



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2017 – 08:15 PM EDT

PDB ID : 2IGK  
Title : Crystal structure of recombinant pyranose 2-oxidase  
Authors : Divne, C.  
Deposited on : unknown  
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

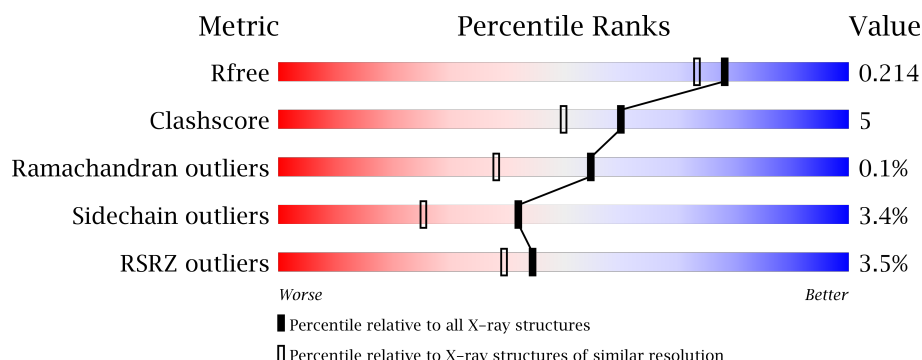
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 4827 (1.80-1.80)                                      |
| Clashscore            | 112137                      | 5742 (1.80-1.80)                                      |
| Ramachandran outliers | 110173                      | 5676 (1.80-1.80)                                      |
| Sidechain outliers    | 110143                      | 5675 (1.80-1.80)                                      |
| RSRZ outliers         | 101464                      | 4906 (1.80-1.80)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 623    | <div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>  |
| 1   | B     | 623    | <div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div> |
| 1   | C     | 623    | <div> <div>4%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>  |
| 1   | D     | 623    | <div> <div>3%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>7%</div> </div> </div>  |
| 1   | E     | 623    | <div> <div>3%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain    |
|-----|-------|--------|---------------------|
| 1   | F     | 623    | <br>3% 82% 9% • 7%  |
| 1   | G     | 623    | <br>4% 82% 10% • 7% |
| 1   | H     | 623    | <br>2% 83% 8% • 7%  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | MES  | A     | 902 | -         | -        | X       | X                |
| 3   | MES  | B     | 901 | -         | -        | X       | X                |
| 3   | MES  | C     | 904 | -         | -        | X       | X                |
| 3   | MES  | D     | 903 | -         | -        | X       | X                |
| 3   | MES  | E     | 905 | -         | -        | -       | X                |
| 3   | MES  | E     | 906 | -         | -        | X       | X                |
| 3   | MES  | G     | 908 | -         | -        | X       | X                |
| 3   | MES  | H     | 907 | -         | -        | X       | X                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39837 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 Pyranose oxidase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |
| 1   | B     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |
| 1   | C     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |
| 1   | D     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |
| 1   | E     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |
| 1   | F     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |
| 1   | G     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |
| 1   | H     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4549  | 2872 | 778 | 874 | 25 |         |         |       |

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 2   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | B     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | C     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | D     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | E     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | E     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | G     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |
| 3   | H     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 417      | Total | O   | 0       | 0       |
|     |       |          | 417   | 417 |         |         |
| 4   | B     | 418      | Total | O   | 0       | 0       |
|     |       |          | 418   | 418 |         |         |
| 4   | C     | 307      | Total | O   | 0       | 0       |
|     |       |          | 307   | 307 |         |         |
| 4   | D     | 354      | Total | O   | 0       | 0       |
|     |       |          | 354   | 354 |         |         |

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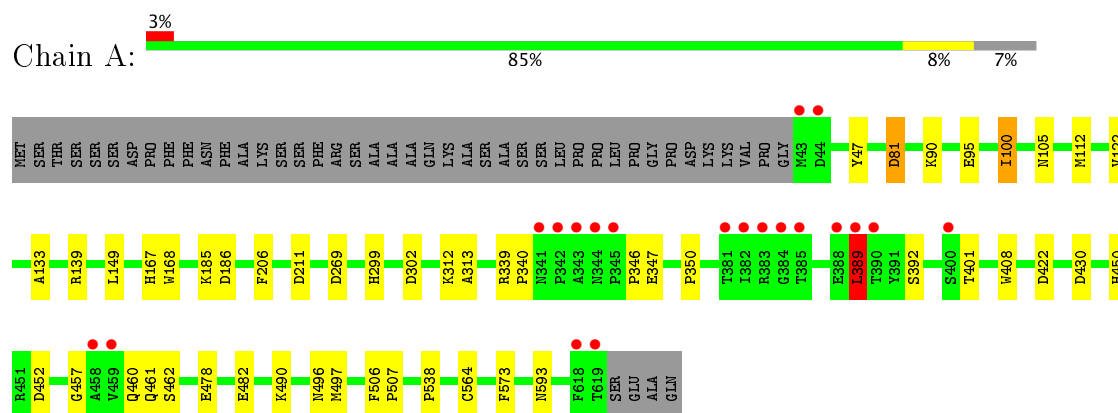
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | E     | 336      | Total<br>336 | O<br>336 | 0       | 0       |
| 4   | F     | 318      | Total<br>318 | O<br>318 | 0       | 0       |
| 4   | G     | 379      | Total<br>379 | O<br>379 | 0       | 0       |
| 4   | H     | 396      | Total<br>396 | O<br>396 | 0       | 0       |

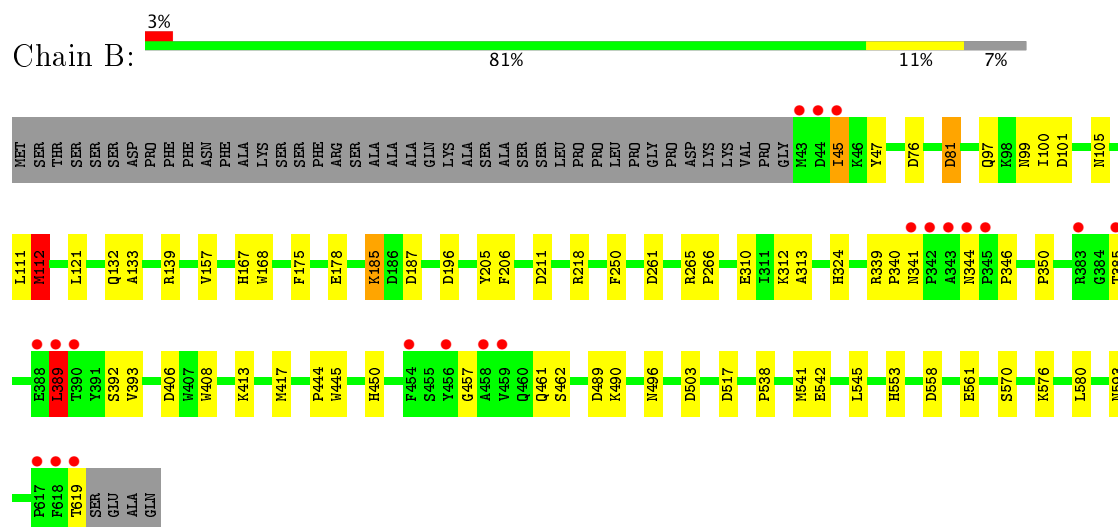
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

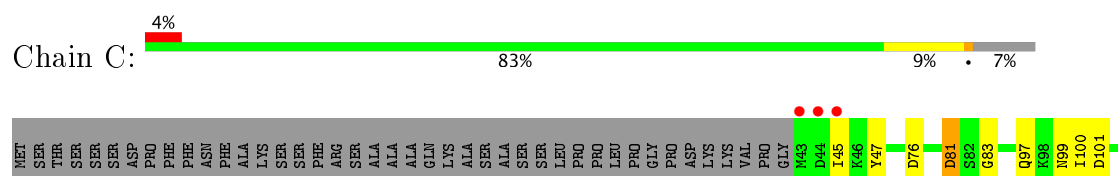
#### • Molecule 1: Pyranose oxidase



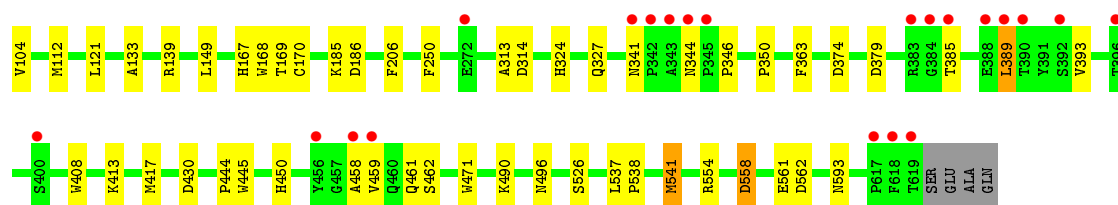
#### • Molecule 1: Pyranose oxidase



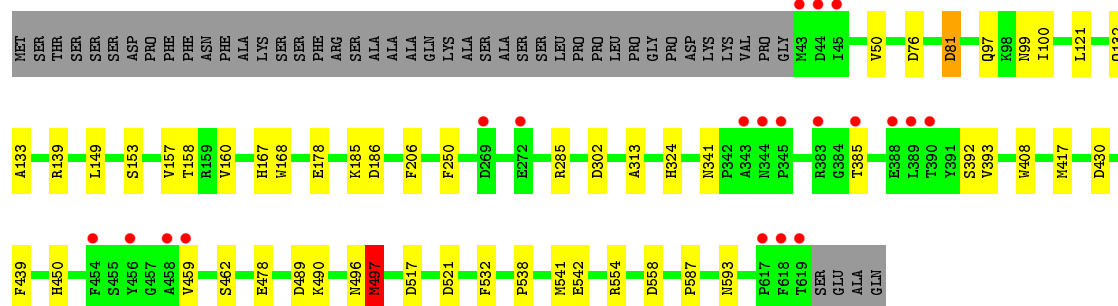
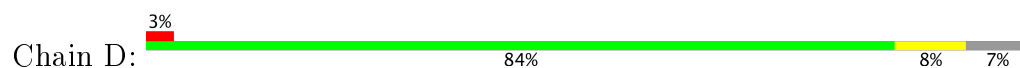
#### • Molecule 1: Pyranose oxidase



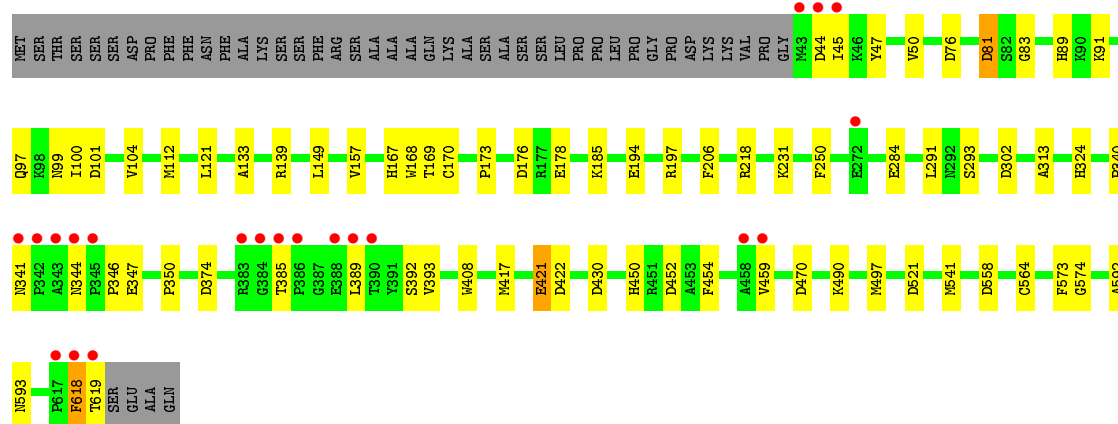
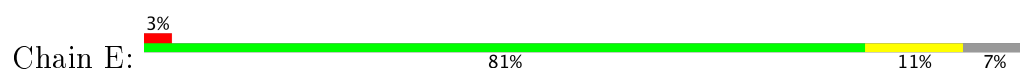




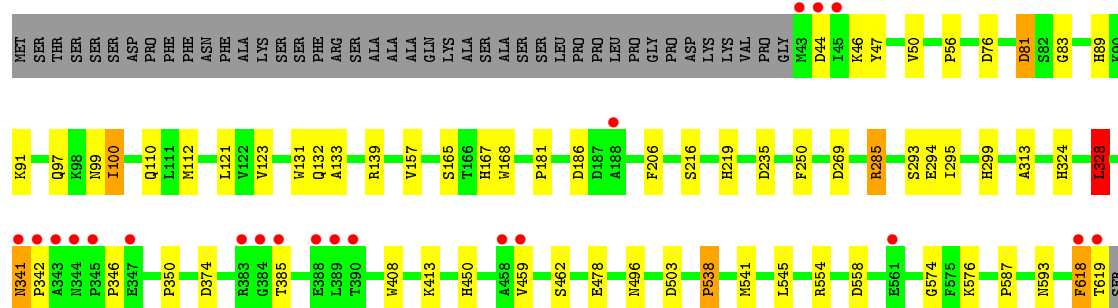
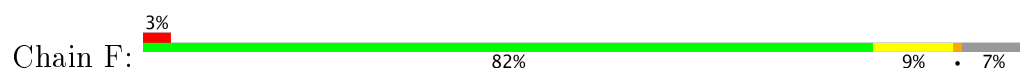
• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase




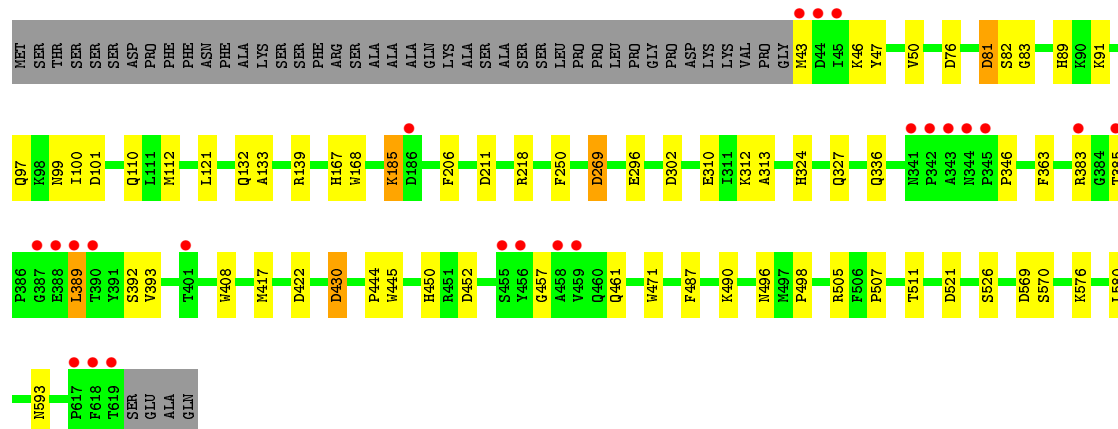
• Molecule 1: Pyranose oxidase




GLU  
ALA  
GLN

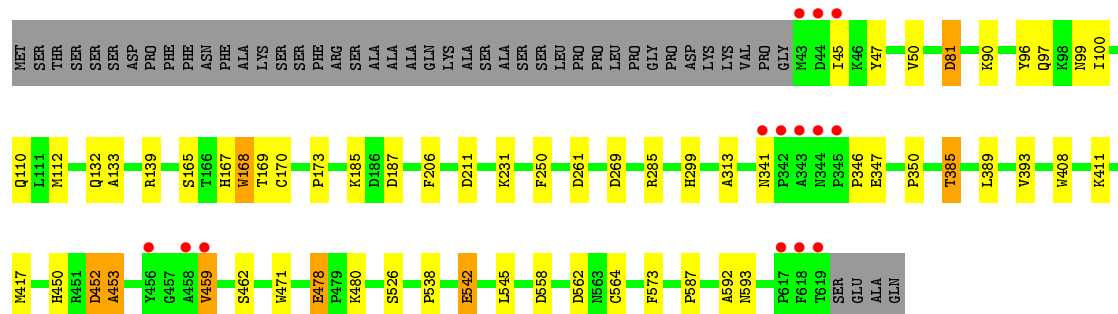
• Molecule 1: Pyranose oxidase

Chain G: 



