| 2:C:276:GLU:HA   | 2:C:279:ARG:NH1    | 2.14                     | 0.63              |
| 1:B:98:LYS:HE2   | 1:B:157:ASN:O      | 1.98                     | 0.62              |
| 2:D:66:ARG:NH2   | 7:D:372:HOH:O      | 2.32                     | 0.62              |
| 1:B:200:TYR:HH   | 4:L:88:TRP:HH2     | 1.47                     | 0.62              |
| 1:B:9:ASN:ND2    | 1:B:12:ASP:H       | 1.97                     | 0.62              |
| 2:C:48:ARG:HG3   | 3:F:11:PHE:CE1     | 2.34                     | 0.62              |
| 1:A:58:MET:HE2   | 1:A:133:MET:HE1    | 1.80                     | 0.62              |
| 2:D:75:ASP:CA    | 2:D:152:MET:CE     | 2.78                     | 0.61              |
| 1:A:337:THR:HG21 | 1:A:376:ARG:NH1    | 2.14                     | 0.61              |
| 1:B:216:TYR:HE1  | 4:L:35:PRO:CD      | 2.12                     | 0.61              |
| 1:B:161:ASP:OD1  | 2:D:22:ARG:NH2     | 2.34                     | 0.61              |
| 1:B:164:HIS:HD2  | 7:D:452:HOH:O      | 1.83                     | 0.61              |
| 1:B:444:PRO:O    | 1:B:448:ILE:HG23   | 2.00                     | 0.61              |
| 2:D:152:MET:CE   | 2:D:263:TRP:HB2    | 2.30                     | 0.61              |
| 2:C:171:ALA:CB   | 2:C:182:LEU:HD13   | 2.31                     | 0.61              |
| 1:A:81:GLN:HE21  | 4:L:36:ALA:HB1     | 1.66                     | 0.61              |
| 2:D:75:ASP:CB    | 2:D:152:MET:CE     | 2.70                     | 0.61              |
| 2:C:225:MET:CE   | 2:C:310:LEU:HD11   | 2.31                     | 0.61              |
| 2:C:318:SER:OG   | 2:C:328:SER:HB2    | 2.01                     | 0.61              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:D:130:GLU:OE1  | 2:D:160:ARG:HD2    | 2.01                     | 0.60              |
| 1:A:494:HIS:HB2  | 7:A:553:HOH:O      | 2.01                     | 0.60              |
| 1:A:122:PHE:CZ   | 1:A:191:LEU:HD22   | 2.37                     | 0.60              |
| 2:D:160:ARG:HH22 | 2:D:223:ASP:CG     | 2.10                     | 0.60              |
| 1:A:138:GLU:HA   | 1:A:138:GLU:OE2    | 2.02                     | 0.60              |
| 1:A:132:GLN:HB3  | 2:C:158:MET:HE1    | 1.83                     | 0.59              |
| 1:B:53:PRO:CB    | 1:B:238:THR:HG22   | 2.32                     | 0.59              |
| 1:B:444:PRO:CD   | 1:B:445[A]:GLU:OE2 | 2.49                     | 0.59              |
| 2:D:152:MET:HE2  | 2:D:263:TRP:HB2    | 1.83                     | 0.59              |
| 1:B:472:GLN:HE22 | 1:B:478:ASN:HD22   | 1.48                     | 0.59              |
| 1:B:273:LEU:O    | 1:B:274:SER:C      | 2.45                     | 0.59              |
| 1:A:274:SER:HB2  | 1:A:335:LEU:CD1    | 2.32                     | 0.59              |
| 1:B:403:GLN:HE22 | 2:D:46:HIS:CD2     | 2.20                     | 0.59              |
| 1:A:488:GLY:H    | 1:A:492:GLN:HE22   | 1.46                     | 0.59              |
| 1:A:164:HIS:HE1  | 1:A:474:TYR:O      | 1.86                     | 0.59              |
| 1:A:215:ALA:HB2  | 1:A:223:VAL:HG21   | 1.85                     | 0.59              |
| 1:B:277:SER:HB2  | 1:B:291:TRP:CG     | 2.38                     | 0.59              |
| 2:D:75:ASP:CG    | 2:D:152:MET:CE     | 2.76                     | 0.58              |
| 1:B:200:TYR:OH   | 4:L:88:TRP:CH2     | 2.57                     | 0.58              |
| 2:D:225:MET:CE   | 2:D:310:LEU:HD11   | 2.33                     | 0.58              |
| 3:F:92:SER:O     | 3:F:96:GLN:HG2     | 2.03                     | 0.58              |
| 2:D:171:ALA:CB   | 2:D:182:LEU:HD13   | 2.30                     | 0.58              |
| 1:B:215:ALA:HB1  | 4:L:35:PRO:HB2     | 1.85                     | 0.58              |
| 1:B:9:ASN:C      | 1:B:9:ASN:HD22     | 2.12                     | 0.57              |
| 2:C:189:TRP:CD1  | 2:C:190:MET:CE     | 2.87                     | 0.57              |
| 1:B:451:TRP:H    | 2:D:46:HIS:CD2     | 2.22                     | 0.57              |
| 1:A:16:TYR:CD2   | 2:C:182:LEU:HD23   | 2.40                     | 0.57              |
| 1:B:281:ASP:O    | 1:B:287:LYS:HE3    | 2.04                     | 0.57              |
| 2:C:194:MET:HE2  | 2:C:303:ALA:HB3    | 1.86                     | 0.57              |
| 2:D:52:ASP:OD2   | 2:D:55:HIS:HD2     | 1.87                     | 0.57              |
