



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 01:44 PM EDT

PDB ID : 2IGO  
Title : Crystal structure of pyranose 2-oxidase H167A mutant with 2-fluoro-2-deoxy-D-glucose  
Authors : Divne, C.  
Deposited on : unknown  
Resolution : 1.95 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  |

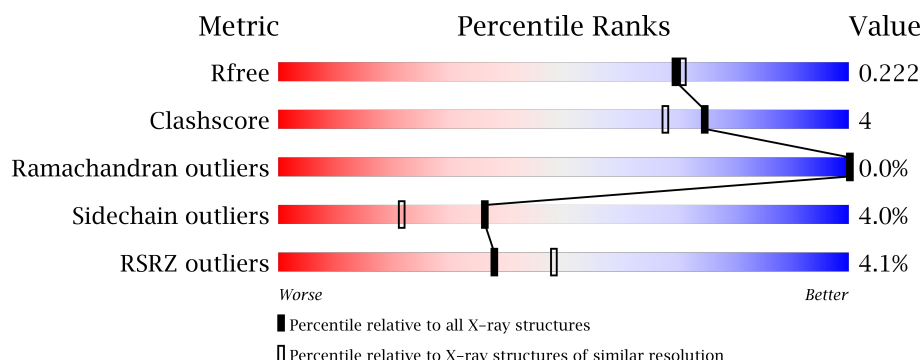
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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                      | 2004 (1.96-1.96)                                      |
| Clashscore            | 112137                      | 2136 (1.96-1.96)                                      |
| Ramachandran outliers | 110173                      | 2117 (1.96-1.96)                                      |
| Sidechain outliers    | 110143                      | 2117 (1.96-1.96)                                      |
| RSRZ outliers         | 101464                      | 2018 (1.96-1.96)                                      |

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>4%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>7%</div> </div> </div> |
| 1   | B     | 623    | <div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>7%</div> </div> </div>  |
| 1   | C     | 623    | <div> <div>4%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div> |
| 1   | D     | 623    | <div> <div>3%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>7%</div> </div> </div> |
| 1   | E     | 623    | <div> <div>4%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>7%</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|-------------------|
| 1   | F     | 623    | <br>5% 81% 9% 7%  |
| 1   | G     | 623    | <br>4% 80% 11% 7% |
| 1   | H     | 623    | <br>4% 80% 12% 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | SHG  | G     | 808 | -         | -        | -       | X                |
| 3   | FAD  | A     | 701 | -         | -        | -       | X                |
| 3   | FAD  | B     | 702 | -         | -        | -       | X                |
| 3   | FAD  | C     | 704 | -         | -        | -       | X                |
| 3   | FAD  | D     | 703 | -         | -        | -       | X                |
| 3   | FAD  | E     | 705 | -         | -        | -       | X                |
| 3   | FAD  | F     | 706 | -         | -        | -       | X                |
| 3   | FAD  | G     | 708 | -         | -        | -       | X                |
| 3   | FAD  | H     | 707 | -         | -        | -       | X                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 38602 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.

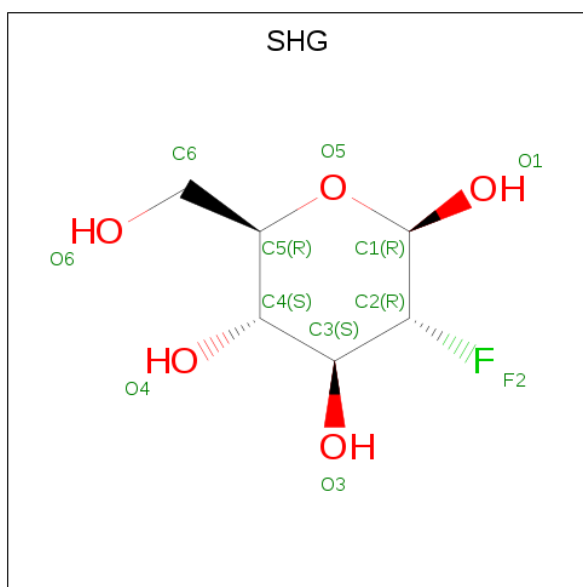
- Molecule 1 is a protein called Pyranose oxidase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |
| 1   | B     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |
| 1   | D     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |
| 1   | C     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |
| 1   | E     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |
| 1   | F     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |
| 1   | H     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |
| 1   | G     | 577      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4544  | 2869 | 776 | 874 | 25 |         |         |       |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment    | Reference  |
|-------|---------|----------|--------|------------|------------|
| A     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |
| B     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |
| C     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |
| D     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |
| E     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |
| F     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |
| G     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |
| H     | 167     | ALA      | HIS    | ENGINEERED | UNP Q7ZA32 |

- Molecule 2 is 2-deoxy-2-fluoro-beta-D-glucopyranose (three-letter code: SHG) (formula: C<sub>6</sub>H<sub>11</sub>FO<sub>5</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |
| 2   | D     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |
| 2   | C     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |
| 2   | E     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |
| 2   | F     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |
| 2   | H     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |
| 2   | G     | 1        | Total | C | F | O | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 5 |         |         |

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | B     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | D     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | C     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | E     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | F     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | H     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |
| 3   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 53    | 27 | 9 | 15 | 2 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4   | A     | 244      | Total | O   | 0       | 0       |
|     |       |          | 244   | 244 |         |         |
| 4   | B     | 251      | Total | O   | 0       | 0       |
|     |       |          | 251   | 251 |         |         |
| 4   | D     | 222      | Total | O   | 0       | 0       |
|     |       |          | 222   | 222 |         |         |
| 4   | C     | 199      | Total | O   | 0       | 0       |
|     |       |          | 199   | 199 |         |         |

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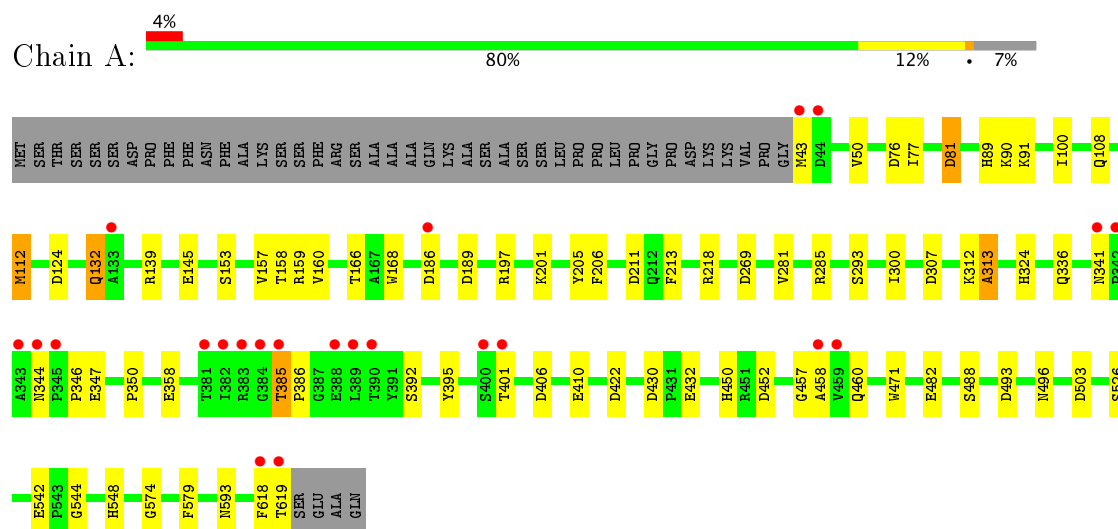
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | E     | 195      | Total<br>195 | O<br>195 | 0       | 0       |
| 4   | F     | 192      | Total<br>192 | O<br>192 | 0       | 0       |
| 4   | H     | 217      | Total<br>217 | O<br>217 | 0       | 0       |
| 4   | G     | 210      | Total<br>210 | O<br>210 | 0       | 0       |

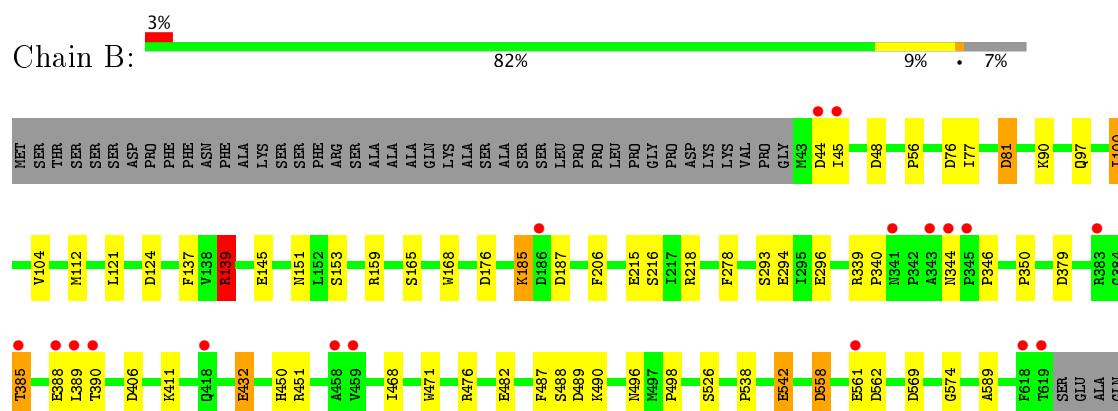
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

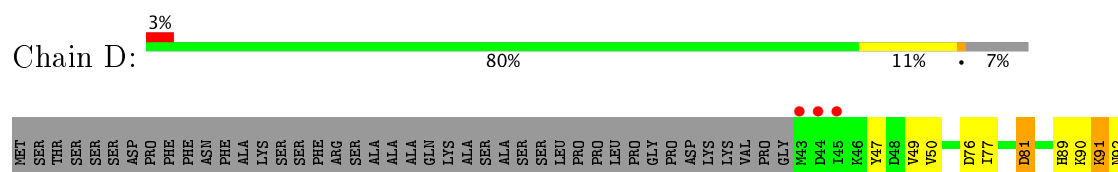
#### • Molecule 1: Pyranose oxidase



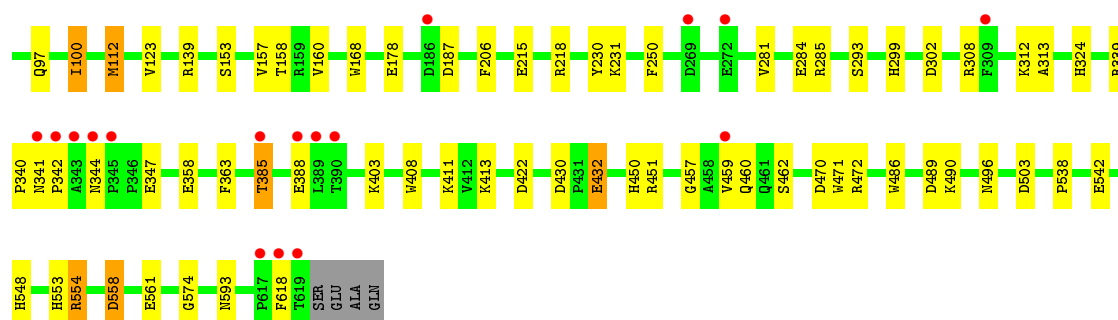
#### • Molecule 1: Pyranose oxidase



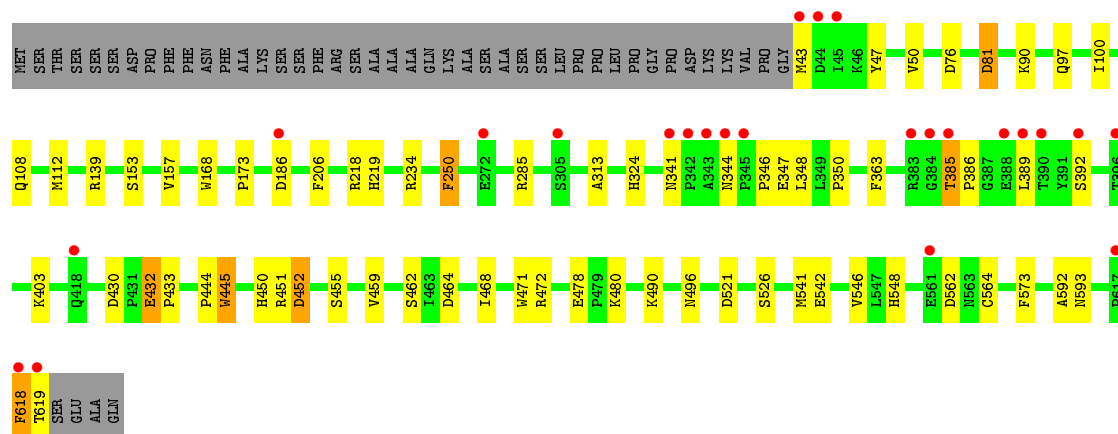
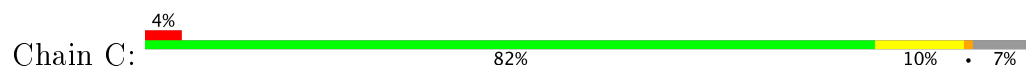
#### • Molecule 1: Pyranose oxidase