• Molecule 1: Pyranose oxidase

Chain H: 



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 168.78Å 103.86Å 169.26Å<br>90.00° 106.36° 90.00°            | Depositor        |
| Resolution (Å)  | 39.20 – 1.80<br>39.17 – 1.80                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (39.20-1.80)<br>99.9 (39.17-1.80)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.08  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.40 (at 1.79Å)   | Xtriage          |
| Refinement program  | REFMAC 5.1.24   | Depositor        |
| R, $R_{free}$   | 0.177 , 0.214<br>0.177 , 0.214                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5182 reflections (1.01%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 19.1  | Xtriage          |
| Anisotropy  | 0.223   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 44.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | 0.017 for l,-k,h  | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 39837   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 23.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.94% 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: FAD, MES

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     | 1.01         | 3/4665 (0.1%)   | 0.95        | 13/6343 (0.2%)   |
| 1   | B     | 0.97         | 3/4665 (0.1%)   | 0.98        | 15/6343 (0.2%)   |
| 1   | C     | 0.87         | 0/4665          | 0.91        | 13/6343 (0.2%)   |
| 1   | D     | 0.90         | 2/4665 (0.0%)   | 0.91        | 12/6343 (0.2%)   |
| 1   | E     | 0.89         | 0/4665          | 0.90        | 14/6343 (0.2%)   |
| 1   | F     | 0.88         | 1/4665 (0.0%)   | 0.92        | 14/6343 (0.2%)   |
| 1   | G     | 0.95         | 1/4665 (0.0%)   | 0.96        | 14/6343 (0.2%)   |
| 1   | H     | 0.96         | 2/4665 (0.0%)   | 0.97        | 13/6343 (0.2%)   |
| All | All   | 0.93         | 12/37320 (0.0%) | 0.94        | 108/50744 (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   | B     | 0                   | 1                   |

All (12) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | B     | 112 | MET  | CB-CG   | 6.50  | 1.72        | 1.51     |
| 1   | D     | 478 | GLU  | CD-OE1  | 5.70  | 1.31        | 1.25     |
| 1   | B     | 205 | TYR  | CD1-CE1 | 5.67  | 1.47        | 1.39     |
| 1   | H     | 96  | TYR  | CD2-CE2 | -5.54 | 1.31        | 1.39     |
| 1   | B     | 175 | PHE  | CE2-CZ  | 5.48  | 1.47        | 1.37     |
| 1   | G     | 81  | ASP  | CA-C    | 5.42  | 1.67        | 1.52     |
| 1   | A     | 482 | GLU  | CD-OE1  | 5.29  | 1.31        | 1.25     |
| 1   | D     | 497 | MET  | SD-CE   | -5.08 | 1.49        | 1.77     |
| 1   | F     | 478 | GLU  | CD-OE1  | 5.08  | 1.31        | 1.25     |
| 1   | A     | 122 | VAL  | CB-CG1  | 5.04  | 1.63        | 1.52     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | H     | 478 | GLU  | CD-OE1 | 5.01 | 1.31        | 1.25     |
| 1   | A     | 478 | GLU  | CD-OE1 | 5.00 | 1.31        | 1.25     |

All (108) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | F     | 139 | ARG  | NE-CZ-NH2 | -19.04 | 110.78      | 120.30   |
| 1   | B     | 139 | ARG  | NE-CZ-NH2 | -15.60 | 112.50      | 120.30   |
| 1   | G     | 139 | ARG  | NE-CZ-NH2 | -14.95 | 112.83      | 120.30   |
| 1   | H     | 389 | LEU  | CA-CB-CG  | 14.62  | 148.93      | 115.30   |
| 1   | B     | 139 | ARG  | NE-CZ-NH1 | 13.94  | 127.27      | 120.30   |
| 1   | F     | 139 | ARG  | NE-CZ-NH1 | 13.24  | 126.92      | 120.30   |
| 1   | D     | 139 | ARG  | NE-CZ-NH2 | -12.78 | 113.91      | 120.30   |
| 1   | C     | 139 | ARG  | NE-CZ-NH2 | -12.73 | 113.93      | 120.30   |
| 1   | E     | 139 | ARG  | NE-CZ-NH2 | -12.48 | 114.06      | 120.30   |
| 1   | G     | 81  | ASP  | CB-CG-OD2 | 12.41  | 129.47      | 118.30   |
| 1   | G     | 139 | ARG  | NE-CZ-NH1 | 12.41  | 126.50      | 120.30   |
| 1   | A     | 139 | ARG  | NE-CZ-NH2 | -11.97 | 114.31      | 120.30   |
| 1   | E     | 81  | ASP  | CB-CG-OD2 | 11.83  | 128.95      | 118.30   |
| 1   | B     | 81  | ASP  | CB-CG-OD2 | 11.81  | 128.93      | 118.30   |
| 1   | C     | 81  | ASP  | CB-CG-OD2 | 11.55  | 128.70      | 118.30   |
| 1   | H     | 139 | ARG  | NE-CZ-NH2 | -11.17 | 114.72      | 120.30   |
| 1   | A     | 81  | ASP  | CB-CG-OD2 | 11.03  | 128.23      | 118.30   |
| 1   | C     | 139 | ARG  | NE-CZ-NH1 | 10.69  | 125.64      | 120.30   |
| 1   | H     | 81  | ASP  | CB-CG-OD2 | 10.63  | 127.87      | 118.30   |
| 1   | H     | 81  | ASP  | CB-CG-OD1 | -10.23 | 109.09      | 118.30   |
| 1   | D     | 81  | ASP  | CB-CG-OD2 | 10.16  | 127.44      | 118.30   |
| 1   | D     | 139 | ARG  | NE-CZ-NH1 | 9.48   | 125.04      | 120.30   |
| 1   | G     | 81  | ASP  | CB-CG-OD1 | -9.15  | 110.06      | 118.30   |
| 1   | F     | 76  | ASP  | CB-CG-OD2 | 9.08   | 126.47      | 118.30   |
| 1   | F     | 81  | ASP  | CB-CG-OD2 | 9.00   | 126.40      | 118.30   |
| 1   | A     | 81  | ASP  | CB-CG-OD1 | -8.92  | 110.27      | 118.30   |
| 1   | B     | 81  | ASP  | CB-CG-OD1 | -8.70  | 110.47      | 118.30   |
| 1   | G     | 76  | ASP  | CB-CG-OD2 | 8.29   | 125.76      | 118.30   |
| 1   | E     | 81  | ASP  | CB-CG-OD1 | -8.18  | 110.94      | 118.30   |
| 1   | H     | 389 | LEU  | CB-CG-CD2 | -7.85  | 97.66       | 111.00   |
| 1   | D     | 302 | ASP  | CB-CG-OD2 | 7.67   | 125.20      | 118.30   |
| 1   | E     | 139 | ARG  | NE-CZ-NH1 | 7.54   | 124.07      | 120.30   |
| 1   | H     | 139 | ARG  | NE-CZ-NH1 | 7.27   | 123.94      | 120.30   |
| 1   | A     | 139 | ARG  | NE-CZ-NH1 | 7.14   | 123.87      | 120.30   |
| 1   | C     | 81  | ASP  | CB-CG-OD1 | -7.08  | 111.93      | 118.30   |
| 1   | H     | 211 | ASP  | CB-CG-OD1 | 7.07   | 124.66      | 118.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 389 | LEU  | CB-CG-CD1  | 6.99  | 122.89      | 111.00   |
| 1   | A     | 186 | ASP  | CB-CG-OD2  | 6.96  | 124.56      | 118.30   |
| 1   | G     | 211 | ASP  | CB-CG-OD1  | 6.84  | 124.46      | 118.30   |
| 1   | B     | 406 | ASP  | CB-CG-OD1  | 6.75  | 124.37      | 118.30   |
| 1   | E     | 521 | ASP  | CB-CG-OD2  | 6.73  | 124.35      | 118.30   |
| 1   | E     | 374 | ASP  | CB-CG-OD2  | 6.72  | 124.35      | 118.30   |
| 1   | F     | 44  | ASP  | CB-CG-OD2  | 6.67  | 124.30      | 118.30   |
| 1   | A     | 269 | ASP  | CB-CG-OD2  | 6.51  | 124.16      | 118.30   |
| 1   | A     | 422 | ASP  | CB-CG-OD2  | 6.50  | 124.15      | 118.30   |
| 1   | B     | 76  | ASP  | CB-CG-OD2  | 6.45  | 124.10      | 118.30   |
| 1   | F     | 328 | LEU  | CA-CB-CG   | 6.34  | 129.89      | 115.30   |
| 1   | B     | 489 | ASP  | CB-CG-OD1  | 6.31  | 123.98      | 118.30   |
| 1   | G     | 101 | ASP  | CB-CG-OD2  | 6.24  | 123.92      | 118.30   |
| 1   | C     | 558 | ASP  | CB-CG-OD2  | 6.17  | 123.85      | 118.30   |
| 1   | B     | 503 | ASP  | CB-CG-OD2  | 6.12  | 123.80      | 118.30   |
| 1   | A     | 389 | LEU  | CA-CB-CG   | 6.06  | 129.25      | 115.30   |
| 1   | C     | 562 | ASP  | CB-CG-OD2  | 6.01  | 123.71      | 118.30   |
| 1   | D     | 517 | ASP  | CB-CG-OD2  | 6.00  | 123.70      | 118.30   |
| 1   | D     | 76  | ASP  | CB-CG-OD2  | 5.99  | 123.69      | 118.30   |
| 1   | D     | 81  | ASP  | CB-CG-OD1  | -5.94 | 112.95      | 118.30   |
| 1   | H     | 562 | ASP  | CB-CG-OD2  | 5.94  | 123.64      | 118.30   |
| 1   | C     | 541 | MET  | CG-SD-CE   | 5.93  | 109.69      | 100.20   |
| 1   | F     | 81  | ASP  | CB-CG-OD1  | -5.92 | 112.97      | 118.30   |
| 1   | G     | 269 | ASP  | CB-CG-OD2  | 5.92  | 123.62      | 118.30   |
| 1   | B     | 517 | ASP  | CB-CG-OD2  | 5.91  | 123.62      | 118.30   |
| 1   | A     | 211 | ASP  | CB-CG-OD1  | 5.87  | 123.58      | 118.30   |
| 1   | G     | 521 | ASP  | CB-CG-OD2  | 5.80  | 123.52      | 118.30   |
| 1   | E     | 76  | ASP  | CB-CG-OD2  | 5.79  | 123.51      | 118.30   |
| 1   | H     | 261 | ASP  | CB-CG-OD2  | 5.77  | 123.50      | 118.30   |
| 1   | D     | 489 | ASP  | CB-CG-OD2  | 5.75  | 123.48      | 118.30   |
| 1   | F     | 558 | ASP  | CB-CG-OD2  | 5.75  | 123.48      | 118.30   |
| 1   | B     | 139 | ARG  | CD-NE-CZ   | 5.72  | 131.60      | 123.60   |
| 1   | G     | 569 | ASP  | CB-CG-OD2  | 5.65  | 123.39      | 118.30   |
| 1   | E     | 452 | ASP  | CB-CG-OD2  | 5.56  | 123.31      | 118.30   |
| 1   | D     | 521 | ASP  | CB-CG-OD2  | 5.52  | 123.27      | 118.30   |
| 1   | E     | 558 | ASP  | CB-CG-OD2  | 5.50  | 123.25      | 118.30   |
| 1   | H     | 385 | THR  | OG1-CB-CG2 | -5.48 | 97.41       | 110.00   |
| 1   | G     | 452 | ASP  | CB-CG-OD2  | 5.43  | 123.18      | 118.30   |
| 1   | C     | 314 | ASP  | CB-CG-OD1  | 5.41  | 123.17      | 118.30   |
| 1   | H     | 558 | ASP  | CB-CG-OD2  | 5.41  | 123.17      | 118.30   |
| 1   | C     | 374 | ASP  | CB-CG-OD2  | 5.40  | 123.16      | 118.30   |
| 1   | B     | 261 | ASP  | CB-CG-OD1  | 5.40  | 123.16      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 187 | ASP  | CB-CG-OD2 | 5.37  | 123.13      | 118.30   |
| 1   | E     | 302 | ASP  | CB-CG-OD2 | 5.36  | 123.12      | 118.30   |
| 1   | B     | 101 | ASP  | CB-CG-OD2 | 5.34  | 123.11      | 118.30   |
| 1   | F     | 374 | ASP  | CB-CG-OD2 | 5.33  | 123.10      | 118.30   |
| 1   | E     | 422 | ASP  | CB-CG-OD2 | 5.32  | 123.08      | 118.30   |
| 1   | A     | 302 | ASP  | CB-CG-OD2 | 5.31  | 123.08      | 118.30   |
| 1   | D     | 558 | ASP  | CB-CG-OD2 | 5.31  | 123.08      | 118.30   |
| 1   | F     | 186 | ASP  | CB-CG-OD2 | 5.29  | 123.06      | 118.30   |
| 1   | G     | 430 | ASP  | CB-CG-OD2 | 5.27  | 123.04      | 118.30   |
| 1   | F     | 269 | ASP  | CB-CG-OD2 | 5.21  | 122.99      | 118.30   |
| 1   | G     | 302 | ASP  | CB-CG-OD2 | 5.21  | 122.99      | 118.30   |
| 1   | G     | 422 | ASP  | CB-CG-OD2 | 5.20  | 122.98      | 118.30   |
| 1   | A     | 139 | ARG  | CG-CD-NE  | -5.18 | 100.92      | 111.80   |
| 1   | A     | 430 | ASP  | CB-CG-OD2 | 5.17  | 122.96      | 118.30   |
| 1   | C     | 379 | ASP  | CB-CG-OD2 | 5.17  | 122.95      | 118.30   |
| 1   | E     | 44  | ASP  | CB-CG-OD2 | 5.16  | 122.94      | 118.30   |
| 1   | F     | 139 | ARG  | CD-NE-CZ  | 5.14  | 130.80      | 123.60   |
| 1   | F     | 503 | ASP  | CB-CG-OD2 | 5.14  | 122.92      | 118.30   |
| 1   | E     | 470 | ASP  | CB-CG-OD1 | 5.12  | 122.91      | 118.30   |
| 1   | B     | 211 | ASP  | CB-CG-OD1 | 5.08  | 122.88      | 118.30   |
| 1   | B     | 196 | ASP  | CB-CG-OD1 | 5.08  | 122.87      | 118.30   |
| 1   | C     | 186 | ASP  | CB-CG-OD2 | 5.08  | 122.87      | 118.30   |
| 1   | F     | 235 | ASP  | CB-CG-OD2 | 5.08  | 122.87      | 118.30   |
| 1   | A     | 452 | ASP  | CB-CG-OD2 | 5.08  | 122.87      | 118.30   |
| 1   | D     | 430 | ASP  | CB-CG-OD2 | 5.06  | 122.86      | 118.30   |
| 1   | D     | 541 | MET  | CG-SD-CE  | 5.04  | 108.27      | 100.20   |
| 1   | C     | 430 | ASP  | CB-CG-OD2 | 5.04  | 122.83      | 118.30   |
| 1   | C     | 76  | ASP  | CB-CG-OD2 | 5.03  | 122.83      | 118.30   |
| 1   | H     | 269 | ASP  | CB-CG-OD2 | 5.02  | 122.82      | 118.30   |
| 1   | E     | 430 | ASP  | CB-CG-OD2 | 5.01  | 122.81      | 118.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B     | 553 | HIS  | 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     | 4549  | 0        | 4395     | 37      | 0            |
| 1   | B     | 4549  | 0        | 4395     | 53      | 0            |
| 1   | C     | 4549  | 0        | 4395     | 44      | 0            |
| 1   | D     | 4549  | 0        | 4395     | 37      | 0            |
| 1   | E     | 4549  | 0        | 4395     | 68      | 1            |
| 1   | F     | 4549  | 0        | 4395     | 52      | 0            |
| 1   | G     | 4549  | 0        | 4395     | 57      | 0            |
| 1   | H     | 4549  | 0        | 4395     | 48      | 0            |
| 2   | A     | 53    | 0        | 31       | 8       | 0            |
| 2   | B     | 53    | 0        | 31       | 8       | 0            |
| 2   | C     | 53    | 0        | 31       | 4       | 0            |
| 2   | D     | 53    | 0        | 31       | 6       | 0            |
| 2   | E     | 53    | 0        | 31       | 7       | 0            |
| 2   | F     | 53    | 0        | 30       | 3       | 0            |
| 2   | G     | 53    | 0        | 30       | 0       | 0            |
| 2   | H     | 53    | 0        | 30       | 3       | 0            |
| 3   | A     | 12    | 0        | 13       | 9       | 0            |
| 3   | B     | 12    | 0        | 13       | 15      | 0            |
| 3   | C     | 12    | 0        | 13       | 12      | 0            |
| 3   | D     | 12    | 0        | 13       | 14      | 0            |
| 3   | E     | 24    | 0        | 26       | 13      | 0            |
| 3   | G     | 12    | 0        | 13       | 13      | 0            |
| 3   | H     | 12    | 0        | 13       | 13      | 0            |
| 4   | A     | 417   | 0        | 0        | 4       | 0            |
| 4   | B     | 418   | 0        | 0        | 6       | 0            |
| 4   | C     | 307   | 0        | 0        | 3       | 0            |
| 4   | D     | 354   | 0        | 0        | 2       | 1            |
| 4   | E     | 336   | 0        | 0        | 14      | 0            |
| 4   | F     | 318   | 0        | 0        | 9       | 0            |
| 4   | G     | 379   | 0        | 0        | 21      | 0            |
| 4   | H     | 396   | 0        | 0        | 5       | 0            |
| All | All   | 39837 | 0        | 35509    | 379     | 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 5.