| 1:B:68:LYS:HD2   | 7:L:1028:HOH:O     | 2.05                     | 0.57              |
| 3:E:116:ASN:ND2  | 7:E:190:HOH:O      | 2.38                     | 0.56              |
| 1:A:446:LYS:NZ   | 2:C:50:GLN:HE22    | 2.03                     | 0.56              |
| 1:B:200:TYR:OH   | 4:L:88:TRP:HH2     | 1.87                     | 0.56              |
| 1:B:71:LYS:NZ    | 4:L:68:ILE:CD1     | 2.67                     | 0.56              |
| 1:A:47:TRP:CE3   | 1:A:124:GLY:HA3    | 2.40                     | 0.56              |
| 1:B:494:HIS:HD2  | 7:B:675:HOH:O      | 1.88                     | 0.56              |
| 2:C:64:ALA:HB3   | 2:C:281:LEU:HD11   | 1.86                     | 0.56              |
| 1:B:288:VAL:HG12 | 1:B:289:MET:HB2    | 1.88                     | 0.55              |
| 1:B:451:TRP:H    | 2:D:46:HIS:HD2     | 1.53                     | 0.55              |
| 1:B:149:MET:HE3  | 1:B:159:LEU:HD23   | 1.89                     | 0.55              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:A:417:LEU:CD2  | 3:F:39:PRO:HD3     | 2.37                     | 0.55              |
| 1:B:231:SER:HB3  | 4:L:70:VAL:HG13    | 1.89                     | 0.55              |
| 1:B:488:GLY:H    | 1:B:492:GLN:NE2    | 2.05                     | 0.55              |
| 1:B:483:ASN:HD22 | 1:B:483:ASN:H      | 1.53                     | 0.54              |
| 2:C:318:SER:OG   | 2:C:328:SER:HB3    | 2.06                     | 0.54              |
| 1:B:72:LEU:CD1   | 1:B:224:THR:HG22   | 2.37                     | 0.54              |
| 1:A:81:GLN:NE2   | 1:B:227[B]:PHE:CE1 | 2.75                     | 0.54              |
| 1:B:216:TYR:CD1  | 1:B:288:VAL:HG22   | 2.42                     | 0.54              |
| 2:D:241:GLN:O    | 7:D:491:HOH:O      | 2.18                     | 0.54              |
| 2:C:294:TYR:CD1  | 2:C:314:ARG:HD2    | 2.43                     | 0.54              |
| 1:A:161:ASP:O    | 1:A:165:MET:HG3    | 2.07                     | 0.54              |
| 1:B:230:GLN:CG   | 4:L:72:SER:N       | 2.62                     | 0.54              |
| 2:C:190:MET:HE2  | 2:C:190:MET:CA     | 2.35                     | 0.54              |
| 2:D:322:LYS:HG3  | 7:D:546:HOH:O      | 2.07                     | 0.54              |
| 1:A:259:GLN:NE2  | 1:A:316:ARG:H      | 2.05                     | 0.53              |
| 1:A:58:MET:HE1   | 1:A:133:MET:HE1    | 1.76                     | 0.53              |
| 1:A:58:MET:H     | 2:C:165:GLN:NE2    | 2.02                     | 0.53              |
| 2:D:194:MET:CE   | 2:D:195:TRP:NE1    | 2.71                     | 0.53              |
| 1:A:446:LYS:HZ2  | 2:C:50:GLN:HE22    | 1.55                     | 0.53              |
| 1:A:132:GLN:HB3  | 2:C:158:MET:CE     | 2.39                     | 0.53              |
| 1:A:140:ARG:CD   | 2:C:81:TYR:CE2     | 2.92                     | 0.53              |
| 1:B:164:HIS:HE1  | 1:B:474:TYR:O      | 1.92                     | 0.53              |
| 1:B:149:MET:HE3  | 1:B:159:LEU:CD2    | 2.38                     | 0.53              |
| 2:D:232:ASP:O    | 2:D:236:GLN:HG3    | 2.09                     | 0.53              |
| 2:C:40:GLU:CD    | 2:C:40:GLU:H       | 2.16                     | 0.52              |
| 3:E:92:SER:OG    | 3:E:95:GLU:HB2     | 2.09                     | 0.52              |
| 3:F:35:LEU:HA    | 3:F:119:TYR:CE2    | 2.43                     | 0.52              |
| 1:A:446:LYS:NZ   | 2:C:50:GLN:NE2     | 2.57                     | 0.52              |
| 1:B:208:VAL:O    | 1:B:212:SER:OG     | 2.26                     | 0.52              |
| 2:D:220:ILE:CD1  | 2:D:264:THR:HB     | 2.40                     | 0.52              |
| 1:A:471:VAL:O    | 1:A:475:TYR:HB2    | 2.10                     | 0.52              |
| 1:B:9:ASN:HD22   | 1:B:12:ASP:H       | 1.57                     | 0.52              |
| 1:B:138:GLU:OE1  | 1:B:199:GLU:OE1    | 2.27                     | 0.52              |
| 2:C:156:THR:O    | 2:C:159:ASP:HB2    | 2.10                     | 0.52              |
| 2:C:131:LEU:O    | 2:C:131:LEU:HG     | 2.07                     | 0.52              |
| 1:A:296:GLU:O    | 1:A:301:GLN:HG3    | 2.10                     | 0.52              |
| 1:A:399:CYS:O    | 1:A:403:GLN:HA     | 2.09                     | 0.52              |
| 2:C:68:GLU:HA    | 2:C:68:GLU:OE1     | 2.09                     | 0.52              |