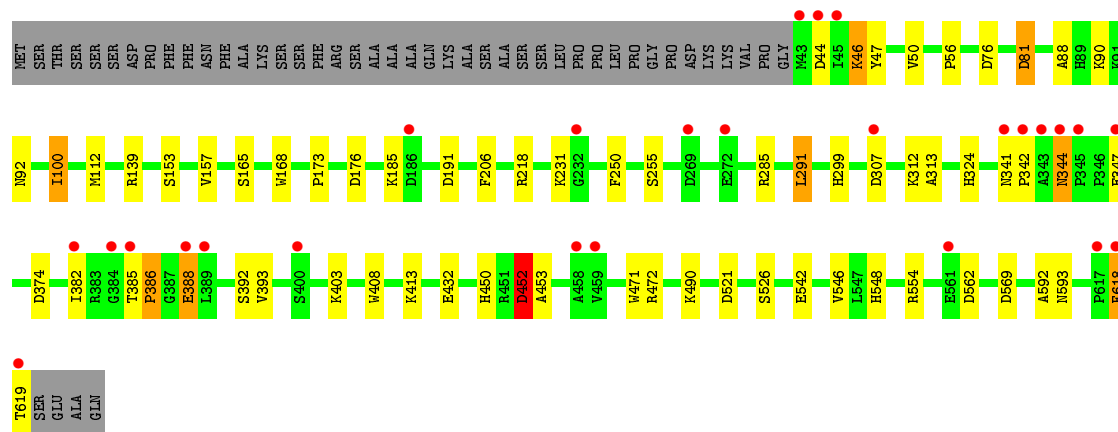
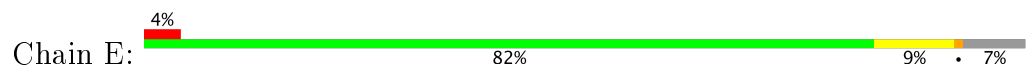




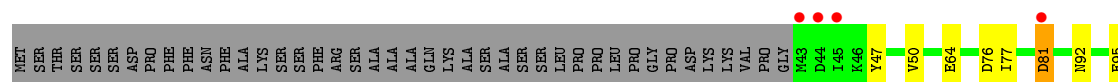
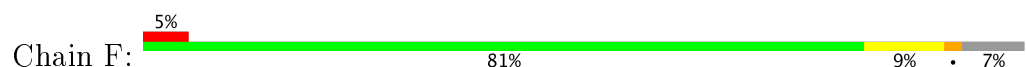
• Molecule 1: Pyranose oxidase

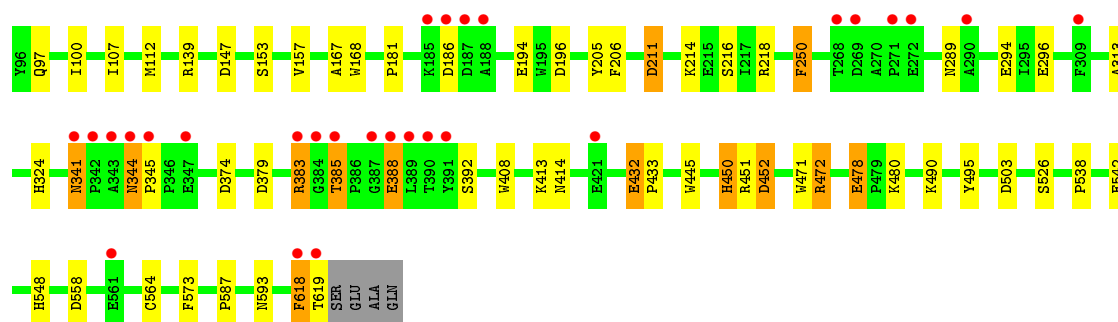


• Molecule 1: Pyranose oxidase

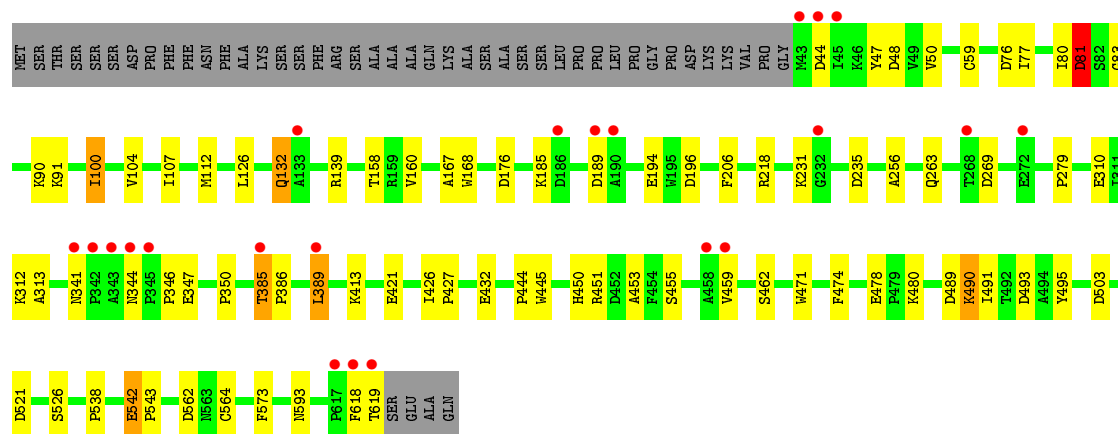
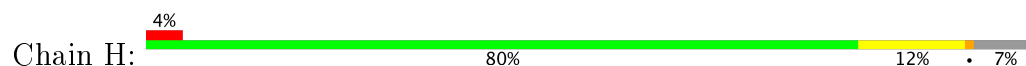


• Molecule 1: Pyranose oxidase

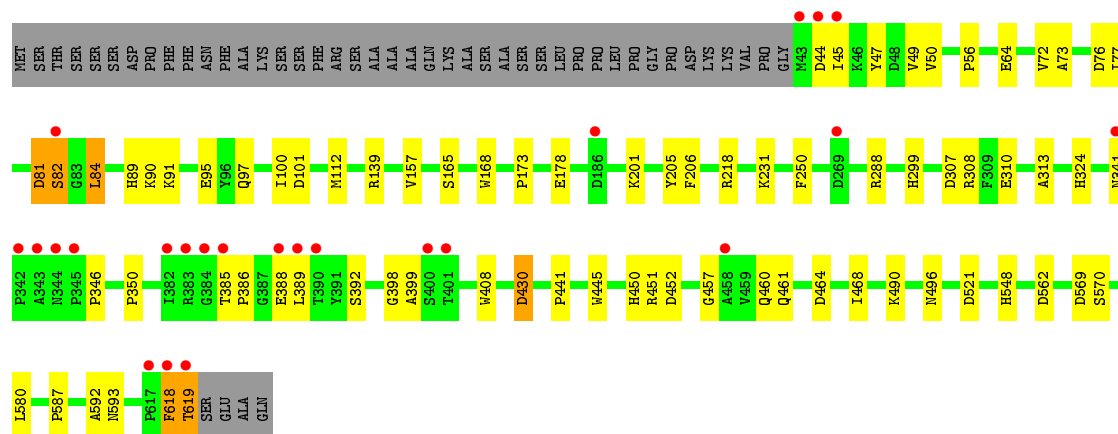
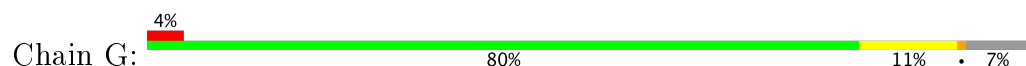




• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 168.59Å 103.08Å 169.04Å<br>90.00° 106.30° 90.00°            | Depositor        |
| Resolution (Å)  | 38.90 – 1.95<br>38.99 – 1.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (38.90-1.95)<br>99.9 (38.99-1.95)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.07  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.86 (at 1.95Å)   | Xtriage          |
| Refinement program  | REFMAC 5.1.24   | Depositor        |
| R, $R_{free}$   | 0.184 , 0.221<br>0.188 , 0.222                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4042 reflections (1.01%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 21.2  | Xtriage          |
| Anisotropy  | 0.222   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 41.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | 0.019 for l,-k,h  | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 38602   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 27.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.84% 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, SHG

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     | 1.14         | 7/4659 (0.2%)   | 1.08        | 20/6335 (0.3%)   |
| 1   | B     | 1.10         | 4/4659 (0.1%)   | 1.08        | 19/6335 (0.3%)   |
| 1   | C     | 1.04         | 3/4659 (0.1%)   | 1.04        | 13/6335 (0.2%)   |
| 1   | D     | 1.08         | 5/4659 (0.1%)   | 1.05        | 19/6335 (0.3%)   |
| 1   | E     | 1.04         | 1/4659 (0.0%)   | 1.04        | 20/6335 (0.3%)   |
| 1   | F     | 1.03         | 3/4659 (0.1%)   | 1.07        | 18/6335 (0.3%)   |
| 1   | G     | 1.05         | 0/4659          | 1.06        | 18/6335 (0.3%)   |
| 1   | H     | 1.07         | 3/4659 (0.1%)   | 1.05        | 23/6335 (0.4%)   |
| All | All   | 1.07         | 26/37272 (0.1%) | 1.06        | 150/50680 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (26) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | E     | 291 | LEU  | CG-CD1 | 7.79 | 1.80        | 1.51     |
| 1   | C     | 541 | MET  | CG-SD  | 6.66 | 1.98        | 1.81     |
| 1   | A     | 482 | GLU  | CD-OE1 | 6.66 | 1.32        | 1.25     |
| 1   | A     | 313 | ALA  | CA-CB  | 6.29 | 1.65        | 1.52     |
| 1   | A     | 112 | MET  | CB-CG  | 5.91 | 1.70        | 1.51     |
| 1   | D     | 486 | TRP  | CB-CG  | 5.88 | 1.60        | 1.50     |
| 1   | C     | 108 | GLN  | CG-CD  | 5.70 | 1.64        | 1.51     |
| 1   | D     | 358 | GLU  | CD-OE2 | 5.63 | 1.31        | 1.25     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 230 | TYR  | CD1-CE1 | 5.54  | 1.47        | 1.39     |
| 1   | F     | 478 | GLU  | CD-OE1  | 5.48  | 1.31        | 1.25     |
| 1   | F     | 250 | PHE  | CE2-CZ  | 5.46  | 1.47        | 1.37     |
| 1   | A     | 108 | GLN  | CG-CD   | 5.34  | 1.63        | 1.51     |
| 1   | B     | 278 | PHE  | CE2-CZ  | 5.32  | 1.47        | 1.37     |
| 1   | A     | 579 | PHE  | CD2-CE2 | 5.24  | 1.49        | 1.39     |
| 1   | H     | 104 | VAL  | CB-CG2  | -5.24 | 1.41        | 1.52     |
| 1   | A     | 81  | ASP  | CB-CG   | -5.23 | 1.40        | 1.51     |
| 1   | H     | 196 | ASP  | CB-CG   | 5.19  | 1.62        | 1.51     |
| 1   | F     | 139 | ARG  | CD-NE   | -5.18 | 1.37        | 1.46     |
| 1   | B     | 482 | GLU  | CD-OE2  | 5.17  | 1.31        | 1.25     |
| 1   | D     | 49  | VAL  | CB-CG1  | 5.14  | 1.63        | 1.52     |
| 1   | A     | 213 | PHE  | CE1-CZ  | 5.14  | 1.47        | 1.37     |
| 1   | H     | 474 | PHE  | CD1-CE1 | 5.14  | 1.49        | 1.39     |
| 1   | C     | 250 | PHE  | CE2-CZ  | 5.14  | 1.47        | 1.37     |
| 1   | B     | 542 | GLU  | CG-CD   | 5.13  | 1.59        | 1.51     |
| 1   | D     | 281 | VAL  | CB-CG2  | 5.09  | 1.63        | 1.52     |
| 1   | B     | 482 | GLU  | CG-CD   | 5.07  | 1.59        | 1.51     |