All (379) 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:D:167:HIS:HE2  | 2:D:801:FAD:C8M  | 0.98                     | 1.61              |
| 1:A:167:HIS:HE2  | 2:A:801:FAD:C8M  | 0.98                     | 1.58              |
| 1:C:167:HIS:HE2  | 2:C:801:FAD:C8M  | 0.91                     | 1.56              |
| 1:E:167:HIS:HE2  | 2:E:801:FAD:C8M  | 0.92                     | 1.56              |
| 1:B:167:HIS:HE2  | 2:B:801:FAD:C8M  | 0.92                     | 1.55              |
| 1:D:133:ALA:HB3  | 3:D:903:MES:C7   | 1.51                     | 1.39              |
| 1:H:133:ALA:HB3  | 3:H:907:MES:C7   | 1.58                     | 1.31              |
| 1:A:167:HIS:NE2  | 2:A:801:FAD:HM82 | 0.97                     | 1.28              |
| 1:B:167:HIS:NE2  | 2:B:801:FAD:HM82 | 0.94                     | 1.27              |
| 1:D:167:HIS:NE2  | 2:D:801:FAD:HM82 | 0.93                     | 1.24              |
| 1:H:133:ALA:CB   | 3:H:907:MES:C7   | 2.15                     | 1.24              |
| 1:E:167:HIS:NE2  | 2:E:801:FAD:HM82 | 0.88                     | 1.21              |
| 1:C:167:HIS:CD2  | 2:C:801:FAD:HM82 | 1.76                     | 1.20              |
| 1:C:133:ALA:HB3  | 3:C:904:MES:C7   | 1.72                     | 1.20              |
| 1:G:133:ALA:HB3  | 3:G:908:MES:C7   | 1.72                     | 1.19              |
| 1:B:133:ALA:HB3  | 3:B:901:MES:C7   | 1.73                     | 1.19              |
| 1:A:133:ALA:HB3  | 3:A:902:MES:C7   | 1.73                     | 1.18              |
| 1:C:167:HIS:NE2  | 2:C:801:FAD:HM82 | 0.86                     | 1.18              |
| 1:D:133:ALA:CB   | 3:D:903:MES:C7   | 2.20                     | 1.18              |
| 1:E:133:ALA:HB3  | 3:E:906:MES:C7   | 1.72                     | 1.17              |
| 1:H:133:ALA:CB   | 3:H:907:MES:H72  | 1.72                     | 1.17              |
| 1:C:133:ALA:HB3  | 3:C:904:MES:H72  | 1.17                     | 1.15              |
| 1:D:133:ALA:CB   | 3:D:903:MES:H72  | 1.77                     | 1.14              |
| 1:E:121:LEU:CD2  | 1:F:459:VAL:HA   | 1.76                     | 1.14              |
| 1:D:133:ALA:HB3  | 3:D:903:MES:H71  | 1.32                     | 1.11              |
| 1:E:167:HIS:CD2  | 2:E:801:FAD:HM82 | 1.87                     | 1.09              |
| 1:B:133:ALA:HB3  | 3:B:901:MES:H72  | 1.29                     | 1.09              |
| 1:A:133:ALA:HB3  | 3:A:902:MES:H72  | 1.28                     | 1.08              |
| 1:H:133:ALA:HB3  | 3:H:907:MES:H72  | 1.13                     | 1.08              |
| 1:B:167:HIS:CD2  | 2:B:801:FAD:HM82 | 1.88                     | 1.07              |
| 1:G:133:ALA:HB3  | 3:G:908:MES:H72  | 1.31                     | 1.07              |
| 1:G:133:ALA:CB   | 3:G:908:MES:C7   | 2.32                     | 1.07              |
| 1:E:133:ALA:HB3  | 3:E:906:MES:H72  | 1.37                     | 1.06              |
| 1:G:81:ASP:CA    | 4:G:3105:HOH:O   | 2.03                     | 1.06              |
| 1:D:133:ALA:HB3  | 3:D:903:MES:H72  | 1.11                     | 1.04              |
| 1:B:133:ALA:CB   | 3:B:901:MES:C7   | 2.34                     | 1.03              |
| 1:H:133:ALA:CB   | 3:H:907:MES:H71  | 1.88                     | 1.03              |
| 1:E:121:LEU:HD23 | 1:F:459:VAL:HA   | 1.37                     | 1.03              |
| 1:D:167:HIS:CD2  | 2:D:801:FAD:HM82 | 1.94                     | 1.02              |
| 1:H:133:ALA:HB3  | 3:H:907:MES:H71  | 1.42                     | 1.02              |
| 1:F:81:ASP:HB2   | 4:F:3658:HOH:O   | 1.60                     | 1.01              |
| 1:E:133:ALA:CB   | 3:E:906:MES:C7   | 2.37                     | 1.01              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:133:ALA:HB3  | 3:E:906:MES:H71  | 1.39                     | 1.00              |
| 1:G:133:ALA:CB   | 3:G:908:MES:H72  | 1.90                     | 0.99              |
| 1:A:167:HIS:CD2  | 2:A:801:FAD:HM82 | 1.98                     | 0.98              |
| 1:C:133:ALA:CB   | 3:C:904:MES:C7   | 2.44                     | 0.96              |
| 1:B:167:HIS:HE2  | 2:B:801:FAD:HM81 | 1.25                     | 0.96              |
| 1:G:81:ASP:CA    | 4:G:3782:HOH:O   | 2.14                     | 0.95              |
| 1:G:110:GLN:HE21 | 1:G:167:HIS:HD1  | 1.15                     | 0.95              |
| 1:C:133:ALA:CB   | 3:C:904:MES:H72  | 1.97                     | 0.95              |
| 1:G:133:ALA:CB   | 3:G:908:MES:H71  | 1.97                     | 0.94              |
| 1:H:393:VAL:H    | 1:H:417:MET:HE1  | 1.33                     | 0.94              |
| 1:B:133:ALA:CB   | 3:B:901:MES:H72  | 1.95                     | 0.93              |
| 1:D:133:ALA:CB   | 3:D:903:MES:H71  | 1.90                     | 0.93              |
| 1:G:133:ALA:HB3  | 3:G:908:MES:H71  | 1.46                     | 0.93              |
| 1:E:133:ALA:CB   | 3:E:906:MES:H72  | 1.98                     | 0.93              |
| 1:E:133:ALA:CB   | 3:E:906:MES:H71  | 1.99                     | 0.92              |
| 1:E:167:HIS:HE2  | 2:E:801:FAD:HM81 | 1.30                     | 0.92              |
| 1:B:393:VAL:H    | 1:B:417:MET:CE   | 1.83                     | 0.92              |
| 1:E:121:LEU:HD21 | 1:F:459:VAL:HG22 | 1.50                     | 0.92              |
| 1:F:110:GLN:HE21 | 1:F:167:HIS:HD1  | 1.11                     | 0.92              |
| 1:G:81:ASP:C     | 4:G:3782:HOH:O   | 2.07                     | 0.91              |
| 1:B:133:ALA:HB3  | 3:B:901:MES:H71  | 1.49                     | 0.91              |
| 4:E:2488:HOH:O   | 1:F:132:GLN:HG2  | 1.69                     | 0.91              |
| 1:B:133:ALA:CB   | 3:B:901:MES:H71  | 2.01                     | 0.90              |
| 1:G:81:ASP:C     | 4:G:3105:HOH:O   | 2.07                     | 0.90              |
| 1:B:393:VAL:H    | 1:B:417:MET:HE2  | 1.35                     | 0.90              |
| 1:A:133:ALA:HB3  | 3:A:902:MES:H71  | 1.53                     | 0.89              |
| 1:D:133:ALA:HB2  | 3:D:903:MES:O1S  | 1.71                     | 0.89              |
| 1:H:133:ALA:HB2  | 3:H:907:MES:C7   | 2.01                     | 0.88              |
| 1:E:167:HIS:CE1  | 2:E:801:FAD:HM82 | 2.03                     | 0.88              |
| 1:C:167:HIS:HE2  | 2:C:801:FAD:HM81 | 1.33                     | 0.88              |
| 1:H:110:GLN:HE21 | 1:H:167:HIS:HD1  | 1.20                     | 0.87              |
| 1:A:167:HIS:CE1  | 2:A:801:FAD:HM82 | 2.09                     | 0.86              |
| 1:G:81:ASP:HA    | 4:G:3782:HOH:O   | 1.70                     | 0.86              |
| 1:A:133:ALA:CB   | 3:A:902:MES:C7   | 2.52                     | 0.85              |
| 1:B:133:ALA:HB2  | 3:B:901:MES:O1S  | 1.77                     | 0.84              |
| 1:B:178:GLU:HG3  | 4:B:3228:HOH:O   | 1.77                     | 0.83              |
| 1:D:393:VAL:H    | 1:D:417:MET:HE2  | 1.42                     | 0.83              |
| 1:G:82:SER:N     | 4:G:3782:HOH:O   | 2.10                     | 0.83              |
| 1:A:167:HIS:HE2  | 2:A:801:FAD:HM81 | 1.39                     | 0.83              |
| 1:C:133:ALA:HB3  | 3:C:904:MES:H71  | 1.60                     | 0.82              |
| 1:E:81:ASP:HA    | 4:F:3642:HOH:O   | 1.78                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:83:GLY:N     | 4:F:3642:HOH:O   | 2.13                     | 0.82              |
| 1:F:83:GLY:HA2   | 4:F:3642:HOH:O   | 1.79                     | 0.81              |
| 1:D:167:HIS:CE1  | 2:D:801:FAD:HM82 | 2.08                     | 0.81              |
| 1:E:393:VAL:H    | 1:E:417:MET:HE1  | 1.45                     | 0.81              |
| 1:G:133:ALA:HB2  | 3:G:908:MES:O1S  | 1.81                     | 0.80              |
| 1:G:505:ARG:NH2  | 4:G:3175:HOH:O   | 2.14                     | 0.80              |
| 1:E:393:VAL:H    | 1:E:417:MET:CE   | 1.95                     | 0.80              |
| 1:G:83:GLY:N     | 4:G:2294:HOH:O   | 1.97                     | 0.79              |
| 1:B:167:HIS:CE1  | 2:B:801:FAD:HM82 | 2.10                     | 0.79              |
| 4:C:3530:HOH:O   | 1:D:81:ASP:HA    | 1.83                     | 0.78              |
| 4:E:3661:HOH:O   | 1:F:81:ASP:HA    | 1.85                     | 0.77              |
| 1:G:393:VAL:H    | 1:G:417:MET:CE   | 1.98                     | 0.77              |
| 1:E:133:ALA:HB2  | 3:E:906:MES:O1S  | 1.85                     | 0.76              |
| 1:F:538:PRO:HG2  | 1:H:538:PRO:HG2  | 1.67                     | 0.76              |
| 1:F:97:GLN:HG3   | 1:F:250:PHE:CD2  | 2.20                     | 0.76              |
| 1:A:133:ALA:CB   | 3:A:902:MES:H72  | 2.12                     | 0.76              |
| 1:C:393:VAL:H    | 1:C:417:MET:HE1  | 1.52                     | 0.74              |
| 1:F:167:HIS:CD2  | 2:F:801:FAD:C8M  | 2.67                     | 0.74              |
| 3:E:906:MES:H52  | 4:E:2112:HOH:O   | 1.87                     | 0.74              |
| 1:E:121:LEU:HD21 | 1:F:459:VAL:CG2  | 2.17                     | 0.73              |
| 1:G:393:VAL:H    | 1:G:417:MET:HE2  | 1.53                     | 0.73              |
| 1:B:576:LYS:HG3  | 4:B:3770:HOH:O   | 1.89                     | 0.73              |
| 1:E:121:LEU:CD2  | 1:F:459:VAL:CA   | 2.63                     | 0.72              |
| 1:D:133:ALA:HB2  | 3:D:903:MES:C7   | 2.19                     | 0.72              |
| 1:H:167:HIS:CD2  | 2:H:801:FAD:C8M  | 2.71                     | 0.72              |
| 1:G:97:GLN:HG3   | 1:G:250:PHE:CD2  | 2.24                     | 0.72              |
| 1:F:83:GLY:CA    | 4:F:3642:HOH:O   | 2.33                     | 0.71              |
| 1:A:133:ALA:HB2  | 3:A:902:MES:O1S  | 1.89                     | 0.71              |
| 1:H:133:ALA:HB2  | 3:H:907:MES:O1S  | 1.91                     | 0.71              |
| 1:A:100:ILE:HD13 | 1:A:100:ILE:O    | 1.92                     | 0.70              |
| 1:E:541:MET:HE2  | 1:E:541:MET:HA   | 1.74                     | 0.70              |
| 1:G:133:ALA:HB2  | 3:G:908:MES:C7   | 2.21                     | 0.70              |
| 3:C:904:MES:H52  | 4:C:1926:HOH:O   | 1.91                     | 0.69              |
| 1:B:133:ALA:HB2  | 3:B:901:MES:C7   | 2.23                     | 0.69              |
| 3:G:908:MES:H52  | 4:G:1962:HOH:O   | 1.93                     | 0.68              |
| 1:G:97:GLN:HG3   | 1:G:250:PHE:CE2  | 2.28                     | 0.68              |
| 1:F:97:GLN:HG3   | 1:F:250:PHE:CE2  | 2.29                     | 0.68              |
| 1:G:132:GLN:HG2  | 4:G:3160:HOH:O   | 1.93                     | 0.68              |
| 1:D:393:VAL:H    | 1:D:417:MET:CE   | 2.06                     | 0.68              |
| 1:G:81:ASP:O     | 4:G:3105:HOH:O   | 2.10                     | 0.67              |
| 1:G:83:GLY:CA    | 4:G:2294:HOH:O   | 2.39                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:167:HIS:HE2  | 2:D:801:FAD:HM81 | 1.43                     | 0.67              |
| 1:G:99:ASN:CB    | 1:H:112:MET:HE1  | 2.25                     | 0.67              |
| 1:A:167:HIS:HE2  | 2:A:801:FAD:C8   | 2.00                     | 0.67              |
| 1:C:133:ALA:CB   | 3:C:904:MES:H71  | 2.18                     | 0.67              |
| 1:A:133:ALA:CB   | 3:A:902:MES:H71  | 2.21                     | 0.66              |
| 1:G:81:ASP:C     | 1:G:81:ASP:OD1   | 2.32                     | 0.65              |
| 4:G:2294:HOH:O   | 1:H:81:ASP:HA    | 1.96                     | 0.65              |
| 1:H:393:VAL:H    | 1:H:417:MET:CE   | 2.08                     | 0.65              |
| 1:H:167:HIS:CE1  | 2:H:801:FAD:C8M  | 2.75                     | 0.65              |
| 1:G:81:ASP:HA    | 4:G:3105:HOH:O   | 1.79                     | 0.65              |
| 1:C:393:VAL:H    | 1:C:417:MET:CE   | 2.09                     | 0.64              |
| 1:E:121:LEU:HD21 | 1:F:459:VAL:CB   | 2.28                     | 0.64              |
| 1:G:81:ASP:CB    | 4:G:3105:HOH:O   | 2.39                     | 0.64              |
| 1:E:497:MET:CE   | 4:E:3557:HOH:O   | 2.47                     | 0.63              |
| 1:E:497:MET:HE3  | 4:E:3557:HOH:O   | 1.98                     | 0.63              |
| 1:B:81:ASP:C     | 1:B:81:ASP:OD1   | 2.35                     | 0.63              |
| 1:F:133:ALA:O    | 4:G:3175:HOH:O   | 2.16                     | 0.63              |
| 1:E:121:LEU:CD2  | 1:F:459:VAL:HG22 | 2.27                     | 0.63              |
| 1:F:299:HIS:HB3  | 4:F:3325:HOH:O   | 1.98                     | 0.63              |
| 1:H:167:HIS:NE2  | 2:H:801:FAD:HM81 | 2.00                     | 0.63              |
| 1:E:83:GLY:N     | 4:E:3661:HOH:O   | 2.23                     | 0.63              |
| 3:E:905:MES:H52  | 4:E:2488:HOH:O   | 1.97                     | 0.63              |
| 1:F:541:MET:CE   | 1:F:545:LEU:HD23 | 2.29                     | 0.62              |
| 1:B:457:GLY:O    | 1:B:461:GLN:HG3  | 2.00                     | 0.61              |
| 1:G:336:GLN:HB2  | 1:G:346:PRO:HG3  | 1.83                     | 0.61              |
| 1:C:112:MET:HE1  | 1:D:99:ASN:CB    | 2.31                     | 0.61              |
| 1:H:50:VAL:HG13  | 1:H:313:ALA:HB2  | 1.83                     | 0.61              |
| 1:G:392:SER:HA   | 1:G:417:MET:HE1  | 1.83                     | 0.60              |
| 3:C:904:MES:H21  | 1:D:462:SER:OG   | 2.01                     | 0.60              |
| 1:G:133:ALA:HB2  | 3:G:908:MES:H71  | 1.79                     | 0.60              |
| 1:F:81:ASP:CA    | 4:F:3658:HOH:O   | 2.50                     | 0.60              |
| 1:E:89:HIS:CE1   | 1:E:91:LYS:HG2   | 2.36                     | 0.60              |
| 1:C:133:ALA:HB2  | 3:C:904:MES:O1S  | 2.01                     | 0.59              |
| 1:C:462:SER:OG   | 3:D:903:MES:H21  | 2.03                     | 0.58              |
| 1:A:462:SER:OG   | 3:B:901:MES:H21  | 2.04                     | 0.58              |
| 1:F:167:HIS:CE1  | 2:F:801:FAD:C8M  | 2.76                     | 0.58              |
| 1:G:83:GLY:HA2   | 4:G:2294:HOH:O   | 2.02                     | 0.58              |
| 1:H:393:VAL:N    | 1:H:417:MET:HE1  | 2.10                     | 0.58              |
| 1:C:97:GLN:HG3   | 1:C:250:PHE:CD2  | 2.38                     | 0.58              |
| 1:B:393:VAL:H    | 1:B:417:MET:HE1  | 1.64                     | 0.57              |
| 3:D:903:MES:H52  | 4:D:1743:HOH:O   | 2.04                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:133:ALA:HB2  | 3:E:906:MES:C7   | 2.30                     | 0.57              |
| 3:E:905:MES:H32  | 3:E:905:MES:O3S  | 2.05                     | 0.57              |
| 1:E:121:LEU:HD21 | 1:F:459:VAL:HG13 | 1.87                     | 0.57              |
| 1:B:393:VAL:N    | 1:B:417:MET:HE2  | 2.12                     | 0.56              |
| 1:E:167:HIS:CE1  | 2:E:801:FAD:C8M  | 2.77                     | 0.56              |
| 1:B:167:HIS:HE2  | 2:B:801:FAD:C8   | 1.99                     | 0.56              |
| 1:B:45:ILE:H     | 1:B:45:ILE:HD12  | 1.71                     | 0.56              |
| 1:H:417:MET:CE   | 4:H:3504:HOH:O   | 2.54                     | 0.55              |
| 1:H:133:ALA:HB2  | 3:H:907:MES:C8   | 2.36                     | 0.55              |
| 1:E:421:GLU:H    | 1:E:421:GLU:CD   | 2.08                     | 0.55              |
| 1:D:133:ALA:HB2  | 3:D:903:MES:H71  | 1.84                     | 0.55              |
| 1:E:393:VAL:N    | 1:E:417:MET:HE1  | 2.20                     | 0.55              |
| 1:A:457:GLY:H    | 1:A:460:GLN:HE21 | 1.52                     | 0.55              |
| 1:H:346:PRO:HG2  | 1:H:350:PRO:HA   | 1.89                     | 0.55              |
| 1:F:541:MET:HE3  | 1:F:545:LEU:HD23 | 1.88                     | 0.55              |
| 1:G:296:GLU:O    | 1:G:312:LYS:HE3  | 2.08                     | 0.54              |
| 1:G:81:ASP:HB2   | 4:G:3105:HOH:O   | 2.02                     | 0.54              |
| 1:D:50:VAL:HG13  | 1:D:313:ALA:HB2  | 1.90                     | 0.54              |
| 1:H:81:ASP:O     | 1:H:90:LYS:HE2   | 2.08                     | 0.54              |
| 1:C:393:VAL:N    | 1:C:417:MET:HE1  | 2.21                     | 0.53              |
| 1:D:97:GLN:HG3   | 1:D:250:PHE:CD2  | 2.42                     | 0.53              |
| 1:B:97:GLN:HG3   | 1:B:250:PHE:CD2  | 2.43                     | 0.53              |
| 1:E:97:GLN:HG3   | 1:E:250:PHE:CE2  | 2.43                     | 0.53              |
| 1:H:133:ALA:HB2  | 3:H:907:MES:H71  | 1.71                     | 0.53              |
| 1:H:564:CYS:HG   | 1:H:573:PHE:HE2  | 1.57                     | 0.53              |