| 2:D:220:ILE:HD11 | 2:D:264:THR:HB     | 1.92                     | 0.52              |
| 1:B:252:GLU:HG2  | 7:B:570:HOH:O      | 2.09                     | 0.52              |
| 1:B:71:LYS:CE    | 4:L:68:ILE:HD11    | 2.39                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:350:THR:O    | 1:A:485:ASP:HA   | 2.11                     | 0.51              |
| 1:B:143:GLN:HE22 | 2:D:151:GLN:HE22 | 1.58                     | 0.51              |
| 1:B:161:ASP:CG   | 2:D:22:ARG:HH22  | 2.19                     | 0.51              |
| 1:B:200:TYR:CE1  | 1:B:306:LEU:HD13 | 2.41                     | 0.51              |
| 1:A:371:LYS:HD2  | 1:A:372:TYR:CE1  | 2.45                     | 0.50              |
| 1:A:68:LYS:NZ    | 1:A:228:SER:O    | 2.42                     | 0.50              |
| 1:B:249:GLU:OE2  | 1:B:313:TYR:HE2  | 1.95                     | 0.50              |
| 1:B:471:VAL:HG13 | 1:B:477:ILE:HB   | 1.94                     | 0.50              |
| 1:B:356:GLU:CD   | 1:B:356:GLU:H    | 2.19                     | 0.50              |
| 1:A:58:MET:CE    | 1:A:133:MET:CE   | 2.74                     | 0.50              |
| 2:C:196:GLN:N    | 2:C:197:PRO:CD   | 2.74                     | 0.50              |
| 1:A:92:ARG:HD2   | 1:A:351:TRP:CE2  | 2.46                     | 0.50              |
| 1:A:140:ARG:HD3  | 2:C:81:TYR:CE2   | 2.46                     | 0.50              |
| 1:B:71:LYS:HZ1   | 4:L:68:ILE:HD11  | 1.76                     | 0.50              |
| 1:A:90:ASP:HB3   | 1:A:285:PRO:HG2  | 1.93                     | 0.50              |
| 1:A:417:LEU:HD21 | 3:F:39:PRO:HD3   | 1.94                     | 0.49              |
| 1:B:196:PHE:CE1  | 1:B:244:ILE:HG12 | 2.47                     | 0.49              |
| 1:B:72:LEU:HD12  | 1:B:224:THR:HG22 | 1.94                     | 0.49              |
| 1:B:68:LYS:HD3   | 4:L:68:ILE:CA    | 2.40                     | 0.49              |
| 1:B:160:HIS:HE1  | 1:B:482:ASP:OD1  | 1.95                     | 0.49              |
| 1:A:358:MET:HG3  | 1:A:369:PHE:CE2  | 2.47                     | 0.49              |
| 3:E:51:SER:HB2   | 3:E:89:ALA:O     | 2.12                     | 0.49              |
| 1:B:230:GLN:HB3  | 4:L:70:VAL:C     | 2.34                     | 0.49              |
| 1:B:341:GLN:HE22 | 3:E:37:CYS:H     | 1.61                     | 0.49              |
| 2:D:243:ALA:O    | 2:D:246:VAL:HG23 | 2.13                     | 0.49              |
| 1:B:58:MET:H     | 2:D:165:GLN:NE2  | 2.01                     | 0.49              |
| 1:A:405:PRO:HB2  | 1:A:407:ILE:HG23 | 1.93                     | 0.48              |
| 1:B:330:HIS:HD2  | 1:B:373:TYR:OH   | 1.94                     | 0.48              |
| 2:C:56:THR:O     | 2:C:62:ARG:NH2   | 2.41                     | 0.48              |
| 2:D:153:HIS:HA   | 2:D:156:THR:HG22 | 1.94                     | 0.48              |
| 3:E:48:MET:HG2   | 3:E:93:LEU:HD22  | 1.96                     | 0.48              |
| 7:B:733:HOH:O    | 4:L:35:PRO:HG3   | 2.12                     | 0.48              |
| 1:A:15:GLN:HG2   | 1:A:19:ARG:NH1   | 2.29                     | 0.48              |
| 3:F:29:TYR:O     | 3:F:31:PRO:HD3   | 2.13                     | 0.48              |
| 1:B:117:LYS:HE2  | 2:D:51:TRP:CZ3   | 2.48                     | 0.48              |
| 1:B:279:MET:SD   | 1:B:279:MET:C    | 2.97                     | 0.48              |
| 1:A:174:VAL:HB   | 1:A:175:PRO:CD   | 2.44                     | 0.48              |
| 1:B:344:GLN:HE21 | 1:B:344:GLN:N    | 2.04                     | 0.48              |
| 1:B:309:ASP:C    | 1:B:309:ASP:OD1  | 2.57                     | 0.47              |
| 1:B:318:PRO:O    | 1:B:321:GLN:HB2  | 2.13                     | 0.47              |
| 1:B:122:PHE:CE2  | 1:B:191:LEU:HD22 | 2.49                     | 0.47              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:B:399:CYS:O    | 1:B:403:GLN:HA     | 2.15                     | 0.47              |
| 2:C:260:SER:HB3  | 7:C:364:HOH:O      | 2.15                     | 0.47              |
| 1:B:51:GLU:O     | 1:B:242:GLU:HG2    | 2.15                     | 0.47              |
| 1:A:358:MET:HG3  | 1:A:369:PHE:CZ     | 2.49                     | 0.47              |
| 1:B:44:ILE:HA    | 1:B:250:GLN:HG3    | 1.97                     | 0.47              |
| 2:C:40:GLU:HG2   | 2:C:145:THR:O      | 2.16                     | 0.46              |