All (150) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | F     | 139 | ARG  | NE-CZ-NH2 | -24.01 | 108.29      | 120.30   |
| 1   | D     | 139 | ARG  | NE-CZ-NH2 | -20.93 | 109.83      | 120.30   |
| 1   | B     | 139 | ARG  | NE-CZ-NH2 | -20.35 | 110.12      | 120.30   |
| 1   | E     | 139 | ARG  | NE-CZ-NH2 | -19.12 | 110.74      | 120.30   |
| 1   | G     | 139 | ARG  | NE-CZ-NH2 | -18.89 | 110.86      | 120.30   |
| 1   | C     | 139 | ARG  | NE-CZ-NH2 | -17.76 | 111.42      | 120.30   |
| 1   | A     | 139 | ARG  | NE-CZ-NH2 | -16.90 | 111.85      | 120.30   |
| 1   | G     | 139 | ARG  | NE-CZ-NH1 | 15.63  | 128.11      | 120.30   |
| 1   | C     | 139 | ARG  | NE-CZ-NH1 | 15.60  | 128.10      | 120.30   |
| 1   | F     | 139 | ARG  | NE-CZ-NH1 | 15.18  | 127.89      | 120.30   |
| 1   | H     | 139 | ARG  | NE-CZ-NH2 | -14.74 | 112.93      | 120.30   |
| 1   | B     | 81  | ASP  | CB-CG-OD2 | 14.54  | 131.39      | 118.30   |
| 1   | D     | 139 | ARG  | NE-CZ-NH1 | 14.11  | 127.36      | 120.30   |
| 1   | E     | 139 | ARG  | NE-CZ-NH1 | 13.50  | 127.05      | 120.30   |
| 1   | B     | 139 | ARG  | NE-CZ-NH1 | 13.20  | 126.90      | 120.30   |
| 1   | G     | 81  | ASP  | CB-CG-OD2 | 12.71  | 129.74      | 118.30   |
| 1   | H     | 139 | ARG  | NE-CZ-NH1 | 12.49  | 126.55      | 120.30   |
| 1   | C     | 81  | ASP  | CB-CG-OD2 | 12.07  | 129.16      | 118.30   |
| 1   | E     | 291 | LEU  | CB-CG-CD2 | -10.88 | 92.51       | 111.00   |
| 1   | G     | 81  | ASP  | CB-CG-OD1 | -10.68 | 108.69      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | B     | 81  | ASP  | CB-CG-OD1 | -10.48 | 108.86      | 118.30   |
| 1   | A     | 139 | ARG  | NE-CZ-NH1 | 10.42  | 125.51      | 120.30   |
| 1   | E     | 81  | ASP  | CB-CG-OD2 | 9.67   | 127.00      | 118.30   |
| 1   | F     | 81  | ASP  | CB-CG-OD2 | 9.62   | 126.96      | 118.30   |
| 1   | C     | 81  | ASP  | CB-CG-OD1 | -9.15  | 110.06      | 118.30   |
| 1   | F     | 558 | ASP  | CB-CG-OD2 | 9.05   | 126.44      | 118.30   |
| 1   | G     | 76  | ASP  | CB-CG-OD2 | 9.04   | 126.44      | 118.30   |
| 1   | F     | 139 | ARG  | CD-NE-CZ  | 8.87   | 136.01      | 123.60   |
| 1   | F     | 76  | ASP  | CB-CG-OD2 | 8.83   | 126.25      | 118.30   |
| 1   | B     | 76  | ASP  | CB-CG-OD2 | 8.62   | 126.06      | 118.30   |
| 1   | E     | 139 | ARG  | CG-CD-NE  | -8.47  | 94.01       | 111.80   |
| 1   | B     | 139 | ARG  | CG-CD-NE  | -8.44  | 94.08       | 111.80   |
| 1   | F     | 472 | ARG  | NE-CZ-NH1 | 8.41   | 124.50      | 120.30   |
| 1   | E     | 76  | ASP  | CB-CG-OD2 | 8.36   | 125.82      | 118.30   |
| 1   | G     | 521 | ASP  | CB-CG-OD2 | 8.32   | 125.79      | 118.30   |
| 1   | H     | 562 | ASP  | CB-CG-OD2 | 8.28   | 125.75      | 118.30   |
| 1   | D     | 81  | ASP  | CB-CG-OD2 | 8.24   | 125.71      | 118.30   |
| 1   | D     | 76  | ASP  | CB-CG-OD2 | 8.21   | 125.69      | 118.30   |
| 1   | A     | 76  | ASP  | CB-CG-OD2 | 8.14   | 125.62      | 118.30   |
| 1   | B     | 558 | ASP  | CB-CG-OD2 | 7.85   | 125.36      | 118.30   |
| 1   | E     | 81  | ASP  | CB-CG-OD1 | -7.85  | 111.24      | 118.30   |
| 1   | C     | 562 | ASP  | CB-CG-OD2 | 7.69   | 125.22      | 118.30   |
| 1   | F     | 139 | ARG  | CG-CD-NE  | -7.68  | 95.67       | 111.80   |
| 1   | H     | 493 | ASP  | CB-CG-OD1 | 7.68   | 125.21      | 118.30   |
| 1   | H     | 81  | ASP  | CB-CG-OD1 | -7.66  | 111.41      | 118.30   |
| 1   | E     | 176 | ASP  | CB-CG-OD2 | 7.65   | 125.18      | 118.30   |
| 1   | A     | 493 | ASP  | CB-CG-OD1 | 7.59   | 125.13      | 118.30   |
| 1   | C     | 139 | ARG  | CD-NE-CZ  | 7.45   | 134.03      | 123.60   |
| 1   | E     | 291 | LEU  | CA-CB-CG  | -7.36  | 98.38       | 115.30   |
| 1   | E     | 452 | ASP  | CB-CG-OD2 | 7.25   | 124.82      | 118.30   |
| 1   | H     | 81  | ASP  | CB-CG-OD2 | 7.18   | 124.76      | 118.30   |
| 1   | G     | 562 | ASP  | CB-CG-OD2 | 7.04   | 124.63      | 118.30   |
| 1   | G     | 430 | ASP  | CB-CG-OD2 | 7.03   | 124.63      | 118.30   |
| 1   | B     | 139 | ARG  | CD-NE-CZ  | 6.99   | 133.39      | 123.60   |
| 1   | A     | 139 | ARG  | CG-CD-NE  | -6.91  | 97.28       | 111.80   |
| 1   | F     | 374 | ASP  | CB-CG-OD2 | 6.90   | 124.51      | 118.30   |
| 1   | D     | 470 | ASP  | CB-CG-OD1 | 6.84   | 124.45      | 118.30   |
| 1   | D     | 503 | ASP  | CB-CG-OD2 | 6.82   | 124.44      | 118.30   |
| 1   | H     | 389 | LEU  | CB-CG-CD2 | -6.81  | 99.43       | 111.00   |
| 1   | H     | 503 | ASP  | CB-CG-OD2 | 6.74   | 124.37      | 118.30   |
| 1   | D     | 97  | GLN  | CA-CB-CG  | -6.74  | 98.58       | 113.40   |
| 1   | F     | 472 | ARG  | NE-CZ-NH2 | -6.69  | 116.96      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 430 | ASP  | CB-CG-OD2 | 6.63  | 124.27      | 118.30   |
| 1   | F     | 196 | ASP  | CB-CG-OD1 | 6.56  | 124.20      | 118.30   |
| 1   | G     | 569 | ASP  | CB-CG-OD2 | 6.55  | 124.20      | 118.30   |
| 1   | C     | 76  | ASP  | CB-CG-OD2 | 6.50  | 124.15      | 118.30   |
| 1   | E     | 44  | ASP  | CB-CG-OD2 | 6.49  | 124.14      | 118.30   |
| 1   | D     | 187 | ASP  | CB-CG-OD2 | 6.48  | 124.14      | 118.30   |
| 1   | H     | 521 | ASP  | CB-CG-OD2 | 6.46  | 124.11      | 118.30   |
| 1   | D     | 139 | ARG  | CG-CD-NE  | -6.39 | 98.38       | 111.80   |
| 1   | G     | 452 | ASP  | CB-CG-OD2 | 6.39  | 124.05      | 118.30   |
| 1   | D     | 139 | ARG  | CD-NE-CZ  | 6.36  | 132.51      | 123.60   |
| 1   | B     | 124 | ASP  | CB-CG-OD2 | 6.36  | 124.02      | 118.30   |
| 1   | F     | 97  | GLN  | CA-CB-CG  | -6.35 | 99.44       | 113.40   |
| 1   | C     | 139 | ARG  | CG-CD-NE  | -6.28 | 98.62       | 111.80   |
| 1   | A     | 211 | ASP  | CB-CG-OD1 | 6.26  | 123.93      | 118.30   |
| 1   | A     | 189 | ASP  | CB-CG-OD2 | 6.22  | 123.90      | 118.30   |
| 1   | A     | 139 | ARG  | CD-NE-CZ  | 6.21  | 132.29      | 123.60   |
| 1   | A     | 81  | ASP  | CB-CG-OD1 | -6.20 | 112.72      | 118.30   |
| 1   | B     | 97  | GLN  | CA-CB-CG  | -6.20 | 99.76       | 113.40   |
| 1   | D     | 558 | ASP  | CB-CG-OD2 | 6.19  | 123.87      | 118.30   |
| 1   | E     | 569 | ASP  | CB-CG-OD2 | 6.18  | 123.87      | 118.30   |
| 1   | H     | 389 | LEU  | CA-CB-CG  | 6.18  | 129.52      | 115.30   |
| 1   | F     | 211 | ASP  | CB-CG-OD2 | 6.17  | 123.85      | 118.30   |
| 1   | G     | 139 | ARG  | CG-CD-NE  | -6.14 | 98.89       | 111.80   |
| 1   | H     | 76  | ASP  | CB-CG-OD2 | 6.13  | 123.82      | 118.30   |
| 1   | B     | 489 | ASP  | CB-CG-OD1 | 6.13  | 123.81      | 118.30   |
| 1   | D     | 472 | ARG  | NE-CZ-NH2 | -6.09 | 117.25      | 120.30   |
| 1   | G     | 44  | ASP  | CB-CG-OD2 | 6.04  | 123.74      | 118.30   |
| 1   | H     | 269 | ASP  | CB-CG-OD2 | 6.04  | 123.73      | 118.30   |
| 1   | E     | 554 | ARG  | NE-CZ-NH1 | 6.00  | 123.30      | 120.30   |
| 1   | G     | 288 | ARG  | NE-CZ-NH2 | -6.00 | 117.30      | 120.30   |
| 1   | A     | 452 | ASP  | CB-CG-OD2 | 5.99  | 123.69      | 118.30   |
| 1   | A     | 81  | ASP  | CB-CG-OD2 | 5.98  | 123.68      | 118.30   |
| 1   | A     | 124 | ASP  | CB-CG-OD2 | 5.97  | 123.68      | 118.30   |
| 1   | B     | 379 | ASP  | CB-CG-OD2 | 5.93  | 123.63      | 118.30   |
| 1   | H     | 235 | ASP  | CB-CG-OD2 | 5.88  | 123.59      | 118.30   |
| 1   | G     | 288 | ARG  | NE-CZ-NH1 | 5.88  | 123.24      | 120.30   |
| 1   | B     | 406 | ASP  | CB-CG-OD1 | 5.86  | 123.58      | 118.30   |
| 1   | G     | 139 | ARG  | CD-NE-CZ  | 5.83  | 131.77      | 123.60   |
| 1   | F     | 503 | ASP  | CB-CG-OD2 | 5.79  | 123.51      | 118.30   |
| 1   | B     | 176 | ASP  | CB-CG-OD2 | 5.76  | 123.49      | 118.30   |
| 1   | E     | 374 | ASP  | CB-CG-OD2 | 5.75  | 123.48      | 118.30   |
| 1   | A     | 197 | ARG  | NE-CZ-NH1 | -5.75 | 117.42      | 120.30   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | H     | 196 | ASP  | CB-CG-OD2  | 5.75  | 123.48      | 118.30   |
| 1   | H     | 489 | ASP  | CB-CG-OD2  | 5.73  | 123.45      | 118.30   |
| 1   | A     | 406 | ASP  | CB-CG-OD1  | 5.71  | 123.44      | 118.30   |
| 1   | A     | 422 | ASP  | CB-CG-OD2  | 5.67  | 123.40      | 118.30   |
| 1   | H     | 176 | ASP  | CB-CG-OD2  | 5.67  | 123.40      | 118.30   |
| 1   | F     | 81  | ASP  | CB-CG-OD1  | -5.65 | 113.22      | 118.30   |
| 1   | C     | 186 | ASP  | CB-CG-OD2  | 5.64  | 123.38      | 118.30   |
| 1   | E     | 291 | LEU  | CB-CG-CD1  | 5.60  | 120.53      | 111.00   |
| 1   | D     | 472 | ARG  | NE-CZ-NH1  | 5.58  | 123.09      | 120.30   |
| 1   | A     | 503 | ASP  | CB-CG-OD2  | 5.58  | 123.32      | 118.30   |
| 1   | A     | 186 | ASP  | CB-CG-OD2  | 5.57  | 123.31      | 118.30   |
| 1   | E     | 307 | ASP  | CB-CG-OD2  | 5.55  | 123.30      | 118.30   |
| 1   | B     | 562 | ASP  | CB-CG-OD2  | 5.54  | 123.29      | 118.30   |
| 1   | G     | 464 | ASP  | CB-CG-OD2  | 5.53  | 123.27      | 118.30   |
| 1   | A     | 307 | ASP  | CB-CG-OD2  | 5.51  | 123.26      | 118.30   |
| 1   | H     | 48  | ASP  | CB-CG-OD2  | 5.49  | 123.24      | 118.30   |
| 1   | H     | 139 | ARG  | CA-CB-CG   | 5.48  | 125.46      | 113.40   |
| 1   | E     | 521 | ASP  | CB-CG-OD2  | 5.46  | 123.21      | 118.30   |
| 1   | F     | 147 | ASP  | CB-CG-OD1  | 5.45  | 123.20      | 118.30   |
| 1   | B     | 44  | ASP  | CB-CG-OD2  | 5.45  | 123.20      | 118.30   |
| 1   | B     | 48  | ASP  | CB-CG-OD2  | 5.42  | 123.18      | 118.30   |
| 1   | G     | 101 | ASP  | CB-CG-OD2  | 5.41  | 123.17      | 118.30   |