| 1:D:393:VAL:N    | 1:D:417:MET:HE2  | 2.19                     | 0.53              |
| 1:B:389:LEU:HD13 | 1:B:389:LEU:H    | 1.74                     | 0.52              |
| 1:B:538:PRO:HG2  | 1:D:538:PRO:HG2  | 1.90                     | 0.52              |
| 1:E:459:VAL:HG12 | 1:F:123:VAL:HG22 | 1.92                     | 0.52              |
| 1:G:112:MET:HE1  | 1:H:99:ASN:CB    | 2.38                     | 0.52              |
| 1:F:346:PRO:HG2  | 1:F:350:PRO:HA   | 1.91                     | 0.52              |
| 1:A:149:LEU:HD22 | 3:D:903:MES:H51  | 1.92                     | 0.52              |
| 1:A:81:ASP:O     | 1:A:90:LYS:HE2   | 2.09                     | 0.51              |
| 3:C:904:MES:O3S  | 3:C:904:MES:H32  | 2.10                     | 0.51              |
| 1:E:618:PHE:CD1  | 1:E:618:PHE:C    | 2.84                     | 0.51              |
| 1:E:97:GLN:HG3   | 1:E:250:PHE:CD2  | 2.45                     | 0.51              |
| 1:E:169:THR:O    | 1:E:170:CYS:HB2  | 2.11                     | 0.51              |
| 1:D:167:HIS:CE1  | 2:D:801:FAD:C8M  | 2.83                     | 0.51              |
| 1:G:487:PHE:HB3  | 1:G:498:PRO:HB2  | 1.93                     | 0.51              |
| 3:B:901:MES:H52  | 4:B:2032:HOH:O   | 2.10                     | 0.51              |
| 1:B:167:HIS:CE1  | 2:B:801:FAD:C8M  | 2.81                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:618:PHE:HD1  | 1:E:618:PHE:C    | 2.15                     | 0.50              |
| 1:H:417:MET:HE2  | 4:H:3504:HOH:O   | 2.10                     | 0.50              |
| 1:B:133:ALA:HB2  | 3:B:901:MES:H71  | 1.84                     | 0.50              |
| 1:G:393:VAL:H    | 1:G:417:MET:HE1  | 1.72                     | 0.50              |
| 1:B:218:ARG:HD2  | 4:B:1194:HOH:O   | 2.12                     | 0.50              |
| 1:C:324:HIS:HD2  | 1:C:327:GLN:OE1  | 1.94                     | 0.50              |
| 1:B:167:HIS:NE2  | 2:B:801:FAD:C8   | 2.66                     | 0.50              |
| 1:G:112:MET:HE1  | 1:H:99:ASN:HB3   | 1.94                     | 0.50              |
| 3:G:908:MES:H21  | 1:H:462:SER:OG   | 2.10                     | 0.50              |
| 1:A:81:ASP:OD1   | 1:A:81:ASP:C     | 2.50                     | 0.49              |
| 1:D:158:THR:HG22 | 1:D:160:VAL:HG22 | 1.94                     | 0.49              |
| 1:C:389:LEU:N    | 1:C:389:LEU:HD13 | 2.28                     | 0.49              |
| 1:D:497:MET:HA   | 1:D:497:MET:HE3  | 1.94                     | 0.49              |
| 1:C:133:ALA:HB2  | 3:C:904:MES:C7   | 2.39                     | 0.49              |
| 1:E:121:LEU:HD21 | 1:F:459:VAL:CG1  | 2.43                     | 0.49              |
| 1:F:285:ARG:HA   | 1:F:328:LEU:HD13 | 1.95                     | 0.49              |
| 1:H:459:VAL:O    | 1:H:462:SER:HB3  | 2.13                     | 0.49              |
| 1:D:178:GLU:CD   | 1:D:439:PHE:HE1  | 2.16                     | 0.49              |
| 1:E:121:LEU:HD23 | 1:F:459:VAL:CA   | 2.27                     | 0.49              |
| 1:G:324:HIS:HD2  | 1:G:327:GLN:OE1  | 1.96                     | 0.49              |
| 1:G:324:HIS:CE1  | 4:G:2467:HOH:O   | 2.66                     | 0.48              |
| 1:A:497:MET:CE   | 4:A:3235:HOH:O   | 2.60                     | 0.48              |
| 1:E:392:SER:HA   | 1:E:417:MET:HE3  | 1.95                     | 0.48              |
| 1:E:176:ASP:OD2  | 1:E:178:GLU:OE2  | 2.31                     | 0.48              |
| 3:B:901:MES:H51  | 1:C:149:LEU:HD22 | 1.96                     | 0.48              |
| 1:B:97:GLN:HG3   | 1:B:250:PHE:CE2  | 2.49                     | 0.48              |
| 1:F:89:HIS:CE1   | 1:F:91:LYS:HB2   | 2.49                     | 0.48              |
| 1:A:538:PRO:HG2  | 1:C:538:PRO:HG2  | 1.95                     | 0.48              |
| 1:B:157:VAL:HG21 | 1:B:324:HIS:HE1  | 1.79                     | 0.48              |
| 1:E:619:THR:HG22 | 4:E:2505:HOH:O   | 2.12                     | 0.48              |
| 1:F:100:ILE:HG22 | 4:F:3798:HOH:O   | 2.14                     | 0.47              |
| 1:H:165:SER:HA   | 1:H:168:TRP:CD1  | 2.49                     | 0.47              |
| 1:G:457:GLY:O    | 1:G:461:GLN:HG3  | 2.14                     | 0.47              |
| 3:C:904:MES:H31  | 3:C:904:MES:H82  | 1.56                     | 0.47              |
| 1:G:444:PRO:HD2  | 1:G:445:TRP:CZ3  | 2.49                     | 0.47              |
| 3:G:908:MES:H32  | 3:G:908:MES:O3S  | 2.15                     | 0.47              |
| 1:F:81:ASP:CB    | 4:F:3658:HOH:O   | 2.32                     | 0.47              |
| 1:G:471:TRP:CH2  | 1:G:526:SER:HA   | 2.49                     | 0.47              |
| 1:A:389:LEU:H    | 1:A:389:LEU:HD13 | 1.80                     | 0.47              |
| 1:C:459:VAL:O    | 1:C:462:SER:CB   | 2.63                     | 0.47              |
| 1:H:478:GLU:OE2  | 1:H:480:LYS:HE2  | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:167:HIS:CE1  | 2:A:801:FAD:C8M  | 2.81                     | 0.47              |
| 1:G:50:VAL:HG13  | 1:G:313:ALA:HB2  | 1.97                     | 0.47              |
| 1:B:346:PRO:HG2  | 1:B:350:PRO:HA   | 1.97                     | 0.47              |
| 1:F:50:VAL:HG13  | 1:F:313:ALA:HB2  | 1.96                     | 0.47              |
| 1:G:576:LYS:HG2  | 4:G:2971:HOH:O   | 2.15                     | 0.47              |
| 1:A:538:PRO:HG2  | 1:C:538:PRO:CG   | 2.44                     | 0.47              |
| 1:E:284:GLU:HA   | 1:E:497:MET:CE   | 2.45                     | 0.46              |
| 1:F:56:PRO:HD3   | 1:F:165:SER:HB3  | 1.96                     | 0.46              |
| 1:G:507:PRO:HD2  | 1:G:511:THR:HG21 | 1.95                     | 0.46              |
| 1:C:459:VAL:O    | 1:C:462:SER:HB3  | 2.15                     | 0.46              |
| 1:E:99:ASN:CB    | 1:F:112:MET:HE1  | 2.45                     | 0.46              |
| 1:H:47:TYR:O     | 1:H:313:ALA:HA   | 2.16                     | 0.46              |
| 1:C:47:TYR:O     | 1:C:313:ALA:HA   | 2.15                     | 0.46              |
| 1:E:157:VAL:HG21 | 1:E:324:HIS:HE1  | 1.81                     | 0.46              |
| 1:E:618:PHE:HD1  | 1:E:619:THR:N    | 2.12                     | 0.46              |
| 1:E:133:ALA:HB2  | 3:E:906:MES:H71  | 1.92                     | 0.46              |
| 1:C:541:MET:CE   | 1:C:541:MET:HA   | 2.46                     | 0.46              |
| 1:D:97:GLN:HG3   | 1:D:250:PHE:CE2  | 2.50                     | 0.46              |
| 1:B:558:ASP:HB3  | 1:B:561:GLU:HB2  | 1.98                     | 0.46              |
| 1:F:538:PRO:HG2  | 1:H:538:PRO:CG   | 2.43                     | 0.46              |
| 1:H:285:ARG:HH22 | 1:H:299:HIS:CE1  | 2.34                     | 0.46              |
| 1:H:478:GLU:CD   | 1:H:480:LYS:HE2  | 2.35                     | 0.46              |
| 1:C:458:ALA:O    | 1:D:121:LEU:HD12 | 2.15                     | 0.46              |
| 1:G:89:HIS:CE1   | 1:G:91:LYS:HB2   | 2.51                     | 0.46              |
| 1:C:97:GLN:HG3   | 1:C:250:PHE:CE2  | 2.52                     | 0.45              |
| 1:E:83:GLY:CA    | 4:E:3661:HOH:O   | 2.64                     | 0.45              |
| 1:H:542:GLU:OE1  | 1:H:545:LEU:HD13 | 2.17                     | 0.45              |
| 1:F:47:TYR:O     | 1:F:313:ALA:HA   | 2.17                     | 0.45              |
| 1:H:97:GLN:HG3   | 1:H:250:PHE:CD2  | 2.52                     | 0.45              |
| 3:E:906:MES:H21  | 1:F:462:SER:OG   | 2.16                     | 0.45              |
| 1:F:541:MET:HE2  | 1:F:545:LEU:HD23 | 1.97                     | 0.45              |
| 1:A:112:MET:HE1  | 1:B:99:ASN:CB    | 2.46                     | 0.45              |
| 1:B:132:GLN:NE2  | 4:B:2718:HOH:O   | 2.41                     | 0.45              |
| 1:B:541:MET:CE   | 1:B:545:LEU:HD23 | 2.47                     | 0.45              |
| 1:F:167:HIS:NE2  | 2:F:801:FAD:HM81 | 2.07                     | 0.45              |
| 3:D:903:MES:H71  | 4:D:1743:HOH:O   | 2.17                     | 0.44              |
| 1:E:194:GLU:CD   | 1:E:197:ARG:HH21 | 2.20                     | 0.44              |
| 1:E:50:VAL:HG13  | 1:E:313:ALA:HB2  | 1.99                     | 0.44              |
| 1:E:497:MET:HE1  | 4:E:3557:HOH:O   | 2.15                     | 0.44              |
| 1:E:393:VAL:H    | 1:E:417:MET:HE3  | 1.81                     | 0.44              |
| 1:H:169:THR:O    | 1:H:170:CYS:HB2  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:149:LEU:HD22 | 3:H:907:MES:H51  | 1.99                     | 0.44              |
| 1:C:83:GLY:N     | 4:C:3530:HOH:O   | 2.27                     | 0.44              |
| 1:C:81:ASP:OD1   | 1:C:81:ASP:C     | 2.54                     | 0.44              |
| 1:F:294:GLU:HG2  | 1:F:295:ILE:N    | 2.32                     | 0.44              |
| 1:H:97:GLN:HG3   | 1:H:250:PHE:CE2  | 2.52                     | 0.44              |
| 1:C:101:ASP:O    | 1:C:104:VAL:HG12 | 2.18                     | 0.43              |
| 1:E:173:PRO:HG2  | 1:E:592:ALA:HB1  | 2.00                     | 0.43              |
| 1:B:47:TYR:O     | 1:B:313:ALA:HA   | 2.18                     | 0.43              |
| 1:D:392:SER:HA   | 1:D:417:MET:HE1  | 2.00                     | 0.43              |
| 1:E:47:TYR:O     | 1:E:313:ALA:HA   | 2.18                     | 0.43              |
| 1:H:173:PRO:HG2  | 1:H:592:ALA:HB1  | 2.00                     | 0.43              |
| 1:C:324:HIS:CD2  | 1:C:327:GLN:OE1  | 2.71                     | 0.43              |
| 1:F:293:SER:HA   | 1:F:574:GLY:O    | 2.18                     | 0.43              |
| 1:G:47:TYR:O     | 1:G:313:ALA:HA   | 2.18                     | 0.43              |
| 3:H:907:MES:H82  | 3:H:907:MES:H31  | 1.36                     | 0.43              |
| 1:A:105:ASN:O    | 1:B:105:ASN:HB3  | 2.19                     | 0.43              |
| 1:B:392:SER:HA   | 1:B:417:MET:HE1  | 2.00                     | 0.43              |
| 1:F:181:PRO:HG3  | 1:F:587:PRO:HD2  | 2.00                     | 0.43              |
| 3:G:908:MES:H31  | 3:G:908:MES:H82  | 1.64                     | 0.43              |
| 1:C:363:PHE:HA   | 1:C:471:TRP:O    | 2.19                     | 0.43              |
| 1:D:153:SER:OG   | 1:D:542:GLU:HG3  | 2.18                     | 0.43              |
| 1:E:346:PRO:HG2  | 1:E:350:PRO:HA   | 1.99                     | 0.43              |
| 1:C:537:LEU:HB3  | 1:C:538:PRO:HD2  | 2.01                     | 0.43              |
| 1:G:389:LEU:N    | 1:G:389:LEU:CD1  | 2.82                     | 0.43              |
| 1:C:346:PRO:HG2  | 1:C:350:PRO:HA   | 2.00                     | 0.43              |
| 1:E:112:MET:HE1  | 1:F:99:ASN:CB    | 2.49                     | 0.43              |
| 1:H:411:LYS:HD3  | 4:H:2747:HOH:O   | 2.18                     | 0.43              |
| 1:B:121:LEU:CD2  | 1:C:121:LEU:CD2  | 2.97                     | 0.42              |
| 1:G:218:ARG:HD2  | 4:G:1363:HOH:O   | 2.19                     | 0.42              |
| 1:A:95:GLU:HG3   | 1:B:112:MET:CE   | 2.49                     | 0.42              |
| 1:E:101:ASP:O    | 1:E:104:VAL:HG12 | 2.19                     | 0.42              |
| 1:E:218:ARG:HD2  | 4:E:1455:HOH:O   | 2.19                     | 0.42              |
| 3:H:907:MES:H52  | 4:H:2336:HOH:O   | 2.18                     | 0.42              |
| 1:A:564:CYS:HG   | 1:A:573:PHE:HE2  | 1.63                     | 0.42              |
| 1:D:157:VAL:HG21 | 1:D:324:HIS:HE1  | 1.84                     | 0.42              |
| 1:F:341:ASN:HD22 | 1:F:342:PRO:HD2  | 1.83                     | 0.42              |
| 1:C:558:ASP:HB3  | 1:C:561:GLU:HB2  | 2.01                     | 0.42              |
| 1:C:112:MET:CE   | 1:D:99:ASN:CG    | 2.87                     | 0.42              |
| 1:B:81:ASP:O     | 1:B:81:ASP:OD1   | 2.38                     | 0.42              |
| 1:A:497:MET:HE1  | 4:A:3235:HOH:O   | 2.19                     | 0.42              |
| 1:G:570:SER:HB3  | 1:G:580:LEU:O    | 2.20                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:452:ASP:O    | 1:H:453:ALA:C    | 2.57                     | 0.42              |
| 1:E:121:LEU:HD12 | 4:E:2793:HOH:O   | 2.20                     | 0.42              |
| 1:A:167:HIS:NE2  | 2:A:801:FAD:C8   | 2.72                     | 0.42              |
| 1:A:339:ARG:HA   | 1:A:340:PRO:HD3  | 1.93                     | 0.42              |
| 1:E:167:HIS:NE2  | 2:E:801:FAD:C8   | 2.71                     | 0.42              |
| 1:A:299:HIS:HB3  | 4:A:2839:HOH:O   | 2.20                     | 0.42              |
| 1:D:532:PHE:CZ   | 1:D:538:PRO:HG3  | 2.55                     | 0.42              |
| 1:F:131:TRP:CH2  | 1:F:133:ALA:HB2  | 2.55                     | 0.42              |
| 1:A:497:MET:HE2  | 4:A:3235:HOH:O   | 2.19                     | 0.41              |
| 1:B:185:LYS:HE3  | 1:B:185:LYS:HB2  | 1.89                     | 0.41              |
| 1:C:471:TRP:CH2  | 1:C:526:SER:HA   | 2.55                     | 0.41              |
| 1:B:339:ARG:HA   | 1:B:340:PRO:HD3  | 1.89                     | 0.41              |
| 3:A:902:MES:H51  | 1:D:149:LEU:HD22 | 2.01                     | 0.41              |
| 1:E:564:CYS:HG   | 1:E:573:PHE:HE2  | 1.66                     | 0.41              |
| 1:G:218:ARG:HG3  | 1:G:430:ASP:OD2  | 2.21                     | 0.41              |
| 1:A:47:TYR:O     | 1:A:313:ALA:HA   | 2.21                     | 0.41              |
| 1:A:95:GLU:HG3   | 1:B:112:MET:HE2  | 2.01                     | 0.41              |
| 1:B:542:GLU:OE1  | 1:B:545:LEU:HD13 | 2.20                     | 0.41              |
| 3:B:901:MES:H71  | 4:B:2032:HOH:O   | 2.20                     | 0.41              |
| 1:F:216:SER:HB3  | 1:F:219:HIS:HB3  | 2.03                     | 0.41              |
| 1:C:444:PRO:HD2  | 1:C:445:TRP:CZ3  | 2.56                     | 0.41              |
| 1:F:618:PHE:CD1  | 1:F:618:PHE:C    | 2.94                     | 0.41              |
| 1:H:471:TRP:CH2  | 1:H:526:SER:HA   | 2.56                     | 0.41              |
| 1:B:444:PRO:HD2  | 1:B:445:TRP:CZ3  | 2.56                     | 0.41              |
| 1:F:157:VAL:HG21 | 1:F:324:HIS:HE1  | 1.86                     | 0.41              |
| 1:G:112:MET:CE   | 1:H:99:ASN:CG    | 2.89                     | 0.41              |
| 1:G:363:PHE:HA   | 1:G:471:TRP:O    | 2.20                     | 0.41              |
| 1:E:83:GLY:HA2   | 4:E:3661:HOH:O   | 2.20                     | 0.41              |
| 1:E:121:LEU:CD2  | 1:F:459:VAL:HG13 | 2.51                     | 0.41              |
| 1:C:112:MET:HE1  | 1:D:99:ASN:CG    | 2.40                     | 0.41              |
| 1:C:169:THR:O    | 1:C:170:CYS:HB2  | 2.21                     | 0.41              |
| 1:D:459:VAL:O    | 1:D:462:SER:HB3  | 2.20                     | 0.41              |
| 1:E:454:PHE:HA   | 4:E:3652:HOH:O   | 2.21                     | 0.41              |
| 1:G:185:LYS:HG2  | 1:G:185:LYS:H    | 1.69                     | 0.41              |
| 1:F:121:LEU:HD21 | 1:G:121:LEU:CD2  | 2.51                     | 0.41              |
| 1:H:285:ARG:NH2  | 1:H:299:HIS:CE1  | 2.89                     | 0.41              |
| 1:B:265:ARG:HA   | 1:B:266:PRO:C    | 2.42                     | 0.40              |
| 1:E:293:SER:HA   | 1:E:574:GLY:O    | 2.21                     | 0.40              |
| 1:B:111:LEU:HD23 | 1:B:111:LEU:HA   | 1.97                     | 0.40              |
| 3:A:902:MES:H21  | 1:B:462:SER:OG   | 2.22                     | 0.40              |
| 1:E:81:ASP:OD1   | 1:E:81:ASP:C     | 2.57                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:99:ASN:CG   | 1:H:112:MET:CE  | 2.90                     | 0.40              |
| 1:A:346:PRO:HG2 | 1:A:350:PRO:HA  | 2.03                     | 0.40              |
| 3:D:903:MES:O3S | 3:D:903:MES:H32 | 2.21                     | 0.40              |
| 1:B:133:ALA:HB2 | 3:B:901:MES:C8  | 2.51                     | 0.40              |
| 1:H:299:HIS:HB3 | 4:H:3326:HOH:O  | 2.20                     | 0.40              |
| 1:A:506:PHE:HA  | 1:A:507:PRO:HD3 | 1.94                     | 0.40              |
| 1:B:570:SER:HB3 | 1:B:580:LEU:O   | 2.21                     | 0.40              |
| 3:B:901:MES:H82 | 3:B:901:MES:H31 | 1.63                     | 0.40              |
| 1:C:541:MET:HE3 | 1:C:541:MET:HA  | 2.04                     | 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) |
|-----------------|-----------------------|--------------------------|-------------------|
| 1:E:291:LEU:CD2 | 4:D:3818:HOH:O[2_665] | 1.77                     | 0.43              |