| 1:B:204:ASN:HD21 | 4:L:6:PHE:HZ       | 1.59                     | 0.46              |
| 1:B:424:HIS:HE1  | 1:B:445[B]:GLU:OE2 | 1.99                     | 0.46              |
| 2:C:52:ASP:OD2   | 2:C:62:ARG:NH1     | 2.49                     | 0.46              |
| 2:C:301:ALA:O    | 2:C:306:GLY:N      | 2.46                     | 0.46              |
| 3:F:81:ASN:O     | 3:F:82:ASP:HB2     | 2.16                     | 0.46              |
| 2:D:126:LEU:CD1  | 2:D:230:VAL:HG11   | 2.46                     | 0.46              |
| 1:A:28:GLN:NE2   | 7:A:607:HOH:O      | 2.48                     | 0.46              |
| 1:B:246:PHE:O    | 1:B:250:GLN:HB2    | 2.16                     | 0.46              |
| 1:A:120:ARG:HG2  | 2:C:139:LYS:HB3    | 1.97                     | 0.46              |
| 1:A:122:PHE:CE2  | 1:A:191:LEU:HD22   | 2.51                     | 0.46              |
| 1:A:379:TYR:HD1  | 3:F:114:MET:HE1    | 1.73                     | 0.46              |
| 1:B:117:LYS:HE2  | 2:D:51:TRP:CE3     | 2.51                     | 0.46              |
| 3:E:70:LYS:HD2   | 3:E:70:LYS:N       | 2.07                     | 0.46              |
| 4:L:34:GLN:O     | 4:L:35:PRO:O       | 2.33                     | 0.46              |
| 1:B:203:THR:HA   | 7:B:743:HOH:O      | 2.15                     | 0.46              |
| 1:B:206:LEU:HD22 | 1:B:276:VAL:HG21   | 1.98                     | 0.46              |
| 1:B:216:TYR:CD1  | 4:L:35:PRO:HG2     | 2.51                     | 0.46              |
| 2:C:229:LEU:HD21 | 2:C:301:ALA:HB2    | 1.98                     | 0.46              |
| 1:B:230:GLN:CB   | 4:L:70:VAL:O       | 2.50                     | 0.46              |
| 2:D:225:MET:HE1  | 2:D:294:TYR:CA     | 2.38                     | 0.46              |
| 2:D:102:CYS:SG   | 2:D:249:LEU:HD21   | 2.56                     | 0.45              |
| 2:C:233:LYS:HE3  | 2:C:312:GLU:HB2    | 1.98                     | 0.45              |
| 1:A:69:GLU:OE1   | 1:A:140:ARG:NH1    | 2.49                     | 0.45              |
| 2:D:244:GLU:HB2  | 7:D:513:HOH:O      | 2.16                     | 0.45              |
| 2:D:45:PHE:CZ    | 2:D:58:ASN:HB2     | 2.52                     | 0.45              |
| 2:C:194:MET:HE1  | 2:C:303:ALA:HB1    | 1.91                     | 0.45              |
| 1:A:472:GLN:HE22 | 1:A:478:ASN:ND2    | 2.11                     | 0.45              |
| 1:B:71:LYS:HZ3   | 4:L:68:ILE:CD1     | 2.30                     | 0.45              |
| 2:C:172:LEU:HD21 | 2:C:182:LEU:HD22   | 1.99                     | 0.45              |
| 2:D:71:CYS:C     | 2:D:73:VAL:N       | 2.72                     | 0.45              |
| 1:B:53:PRO:O     | 1:B:238:THR:HG21   | 2.17                     | 0.45              |
| 2:D:225:MET:HE3  | 2:D:310:LEU:CD1    | 2.43                     | 0.45              |
| 3:F:33:HIS:HD2   | 3:F:65:HIS:CE1     | 2.34                     | 0.45              |
| 1:B:292:SER:HB2  | 1:B:365:TYR:CE2    | 2.52                     | 0.45              |
| 1:A:58:MET:HE3   | 2:C:161:LEU:HD23   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:104:ILE:O    | 1:A:107:LEU:HB2  | 2.17                     | 0.45              |
| 2:C:137:ASN:HD22 | 2:C:153:HIS:HD2  | 1.64                     | 0.45              |
| 3:E:27:TYR:HA    | 3:E:40:PHE:O     | 2.17                     | 0.45              |
| 1:A:451:TRP:CE2  | 1:A:456:GLN:HG3  | 2.53                     | 0.44              |
| 1:B:134:GLN:HB2  | 7:B:667:HOH:O    | 2.18                     | 0.44              |
| 1:B:443:GLU:HB3  | 3:E:3:VAL:HG22   | 1.99                     | 0.44              |
| 1:A:57:THR:OG1   | 1:A:59:ASP:OD1   | 2.32                     | 0.44              |
| 1:B:50:TRP:HH2   | 1:B:239:LEU:HD12 | 1.82                     | 0.44              |
| 1:B:139:LEU:HD21 | 2:D:151:GLN:HB2  | 1.99                     | 0.44              |
| 2:D:121:ARG:NH1  | 7:D:357:HOH:O    | 2.23                     | 0.44              |
| 1:B:209:PRO:HB3  | 1:B:280:MET:HB3  | 2.00                     | 0.44              |
| 2:D:48:ARG:HG3   | 3:E:11:PHE:CE1   | 2.52                     | 0.44              |
| 7:D:411:HOH:O    | 3:E:14:LYS:HE3   | 2.18                     | 0.44              |
| 1:A:341:GLN:HE22 | 3:F:37:CYS:H     | 1.65                     | 0.44              |
| 1:A:274:SER:HB2  | 1:A:335:LEU:HD11 | 1.98                     | 0.44              |