| 1   | C     | 464 | ASP  | CB-CG-OD2  | 5.36  | 123.12      | 118.30   |
| 1   | D     | 554 | ARG  | NE-CZ-NH1  | 5.36  | 122.98      | 120.30   |
| 1   | C     | 452 | ASP  | CB-CG-OD2  | 5.35  | 123.11      | 118.30   |
| 1   | B     | 104 | VAL  | CG1-CB-CG2 | -5.34 | 102.36      | 110.90   |
| 1   | D     | 422 | ASP  | CB-CG-OD2  | 5.32  | 123.08      | 118.30   |
| 1   | A     | 269 | ASP  | CB-CG-OD2  | 5.31  | 123.08      | 118.30   |
| 1   | H     | 279 | PRO  | N-CD-CG    | -5.30 | 95.25       | 103.20   |
| 1   | H     | 189 | ASP  | CB-CG-OD2  | 5.29  | 123.06      | 118.30   |
| 1   | H     | 104 | VAL  | CG1-CB-CG2 | -5.26 | 102.48      | 110.90   |
| 1   | H     | 139 | ARG  | CD-NE-CZ   | 5.24  | 130.94      | 123.60   |
| 1   | H     | 44  | ASP  | CB-CG-OD2  | 5.23  | 123.01      | 118.30   |
| 1   | E     | 191 | ASP  | CB-CG-OD2  | 5.21  | 122.99      | 118.30   |
| 1   | F     | 379 | ASP  | CB-CG-OD2  | 5.20  | 122.98      | 118.30   |
| 1   | C     | 521 | ASP  | CB-CG-OD2  | 5.19  | 122.97      | 118.30   |
| 1   | G     | 307 | ASP  | CB-CG-OD2  | 5.19  | 122.97      | 118.30   |
| 1   | E     | 554 | ARG  | NE-CZ-NH2  | -5.17 | 117.72      | 120.30   |
| 1   | F     | 186 | ASP  | CB-CG-OD2  | 5.17  | 122.95      | 118.30   |
| 1   | D     | 112 | MET  | CG-SD-CE   | 5.15  | 108.44      | 100.20   |
| 1   | C     | 234 | ARG  | NE-CZ-NH1  | -5.11 | 117.74      | 120.30   |
| 1   | D     | 489 | ASP  | CB-CG-OD1  | 5.10  | 122.89      | 118.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 302 | ASP  | CB-CG-OD2 | 5.07  | 122.86      | 118.30   |
| 1   | B     | 569 | ASP  | CB-CG-OD2 | 5.07  | 122.86      | 118.30   |
| 1   | D     | 81  | ASP  | CB-CG-OD1 | -5.01 | 113.79      | 118.30   |
| 1   | E     | 562 | ASP  | CB-CG-OD2 | 5.00  | 122.80      | 118.30   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B     | 151 | ASN  | Peptide |
| 1   | D     | 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     | 4544  | 0        | 4393     | 28      | 0            |
| 1   | B     | 4544  | 0        | 4393     | 31      | 0            |
| 1   | C     | 4544  | 0        | 4393     | 33      | 0            |
| 1   | D     | 4544  | 0        | 4393     | 32      | 0            |
| 1   | E     | 4544  | 0        | 4393     | 36      | 0            |
| 1   | F     | 4544  | 0        | 4393     | 35      | 0            |
| 1   | G     | 4544  | 0        | 4393     | 42      | 0            |
| 1   | H     | 4544  | 0        | 4393     | 30      | 0            |
| 2   | A     | 12    | 0        | 11       | 4       | 0            |
| 2   | B     | 12    | 0        | 11       | 1       | 0            |
| 2   | C     | 12    | 0        | 11       | 5       | 0            |
| 2   | D     | 12    | 0        | 11       | 3       | 0            |
| 2   | E     | 12    | 0        | 11       | 4       | 0            |
| 2   | F     | 12    | 0        | 10       | 2       | 0            |
| 2   | G     | 12    | 0        | 11       | 4       | 0            |
| 2   | H     | 12    | 0        | 11       | 0       | 0            |
| 3   | A     | 53    | 0        | 31       | 4       | 0            |
| 3   | B     | 53    | 0        | 31       | 4       | 0            |
| 3   | C     | 53    | 0        | 31       | 1       | 0            |
| 3   | D     | 53    | 0        | 31       | 2       | 0            |
| 3   | E     | 53    | 0        | 31       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | F     | 53    | 0        | 31       | 0       | 0            |
| 3   | G     | 53    | 0        | 31       | 2       | 0            |
| 3   | H     | 53    | 0        | 31       | 0       | 0            |
| 4   | A     | 244   | 0        | 0        | 3       | 0            |
| 4   | B     | 251   | 0        | 0        | 1       | 0            |
| 4   | C     | 199   | 0        | 0        | 2       | 0            |
| 4   | D     | 222   | 0        | 0        | 1       | 0            |
| 4   | E     | 195   | 0        | 0        | 2       | 0            |
| 4   | F     | 192   | 0        | 0        | 1       | 0            |
| 4   | G     | 210   | 0        | 0        | 6       | 0            |
| 4   | H     | 217   | 0        | 0        | 3       | 0            |
| All | All   | 38602 | 0        | 35479    | 269     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (269) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:E:291:LEU:CG   | 1:E:291:LEU:CD1 | 1.80                     | 1.56              |
| 1:G:81:ASP:HA    | 4:G:2497:HOH:O  | 1.42                     | 1.16              |
| 1:C:432:GLU:HG3  | 4:C:2381:HOH:O  | 1.48                     | 1.12              |
| 1:G:81:ASP:CA    | 4:G:2497:HOH:O  | 2.04                     | 0.98              |
| 1:E:291:LEU:CD1  | 1:E:291:LEU:HG  | 2.01                     | 0.88              |
| 1:C:97:GLN:HG3   | 1:C:250:PHE:CE2 | 2.10                     | 0.87              |
| 1:G:81:ASP:C     | 4:G:2497:HOH:O  | 2.15                     | 0.84              |
| 1:G:82:SER:N     | 4:G:2497:HOH:O  | 2.10                     | 0.83              |
| 1:H:312:LYS:HE3  | 4:H:1958:HOH:O  | 1.84                     | 0.77              |
| 1:C:97:GLN:HG3   | 1:C:250:PHE:CD2 | 2.19                     | 0.77              |
| 1:G:385:THR:O    | 1:G:388:GLU:HG2 | 1.86                     | 0.75              |
| 1:D:385:THR:OG1  | 1:D:388:GLU:OE1 | 2.07                     | 0.72              |
| 1:H:81:ASP:O     | 1:H:90:LYS:HE2  | 1.91                     | 0.70              |
| 1:F:157:VAL:HG21 | 1:F:324:HIS:HE1 | 1.58                     | 0.69              |
| 1:F:548:HIS:NE2  | 2:F:806:SHG:O3  | 2.25                     | 0.69              |
| 1:G:385:THR:HG22 | 1:G:386:PRO:HD2 | 1.75                     | 0.69              |
| 1:D:548:HIS:CE1  | 2:D:803:SHG:HO3 | 2.10                     | 0.69              |
| 1:F:385:THR:O    | 1:F:388:GLU:HG3 | 1.93                     | 0.69              |
| 1:F:538:PRO:HG2  | 1:H:538:PRO:HG2 | 1.77                     | 0.67              |
| 1:E:56:PRO:HD3   | 1:E:165:SER:HB3 | 1.76                     | 0.67              |
| 1:C:548:HIS:NE2  | 2:C:804:SHG:O3  | 2.27                     | 0.65              |
| 1:C:50:VAL:HG13  | 1:C:313:ALA:HB2 | 1.76                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:385:THR:HB   | 1:G:388:GLU:OE2  | 1.97                     | 0.65              |
| 1:H:126:LEU:HD12 | 1:H:132:GLN:HG3  | 1.78                     | 0.64              |
| 1:E:81:ASP:O     | 1:E:90:LYS:HE2   | 1.97                     | 0.63              |
| 1:A:132:GLN:HG2  | 4:A:1684:HOH:O   | 1.98                     | 0.63              |
| 1:F:64:GLU:OE2   | 1:F:205:TYR:OH   | 2.15                     | 0.62              |
| 1:H:490:LYS:HD2  | 1:H:491:ILE:HD13 | 1.80                     | 0.62              |
| 1:A:77:ILE:HG22  | 3:A:701:FAD:C4A  | 2.29                     | 0.62              |
| 1:G:201:LYS:HE2  | 1:G:205:TYR:OH   | 1.99                     | 0.61              |
| 1:E:548:HIS:NE2  | 2:E:805:SHG:O3   | 2.29                     | 0.61              |
| 1:C:546:VAL:HA   | 2:C:804:SHG:H6A  | 1.83                     | 0.60              |
| 1:E:291:LEU:H    | 1:E:291:LEU:HD12 | 1.65                     | 0.60              |
| 1:F:413:LYS:NZ   | 1:F:414:ASN:OD1  | 2.34                     | 0.60              |
| 1:H:478:GLU:HG2  | 1:H:480:LYS:HE2  | 1.82                     | 0.60              |
| 1:F:50:VAL:HG13  | 1:F:313:ALA:HB2  | 1.83                     | 0.60              |
| 1:B:77:ILE:HG22  | 3:B:702:FAD:C4A  | 2.33                     | 0.59              |
| 1:C:218:ARG:HD2  | 4:C:1541:HOH:O   | 2.02                     | 0.59              |
| 1:B:385:THR:N    | 1:B:388:GLU:OE1  | 2.34                     | 0.59              |
| 1:D:548:HIS:CE1  | 2:D:803:SHG:O3   | 2.56                     | 0.58              |
| 1:E:618:PHE:HD1  | 1:E:619:THR:N    | 2.01                     | 0.58              |
| 1:B:153:SER:OG   | 1:B:542:GLU:HG3  | 2.03                     | 0.58              |
| 1:C:47:TYR:O     | 1:C:313:ALA:HA   | 2.03                     | 0.58              |
| 1:B:100:ILE:O    | 1:B:100:ILE:HD13 | 2.04                     | 0.58              |
| 1:G:81:ASP:OD1   | 1:G:81:ASP:C     | 2.42                     | 0.57              |
| 1:A:50:VAL:HG13  | 1:A:313:ALA:HB2  | 1.86                     | 0.57              |
| 1:D:89:HIS:CE1   | 1:D:91:LYS:HE2   | 2.40                     | 0.57              |
| 1:B:346:PRO:HG2  | 1:B:350:PRO:HA   | 1.87                     | 0.56              |
| 1:C:452:ASP:OD1  | 1:C:472:ARG:NH1  | 2.38                     | 0.56              |
| 1:G:81:ASP:O     | 1:G:90:LYS:HE2   | 2.05                     | 0.56              |
| 1:A:336:GLN:NE2  | 1:A:344:ASN:O    | 2.38                     | 0.56              |
| 1:A:218:ARG:HD2  | 4:A:1630:HOH:O   | 2.06                     | 0.56              |
| 1:C:548:HIS:CE1  | 2:C:804:SHG:HO3  | 2.22                     | 0.56              |
| 1:F:181:PRO:HG3  | 1:F:587:PRO:HD2  | 1.86                     | 0.56              |
| 1:E:50:VAL:HG13  | 1:E:313:ALA:HB2  | 1.87                     | 0.56              |
| 1:G:56:PRO:HD3   | 1:G:165:SER:HB3  | 1.89                     | 0.55              |
| 1:C:548:HIS:CE1  | 2:C:804:SHG:O3   | 2.59                     | 0.55              |
| 1:H:346:PRO:HG2  | 1:H:350:PRO:HA   | 1.89                     | 0.55              |
| 2:D:803:SHG:H3   | 3:D:703:FAD:N5   | 2.22                     | 0.55              |