## 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     | 575/623 (92%)   | 556 (97%)  | 19 (3%)  | 0        | 100         | 100 |
| 1   | B     | 575/623 (92%)   | 562 (98%)  | 12 (2%)  | 1 (0%)   | 51          | 35  |
| 1   | C     | 575/623 (92%)   | 559 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| 1   | D     | 575/623 (92%)   | 561 (98%)  | 14 (2%)  | 0        | 100         | 100 |
| 1   | E     | 575/623 (92%)   | 555 (96%)  | 20 (4%)  | 0        | 100         | 100 |
| 1   | F     | 575/623 (92%)   | 559 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| 1   | G     | 575/623 (92%)   | 557 (97%)  | 17 (3%)  | 1 (0%)   | 51          | 35  |
| 1   | H     | 575/623 (92%)   | 561 (98%)  | 12 (2%)  | 2 (0%)   | 44          | 29  |
| All | All   | 4600/4984 (92%) | 4470 (97%) | 126 (3%) | 4 (0%)   | 55          | 38  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 46  | LYS  |
| 1   | H     | 187 | ASP  |
| 1   | H     | 453 | ALA  |
| 1   | B     | 389 | LEU  |

### 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     | 505/542 (93%)   | 490 (97%)  | 15 (3%)  | 46          | 30 |
| 1   | B     | 505/542 (93%)   | 486 (96%)  | 19 (4%)  | 38          | 21 |
| 1   | C     | 505/542 (93%)   | 487 (96%)  | 18 (4%)  | 40          | 23 |
| 1   | D     | 505/542 (93%)   | 488 (97%)  | 17 (3%)  | 42          | 25 |
| 1   | E     | 505/542 (93%)   | 487 (96%)  | 18 (4%)  | 40          | 23 |
| 1   | F     | 505/542 (93%)   | 487 (96%)  | 18 (4%)  | 40          | 23 |
| 1   | G     | 505/542 (93%)   | 490 (97%)  | 15 (3%)  | 46          | 30 |
| 1   | H     | 505/542 (93%)   | 488 (97%)  | 17 (3%)  | 42          | 25 |
| All | All   | 4040/4336 (93%) | 3903 (97%) | 137 (3%) | 42          | 25 |