| 2:C:131:LEU:O    | 2:C:135:MET:HG3  | 2.17                     | 0.44              |
| 1:A:134:GLN:O    | 1:A:138:GLU:HG2  | 2.18                     | 0.44              |
| 1:B:19:ARG:NH1   | 1:B:50:TRP:HD1   | 2.16                     | 0.44              |
| 2:C:126:LEU:CD1  | 2:C:230:VAL:HG11 | 2.48                     | 0.44              |
| 2:D:172:LEU:CD2  | 2:D:182:LEU:HD22 | 2.48                     | 0.43              |
| 1:B:11:LYS:O     | 1:B:15:GLN:HG3   | 2.17                     | 0.43              |
| 2:C:234:MET:HE2  | 2:C:234:MET:HB2  | 1.71                     | 0.43              |
| 2:C:294:TYR:OH   | 2:C:307:ILE:HD11 | 2.18                     | 0.43              |
| 1:A:143:GLN:NE2  | 2:C:151:GLN:NE2  | 2.63                     | 0.43              |
| 1:B:26:THR:HG1   | 2:D:199:ARG:HH22 | 1.56                     | 0.43              |
| 1:A:365:TYR:HB2  | 1:A:369:PHE:HB2  | 2.01                     | 0.43              |
| 1:B:458:TYR:C    | 1:B:460:GLY:H    | 2.26                     | 0.43              |
| 1:B:471:VAL:O    | 1:B:475:TYR:HB2  | 2.18                     | 0.43              |
| 1:A:215:ALA:HB1  | 2:D:7:THR:HG23   | 2.00                     | 0.43              |
| 1:B:230:GLN:CG   | 4:L:70:VAL:C     | 2.88                     | 0.43              |
| 3:F:72:ASP:OD2   | 3:F:75:ASN:HB2   | 2.18                     | 0.43              |
| 2:C:328:SER:O    | 2:C:329:ARG:HB2  | 2.19                     | 0.43              |
| 2:D:213:GLU:O    | 2:D:217:VAL:HG23 | 2.19                     | 0.43              |
| 1:B:216:TYR:CG   | 1:B:288:VAL:HG22 | 2.54                     | 0.43              |
| 1:A:9:ASN:HD22   | 1:A:9:ASN:HA     | 1.38                     | 0.43              |
| 1:A:97:LEU:HD22  | 1:A:149:MET:HE1  | 2.01                     | 0.43              |
| 1:B:134:GLN:NE2  | 1:B:199:GLU:OE1  | 2.52                     | 0.43              |
| 1:B:496:LEU:HD23 | 1:B:496:LEU:HA   | 1.89                     | 0.43              |
| 1:A:33:ILE:O     | 1:A:120:ARG:NH1  | 2.51                     | 0.42              |
| 1:A:274:SER:HB2  | 1:A:335:LEU:HD13 | 2.00                     | 0.42              |
| 1:B:277:SER:HB2  | 1:B:291:TRP:CD2  | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:117:LYS:HE3  | 2:D:184:GLU:OE1  | 2.19                     | 0.42              |
| 1:A:361:MET:HE2  | 1:A:369:PHE:CZ   | 2.54                     | 0.42              |
| 1:B:472:GLN:HE22 | 1:B:478:ASN:ND2  | 2.15                     | 0.42              |
| 2:C:212:PHE:CD2  | 2:C:212:PHE:O    | 2.72                     | 0.42              |
| 2:D:234:MET:HE2  | 2:D:234:MET:HB2  | 1.87                     | 0.42              |
| 1:A:132:GLN:OE1  | 2:C:158:MET:HE1  | 2.20                     | 0.42              |
| 1:A:356:GLU:CD   | 1:A:356:GLU:N    | 2.71                     | 0.42              |
| 1:A:253:ASP:O    | 1:A:256:PRO:HD2  | 2.19                     | 0.42              |
| 2:C:38:ASP:OD1   | 2:C:42:LYS:NZ    | 2.44                     | 0.42              |
| 1:B:488:GLY:H    | 1:B:492:GLN:HE22 | 1.68                     | 0.42              |
| 1:B:244:ILE:HD12 | 1:B:245:LYS:N    | 2.33                     | 0.42              |
| 1:B:379:TYR:HD1  | 3:E:114:MET:HE1  | 1.78                     | 0.42              |
| 1:B:417:LEU:CD2  | 3:E:29:TYR:CE2   | 3.03                     | 0.42              |
| 3:F:65:HIS:HA    | 3:F:66:PRO:HD2   | 1.87                     | 0.42              |
| 2:C:89:ALA:HA    | 2:C:92:GLN:HG3   | 2.01                     | 0.42              |
| 2:D:152:MET:HE2  | 2:D:263:TRP:CB   | 2.49                     | 0.42              |
| 2:D:291:PRO:O    | 2:D:295:GLU:HG2  | 2.20                     | 0.42              |
| 1:A:98:LYS:HE2   | 1:A:157:ASN:O    | 2.21                     | 0.41              |
| 2:C:45:PHE:CZ    | 2:C:58:ASN:HB2   | 2.55                     | 0.41              |
| 2:C:228:PRO:O    | 2:C:232:ASP:HB2  | 2.20                     | 0.41              |
| 3:F:39:PRO:HG2   | 3:F:103:MET:HE1  | 2.02                     | 0.41              |
| 1:B:309:ASP:OD1  | 1:B:309:ASP:O    | 2.38                     | 0.41              |
| 3:E:99:ASP:OD1   | 3:E:102:SER:OG   | 2.38                     | 0.41              |
| 1:A:105:SER:N    | 1:A:106:PRO:CD   | 2.84                     | 0.41              |