| 1:G:618:PHE:C    | 1:G:618:PHE:HD1  | 2.10                     | 0.55              |
| 2:A:801:SHG:H3   | 3:A:701:FAD:N5   | 2.21                     | 0.54              |
| 1:B:538:PRO:HG2  | 1:D:538:PRO:HG2  | 1.89                     | 0.54              |
| 1:G:64:GLU:OE2   | 1:G:205:TYR:OH   | 2.18                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:47:TYR:O     | 1:G:313:ALA:HA   | 2.08                     | 0.54              |
| 1:E:153:SER:OG   | 1:E:542:GLU:HG3  | 2.07                     | 0.54              |
| 1:G:97:GLN:HG3   | 1:G:250:PHE:CE2  | 2.43                     | 0.54              |
| 1:C:564:CYS:HG   | 1:C:573:PHE:HE2  | 1.55                     | 0.54              |
| 1:F:92:ASN:O     | 1:F:250:PHE:HZ   | 1.91                     | 0.54              |
| 1:B:81:ASP:C     | 1:B:81:ASP:OD1   | 2.45                     | 0.54              |
| 1:F:153:SER:OG   | 1:F:542:GLU:HG2  | 2.08                     | 0.53              |
| 1:G:346:PRO:HG2  | 1:G:350:PRO:HA   | 1.90                     | 0.53              |
| 1:G:49:VAL:HB    | 1:G:72:VAL:HG22  | 1.90                     | 0.52              |
| 1:D:50:VAL:HG13  | 1:D:313:ALA:HB2  | 1.90                     | 0.52              |
| 1:D:81:ASP:O     | 1:D:90:LYS:HE2   | 2.10                     | 0.52              |
| 1:E:452:ASP:OD1  | 1:E:472:ARG:NH1  | 2.42                     | 0.52              |
| 1:G:548:HIS:CE1  | 2:G:808:SHG:HO3  | 2.26                     | 0.52              |
| 1:D:153:SER:OG   | 1:D:542:GLU:HG3  | 2.09                     | 0.52              |
| 1:E:291:LEU:H    | 1:E:291:LEU:CD1  | 2.23                     | 0.52              |
| 1:E:548:HIS:CE1  | 2:E:805:SHG:O3   | 2.63                     | 0.52              |
| 1:D:100:ILE:HD13 | 1:D:100:ILE:C    | 2.30                     | 0.52              |
| 1:G:618:PHE:C    | 1:G:618:PHE:CD1  | 2.82                     | 0.51              |
| 1:G:618:PHE:HD1  | 1:G:619:THR:N    | 2.08                     | 0.51              |
| 1:G:50:VAL:HG13  | 1:G:313:ALA:HB2  | 1.93                     | 0.51              |
| 1:G:218:ARG:HD2  | 4:G:1593:HOH:O   | 2.10                     | 0.51              |
| 1:B:137:PHE:CE2  | 1:B:139:ARG:HG2  | 2.46                     | 0.51              |
| 1:A:81:ASP:O     | 1:A:90:LYS:HE2   | 2.12                     | 0.50              |
| 1:C:157:VAL:HG21 | 1:C:324:HIS:HE1  | 1.76                     | 0.50              |
| 1:D:77:ILE:HG22  | 3:D:703:FAD:C4A  | 2.40                     | 0.50              |
| 1:E:157:VAL:HG21 | 1:E:324:HIS:HE1  | 1.76                     | 0.50              |
| 1:G:157:VAL:HG21 | 1:G:324:HIS:HE1  | 1.76                     | 0.50              |
| 1:B:153:SER:OG   | 1:B:542:GLU:CG   | 2.58                     | 0.50              |
| 1:B:159:ARG:HA   | 3:B:702:FAD:O2B  | 2.10                     | 0.50              |
| 2:C:804:SHG:H3   | 3:C:704:FAD:N5   | 2.26                     | 0.50              |
| 1:D:157:VAL:HG21 | 1:D:324:HIS:HE1  | 1.77                     | 0.49              |
| 1:B:100:ILE:C    | 1:B:100:ILE:HD13 | 2.32                     | 0.49              |
| 1:F:289:ASN:HB3  | 1:F:296:GLU:OE2  | 2.12                     | 0.49              |
| 1:G:548:HIS:NE2  | 2:G:808:SHG:O3   | 2.38                     | 0.49              |
| 1:E:618:PHE:HD1  | 1:E:619:THR:H    | 1.60                     | 0.49              |
| 1:E:291:LEU:HD13 | 4:E:2441:HOH:O   | 2.13                     | 0.49              |
| 1:G:84:LEU:N     | 1:G:84:LEU:HD23  | 2.28                     | 0.49              |
| 1:C:173:PRO:HG2  | 1:C:592:ALA:HB1  | 1.93                     | 0.49              |
| 1:E:385:THR:O    | 1:E:388:GLU:HG2  | 2.12                     | 0.49              |
| 1:H:312:LYS:CE   | 4:H:1958:HOH:O   | 2.54                     | 0.49              |
| 1:A:457:GLY:H    | 1:A:460:GLN:HE21 | 1.61                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:126:LEU:CD1  | 1:H:132:GLN:HG3  | 2.42                     | 0.49              |
| 1:H:218:ARG:HD2  | 4:H:1173:HOH:O   | 2.13                     | 0.49              |
| 1:E:471:TRP:CH2  | 1:E:526:SER:HA   | 2.47                     | 0.48              |
| 1:F:218:ARG:HD2  | 4:F:2063:HOH:O   | 2.12                     | 0.48              |
| 1:F:47:TYR:O     | 1:F:313:ALA:HA   | 2.14                     | 0.48              |
| 1:H:432:GLU:HB3  | 1:H:451:ARG:HB2  | 1.96                     | 0.48              |
| 1:F:452:ASP:OD1  | 1:F:452:ASP:N    | 2.47                     | 0.48              |
| 1:C:153:SER:OG   | 1:C:542:GLU:HG3  | 2.13                     | 0.48              |
| 1:F:548:HIS:CE1  | 2:F:806:SHG:O3   | 2.66                     | 0.48              |
| 1:B:432:GLU:HG2  | 1:B:432:GLU:H    | 1.39                     | 0.47              |
| 1:D:457:GLY:H    | 1:D:460:GLN:HE21 | 1.62                     | 0.47              |
| 1:E:47:TYR:O     | 1:E:313:ALA:HA   | 2.14                     | 0.47              |
| 1:A:157:VAL:HG21 | 1:A:324:HIS:HE1  | 1.79                     | 0.47              |
| 1:B:81:ASP:O     | 1:B:90:LYS:HE2   | 2.14                     | 0.47              |
| 1:H:59:CYS:SG    | 1:H:256:ALA:HB1  | 2.55                     | 0.47              |
| 1:B:218:ARG:HD2  | 4:B:948:HOH:O    | 2.15                     | 0.47              |
| 1:E:342:PRO:C    | 1:E:344:ASN:H    | 2.18                     | 0.47              |
| 1:D:123:VAL:HG22 | 1:C:459:VAL:CG1  | 2.44                     | 0.47              |
| 1:G:457:GLY:O    | 1:G:461:GLN:HG3  | 2.15                     | 0.47              |
| 1:B:56:PRO:HD3   | 1:B:165:SER:HB3  | 1.97                     | 0.46              |
| 1:D:158:THR:HG22 | 1:D:160:VAL:HG22 | 1.96                     | 0.46              |
| 1:D:284:GLU:HB2  | 1:D:299:HIS:HD2  | 1.80                     | 0.46              |
| 1:A:158:THR:HG22 | 1:A:160:VAL:HG22 | 1.96                     | 0.46              |
| 1:C:432:GLU:H    | 1:C:432:GLU:HG2  | 1.45                     | 0.46              |
| 1:D:218:ARG:HG3  | 1:D:430:ASP:OD2  | 2.16                     | 0.46              |
| 1:F:92:ASN:O     | 1:F:250:PHE:CZ   | 2.68                     | 0.46              |
| 2:E:805:SHG:H3   | 3:E:705:FAD:N5   | 2.31                     | 0.46              |
| 1:A:77:ILE:CG2   | 3:A:701:FAD:C4A  | 2.93                     | 0.46              |
| 1:F:344:ASN:N    | 1:F:345:PRO:CD   | 2.78                     | 0.46              |
| 1:G:299:HIS:CE1  | 1:G:308:ARG:HB3  | 2.51                     | 0.46              |
| 1:A:159:ARG:HA   | 3:A:701:FAD:O2B  | 2.16                     | 0.46              |
| 1:B:487:PHE:HB3  | 1:B:498:PRO:HB2  | 1.98                     | 0.46              |
| 1:H:471:TRP:CH2  | 1:H:526:SER:HA   | 2.51                     | 0.46              |
| 1:F:618:PHE:C    | 1:F:618:PHE:CD1  | 2.89                     | 0.46              |
| 1:B:451:ARG:HD3  | 1:B:468:ILE:O    | 2.16                     | 0.45              |
| 1:G:178:GLU:OE1  | 1:G:441:PRO:HG3  | 2.16                     | 0.45              |
| 1:A:548:HIS:CE1  | 2:A:801:SHG:HO3  | 2.32                     | 0.45              |
| 1:B:294:GLU:OE1  | 1:B:296:GLU:OE2  | 2.35                     | 0.45              |
| 1:G:173:PRO:HG2  | 1:G:592:ALA:HB1  | 1.98                     | 0.45              |
| 1:H:490:LYS:HD2  | 1:H:491:ILE:CD1  | 2.45                     | 0.45              |
| 1:B:471:TRP:CH2  | 1:B:526:SER:HA   | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:293:SER:HA   | 1:D:574:GLY:O    | 2.17                     | 0.45              |
| 1:H:80:ILE:O     | 1:H:81:ASP:HB3   | 2.15                     | 0.45              |
| 1:B:45:ILE:HG13  | 1:B:45:ILE:H     | 1.65                     | 0.45              |
| 1:E:619:THR:O    | 1:E:619:THR:HG23 | 2.17                     | 0.45              |
| 1:H:459:VAL:O    | 1:H:462:SER:HB3  | 2.16                     | 0.45              |
| 1:C:478:GLU:OE2  | 1:C:480:LYS:HE2  | 2.15                     | 0.45              |
| 1:E:218:ARG:HD2  | 4:E:1659:HOH:O   | 2.16                     | 0.45              |
| 1:H:77:ILE:HD11  | 1:H:495:TYR:CD2  | 2.52                     | 0.45              |
| 1:D:100:ILE:HD13 | 1:D:100:ILE:O    | 2.17                     | 0.45              |
| 1:E:385:THR:HG22 | 1:E:386:PRO:HD2  | 1.99                     | 0.45              |
| 2:G:808:SHG:H3   | 3:G:708:FAD:N5   | 2.32                     | 0.45              |
| 1:E:291:LEU:HD12 | 1:E:291:LEU:N    | 2.32                     | 0.45              |
| 1:C:451:ARG:HD3  | 1:C:468:ILE:O    | 2.17                     | 0.44              |
| 1:E:546:VAL:HA   | 2:E:805:SHG:H6   | 1.98                     | 0.44              |
| 1:H:107:ILE:HG12 | 1:H:167:ALA:HB1  | 1.98                     | 0.44              |
| 1:H:50:VAL:HG13  | 1:H:313:ALA:HB2  | 1.98                     | 0.44              |
| 1:F:432:GLU:HB3  | 1:F:451:ARG:HB2  | 1.99                     | 0.44              |
| 1:F:77:ILE:HD11  | 1:F:495:TYR:CD2  | 2.52                     | 0.44              |
| 1:A:548:HIS:CE1  | 2:A:801:SHG:O3   | 2.70                     | 0.44              |
| 1:E:81:ASP:CG    | 1:E:81:ASP:O     | 2.55                     | 0.44              |
| 1:H:100:ILE:HD13 | 1:H:453:ALA:HA   | 1.99                     | 0.44              |
| 1:F:471:TRP:CH2  | 1:F:526:SER:HA   | 2.52                     | 0.44              |
| 1:G:77:ILE:HG22  | 3:G:708:FAD:C4A  | 2.48                     | 0.44              |
| 1:B:185:LYS:HE3  | 1:B:185:LYS:HB2  | 1.59                     | 0.44              |