All (137) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 100 | ILE  |
| 1   | A     | 168 | TRP  |
| 1   | A     | 185 | LYS  |
| 1   | A     | 206 | PHE  |
| 1   | A     | 312 | LYS  |
| 1   | A     | 347 | GLU  |
| 1   | A     | 389 | LEU  |
| 1   | A     | 392 | SER  |
| 1   | A     | 401 | THR  |
| 1   | A     | 408 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 450 | HIS  |
| 1   | A     | 461 | GLN  |
| 1   | A     | 490 | LYS  |
| 1   | A     | 496 | ASN  |
| 1   | A     | 593 | ASN  |
| 1   | B     | 45  | ILE  |
| 1   | B     | 100 | ILE  |
| 1   | B     | 112 | MET  |
| 1   | B     | 168 | TRP  |
| 1   | B     | 185 | LYS  |
| 1   | B     | 206 | PHE  |
| 1   | B     | 310 | GLU  |
| 1   | B     | 312 | LYS  |
| 1   | B     | 341 | ASN  |
| 1   | B     | 344 | ASN  |
| 1   | B     | 385 | THR  |
| 1   | B     | 389 | LEU  |
| 1   | B     | 408 | TRP  |
| 1   | B     | 413 | LYS  |
| 1   | B     | 450 | HIS  |
| 1   | B     | 490 | LYS  |
| 1   | B     | 496 | ASN  |
| 1   | B     | 593 | ASN  |
| 1   | B     | 619 | THR  |
| 1   | C     | 45  | ILE  |
| 1   | C     | 99  | ASN  |
| 1   | C     | 100 | ILE  |
| 1   | C     | 168 | TRP  |
| 1   | C     | 185 | LYS  |
| 1   | C     | 206 | PHE  |
| 1   | C     | 341 | ASN  |
| 1   | C     | 344 | ASN  |
| 1   | C     | 385 | THR  |
| 1   | C     | 389 | LEU  |
| 1   | C     | 408 | TRP  |
| 1   | C     | 413 | LYS  |
| 1   | C     | 450 | HIS  |
| 1   | C     | 461 | GLN  |
| 1   | C     | 490 | LYS  |
| 1   | C     | 496 | ASN  |
| 1   | C     | 554 | ARG  |
| 1   | C     | 593 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 100 | ILE  |
| 1   | D     | 132 | GLN  |
| 1   | D     | 168 | TRP  |
| 1   | D     | 185 | LYS  |
| 1   | D     | 186 | ASP  |
| 1   | D     | 206 | PHE  |
| 1   | D     | 285 | ARG  |
| 1   | D     | 341 | ASN  |
| 1   | D     | 385 | THR  |
| 1   | D     | 408 | TRP  |
| 1   | D     | 450 | HIS  |
| 1   | D     | 490 | LYS  |
| 1   | D     | 496 | ASN  |
| 1   | D     | 497 | MET  |
| 1   | D     | 554 | ARG  |
| 1   | D     | 587 | PRO  |
| 1   | D     | 593 | ASN  |
| 1   | E     | 45  | ILE  |
| 1   | E     | 100 | ILE  |
| 1   | E     | 168 | TRP  |
| 1   | E     | 185 | LYS  |
| 1   | E     | 206 | PHE  |
| 1   | E     | 231 | LYS  |
| 1   | E     | 340 | PRO  |
| 1   | E     | 341 | ASN  |
| 1   | E     | 344 | ASN  |
| 1   | E     | 347 | GLU  |
| 1   | E     | 385 | THR  |
| 1   | E     | 389 | LEU  |
| 1   | E     | 408 | TRP  |
| 1   | E     | 421 | GLU  |
| 1   | E     | 450 | HIS  |
| 1   | E     | 490 | LYS  |
| 1   | E     | 593 | ASN  |
| 1   | E     | 618 | PHE  |
| 1   | F     | 46  | LYS  |
| 1   | F     | 100 | ILE  |
| 1   | F     | 168 | TRP  |
| 1   | F     | 206 | PHE  |
| 1   | F     | 285 | ARG  |
| 1   | F     | 328 | LEU  |
| 1   | F     | 341 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 385 | THR  |
| 1   | F     | 408 | TRP  |
| 1   | F     | 413 | LYS  |
| 1   | F     | 450 | HIS  |
| 1   | F     | 496 | ASN  |
| 1   | F     | 538 | PRO  |
| 1   | F     | 554 | ARG  |
| 1   | F     | 576 | LYS  |
| 1   | F     | 593 | ASN  |
| 1   | F     | 618 | PHE  |
| 1   | F     | 619 | THR  |
| 1   | G     | 43  | MET  |
| 1   | G     | 100 | ILE  |
| 1   | G     | 168 | TRP  |
| 1   | G     | 185 | LYS  |
| 1   | G     | 206 | PHE  |
| 1   | G     | 269 | ASP  |
| 1   | G     | 310 | GLU  |
| 1   | G     | 383 | ARG  |
| 1   | G     | 385 | THR  |
| 1   | G     | 389 | LEU  |
| 1   | G     | 408 | TRP  |
| 1   | G     | 450 | HIS  |
| 1   | G     | 490 | LYS  |
| 1   | G     | 496 | ASN  |
| 1   | G     | 593 | ASN  |
| 1   | H     | 45  | ILE  |
| 1   | H     | 100 | ILE  |
| 1   | H     | 132 | GLN  |
| 1   | H     | 168 | TRP  |
| 1   | H     | 185 | LYS  |
| 1   | H     | 206 | PHE  |
| 1   | H     | 231 | LYS  |
| 1   | H     | 341 | ASN  |
| 1   | H     | 347 | GLU  |
| 1   | H     | 385 | THR  |
| 1   | H     | 408 | TRP  |
| 1   | H     | 450 | HIS  |
| 1   | H     | 452 | ASP  |
| 1   | H     | 459 | VAL  |
| 1   | H     | 542 | GLU  |
| 1   | H     | 587 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 593 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 132 | GLN  |
| 1   | A     | 324 | HIS  |
| 1   | A     | 341 | ASN  |
| 1   | A     | 460 | GLN  |
| 1   | B     | 263 | GLN  |
| 1   | B     | 324 | HIS  |
| 1   | B     | 341 | ASN  |
| 1   | B     | 460 | GLN  |
| 1   | C     | 99  | ASN  |
| 1   | C     | 263 | GLN  |
| 1   | C     | 324 | HIS  |
| 1   | C     | 341 | ASN  |
| 1   | D     | 263 | GLN  |
| 1   | D     | 324 | HIS  |
| 1   | D     | 331 | ASN  |
| 1   | D     | 341 | ASN  |
| 1   | D     | 460 | GLN  |
| 1   | D     | 461 | GLN  |
| 1   | E     | 99  | ASN  |
| 1   | E     | 263 | GLN  |
| 1   | E     | 324 | HIS  |
| 1   | E     | 341 | ASN  |
| 1   | E     | 460 | GLN  |
| 1   | E     | 461 | GLN  |
| 1   | F     | 324 | HIS  |
| 1   | F     | 341 | ASN  |
| 1   | F     | 460 | GLN  |
| 1   | G     | 263 | GLN  |
| 1   | G     | 324 | HIS  |
| 1   | G     | 341 | ASN  |
| 1   | G     | 460 | GLN  |
| 1   | G     | 611 | GLN  |
| 1   | H     | 324 | HIS  |
| 1   | H     | 341 | ASN  |
| 1   | H     | 460 | GLN  |
| 1   | H     | 611 | 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |       |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|-------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ  | # $ Z  > 2$ |
| 2   | FAD  | A     | 801 | 1    | 51,58,58     | 1.71 | 8 (15%)     | 54,89,89    | 2.71  | 9 (16%)     |
| 3   | MES  | A     | 902 | -    | 12,12,12     | 1.21 | 2 (16%)     | 14,16,16    | 15.65 | 9 (64%)     |
| 2   | FAD  | B     | 801 | 1    | 51,58,58     | 1.43 | 8 (15%)     | 54,89,89    | 2.22  | 11 (20%)    |
| 3   | MES  | B     | 901 | -    | 12,12,12     | 1.26 | 2 (16%)     | 14,16,16    | 17.65 | 8 (57%)     |
| 2   | FAD  | C     | 801 | 1    | 51,58,58     | 1.53 | 8 (15%)     | 54,89,89    | 2.53  | 9 (16%)     |
| 3   | MES  | C     | 904 | -    | 12,12,12     | 1.34 | 1 (8%)      | 14,16,16    | 18.37 | 9 (64%)     |
| 2   | FAD  | D     | 801 | 1    | 51,58,58     | 1.48 | 7 (13%)     | 54,89,89    | 2.13  | 11 (20%)    |
| 3   | MES  | D     | 903 | -    | 12,12,12     | 1.14 | 1 (8%)      | 14,16,16    | 20.09 | 9 (64%)     |
| 2   | FAD  | E     | 801 | 1    | 51,58,58     | 1.55 | 8 (15%)     | 54,89,89    | 2.01  | 5 (9%)      |
| 3   | MES  | E     | 905 | -    | 12,12,12     | 1.11 | 1 (8%)      | 14,16,16    | 16.83 | 8 (57%)     |
| 3   | MES  | E     | 906 | -    | 12,12,12     | 0.88 | 1 (8%)      | 14,16,16    | 17.72 | 9 (64%)     |
| 2   | FAD  | F     | 801 | 1    | 51,58,58     | 1.51 | 7 (13%)     | 54,89,89    | 2.32  | 12 (22%)    |
| 2   | FAD  | G     | 801 | 1    | 51,58,58     | 1.54 | 7 (13%)     | 54,89,89    | 2.33  | 9 (16%)     |
| 3   | MES  | G     | 908 | -    | 12,12,12     | 1.09 | 2 (16%)     | 14,16,16    | 17.96 | 10 (71%)    |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |       |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|-------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ  | # Z  > 2 |
| 2   | FAD  | H     | 801 | 1    | 51,58,58     | 1.50 | 8 (15%)  | 54,89,89    | 2.43  | 7 (12%)  |
| 3   | MES  | H     | 907 | -    | 12,12,12     | 0.95 | 1 (8%)   | 14,16,16    | 16.25 | 8 (57%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | FAD  | A     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 3   | MES  | A     | 902 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 2   | FAD  | B     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 3   | MES  | B     | 901 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 2   | FAD  | C     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 3   | MES  | C     | 904 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 2   | FAD  | D     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 3   | MES  | D     | 903 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 2   | FAD  | E     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 3   | MES  | E     | 905 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 3   | MES  | E     | 906 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 2   | FAD  | F     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | FAD  | G     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 3   | MES  | G     | 908 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 2   | FAD  | H     | 801 | 1    | -       | 0/28/50/50 | 0/6/6/6 |
| 3   | MES  | H     | 907 | -    | -       | 0/6/14/14  | 0/1/1/1 |

All (72) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | C     | 801 | FAD  | PA-O1A  | -2.04 | 1.43        | 1.50     |
| 2   | G     | 801 | FAD  | C2A-N1A | 2.03  | 1.37        | 1.33     |
| 3   | B     | 901 | MES  | O1S-S   | 2.03  | 1.51        | 1.45     |
| 3   | A     | 902 | MES  | O1S-S   | 2.06  | 1.51        | 1.45     |
| 3   | E     | 906 | MES  | C8-S    | 2.07  | 1.80        | 1.77     |
| 3   | G     | 908 | MES  | O1S-S   | 2.11  | 1.51        | 1.45     |
| 2   | B     | 801 | FAD  | C1'-N10 | 2.11  | 1.50        | 1.48     |
| 2   | B     | 801 | FAD  | C9A-N10 | 2.18  | 1.41        | 1.38     |
| 2   | E     | 801 | FAD  | O4B-C1B | 2.20  | 1.44        | 1.41     |
| 2   | C     | 801 | FAD  | C9A-N10 | 2.21  | 1.41        | 1.38     |
| 2   | C     | 801 | FAD  | C1'-N10 | 2.28  | 1.50        | 1.48     |
| 2   | H     | 801 | FAD  | C5'-C4' | 2.30  | 1.55        | 1.51     |
| 2   | E     | 801 | FAD  | C5X-N5  | 2.31  | 1.38        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | A     | 801 | FAD  | O4B-C1B | 2.33 | 1.44        | 1.41     |
| 3   | G     | 908 | MES  | C8-S    | 2.34 | 1.81        | 1.77     |
| 3   | H     | 907 | MES  | C8-S    | 2.39 | 1.81        | 1.77     |
| 2   | D     | 801 | FAD  | C1'-N10 | 2.45 | 1.50        | 1.48     |
| 2   | B     | 801 | FAD  | C2A-N1A | 2.45 | 1.38        | 1.33     |
| 2   | A     | 801 | FAD  | C5'-C4' | 2.49 | 1.55        | 1.51     |
| 2   | H     | 801 | FAD  | C5X-N5  | 2.52 | 1.39        | 1.35     |
| 2   | G     | 801 | FAD  | C5'-C4' | 2.56 | 1.55        | 1.51     |
| 2   | B     | 801 | FAD  | C5'-C4' | 2.56 | 1.55        | 1.51     |
| 2   | G     | 801 | FAD  | C9A-N10 | 2.58 | 1.42        | 1.38     |
| 2   | D     | 801 | FAD  | C5X-N5  | 2.71 | 1.39        | 1.35     |
| 2   | F     | 801 | FAD  | C9A-N10 | 2.77 | 1.42        | 1.38     |
| 3   | D     | 903 | MES  | C8-S    | 2.80 | 1.81        | 1.77     |
| 2   | H     | 801 | FAD  | C4-N3   | 2.85 | 1.38        | 1.33     |
| 2   | B     | 801 | FAD  | C2A-N3A | 2.88 | 1.37        | 1.32     |
| 3   | E     | 905 | MES  | C8-S    | 2.89 | 1.81        | 1.77     |
| 2   | C     | 801 | FAD  | C2A-N1A | 2.90 | 1.39        | 1.33     |
| 2   | H     | 801 | FAD  | C4X-N5  | 2.91 | 1.37        | 1.33     |
| 2   | D     | 801 | FAD  | C2A-N3A | 2.92 | 1.37        | 1.32     |
| 2   | H     | 801 | FAD  | C2A-N1A | 3.03 | 1.39        | 1.33     |
| 2   | F     | 801 | FAD  | C5X-N5  | 3.04 | 1.40        | 1.35     |
| 2   | F     | 801 | FAD  | C2A-N3A | 3.06 | 1.37        | 1.32     |
| 3   | A     | 902 | MES  | C8-S    | 3.13 | 1.82        | 1.77     |
| 2   | H     | 801 | FAD  | C1'-N10 | 3.14 | 1.51        | 1.48     |
| 2   | C     | 801 | FAD  | C2A-N3A | 3.16 | 1.37        | 1.32     |
| 2   | F     | 801 | FAD  | C2A-N1A | 3.18 | 1.39        | 1.33     |
| 2   | E     | 801 | FAD  | C2A-N1A | 3.20 | 1.39        | 1.33     |
| 2   | C     | 801 | FAD  | C4-N3   | 3.21 | 1.38        | 1.33     |
| 2   | E     | 801 | FAD  | C10-N1  | 3.25 | 1.37        | 1.33     |
| 3   | B     | 901 | MES  | C8-S    | 3.32 | 1.82        | 1.77     |
| 2   | A     | 801 | FAD  | C10-N1  | 3.34 | 1.37        | 1.33     |
| 2   | D     | 801 | FAD  | O4B-C1B | 3.34 | 1.45        | 1.41     |
| 2   | A     | 801 | FAD  | C9A-N10 | 3.51 | 1.43        | 1.38     |
| 2   | A     | 801 | FAD  | C4-N3   | 3.53 | 1.39        | 1.33     |
| 2   | E     | 801 | FAD  | C4X-N5  | 3.53 | 1.38        | 1.33     |
| 2   | F     | 801 | FAD  | C10-N1  | 3.58 | 1.38        | 1.33     |
| 2   | B     | 801 | FAD  | C4-N3   | 3.70 | 1.39        | 1.33     |
| 2   | F     | 801 | FAD  | C4-N3   | 3.78 | 1.39        | 1.33     |
| 2   | B     | 801 | FAD  | C10-N1  | 3.78 | 1.38        | 1.33     |
| 2   | D     | 801 | FAD  | C10-N1  | 3.85 | 1.38        | 1.33     |
| 2   | E     | 801 | FAD  | C2A-N3A | 3.85 | 1.38        | 1.32     |
| 2   | D     | 801 | FAD  | C4-N3   | 3.86 | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | G     | 801 | FAD  | C4X-N5  | 3.88 | 1.38        | 1.33     |
| 3   | C     | 904 | MES  | C8-S    | 3.92 | 1.83        | 1.77     |
| 2   | H     | 801 | FAD  | C10-N1  | 3.97 | 1.38        | 1.33     |
| 2   | G     | 801 | FAD  | C4-N3   | 4.14 | 1.40        | 1.33     |
| 2   | G     | 801 | FAD  | C10-N1  | 4.15 | 1.39        | 1.33     |
| 2   | E     | 801 | FAD  | C4-N3   | 4.34 | 1.40        | 1.33     |
| 2   | A     | 801 | FAD  | C1'-N10 | 4.41 | 1.52        | 1.48     |
| 2   | E     | 801 | FAD  | C1'-N10 | 4.53 | 1.53        | 1.48     |
| 2   | C     | 801 | FAD  | C4X-N5  | 4.69 | 1.40        | 1.33     |
| 2   | G     | 801 | FAD  | C2A-N3A | 4.79 | 1.40        | 1.32     |
| 2   | A     | 801 | FAD  | C2A-N3A | 4.89 | 1.40        | 1.32     |
| 2   | A     | 801 | FAD  | C4X-N5  | 4.91 | 1.40        | 1.33     |
| 2   | H     | 801 | FAD  | C2A-N3A | 4.96 | 1.40        | 1.32     |
| 2   | B     | 801 | FAD  | C4X-N5  | 4.98 | 1.40        | 1.33     |
| 2   | F     | 801 | FAD  | C4X-N5  | 5.01 | 1.40        | 1.33     |
| 2   | C     | 801 | FAD  | C10-N1  | 5.30 | 1.40        | 1.33     |
| 2   | D     | 801 | FAD  | C4X-N5  | 5.53 | 1.41        | 1.33     |