| 1:A:278:MET:HE3  | 1:A:283:MET:HE3  | 2.03                     | 0.41              |
| 1:A:371:LYS:HD2  | 1:A:372:TYR:CZ   | 2.56                     | 0.41              |
| 1:A:442:HIS:HE1  | 7:F:131:HOH:O    | 2.04                     | 0.41              |
| 1:A:477:ILE:HG23 | 1:A:482:ASP:HB2  | 2.03                     | 0.41              |
| 1:B:10:LEU:HD23  | 1:B:10:LEU:HA    | 1.87                     | 0.41              |
| 2:D:198:MET:HA   | 2:D:296:ALA:HB1  | 2.03                     | 0.41              |
| 1:B:102:SER:HB3  | 1:B:172:LEU:HD11 | 2.03                     | 0.41              |
| 2:D:277:THR:HG22 | 7:D:384:HOH:O    | 2.21                     | 0.41              |
| 1:B:61:TYR:OH    | 1:B:136:ILE:HG23 | 2.20                     | 0.41              |
| 1:B:141:HIS:O    | 1:B:145:GLN:HG3  | 2.21                     | 0.41              |
| 1:B:216:TYR:CE1  | 4:L:35:PRO:CG    | 3.04                     | 0.41              |
| 1:B:255:VAL:HG13 | 1:B:315:ILE:HD13 | 2.02                     | 0.41              |
| 2:D:295:GLU:O    | 2:D:299:PRO:HD3  | 2.21                     | 0.41              |
| 1:B:413:ALA:C    | 1:B:415:THR:H    | 2.27                     | 0.41              |
| 2:D:40:GLU:HG2   | 2:D:145:THR:O    | 2.20                     | 0.41              |
| 2:D:156:THR:O    | 2:D:160:ARG:HG2  | 2.21                     | 0.41              |
| 3:F:78:TRP:CZ3   | 3:F:106:VAL:HB   | 2.56                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 4:L:33:HIS:NE2     | 4:L:38:ILE:HG12  | 2.35                     | 0.41              |
| 1:A:455:HIS:O      | 1:A:459:GLN:HG3  | 2.21                     | 0.41              |
| 3:E:28:VAL:HA      | 3:E:104:LEU:O    | 2.22                     | 0.40              |
| 1:A:133:MET:HB2    | 1:A:133:MET:HE3  | 1.58                     | 0.40              |
| 1:A:349:HIS:HB3    | 1:A:486:TYR:N    | 2.35                     | 0.40              |
| 1:B:494:HIS:HB3    | 7:B:674:HOH:O    | 2.21                     | 0.40              |
| 2:C:175:ASP:O      | 2:C:178:THR:HG23 | 2.21                     | 0.40              |
| 1:A:90:ASP:OD1     | 1:A:92:ARG:HB2   | 2.20                     | 0.40              |
| 1:A:283:MET:O      | 1:A:285:PRO:HD3  | 2.22                     | 0.40              |
| 1:B:445[A]:GLU:OE1 | 3:E:3:VAL:HG23   | 2.22                     | 0.40              |
| 3:E:56:GLU:C       | 3:E:57:ILE:HD13  | 2.46                     | 0.40              |
| 3:F:59:LYS:N       | 3:F:60:PRO:HD2   | 2.36                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 7:A:686:HOH:O | 7:E:140:HOH:O[3_645] | 2.06                     | 0.14              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 492/494 (100%) | 472 (96%) | 19 (4%) | 1 (0%)   | 43          | 55  |
| 1   | B     | 495/494 (100%) | 475 (96%) | 20 (4%) | 0        | 100         | 100 |
| 2   | C     | 316/328 (96%)  | 303 (96%) | 13 (4%) | 0        | 100         | 100 |
| 2   | D     | 326/328 (99%)  | 314 (96%) | 12 (4%) | 0        | 100         | 100 |
| 3   | E     | 116/118 (98%)  | 112 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 3   | F     | 116/118 (98%)  | 106 (91%) | 8 (7%)  | 2 (2%)   | 7           | 7   |
| 4   | L     | 77/89 (86%)    | 65 (84%)  | 5 (6%)  | 7 (9%)   | 0           | 0   |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| All | All   | 1938/1969 (98%) | 1847 (95%) | 81 (4%) | 10 (0%)  | 24          | 31 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ASN  |
| 4   | L     | 35  | PRO  |
| 4   | L     | 11  | ASP  |
| 4   | L     | 42  | ALA  |
| 3   | F     | 74  | LEU  |
| 4   | L     | 44  | LYS  |
| 3   | F     | 34  | LEU  |
| 4   | L     | 25  | ASP  |
| 4   | L     | 27  | PRO  |
| 4   | L     | 64  | GLN  |

### 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     | 433/434 (100%)  | 402 (93%)  | 31 (7%)  | 13          | 18 |
| 1   | B     | 436/434 (100%)  | 405 (93%)  | 31 (7%)  | 13          | 19 |
| 2   | C     | 272/281 (97%)   | 254 (93%)  | 18 (7%)  | 15          | 21 |
| 2   | D     | 280/281 (100%)  | 266 (95%)  | 14 (5%)  | 22          | 33 |
| 3   | E     | 98/98 (100%)    | 89 (91%)   | 9 (9%)   | 8           | 11 |
| 3   | F     | 98/98 (100%)    | 89 (91%)   | 9 (9%)   | 8           | 11 |
| 4   | L     | 60/81 (74%)     | 49 (82%)   | 11 (18%) | 2           | 2  |
| All | All   | 1677/1707 (98%) | 1554 (93%) | 123 (7%) | 13          | 18 |