| 1:F:432:GLU:HG2  | 1:F:432:GLU:H    | 1.50                     | 0.44              |
| 1:F:618:PHE:HD1  | 1:F:619:THR:N    | 2.16                     | 0.44              |
| 1:C:471:TRP:CH2  | 1:C:526:SER:HA   | 2.52                     | 0.44              |
| 1:C:81:ASP:OD1   | 1:C:81:ASP:C     | 2.52                     | 0.44              |
| 1:E:285:ARG:HG3  | 1:E:299:HIS:HB3  | 2.00                     | 0.44              |
| 1:G:89:HIS:CE1   | 1:G:91:LYS:HB2   | 2.52                     | 0.44              |
| 1:H:444:PRO:HD2  | 1:H:445:TRP:CZ3  | 2.52                     | 0.44              |
| 1:A:358:GLU:HG2  | 1:A:544:GLY:HA2  | 1.99                     | 0.44              |
| 1:E:291:LEU:CD1  | 1:E:291:LEU:N    | 2.81                     | 0.44              |
| 1:H:158:THR:HG22 | 1:H:160:VAL:HG22 | 2.00                     | 0.44              |
| 1:F:452:ASP:OD1  | 1:F:472:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:548:HIS:NE2  | 2:A:801:SHG:O3   | 2.41                     | 0.43              |
| 1:C:459:VAL:O    | 1:C:462:SER:HB3  | 2.18                     | 0.43              |
| 1:D:432:GLU:HG2  | 1:D:432:GLU:H    | 1.31                     | 0.43              |
| 1:G:385:THR:CG2  | 1:G:386:PRO:HD2  | 2.45                     | 0.43              |
| 1:A:293:SER:HA   | 1:A:574:GLY:O    | 2.18                     | 0.43              |
| 1:F:564:CYS:HG   | 1:F:573:PHE:HE2  | 1.67                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:542:GLU:HB2  | 4:A:2369:HOH:O   | 2.18                     | 0.43              |
| 1:B:339:ARG:HA   | 1:B:340:PRO:HD3  | 1.93                     | 0.43              |
| 1:C:219:HIS:HA   | 1:C:433:PRO:HA   | 2.01                     | 0.43              |
| 1:C:346:PRO:HG2  | 1:C:350:PRO:HA   | 2.01                     | 0.43              |
| 1:F:107:ILE:HG12 | 1:F:167:ALA:HB1  | 1.99                     | 0.43              |
| 1:A:471:TRP:CH2  | 1:A:526:SER:HA   | 2.54                     | 0.43              |
| 1:B:558:ASP:OD2  | 1:B:561:GLU:HG3  | 2.18                     | 0.43              |
| 1:E:46:LYS:HD3   | 1:E:312:LYS:HG2  | 2.00                     | 0.43              |
| 1:G:385:THR:O    | 1:G:388:GLU:CG   | 2.62                     | 0.43              |
| 1:A:90:LYS:HG3   | 1:A:166:THR:HB   | 2.00                     | 0.43              |
| 1:D:47:TYR:O     | 1:D:313:ALA:HA   | 2.18                     | 0.43              |
| 1:D:432:GLU:HB3  | 1:D:451:ARG:HB2  | 2.01                     | 0.43              |
| 1:E:382:ILE:HG12 | 1:E:393:VAL:HG22 | 2.01                     | 0.43              |
| 1:E:92:ASN:O     | 1:E:250:PHE:HZ   | 2.01                     | 0.42              |
| 2:B:802:SHG:H3   | 3:B:702:FAD:N5   | 2.33                     | 0.42              |
| 1:D:558:ASP:HB3  | 1:D:561:GLU:HB2  | 2.01                     | 0.42              |
| 1:A:89:HIS:ND1   | 1:A:91:LYS:HB3   | 2.34                     | 0.42              |
| 1:C:363:PHE:HA   | 1:C:471:TRP:O    | 2.20                     | 0.42              |
| 1:F:341:ASN:HD22 | 1:F:341:ASN:C    | 2.23                     | 0.42              |
| 1:G:89:HIS:ND1   | 1:G:91:LYS:HB2   | 2.34                     | 0.42              |
| 1:B:81:ASP:O     | 1:B:81:ASP:OD1   | 2.38                     | 0.42              |
| 1:D:215:GLU:O    | 1:D:411:LYS:NZ   | 2.53                     | 0.42              |
| 1:E:452:ASP:OD1  | 1:E:452:ASP:N    | 2.53                     | 0.42              |
| 1:F:289:ASN:ND2  | 1:F:294:GLU:HB3  | 2.35                     | 0.42              |
| 1:B:77:ILE:CG2   | 3:B:702:FAD:C4A  | 2.97                     | 0.42              |
| 1:G:451:ARG:HD3  | 1:G:468:ILE:O    | 2.19                     | 0.42              |
| 1:B:476:ARG:HB2  | 1:B:589:ALA:HB1  | 2.01                     | 0.42              |
| 1:D:299:HIS:CE1  | 1:D:308:ARG:HB3  | 2.55                     | 0.42              |
| 1:F:81:ASP:C     | 1:F:81:ASP:OD1   | 2.56                     | 0.42              |
| 1:G:299:HIS:HB2  | 1:G:310:GLU:OE1  | 2.20                     | 0.42              |
| 1:B:215:GLU:O    | 1:B:411:LYS:NZ   | 2.53                     | 0.42              |
| 1:D:341:ASN:HA   | 1:D:342:PRO:HD3  | 1.92                     | 0.42              |
| 1:C:385:THR:HA   | 1:C:386:PRO:HD3  | 1.97                     | 0.42              |
| 1:C:432:GLU:HB3  | 1:C:451:ARG:HB2  | 2.01                     | 0.42              |
| 1:F:211:ASP:O    | 1:F:214:LYS:HG2  | 2.19                     | 0.42              |
| 1:H:426:ILE:HA   | 1:H:427:PRO:HD3  | 1.88                     | 0.42              |
| 1:A:346:PRO:HG2  | 1:A:350:PRO:HA   | 2.01                     | 0.41              |
| 1:C:157:VAL:HG21 | 1:C:324:HIS:CE1  | 2.55                     | 0.41              |
| 1:C:218:ARG:HG3  | 1:C:430:ASP:OD2  | 2.20                     | 0.41              |
| 1:D:312:LYS:HG3  | 1:D:313:ALA:N    | 2.35                     | 0.41              |
| 1:C:444:PRO:HD2  | 1:C:445:TRP:CZ3  | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:383:ARG:HB3  | 1:F:392:SER:HB3  | 2.03                     | 0.41              |
| 1:G:548:HIS:CE1  | 2:G:808:SHG:O3   | 2.74                     | 0.41              |
| 1:E:618:PHE:CD1  | 1:E:619:THR:N    | 2.86                     | 0.41              |
| 1:F:157:VAL:HG21 | 1:F:324:HIS:CE1  | 2.47                     | 0.41              |
| 1:G:218:ARG:HG3  | 1:G:430:ASP:OD2  | 2.20                     | 0.41              |
| 1:H:564:CYS:HG   | 1:H:573:PHE:HE2  | 1.65                     | 0.41              |
| 1:H:83:GLY:N     | 4:G:2497:HOH:O   | 2.53                     | 0.41              |
| 1:A:395:TYR:OH   | 1:A:410:GLU:HB2  | 2.21                     | 0.41              |
| 1:E:173:PRO:HG2  | 1:E:592:ALA:HB1  | 2.02                     | 0.41              |
| 1:F:194:GLU:HA   | 1:F:194:GLU:OE1  | 2.19                     | 0.41              |
| 1:F:433:PRO:O    | 1:F:450:HIS:HA   | 2.20                     | 0.41              |
| 1:G:457:GLY:H    | 1:G:460:GLN:HE21 | 1.68                     | 0.41              |
| 1:G:47:TYR:CE2   | 1:G:73:ALA:HB2   | 2.55                     | 0.41              |
| 1:H:263:GLN:HE21 | 1:H:263:GLN:HB3  | 1.68                     | 0.41              |
| 1:A:201:LYS:HE2  | 1:A:205:TYR:OH   | 2.21                     | 0.41              |
| 1:B:137:PHE:O    | 1:B:139:ARG:HG3  | 2.20                     | 0.41              |
| 1:F:478:GLU:HG2  | 1:F:480:LYS:HE2  | 2.03                     | 0.41              |
| 1:G:570:SER:HB3  | 1:G:580:LEU:O    | 2.20                     | 0.41              |
| 1:H:421:GLU:CD   | 1:H:421:GLU:H    | 2.23                     | 0.41              |
| 1:A:281:VAL:CG1  | 1:A:300:ILE:HB   | 2.51                     | 0.41              |
| 1:H:385:THR:HA   | 1:H:386:PRO:HD3  | 1.96                     | 0.41              |
| 1:A:145:GLU:HG3  | 1:A:488:SER:HB2  | 2.03                     | 0.41              |
| 1:A:385:THR:HA   | 1:A:386:PRO:HD3  | 1.99                     | 0.41              |
| 1:A:153:SER:OG   | 1:A:542:GLU:CG   | 2.69                     | 0.41              |
| 1:B:145:GLU:HG3  | 1:B:488:SER:HB2  | 2.03                     | 0.41              |
| 1:D:339:ARG:HA   | 1:D:340:PRO:HD3  | 1.92                     | 0.41              |
| 1:H:47:TYR:O     | 1:H:313:ALA:HA   | 2.21                     | 0.41              |
| 1:A:458:ALA:O    | 1:B:121:LEU:HD12 | 2.20                     | 0.40              |
| 1:C:618:PHE:C    | 1:C:618:PHE:HD1  | 2.25                     | 0.40              |
| 1:D:157:VAL:HG21 | 1:D:324:HIS:CE1  | 2.57                     | 0.40              |
| 1:D:218:ARG:HD2  | 4:D:1005:HOH:O   | 2.19                     | 0.40              |
| 1:D:363:PHE:HA   | 1:D:471:TRP:O    | 2.21                     | 0.40              |
| 1:H:542:GLU:HA   | 1:H:543:PRO:HD3  | 1.95                     | 0.40              |
| 1:E:618:PHE:C    | 1:E:618:PHE:CD1  | 2.94                     | 0.40              |
| 1:D:92:ASN:O     | 1:D:250:PHE:HZ   | 2.03                     | 0.40              |
| 1:G:398:GLY:O    | 1:G:399:ALA:C    | 2.60                     | 0.40              |
| 1:B:293:SER:HA   | 1:B:574:GLY:O    | 2.21                     | 0.40              |
| 1:E:88:ALA:HA    | 1:E:255:SER:OG   | 2.21                     | 0.40              |
| 1:C:347:GLU:HG2  | 1:C:348:LEU:HG   | 2.02                     | 0.40              |
| 1:C:81:ASP:O     | 1:C:90:LYS:HE2   | 2.22                     | 0.40              |
| 1:D:459:VAL:O    | 1:D:462:SER:HB3  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------|--------------------------|-------------------|
| 1:E:100:ILE:HD13 | 1:E:453:ALA:HA | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 575/623 (92%)   | 558 (97%)  | 17 (3%)  | 0        | 100         | 100 |
| 1   | B     | 575/623 (92%)   | 563 (98%)  | 11 (2%)  | 1 (0%)   | 51          | 41  |
| 1   | C     | 575/623 (92%)   | 554 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 1   | D     | 575/623 (92%)   | 561 (98%)  | 14 (2%)  | 0        | 100         | 100 |
| 1   | E     | 575/623 (92%)   | 558 (97%)  | 17 (3%)  | 0        | 100         | 100 |
| 1   | F     | 575/623 (92%)   | 559 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| 1   | G     | 575/623 (92%)   | 558 (97%)  | 17 (3%)  | 0        | 100         | 100 |
| 1   | H     | 575/623 (92%)   | 559 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| All | All   | 4600/4984 (92%) | 4470 (97%) | 129 (3%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 187 | ASP  |