All (143) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 2   | A     | 801 | FAD  | N3A-C2A-N1A | -14.68 | 116.08      | 128.86   |
| 3   | G     | 908 | MES  | O3S-S-C8    | -12.76 | 90.37       | 106.06   |
| 3   | D     | 903 | MES  | O3S-S-C8    | -12.05 | 91.23       | 106.06   |
| 2   | H     | 801 | FAD  | N3A-C2A-N1A | -11.87 | 118.52      | 128.86   |
| 3   | C     | 904 | MES  | O3S-S-C8    | -10.90 | 92.65       | 106.06   |
| 2   | B     | 801 | FAD  | N3A-C2A-N1A | -10.73 | 119.51      | 128.86   |
| 2   | G     | 801 | FAD  | N3A-C2A-N1A | -10.28 | 119.90      | 128.86   |
| 2   | E     | 801 | FAD  | N3A-C2A-N1A | -9.89  | 120.24      | 128.86   |
| 3   | D     | 903 | MES  | O1S-S-C8    | -9.75  | 98.42       | 106.79   |
| 2   | F     | 801 | FAD  | N3A-C2A-N1A | -9.58  | 120.51      | 128.86   |
| 3   | G     | 908 | MES  | O1S-S-C8    | -9.48  | 98.65       | 106.79   |
| 3   | B     | 901 | MES  | O3S-S-O2S   | -9.31  | 90.03       | 111.37   |
| 2   | C     | 801 | FAD  | N3A-C2A-N1A | -9.25  | 120.81      | 128.86   |
| 3   | E     | 905 | MES  | O1S-S-C8    | -9.17  | 98.91       | 106.79   |
| 3   | E     | 906 | MES  | O3S-S-C8    | -9.16  | 94.79       | 106.06   |
| 3   | E     | 905 | MES  | O3S-S-C8    | -8.77  | 95.27       | 106.06   |
| 3   | D     | 903 | MES  | O3S-S-O2S   | -8.59  | 91.67       | 111.37   |
| 3   | H     | 907 | MES  | O3S-S-O2S   | -8.25  | 92.47       | 111.37   |
| 3   | B     | 901 | MES  | O1S-S-C8    | -8.12  | 99.82       | 106.79   |
| 3   | E     | 906 | MES  | O3S-S-O2S   | -8.01  | 93.01       | 111.37   |
| 3   | A     | 902 | MES  | O3S-S-C8    | -7.91  | 96.33       | 106.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | C     | 904 | MES  | O3S-S-O2S   | -7.89 | 93.29       | 111.37   |
| 3   | C     | 904 | MES  | O1S-S-C8    | -7.86 | 100.04      | 106.79   |
| 3   | E     | 906 | MES  | O1S-S-C8    | -6.92 | 100.85      | 106.79   |
| 3   | B     | 901 | MES  | O3S-S-C8    | -6.89 | 97.58       | 106.06   |
| 3   | E     | 905 | MES  | O3S-S-O2S   | -6.66 | 96.11       | 111.37   |
| 3   | D     | 903 | MES  | O2S-S-O1S   | -6.61 | 90.94       | 113.86   |
| 3   | A     | 902 | MES  | O3S-S-O2S   | -6.60 | 96.23       | 111.37   |
| 3   | G     | 908 | MES  | O3S-S-O2S   | -6.38 | 96.74       | 111.37   |
| 2   | D     | 801 | FAD  | N3A-C2A-N1A | -6.36 | 123.32      | 128.86   |
| 3   | H     | 907 | MES  | O3S-S-C8    | -6.14 | 98.50       | 106.06   |
| 3   | A     | 902 | MES  | O3S-S-O1S   | -6.04 | 97.53       | 111.37   |
| 3   | C     | 904 | MES  | O2S-S-O1S   | -5.94 | 93.28       | 113.86   |
| 3   | B     | 901 | MES  | O3S-S-O1S   | -5.74 | 98.22       | 111.37   |
| 3   | E     | 906 | MES  | O2S-S-O1S   | -5.66 | 94.23       | 113.86   |
| 3   | E     | 906 | MES  | O3S-S-O1S   | -5.65 | 98.42       | 111.37   |
| 3   | G     | 908 | MES  | O3S-S-O1S   | -5.54 | 98.68       | 111.37   |
| 3   | H     | 907 | MES  | O1S-S-C8    | -5.51 | 102.06      | 106.79   |
| 3   | H     | 907 | MES  | O2S-S-O1S   | -5.36 | 95.28       | 113.86   |
| 3   | B     | 901 | MES  | O2S-S-O1S   | -5.25 | 95.65       | 113.86   |
| 3   | E     | 905 | MES  | O2S-S-O1S   | -5.00 | 96.52       | 113.86   |
| 3   | G     | 908 | MES  | O2S-S-O1S   | -4.97 | 96.62       | 113.86   |
| 3   | A     | 902 | MES  | O2S-S-O1S   | -4.96 | 96.66       | 113.86   |
| 3   | A     | 902 | MES  | O1S-S-C8    | -4.92 | 102.56      | 106.79   |
| 3   | H     | 907 | MES  | O3S-S-O1S   | -4.84 | 100.26      | 111.37   |
| 3   | E     | 905 | MES  | O3S-S-O1S   | -4.83 | 100.29      | 111.37   |
| 2   | H     | 801 | FAD  | C4X-C4-N3   | -4.66 | 116.84      | 123.48   |
| 2   | G     | 801 | FAD  | C4X-C4-N3   | -4.59 | 116.95      | 123.48   |
| 2   | C     | 801 | FAD  | C4X-C4-N3   | -4.50 | 117.07      | 123.48   |
| 2   | A     | 801 | FAD  | C4X-C4-N3   | -4.16 | 117.56      | 123.48   |
| 3   | B     | 901 | MES  | O1-C6-C5    | -3.87 | 103.17      | 111.83   |
| 2   | D     | 801 | FAD  | C4X-C4-N3   | -3.72 | 118.19      | 123.48   |
| 3   | H     | 907 | MES  | O1-C6-C5    | -3.67 | 103.61      | 111.83   |
| 2   | D     | 801 | FAD  | C4A-C5A-N7A | -3.63 | 105.91      | 109.41   |
| 3   | C     | 904 | MES  | O3S-S-O1S   | -3.55 | 103.22      | 111.37   |
| 3   | C     | 904 | MES  | O1-C6-C5    | -3.38 | 104.26      | 111.83   |
| 2   | A     | 801 | FAD  | C1B-N9A-C4A | -3.37 | 120.82      | 126.64   |
| 2   | F     | 801 | FAD  | C4-C4X-C10  | -3.03 | 117.51      | 119.96   |
| 2   | B     | 801 | FAD  | C1'-N10-C10 | -2.92 | 115.51      | 118.50   |
| 2   | F     | 801 | FAD  | C4X-C4-N3   | -2.82 | 119.46      | 123.48   |
| 2   | B     | 801 | FAD  | C4X-C4-N3   | -2.76 | 119.56      | 123.48   |
| 3   | E     | 906 | MES  | O1-C6-C5    | -2.71 | 105.77      | 111.83   |
| 2   | G     | 801 | FAD  | C4A-C5A-N7A | -2.70 | 106.80      | 109.41   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 801 | FAD  | C4X-C4-N3   | -2.65 | 119.71      | 123.48   |
| 3   | D     | 903 | MES  | O1-C6-C5    | -2.64 | 105.93      | 111.83   |
| 2   | A     | 801 | FAD  | C4B-O4B-C1B | -2.50 | 107.10      | 109.77   |
| 2   | F     | 801 | FAD  | C1'-N10-C10 | -2.50 | 115.94      | 118.50   |
| 3   | E     | 906 | MES  | O1-C2-C3    | -2.47 | 106.30      | 111.83   |
| 3   | G     | 908 | MES  | O1-C2-C3    | -2.45 | 106.35      | 111.83   |
| 2   | C     | 801 | FAD  | C1B-N9A-C4A | -2.42 | 122.45      | 126.64   |
| 2   | B     | 801 | FAD  | C1B-N9A-C4A | -2.37 | 122.53      | 126.64   |
| 2   | F     | 801 | FAD  | C1B-N9A-C4A | -2.32 | 122.62      | 126.64   |
| 2   | D     | 801 | FAD  | C4B-O4B-C1B | -2.29 | 107.33      | 109.77   |
| 2   | G     | 801 | FAD  | C1B-N9A-C4A | -2.25 | 122.74      | 126.64   |
| 3   | D     | 903 | MES  | O3S-S-O1S   | -2.25 | 106.22      | 111.37   |
| 2   | B     | 801 | FAD  | C6-C5X-N5   | -2.17 | 116.42      | 118.97   |
| 3   | A     | 902 | MES  | O1-C6-C5    | -2.13 | 107.05      | 111.83   |
| 2   | B     | 801 | FAD  | C7-C6-C5X   | -2.09 | 117.85      | 121.08   |
| 3   | C     | 904 | MES  | O1-C2-C3    | -2.04 | 107.28      | 111.83   |
| 3   | G     | 908 | MES  | O1-C6-C5    | -2.03 | 107.29      | 111.83   |
| 2   | A     | 801 | FAD  | C4X-N5-C5X  | 2.01  | 118.88      | 116.76   |
| 2   | D     | 801 | FAD  | C4X-N5-C5X  | 2.02  | 118.89      | 116.76   |
| 2   | F     | 801 | FAD  | C2A-N1A-C6A | 2.04  | 122.34      | 118.77   |
| 2   | G     | 801 | FAD  | C6-C5X-C9A  | 2.12  | 121.75      | 119.00   |
| 2   | F     | 801 | FAD  | C4X-N5-C5X  | 2.25  | 119.13      | 116.76   |
| 2   | F     | 801 | FAD  | C6-C5X-C9A  | 2.31  | 122.00      | 119.00   |
| 3   | G     | 908 | MES  | C2-C3-N4    | 2.34  | 113.39      | 110.11   |
| 2   | D     | 801 | FAD  | O4'-C4'-C3' | 2.43  | 115.12      | 109.09   |
| 2   | H     | 801 | FAD  | C1'-N10-C9A | 2.44  | 120.58      | 118.35   |
| 2   | A     | 801 | FAD  | C1'-N10-C10 | 2.45  | 121.01      | 118.50   |
| 3   | E     | 905 | MES  | C2-C3-N4    | 2.48  | 113.59      | 110.11   |
| 2   | H     | 801 | FAD  | O2B-C2B-C3B | 2.50  | 119.82      | 111.83   |
| 3   | A     | 902 | MES  | C2-C3-N4    | 2.53  | 113.66      | 110.11   |
| 3   | D     | 903 | MES  | C2-C3-N4    | 2.58  | 113.72      | 110.11   |
| 2   | H     | 801 | FAD  | C2A-N1A-C6A | 2.68  | 123.46      | 118.77   |
| 2   | B     | 801 | FAD  | C2A-N1A-C6A | 2.72  | 123.52      | 118.77   |
| 2   | C     | 801 | FAD  | C2B-C3B-C4B | 2.76  | 107.99      | 102.62   |
| 2   | D     | 801 | FAD  | C4-C4X-N5   | 2.85  | 121.81      | 118.68   |
| 2   | D     | 801 | FAD  | C5A-C6A-N6A | 2.88  | 126.33      | 120.47   |
| 2   | F     | 801 | FAD  | C4-C4X-N5   | 2.97  | 121.93      | 118.68   |
| 2   | G     | 801 | FAD  | C5X-C9A-N10 | 2.98  | 119.87      | 117.66   |
| 2   | C     | 801 | FAD  | C6-C5X-C9A  | 3.00  | 122.89      | 119.00   |
| 3   | E     | 906 | MES  | C5-N4-C3    | 3.09  | 115.87      | 108.87   |
| 2   | A     | 801 | FAD  | C5X-C9A-N10 | 3.16  | 120.01      | 117.66   |
| 2   | A     | 801 | FAD  | C2A-N1A-C6A | 3.22  | 124.41      | 118.77   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 801 | FAD  | C6-C5X-C9A  | 3.30  | 123.29      | 119.00   |
| 2   | B     | 801 | FAD  | C4X-N5-C5X  | 3.45  | 120.40      | 116.76   |
| 2   | C     | 801 | FAD  | C4X-N5-C5X  | 3.57  | 120.53      | 116.76   |
| 2   | G     | 801 | FAD  | C1'-N10-C9A | 3.59  | 121.64      | 118.35   |
| 2   | E     | 801 | FAD  | C1'-N10-C9A | 3.74  | 121.77      | 118.35   |
| 3   | B     | 901 | MES  | C5-N4-C3    | 3.80  | 117.48      | 108.87   |
| 2   | D     | 801 | FAD  | C5X-C9A-N10 | 3.87  | 120.53      | 117.66   |
| 2   | C     | 801 | FAD  | C5X-C9A-N10 | 3.93  | 120.58      | 117.66   |
| 2   | F     | 801 | FAD  | C5X-C9A-N10 | 4.07  | 120.68      | 117.66   |
| 3   | H     | 907 | MES  | C5-N4-C3    | 4.07  | 118.09      | 108.87   |
| 3   | C     | 904 | MES  | C5-N4-C3    | 4.15  | 118.28      | 108.87   |
| 3   | D     | 903 | MES  | C5-N4-C3    | 4.22  | 118.44      | 108.87   |
| 2   | G     | 801 | FAD  | C4X-N5-C5X  | 4.24  | 121.24      | 116.76   |
| 2   | B     | 801 | FAD  | C4-N3-C2    | 4.28  | 118.90      | 115.16   |
| 2   | H     | 801 | FAD  | C4X-N5-C5X  | 4.35  | 121.35      | 116.76   |
| 3   | G     | 908 | MES  | C5-N4-C3    | 4.47  | 118.98      | 108.87   |
| 3   | A     | 902 | MES  | C5-N4-C3    | 4.47  | 119.00      | 108.87   |
| 3   | E     | 905 | MES  | C5-N4-C3    | 4.55  | 119.19      | 108.87   |
| 2   | D     | 801 | FAD  | C1'-N10-C9A | 4.57  | 122.54      | 118.35   |
| 2   | F     | 801 | FAD  | C1'-N10-C9A | 4.91  | 122.85      | 118.35   |
| 2   | E     | 801 | FAD  | C5X-C9A-N10 | 4.95  | 121.33      | 117.66   |
| 2   | E     | 801 | FAD  | C4-N3-C2    | 5.34  | 119.83      | 115.16   |
| 2   | C     | 801 | FAD  | C1'-N10-C9A | 5.43  | 123.32      | 118.35   |
| 2   | B     | 801 | FAD  | C1'-N10-C9A | 5.55  | 123.44      | 118.35   |
| 2   | D     | 801 | FAD  | C4-N3-C2    | 8.18  | 122.31      | 115.16   |
| 2   | H     | 801 | FAD  | C4-N3-C2    | 8.34  | 122.46      | 115.16   |
| 2   | G     | 801 | FAD  | C4-N3-C2    | 8.63  | 122.71      | 115.16   |
| 2   | F     | 801 | FAD  | C4-N3-C2    | 8.76  | 122.82      | 115.16   |
| 2   | A     | 801 | FAD  | C4-N3-C2    | 9.27  | 123.27      | 115.16   |
| 2   | C     | 801 | FAD  | C4-N3-C2    | 10.65 | 124.47      | 115.16   |
| 3   | A     | 902 | MES  | O2S-S-C8    | 56.58 | 155.39      | 106.79   |
| 3   | H     | 907 | MES  | O2S-S-C8    | 58.93 | 157.41      | 106.79   |
| 3   | E     | 905 | MES  | O2S-S-C8    | 60.61 | 158.85      | 106.79   |
| 3   | B     | 901 | MES  | O2S-S-C8    | 63.76 | 161.56      | 106.79   |
| 3   | E     | 906 | MES  | O2S-S-C8    | 64.04 | 161.79      | 106.79   |
| 3   | G     | 908 | MES  | O2S-S-C8    | 64.26 | 161.99      | 106.79   |
| 3   | C     | 904 | MES  | O2S-S-C8    | 66.33 | 163.77      | 106.79   |
| 3   | D     | 903 | MES  | O2S-S-C8    | 72.43 | 169.00      | 106.79   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 128 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 801 | FAD  | 8       | 0            |
| 3   | A     | 902 | MES  | 9       | 0            |
| 2   | B     | 801 | FAD  | 8       | 0            |
| 3   | B     | 901 | MES  | 15      | 0            |
| 2   | C     | 801 | FAD  | 4       | 0            |
| 3   | C     | 904 | MES  | 12      | 0            |
| 2   | D     | 801 | FAD  | 6       | 0            |
| 3   | D     | 903 | MES  | 14      | 0            |
| 2   | E     | 801 | FAD  | 7       | 0            |
| 3   | E     | 905 | MES  | 2       | 0            |
| 3   | E     | 906 | MES  | 11      | 0            |
| 2   | F     | 801 | FAD  | 3       | 0            |
| 3   | G     | 908 | MES  | 13      | 0            |
| 2   | H     | 801 | FAD  | 3       | 0            |
| 3   | H     | 907 | MES  | 13      | 0            |