All (123) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ASN  |
| 1   | A     | 43  | LYS  |
| 1   | A     | 101 | ILE  |
| 1   | A     | 104 | ILE  |
| 1   | A     | 105 | SER  |
| 1   | A     | 107 | LEU  |
| 1   | A     | 118 | VAL  |
| 1   | A     | 120 | ARG  |
| 1   | A     | 133 | MET  |
| 1   | A     | 161 | ASP  |
| 1   | A     | 179 | PHE  |
| 1   | A     | 191 | LEU  |
| 1   | A     | 223 | VAL  |
| 1   | A     | 241 | LEU  |
| 1   | A     | 243 | VAL  |
| 1   | A     | 244 | ILE  |
| 1   | A     | 296 | GLU  |
| 1   | A     | 319 | LYS  |
| 1   | A     | 335 | LEU  |
| 1   | A     | 344 | GLN  |
| 1   | A     | 355 | LYS  |
| 1   | A     | 356 | GLU  |
| 1   | A     | 358 | MET  |
| 1   | A     | 361 | MET  |
| 1   | A     | 389 | ARG  |
| 1   | A     | 415 | THR  |
| 1   | A     | 417 | LEU  |
| 1   | A     | 422 | ILE  |
| 1   | A     | 425 | GLU  |
| 1   | A     | 497 | SER  |
| 1   | B     | 9   | ASN  |
| 1   | B     | 30  | LYS  |
| 1   | B     | 67  | GLU  |
| 1   | B     | 68  | LYS  |
| 1   | B     | 81  | GLN  |
| 1   | B     | 90  | ASP  |
| 1   | B     | 107 | LEU  |
| 1   | B     | 118 | VAL  |
| 1   | B     | 123 | SER  |
| 1   | B     | 136 | ILE  |
| 1   | B     | 179 | PHE  |
| 1   | B     | 199 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 206 | LEU  |
| 1   | B     | 223 | VAL  |
| 1   | B     | 228 | SER  |
| 1   | B     | 230 | GLN  |
| 1   | B     | 241 | LEU  |
| 1   | B     | 244 | ILE  |
| 1   | B     | 250 | GLN  |
| 1   | B     | 274 | SER  |
| 1   | B     | 315 | ILE  |
| 1   | B     | 316 | ARG  |
| 1   | B     | 319 | LYS  |
| 1   | B     | 344 | GLN  |
| 1   | B     | 356 | GLU  |
| 1   | B     | 382 | LYS  |
| 1   | B     | 415 | THR  |
| 1   | B     | 417 | LEU  |
| 1   | B     | 468 | GLU  |
| 1   | B     | 483 | ASN  |
| 1   | B     | 498 | ILE  |
| 2   | C     | 40  | GLU  |
| 2   | C     | 54  | GLU  |
| 2   | C     | 57  | LEU  |
| 2   | C     | 66  | ARG  |
| 2   | C     | 68  | GLU  |
| 2   | C     | 74  | SER  |
| 2   | C     | 139 | LYS  |
| 2   | C     | 154 | ILE  |
| 2   | C     | 156 | THR  |
| 2   | C     | 182 | LEU  |
| 2   | C     | 207 | VAL  |
| 2   | C     | 261 | LEU  |
| 2   | C     | 276 | GLU  |
| 2   | C     | 281 | LEU  |
| 2   | C     | 290 | GLU  |
| 2   | C     | 298 | LYS  |
| 2   | C     | 307 | ILE  |
| 2   | C     | 328 | SER  |
| 2   | D     | 7   | THR  |
| 2   | D     | 14  | ARG  |
| 2   | D     | 40  | GLU  |
| 2   | D     | 57  | LEU  |
| 2   | D     | 68  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | D     | 74  | SER  |
| 2   | D     | 114 | GLU  |
| 2   | D     | 151 | GLN  |
| 2   | D     | 182 | LEU  |
| 2   | D     | 193 | GLU  |
| 2   | D     | 207 | VAL  |
| 2   | D     | 246 | VAL  |
| 2   | D     | 261 | LEU  |
| 2   | D     | 279 | ARG  |
| 3   | E     | 6   | LEU  |
| 3   | E     | 10  | LYS  |
| 3   | E     | 24  | GLN  |
| 3   | E     | 70  | LYS  |
| 3   | E     | 74  | LEU  |
| 3   | E     | 79  | LEU  |
| 3   | E     | 80  | LEU  |
| 3   | E     | 93  | LEU  |
| 3   | E     | 112 | LYS  |
| 3   | F     | 6   | LEU  |
| 3   | F     | 23  | MET  |
| 3   | F     | 44  | VAL  |
| 3   | F     | 48  | MET  |
| 3   | F     | 59  | LYS  |
| 3   | F     | 74  | LEU  |
| 3   | F     | 77  | GLU  |
| 3   | F     | 93  | LEU  |
| 3   | F     | 95  | GLU  |
| 4   | L     | 28  | ASP  |
| 4   | L     | 32  | GLN  |
| 4   | L     | 51  | GLU  |
| 4   | L     | 55  | GLU  |
| 4   | L     | 59  | ARG  |
| 4   | L     | 62  | ASP  |
| 4   | L     | 63  | VAL  |
| 4   | L     | 67  | LEU  |
| 4   | L     | 68  | ILE  |
| 4   | L     | 70  | VAL  |
| 4   | L     | 73  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | ASN  |
| 1   | A     | 28  | GLN  |
| 1   | A     | 49  | GLN  |
| 1   | A     | 65  | GLN  |
| 1   | A     | 81  | GLN  |
| 1   | A     | 87  | ASN  |
| 1   | A     | 146 | GLN  |
| 1   | A     | 153 | ASN  |
| 1   | A     | 164 | HIS  |
| 1   | A     | 259 | GLN  |
| 1   | A     | 321 | GLN  |
| 1   | A     | 341 | GLN  |
| 1   | A     | 344 | GLN  |
| 1   | A     | 397 | GLN  |
| 1   | A     | 400 | GLN  |
| 1   | A     | 442 | HIS  |
| 1   | A     | 455 | HIS  |
| 1   | A     | 478 | ASN  |
| 1   | A     | 492 | GLN  |
| 1   | B     | 9   | ASN  |
| 1   | B     | 15  | GLN  |
| 1   | B     | 28  | GLN  |
| 1   | B     | 65  | GLN  |
| 1   | B     | 86  | GLN  |
| 1   | B     | 87  | ASN  |