### 5.3.2 Protein sidechains [i](#)

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     | 504/541 (93%)   | 485 (96%)  | 19 (4%)  | 38          | 24 |
| 1   | B     | 504/541 (93%)   | 489 (97%)  | 15 (3%)  | 46          | 34 |
| 1   | C     | 504/541 (93%)   | 483 (96%)  | 21 (4%)  | 34          | 20 |
| 1   | D     | 504/541 (93%)   | 483 (96%)  | 21 (4%)  | 34          | 20 |
| 1   | E     | 504/541 (93%)   | 482 (96%)  | 22 (4%)  | 33          | 18 |
| 1   | F     | 504/541 (93%)   | 485 (96%)  | 19 (4%)  | 38          | 24 |
| 1   | G     | 504/541 (93%)   | 483 (96%)  | 21 (4%)  | 34          | 20 |
| 1   | H     | 504/541 (93%)   | 480 (95%)  | 24 (5%)  | 30          | 14 |
| All | All   | 4032/4328 (93%) | 3870 (96%) | 162 (4%) | 36          | 21 |

All (162) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 43  | MET  |
| 1   | A     | 100 | ILE  |
| 1   | A     | 112 | MET  |
| 1   | A     | 132 | GLN  |
| 1   | A     | 168 | TRP  |
| 1   | A     | 206 | PHE  |
| 1   | A     | 285 | ARG  |
| 1   | A     | 312 | LYS  |
| 1   | A     | 341 | ASN  |
| 1   | A     | 347 | GLU  |
| 1   | A     | 385 | THR  |
| 1   | A     | 392 | SER  |
| 1   | A     | 401 | THR  |
| 1   | A     | 432 | GLU  |
| 1   | A     | 450 | HIS  |
| 1   | A     | 496 | ASN  |
| 1   | A     | 593 | ASN  |
| 1   | A     | 618 | PHE  |
| 1   | A     | 619 | THR  |
| 1   | B     | 100 | ILE  |
| 1   | B     | 112 | MET  |
| 1   | B     | 139 | ARG  |
| 1   | B     | 168 | TRP  |
| 1   | B     | 185 | LYS  |
| 1   | B     | 206 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 216 | SER  |
| 1   | B     | 344 | ASN  |
| 1   | B     | 385 | THR  |
| 1   | B     | 389 | LEU  |
| 1   | B     | 390 | THR  |
| 1   | B     | 432 | GLU  |
| 1   | B     | 450 | HIS  |
| 1   | B     | 490 | LYS  |
| 1   | B     | 496 | ASN  |
| 1   | D     | 91  | LYS  |
| 1   | D     | 100 | ILE  |
| 1   | D     | 112 | MET  |
| 1   | D     | 168 | TRP  |
| 1   | D     | 178 | GLU  |
| 1   | D     | 206 | PHE  |
| 1   | D     | 231 | LYS  |
| 1   | D     | 285 | ARG  |
| 1   | D     | 344 | ASN  |
| 1   | D     | 347 | GLU  |
| 1   | D     | 385 | THR  |
| 1   | D     | 403 | LYS  |
| 1   | D     | 408 | TRP  |
| 1   | D     | 413 | LYS  |
| 1   | D     | 432 | GLU  |
| 1   | D     | 450 | HIS  |
| 1   | D     | 490 | LYS  |
| 1   | D     | 496 | ASN  |
| 1   | D     | 554 | ARG  |
| 1   | D     | 593 | ASN  |
| 1   | D     | 618 | PHE  |
| 1   | C     | 43  | MET  |
| 1   | C     | 100 | ILE  |
| 1   | C     | 112 | MET  |
| 1   | C     | 168 | TRP  |
| 1   | C     | 206 | PHE  |
| 1   | C     | 285 | ARG  |
| 1   | C     | 341 | ASN  |
| 1   | C     | 344 | ASN  |
| 1   | C     | 385 | THR  |
| 1   | C     | 389 | LEU  |
| 1   | C     | 392 | SER  |
| 1   | C     | 403 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 432 | GLU  |
| 1   | C     | 445 | TRP  |
| 1   | C     | 450 | HIS  |
| 1   | C     | 455 | SER  |
| 1   | C     | 490 | LYS  |
| 1   | C     | 496 | ASN  |
| 1   | C     | 593 | ASN  |
| 1   | C     | 618 | PHE  |
| 1   | C     | 619 | THR  |
| 1   | E     | 46  | LYS  |
| 1   | E     | 100 | ILE  |
| 1   | E     | 112 | MET  |
| 1   | E     | 168 | TRP  |
| 1   | E     | 185 | LYS  |
| 1   | E     | 206 | PHE  |
| 1   | E     | 231 | LYS  |
| 1   | E     | 341 | ASN  |
| 1   | E     | 344 | ASN  |
| 1   | E     | 347 | GLU  |
| 1   | E     | 386 | PRO  |
| 1   | E     | 388 | GLU  |
| 1   | E     | 392 | SER  |
| 1   | E     | 403 | LYS  |
| 1   | E     | 408 | TRP  |
| 1   | E     | 413 | LYS  |
| 1   | E     | 432 | GLU  |
| 1   | E     | 450 | HIS  |
| 1   | E     | 452 | ASP  |
| 1   | E     | 490 | LYS  |
| 1   | E     | 593 | ASN  |
| 1   | E     | 618 | PHE  |
| 1   | F     | 95  | GLU  |
| 1   | F     | 100 | ILE  |
| 1   | F     | 112 | MET  |
| 1   | F     | 168 | TRP  |
| 1   | F     | 206 | PHE  |
| 1   | F     | 216 | SER  |
| 1   | F     | 341 | ASN  |
| 1   | F     | 344 | ASN  |
| 1   | F     | 383 | ARG  |
| 1   | F     | 385 | THR  |
| 1   | F     | 388 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 408 | TRP  |
| 1   | F     | 432 | GLU  |
| 1   | F     | 445 | TRP  |
| 1   | F     | 450 | HIS  |
| 1   | F     | 452 | ASP  |
| 1   | F     | 490 | LYS  |
| 1   | F     | 593 | ASN  |
| 1   | F     | 618 | PHE  |
| 1   | H     | 81  | ASP  |
| 1   | H     | 91  | LYS  |
| 1   | H     | 100 | ILE  |
| 1   | H     | 112 | MET  |
| 1   | H     | 132 | GLN  |
| 1   | H     | 168 | TRP  |
| 1   | H     | 185 | LYS  |
| 1   | H     | 194 | GLU  |
| 1   | H     | 206 | PHE  |
| 1   | H     | 231 | LYS  |
| 1   | H     | 310 | GLU  |
| 1   | H     | 341 | ASN  |
| 1   | H     | 344 | ASN  |
| 1   | H     | 347 | GLU  |
| 1   | H     | 385 | THR  |
| 1   | H     | 389 | LEU  |
| 1   | H     | 413 | LYS  |
| 1   | H     | 450 | HIS  |
| 1   | H     | 455 | SER  |
| 1   | H     | 490 | LYS  |
| 1   | H     | 542 | GLU  |
| 1   | H     | 593 | ASN  |
| 1   | H     | 618 | PHE  |
| 1   | H     | 619 | THR  |
| 1   | G     | 45  | ILE  |
| 1   | G     | 82  | SER  |
| 1   | G     | 84  | LEU  |
| 1   | G     | 95  | GLU  |
| 1   | G     | 100 | ILE  |
| 1   | G     | 112 | MET  |
| 1   | G     | 168 | TRP  |
| 1   | G     | 206 | PHE  |
| 1   | G     | 231 | LYS  |
| 1   | G     | 341 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 389 | LEU  |
| 1   | G     | 392 | SER  |
| 1   | G     | 408 | TRP  |
| 1   | G     | 445 | TRP  |
| 1   | G     | 450 | HIS  |
| 1   | G     | 490 | LYS  |
| 1   | G     | 496 | ASN  |
| 1   | G     | 587 | PRO  |
| 1   | G     | 593 | ASN  |
| 1   | G     | 618 | PHE  |
| 1   | G     | 619 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 341 | ASN  |
| 1   | A     | 460 | GLN  |
| 1   | B     | 341 | ASN  |
| 1   | B     | 460 | GLN  |
| 1   | D     | 299 | HIS  |
| 1   | D     | 324 | HIS  |
| 1   | D     | 341 | ASN  |
| 1   | D     | 460 | GLN  |
| 1   | C     | 341 | ASN  |
| 1   | E     | 263 | GLN  |
| 1   | E     | 341 | ASN  |
| 1   | E     | 460 | GLN  |
| 1   | F     | 341 | ASN  |
| 1   | F     | 460 | GLN  |
| 1   | H     | 263 | GLN  |
| 1   | H     | 341 | ASN  |
| 1   | H     | 460 | GLN  |
| 1   | G     | 263 | GLN  |
| 1   | G     | 299 | HIS  |
| 1   | G     | 460 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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$ |
| 3   | FAD  | A     | 701 | -    | 51,58,58     | 1.73 | 9 (17%)     | 54,89,89    | 2.67 | 9 (16%)     |
| 2   | SHG  | A     | 801 | -    | 11,12,12     | 0.85 | 0           | 14,17,17    | 4.64 | 8 (57%)     |
| 3   | FAD  | B     | 702 | -    | 51,58,58     | 1.51 | 6 (11%)     | 54,89,89    | 2.38 | 8 (14%)     |
| 2   | SHG  | B     | 802 | -    | 11,12,12     | 0.86 | 1 (9%)      | 14,17,17    | 3.73 | 7 (50%)     |
| 3   | FAD  | C     | 704 | -    | 51,58,58     | 1.65 | 9 (17%)     | 54,89,89    | 2.34 | 7 (12%)     |
| 2   | SHG  | C     | 804 | -    | 11,12,12     | 0.62 | 0           | 14,17,17    | 5.36 | 9 (64%)     |
| 3   | FAD  | D     | 703 | -    | 51,58,58     | 1.48 | 6 (11%)     | 54,89,89    | 2.14 | 8 (14%)     |
| 2   | SHG  | D     | 803 | -    | 11,12,12     | 1.04 | 1 (9%)      | 14,17,17    | 3.69 | 7 (50%)     |
| 3   | FAD  | E     | 705 | -    | 51,58,58     | 1.38 | 7 (13%)     | 54,89,89    | 2.67 | 8 (14%)     |
| 2   | SHG  | E     | 805 | -    | 11,12,12     | 0.80 | 0           | 14,17,17    | 4.78 | 7 (50%)     |
| 3   | FAD  | F     | 706 | -    | 51,58,58     | 1.34 | 7 (13%)     | 54,89,89    | 2.42 | 11 (20%)    |
| 2   | SHG  | F     | 806 | -    | 11,12,12     | 0.75 | 0           | 14,17,17    | 4.34 | 7 (50%)     |
| 3   | FAD  | G     | 708 | -    | 51,58,58     | 1.59 | 8 (15%)     | 54,89,89    | 2.31 | 6 (11%)     |
| 2   | SHG  | G     | 808 | -    | 11,12,12     | 0.89 | 0           | 14,17,17    | 5.30 | 7 (50%)     |
| 3   | FAD  | H     | 707 | -    | 51,58,58     | 1.43 | 5 (9%)      | 54,89,89    | 2.33 | 8 (14%)     |
| 2   | SHG  | H     | 807 | -    | 11,12,12     | 0.55 | 0           | 14,17,17    | 4.09 | 11 (78%)    |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | FAD  | A     | 701 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | A     | 801 | -    | -       | 0/2/22/22  | 0/1/1/1 |
| 3   | FAD  | B     | 702 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | B     | 802 | -    | -       | 0/2/22/22  | 0/1/1/1 |
| 3   | FAD  | C     | 704 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | C     | 804 | -    | -       | 0/2/22/22  | 0/1/1/1 |
| 3   | FAD  | D     | 703 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | D     | 803 | -    | -       | 0/2/22/22  | 0/1/1/1 |
| 3   | FAD  | E     | 705 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | E     | 805 | -    | -       | 0/2/22/22  | 0/1/1/1 |
| 3   | FAD  | F     | 706 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | F     | 806 | -    | -       | 0/2/22/22  | 0/1/1/1 |
| 3   | FAD  | G     | 708 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | G     | 808 | -    | -       | 0/2/22/22  | 0/1/1/1 |
| 3   | FAD  | H     | 707 | -    | -       | 0/28/50/50 | 0/6/6/6 |
| 2   | SHG  | H     | 807 | -    | -       | 0/2/22/22  | 0/1/1/1 |