## 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     | 577/623 (92%)   | -0.44  | 20 (3%) 44 39  | 10, 17, 42, 61        | 0     |
| 1   | B     | 577/623 (92%)   | -0.45  | 20 (3%) 44 39  | 10, 17, 39, 61        | 0     |
| 1   | C     | 577/623 (92%)   | -0.23  | 24 (4%) 37 31  | 13, 23, 47, 67        | 0     |
| 1   | D     | 577/623 (92%)   | -0.36  | 20 (3%) 44 39  | 12, 21, 42, 63        | 0     |
| 1   | E     | 577/623 (92%)   | -0.33  | 21 (3%) 43 38  | 13, 21, 43, 64        | 0     |
| 1   | F     | 577/623 (92%)   | -0.32  | 21 (3%) 43 38  | 11, 22, 43, 65        | 0     |
| 1   | G     | 577/623 (92%)   | -0.38  | 23 (3%) 39 33  | 12, 19, 43, 66        | 0     |
| 1   | H     | 577/623 (92%)   | -0.49  | 14 (2%) 59 55  | 11, 18, 39, 62        | 0     |
| All | All   | 4616/4984 (92%) | -0.38  | 163 (3%) 44 39 | 10, 20, 43, 67        | 0     |

All (163) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 619 | THR  | 11.2 |
| 1   | H     | 619 | THR  | 10.2 |
| 1   | A     | 619 | THR  | 9.6  |
| 1   | G     | 619 | THR  | 8.6  |
| 1   | B     | 619 | THR  | 8.6  |
| 1   | D     | 619 | THR  | 8.3  |
| 1   | A     | 459 | VAL  | 8.1  |
| 1   | G     | 44  | ASP  | 7.5  |
| 1   | C     | 45  | ILE  | 7.1  |
| 1   | F     | 459 | VAL  | 7.1  |
| 1   | E     | 43  | MET  | 7.0  |
| 1   | E     | 619 | THR  | 7.0  |
| 1   | C     | 459 | VAL  | 6.7  |
| 1   | C     | 389 | LEU  | 6.6  |
| 1   | F     | 343 | ALA  | 6.6  |
| 1   | F     | 619 | THR  | 6.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 45  | ILE  | 6.2  |
| 1   | D     | 459 | VAL  | 6.2  |
| 1   | C     | 618 | PHE  | 6.1  |
| 1   | H     | 343 | ALA  | 6.0  |
| 1   | H     | 459 | VAL  | 5.9  |
| 1   | C     | 343 | ALA  | 5.8  |
| 1   | A     | 343 | ALA  | 5.7  |
| 1   | B     | 43  | MET  | 5.6  |
| 1   | G     | 458 | ALA  | 5.6  |
| 1   | G     | 343 | ALA  | 5.6  |
| 1   | G     | 459 | VAL  | 5.5  |
| 1   | D     | 343 | ALA  | 5.5  |
| 1   | E     | 389 | LEU  | 5.5  |
| 1   | D     | 458 | ALA  | 5.4  |
| 1   | C     | 44  | ASP  | 5.4  |
| 1   | B     | 343 | ALA  | 5.3  |
| 1   | E     | 385 | THR  | 5.1  |
| 1   | F     | 342 | PRO  | 5.1  |
| 1   | H     | 44  | ASP  | 5.1  |
| 1   | F     | 389 | LEU  | 5.0  |
| 1   | F     | 43  | MET  | 4.9  |
| 1   | H     | 344 | ASN  | 4.9  |
| 1   | B     | 458 | ALA  | 4.9  |
| 1   | A     | 389 | LEU  | 4.9  |
| 1   | F     | 44  | ASP  | 4.9  |
| 1   | B     | 459 | VAL  | 4.8  |
| 1   | E     | 459 | VAL  | 4.8  |
| 1   | A     | 43  | MET  | 4.8  |
| 1   | C     | 345 | PRO  | 4.8  |
| 1   | G     | 43  | MET  | 4.7  |
| 1   | D     | 618 | PHE  | 4.7  |
| 1   | E     | 343 | ALA  | 4.7  |
| 1   | B     | 44  | ASP  | 4.7  |
| 1   | B     | 618 | PHE  | 4.6  |
| 1   | D     | 45  | ILE  | 4.6  |
| 1   | D     | 345 | PRO  | 4.6  |
| 1   | G     | 389 | LEU  | 4.5  |
| 1   | D     | 44  | ASP  | 4.4  |
| 1   | C     | 43  | MET  | 4.4  |
| 1   | F     | 45  | ILE  | 4.4  |
| 1   | F     | 385 | THR  | 4.3  |
| 1   | B     | 45  | ILE  | 4.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 344 | ASN  | 4.2  |
| 1   | H     | 45  | ILE  | 4.2  |
| 1   | H     | 43  | MET  | 4.2  |
| 1   | G     | 618 | PHE  | 4.1  |
| 1   | A     | 385 | THR  | 4.1  |
| 1   | F     | 458 | ALA  | 4.1  |
| 1   | H     | 458 | ALA  | 4.1  |
| 1   | C     | 383 | ARG  | 4.0  |
| 1   | A     | 345 | PRO  | 4.0  |
| 1   | D     | 389 | LEU  | 4.0  |
| 1   | F     | 344 | ASN  | 4.0  |
| 1   | C     | 617 | PRO  | 4.0  |
| 1   | E     | 458 | ALA  | 4.0  |
| 1   | G     | 344 | ASN  | 3.9  |
| 1   | A     | 458 | ALA  | 3.9  |
| 1   | C     | 390 | THR  | 3.9  |
| 1   | E     | 384 | GLY  | 3.8  |
| 1   | G     | 342 | PRO  | 3.8  |
| 1   | D     | 43  | MET  | 3.8  |
| 1   | H     | 618 | PHE  | 3.8  |
| 1   | A     | 388 | GLU  | 3.7  |
| 1   | F     | 345 | PRO  | 3.7  |
| 1   | E     | 388 | GLU  | 3.7  |
| 1   | E     | 618 | PHE  | 3.7  |
| 1   | E     | 345 | PRO  | 3.7  |
| 1   | G     | 388 | GLU  | 3.7  |
| 1   | E     | 342 | PRO  | 3.6  |
| 1   | H     | 345 | PRO  | 3.6  |
| 1   | E     | 44  | ASP  | 3.6  |
| 1   | B     | 389 | LEU  | 3.6  |
| 1   | D     | 388 | GLU  | 3.5  |
| 1   | A     | 344 | ASN  | 3.5  |
| 1   | G     | 345 | PRO  | 3.5  |
| 1   | D     | 385 | THR  | 3.5  |
| 1   | C     | 384 | GLY  | 3.4  |
| 1   | H     | 456 | TYR  | 3.4  |
| 1   | B     | 456 | TYR  | 3.4  |
| 1   | F     | 618 | PHE  | 3.4  |
| 1   | H     | 342 | PRO  | 3.4  |
| 1   | A     | 390 | THR  | 3.4  |
| 1   | A     | 44  | ASP  | 3.4  |
| 1   | F     | 390 | THR  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 385 | THR  | 3.2  |
| 1   | C     | 458 | ALA  | 3.2  |
| 1   | C     | 385 | THR  | 3.1  |
| 1   | C     | 456 | TYR  | 3.1  |
| 1   | C     | 388 | GLU  | 3.1  |
| 1   | E     | 383 | ARG  | 3.1  |
| 1   | F     | 384 | GLY  | 3.1  |
| 1   | F     | 341 | ASN  | 3.0  |
| 1   | E     | 386 | PRO  | 3.0  |
| 1   | D     | 344 | ASN  | 3.0  |
| 1   | E     | 344 | ASN  | 3.0  |
| 1   | G     | 341 | ASN  | 3.0  |
| 1   | A     | 618 | PHE  | 2.9  |
| 1   | C     | 344 | ASN  | 2.8  |
| 1   | G     | 45  | ILE  | 2.8  |
| 1   | B     | 388 | GLU  | 2.8  |
| 1   | F     | 383 | ARG  | 2.8  |
| 1   | D     | 617 | PRO  | 2.7  |
| 1   | G     | 186 | ASP  | 2.7  |
| 1   | G     | 387 | GLY  | 2.7  |
| 1   | G     | 617 | PRO  | 2.7  |
| 1   | C     | 392 | SER  | 2.7  |
| 1   | D     | 272 | GLU  | 2.6  |
| 1   | B     | 342 | PRO  | 2.6  |
| 1   | B     | 341 | ASN  | 2.6  |
| 1   | H     | 617 | PRO  | 2.6  |
| 1   | D     | 383 | ARG  | 2.6  |
| 1   | F     | 388 | GLU  | 2.6  |
| 1   | E     | 617 | PRO  | 2.6  |
| 1   | C     | 272 | GLU  | 2.5  |
| 1   | E     | 390 | THR  | 2.5  |
| 1   | C     | 400 | SER  | 2.5  |
| 1   | B     | 345 | PRO  | 2.5  |
| 1   | D     | 454 | PHE  | 2.4  |
| 1   | C     | 342 | PRO  | 2.4  |
| 1   | G     | 390 | THR  | 2.4  |
| 1   | F     | 188 | ALA  | 2.3  |
| 1   | A     | 382 | ILE  | 2.3  |
| 1   | G     | 383 | ARG  | 2.3  |
| 1   | A     | 341 | ASN  | 2.3  |
| 1   | A     | 384 | GLY  | 2.3  |
| 1   | A     | 383 | ARG  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 269 | ASP  | 2.3  |
| 1   | F     | 347 | GLU  | 2.3  |
| 1   | G     | 401 | THR  | 2.3  |
| 1   | A     | 342 | PRO  | 2.3  |
| 1   | A     | 381 | THR  | 2.3  |
| 1   | G     | 456 | TYR  | 2.2  |
| 1   | E     | 341 | ASN  | 2.2  |
| 1   | A     | 400 | SER  | 2.2  |
| 1   | B     | 390 | THR  | 2.2  |
| 1   | B     | 617 | PRO  | 2.2  |
| 1   | C     | 396 | THR  | 2.2  |
| 1   | B     | 385 | THR  | 2.1  |
| 1   | E     | 272 | GLU  | 2.1  |
| 1   | C     | 341 | ASN  | 2.1  |
| 1   | H     | 341 | ASN  | 2.1  |
| 1   | F     | 561 | GLU  | 2.1  |
| 1   | D     | 456 | TYR  | 2.0  |
| 1   | B     | 454 | PHE  | 2.0  |
| 1   | B     | 383 | ARG  | 2.0  |
| 1   | D     | 390 | THR  | 2.0  |
| 1   | G     | 455 | SER  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 3   | MES  | C     | 904 | 12/12 | 0.85 | 0.32 | 7.77 | 27,37,45,46                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 3   | MES  | D     | 903 | 12/12 | 0.89 | 0.29 | 7.32  | 32,37,41,44                 | 0     |
| 3   | MES  | G     | 908 | 12/12 | 0.85 | 0.28 | 6.95  | 28,37,41,41                 | 0     |
| 3   | MES  | E     | 906 | 12/12 | 0.85 | 0.28 | 6.27  | 31,38,41,42                 | 0     |
| 3   | MES  | B     | 901 | 12/12 | 0.88 | 0.27 | 5.95  | 28,35,38,39                 | 0     |
| 3   | MES  | A     | 902 | 12/12 | 0.92 | 0.20 | 3.60  | 24,29,34,34                 | 0     |
| 3   | MES  | H     | 907 | 12/12 | 0.92 | 0.19 | 3.43  | 29,33,37,37                 | 0     |
| 3   | MES  | E     | 905 | 12/12 | 0.95 | 0.18 | 2.17  | 21,29,32,32                 | 0     |
| 2   | FAD  | D     | 801 | 53/53 | 0.98 | 0.10 | 0.11  | 14,17,20,22                 | 0     |
| 2   | FAD  | F     | 801 | 53/53 | 0.98 | 0.09 | 0.01  | 15,18,21,21                 | 0     |
| 2   | FAD  | H     | 801 | 53/53 | 0.98 | 0.09 | -0.03 | 11,14,17,19                 | 0     |
| 2   | FAD  | A     | 801 | 53/53 | 0.98 | 0.09 | -0.09 | 9,13,17,18                  | 0     |
| 2   | FAD  | G     | 801 | 53/53 | 0.98 | 0.08 | -0.20 | 12,14,18,19                 | 0     |
| 2   | FAD  | B     | 801 | 53/53 | 0.99 | 0.09 | -0.20 | 9,14,16,17                  | 0     |
| 2   | FAD  | C     | 801 | 53/53 | 0.98 | 0.09 | -0.21 | 16,20,22,24                 | 0     |
| 2   | FAD  | E     | 801 | 53/53 | 0.97 | 0.09 | -0.22 | 15,18,21,22                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.