| 1   | B     | 134 | GLN  |
| 1   | B     | 153 | ASN  |
| 1   | B     | 160 | HIS  |
| 1   | B     | 164 | HIS  |
| 1   | B     | 301 | GLN  |
| 1   | B     | 330 | HIS  |
| 1   | B     | 341 | GLN  |
| 1   | B     | 344 | GLN  |
| 1   | B     | 400 | GLN  |
| 1   | B     | 424 | HIS  |
| 1   | B     | 455 | HIS  |
| 1   | B     | 478 | ASN  |
| 1   | B     | 483 | ASN  |
| 1   | B     | 492 | GLN  |
| 1   | B     | 494 | HIS  |
| 2   | C     | 50  | GLN  |
| 2   | C     | 78  | GLN  |
| 2   | C     | 137 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 151 | GLN  |
| 2   | C     | 165 | GLN  |
| 2   | C     | 219 | ASN  |
| 2   | C     | 241 | GLN  |
| 2   | C     | 311 | ASN  |
| 2   | D     | 46  | HIS  |
| 2   | D     | 50  | GLN  |
| 2   | D     | 55  | HIS  |
| 2   | D     | 78  | GLN  |
| 2   | D     | 136 | ASN  |
| 2   | D     | 137 | ASN  |
| 2   | D     | 151 | GLN  |
| 2   | D     | 165 | GLN  |
| 2   | D     | 219 | ASN  |
| 2   | D     | 241 | GLN  |
| 2   | D     | 288 | HIS  |
| 2   | D     | 327 | GLN  |
| 3   | F     | 24  | GLN  |
| 3   | F     | 96  | GLN  |
| 4   | L     | 10  | GLN  |
| 4   | L     | 32  | GLN  |
| 4   | L     | 69  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|-----------------|--------|---------------|-----------------------|----------|
| 1   | A     | 494/494 (100%)  | -0.52  | 2 (0%) 88 89  | 24, 36, 53, 67        | 0        |
| 1   | B     | 493/494 (99%)   | -0.42  | 6 (1%) 76 77  | 15, 37, 58, 69        | 4 (0%)   |
| 2   | C     | 318/328 (96%)   | -0.30  | 0 100 100     | 25, 39, 59, 78        | 0        |
| 2   | D     | 328/328 (100%)  | -0.50  | 3 (0%) 81 82  | 26, 37, 56, 82        | 0        |
| 3   | E     | 118/118 (100%)  | -0.49  | 0 100 100     | 28, 37, 51, 58        | 0        |
| 3   | F     | 118/118 (100%)  | 0.14   | 1 (0%) 82 83  | 39, 55, 70, 74        | 0        |
| 4   | L     | 83/89 (93%)     | 1.84   | 28 (33%) 1 1  | 23, 28, 33, 83        | 81 (97%) |
| All | All   | 1952/1969 (99%) | -0.31  | 40 (2%) 65 66 | 15, 37, 59, 83        | 85 (4%)  |

All (40) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4   | L     | 36  | ALA  | 5.5  |
| 4   | L     | 35  | PRO  | 5.0  |
| 4   | L     | 67  | LEU  | 4.7  |
| 4   | L     | 80  | ASP  | 4.3  |
| 4   | L     | 88  | TRP  | 3.9  |
| 4   | L     | 3   | GLN  | 3.9  |
| 4   | L     | 37  | MET  | 3.7  |
| 4   | L     | 33  | HIS  | 3.6  |
| 4   | L     | 58  | GLY  | 3.6  |
| 4   | L     | 70  | VAL  | 3.5  |
| 4   | L     | 73  | ILE  | 3.5  |
| 2   | D     | 331 | VAL  | 3.3  |
| 4   | L     | 68  | ILE  | 3.3  |
| 4   | L     | 34  | GLN  | 3.3  |
| 4   | L     | 57  | LEU  | 3.2  |
| 1   | B     | 231 | SER  | 3.2  |
| 1   | B     | 207 | PHE  | 3.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | B     | 498    | ILE  | 3.0  |
| 3   | F     | 117    | ALA  | 3.0  |
| 1   | A     | 499    | LYS  | 2.9  |
| 4   | L     | 4      | LEU  | 2.8  |
| 4   | L     | 63     | VAL  | 2.8  |
| 4   | L     | 39     | ARG  | 2.5  |
| 4   | L     | 50     | ARG  | 2.5  |
| 4   | L     | 59     | ARG  | 2.4  |
| 4   | L     | 72     | SER  | 2.4  |
| 2   | D     | 10     | VAL  | 2.4  |
| 1   | B     | 234    | ALA  | 2.4  |
| 1   | A     | 466    | ASP  | 2.3  |
| 4   | L     | 77     | VAL  | 2.3  |
| 4   | L     | 85     | ILE  | 2.3  |
| 4   | L     | 64     | GLN  | 2.3  |
| 4   | L     | 16     | ARG  | 2.3  |
| 4   | L     | 48     | ILE  | 2.3  |
| 1   | B     | 227[A] | PHE  | 2.3  |
| 2   | D     | 6      | LYS  | 2.2  |
| 4   | L     | 52     | THR  | 2.2  |
| 4   | L     | 53     | MET  | 2.2  |
| 4   | L     | 43     | GLU  | 2.0  |
| 1   | B     | 225[A] | PHE  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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.

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | FE   | B     | 5   | 1/1   | 0.94 | 0.07 | 60,60,60,60                 | 0     |
| 5   | FE   | B     | 4   | 1/1   | 0.98 | 0.03 | 37,37,37,37                 | 0     |
| 5   | FE   | A     | 1   | 1/1   | 0.99 | 0.03 | 45,45,45,45                 | 0     |
| 5   | FE   | A     | 3   | 1/1   | 0.99 | 0.02 | 41,41,41,41                 | 0     |
| 6   | ZN   | B     | 500 | 1/1   | 0.99 | 0.02 | 33,33,33,33                 | 0     |
| 6   | ZN   | A     | 2   | 1/1   | 1.00 | 0.04 | 36,36,36,36                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.