All (59) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 803 | SHG  | C2-C3   | -2.50 | 1.50        | 1.52     |
| 3   | C     | 704 | FAD  | P-O1P   | -2.15 | 1.42        | 1.50     |
| 2   | B     | 802 | SHG  | O3-C3   | -2.11 | 1.38        | 1.43     |
| 3   | F     | 706 | FAD  | O4B-C4B | -2.09 | 1.40        | 1.45     |
| 3   | E     | 705 | FAD  | C2A-N1A | 2.02  | 1.37        | 1.33     |
| 3   | C     | 704 | FAD  | C8M-C8  | 2.07  | 1.55        | 1.51     |
| 3   | G     | 708 | FAD  | C5X-N5  | 2.14  | 1.38        | 1.35     |
| 3   | G     | 708 | FAD  | C2A-N1A | 2.20  | 1.38        | 1.33     |
| 3   | F     | 706 | FAD  | C2A-N1A | 2.23  | 1.38        | 1.33     |
| 3   | H     | 707 | FAD  | C2A-N1A | 2.31  | 1.38        | 1.33     |
| 3   | F     | 706 | FAD  | C4-N3   | 2.34  | 1.37        | 1.33     |
| 3   | C     | 704 | FAD  | C4-N3   | 2.38  | 1.37        | 1.33     |
| 3   | G     | 708 | FAD  | C4-N3   | 2.38  | 1.37        | 1.33     |
| 3   | A     | 701 | FAD  | C4-N3   | 2.52  | 1.37        | 1.33     |
| 3   | E     | 705 | FAD  | C5X-N5  | 2.72  | 1.39        | 1.35     |
| 3   | D     | 703 | FAD  | C2A-N1A | 2.73  | 1.39        | 1.33     |
| 3   | H     | 707 | FAD  | C4X-N5  | 2.75  | 1.37        | 1.33     |
| 3   | C     | 704 | FAD  | C2A-N1A | 2.77  | 1.39        | 1.33     |
| 3   | C     | 704 | FAD  | C5X-N5  | 2.79  | 1.39        | 1.35     |
| 3   | A     | 701 | FAD  | C5'-C4' | 2.83  | 1.56        | 1.51     |
| 3   | B     | 702 | FAD  | C2A-N1A | 2.89  | 1.39        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | F     | 706 | FAD  | C9A-N10 | 2.94 | 1.42        | 1.38     |
| 3   | A     | 701 | FAD  | C9A-N10 | 2.98 | 1.42        | 1.38     |
| 3   | E     | 705 | FAD  | C4-N3   | 3.01 | 1.38        | 1.33     |
| 3   | A     | 701 | FAD  | C2A-N3A | 3.03 | 1.37        | 1.32     |
| 3   | D     | 703 | FAD  | C10-N1  | 3.05 | 1.37        | 1.33     |
| 3   | G     | 708 | FAD  | C2A-N3A | 3.05 | 1.37        | 1.32     |
| 3   | G     | 708 | FAD  | C4X-N5  | 3.08 | 1.37        | 1.33     |
| 3   | E     | 705 | FAD  | C4X-N5  | 3.12 | 1.37        | 1.33     |
| 3   | F     | 706 | FAD  | C4X-N5  | 3.13 | 1.37        | 1.33     |
| 3   | E     | 705 | FAD  | C1'-N10 | 3.15 | 1.51        | 1.48     |
| 3   | C     | 704 | FAD  | C5'-C4' | 3.16 | 1.56        | 1.51     |
| 3   | B     | 702 | FAD  | C4X-N5  | 3.16 | 1.37        | 1.33     |
| 3   | A     | 701 | FAD  | C1'-N10 | 3.17 | 1.51        | 1.48     |
| 3   | F     | 706 | FAD  | C2A-N3A | 3.26 | 1.37        | 1.32     |
| 3   | H     | 707 | FAD  | C2A-N3A | 3.26 | 1.37        | 1.32     |
| 3   | B     | 702 | FAD  | C4-N3   | 3.31 | 1.39        | 1.33     |
| 3   | A     | 701 | FAD  | C2A-N1A | 3.34 | 1.40        | 1.33     |
| 3   | E     | 705 | FAD  | C2A-N3A | 3.36 | 1.37        | 1.32     |
| 3   | C     | 704 | FAD  | C2A-N3A | 3.39 | 1.37        | 1.32     |
| 3   | A     | 701 | FAD  | C5X-N5  | 3.44 | 1.40        | 1.35     |
| 3   | F     | 706 | FAD  | C10-N1  | 3.47 | 1.38        | 1.33     |
| 3   | D     | 703 | FAD  | C4-N3   | 3.53 | 1.39        | 1.33     |
| 3   | G     | 708 | FAD  | C5'-C4' | 3.55 | 1.57        | 1.51     |
| 3   | H     | 707 | FAD  | C1'-N10 | 3.56 | 1.52        | 1.48     |
| 3   | D     | 703 | FAD  | C2A-N3A | 3.58 | 1.38        | 1.32     |
| 3   | D     | 703 | FAD  | C4X-N5  | 3.63 | 1.38        | 1.33     |
| 3   | B     | 702 | FAD  | C1'-N10 | 3.64 | 1.52        | 1.48     |
| 3   | B     | 702 | FAD  | C2A-N3A | 3.68 | 1.38        | 1.32     |
| 3   | G     | 708 | FAD  | C1'-N10 | 3.83 | 1.52        | 1.48     |
| 3   | A     | 701 | FAD  | C4X-N5  | 3.97 | 1.39        | 1.33     |
| 3   | D     | 703 | FAD  | C5X-N5  | 4.05 | 1.41        | 1.35     |
| 3   | B     | 702 | FAD  | C10-N1  | 4.25 | 1.39        | 1.33     |
| 3   | H     | 707 | FAD  | C10-N1  | 4.37 | 1.39        | 1.33     |
| 3   | C     | 704 | FAD  | C10-N1  | 4.66 | 1.39        | 1.33     |
| 3   | E     | 705 | FAD  | C10-N1  | 4.72 | 1.39        | 1.33     |
| 3   | C     | 704 | FAD  | C4X-N5  | 5.27 | 1.40        | 1.33     |
| 3   | A     | 701 | FAD  | C10-N1  | 5.86 | 1.41        | 1.33     |
| 3   | G     | 708 | FAD  | C10-N1  | 6.21 | 1.42        | 1.33     |

All (128) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|---|-------------|----------|
|-----|-------|-----|------|-------|---|-------------|----------|

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | A     | 701 | FAD  | N3A-C2A-N1A | -11.63 | 118.73      | 128.86   |
| 3   | H     | 707 | FAD  | N3A-C2A-N1A | -11.12 | 119.18      | 128.86   |
| 3   | E     | 705 | FAD  | N3A-C2A-N1A | -10.89 | 119.37      | 128.86   |
| 3   | G     | 708 | FAD  | N3A-C2A-N1A | -10.85 | 119.41      | 128.86   |
| 3   | D     | 703 | FAD  | N3A-C2A-N1A | -10.59 | 119.64      | 128.86   |
| 3   | C     | 704 | FAD  | N3A-C2A-N1A | -10.47 | 119.74      | 128.86   |
| 3   | F     | 706 | FAD  | N3A-C2A-N1A | -10.44 | 119.77      | 128.86   |
| 3   | B     | 702 | FAD  | N3A-C2A-N1A | -10.27 | 119.91      | 128.86   |
| 3   | E     | 705 | FAD  | C4X-C4-N3   | -4.87  | 116.55      | 123.48   |
| 3   | A     | 701 | FAD  | C4X-C4-N3   | -4.75  | 116.73      | 123.48   |
| 3   | G     | 708 | FAD  | C4X-C4-N3   | -4.34  | 117.30      | 123.48   |
| 3   | C     | 704 | FAD  | C4X-C4-N3   | -4.14  | 117.59      | 123.48   |
| 3   | B     | 702 | FAD  | C4X-C4-N3   | -3.94  | 117.87      | 123.48   |
| 3   | H     | 707 | FAD  | C4X-C4-N3   | -3.50  | 118.50      | 123.48   |
| 3   | F     | 706 | FAD  | C4X-C4-N3   | -3.39  | 118.66      | 123.48   |
| 3   | D     | 703 | FAD  | C4X-C4-N3   | -3.03  | 119.17      | 123.48   |
| 3   | E     | 705 | FAD  | C1'-N10-C10 | -2.80  | 115.63      | 118.50   |
| 3   | A     | 701 | FAD  | O3'-C3'-C4' | -2.57  | 102.45      | 108.82   |
| 3   | F     | 706 | FAD  | C8M-C8-C9   | -2.36  | 114.41      | 120.34   |
| 3   | G     | 708 | FAD  | C4X-C10-N10 | -2.36  | 118.88      | 120.52   |
| 3   | B     | 702 | FAD  | C10-C4X-N5  | -2.34  | 117.90      | 120.59   |
| 3   | A     | 701 | FAD  | C9A-C5X-N5  | -2.31  | 118.79      | 122.24   |
| 3   | H     | 707 | FAD  | C9A-C5X-N5  | -2.25  | 118.89      | 122.24   |
| 3   | D     | 703 | FAD  | O5'-P-O1P   | -2.23  | 100.25      | 109.25   |
| 2   | C     | 804 | SHG  | O6-C6-C5    | -2.19  | 103.96      | 111.34   |
| 2   | H     | 807 | SHG  | O6-C6-C5    | -2.16  | 104.08      | 111.34   |
| 3   | H     | 707 | FAD  | O3'-C3'-C2' | -2.12  | 103.56      | 108.82   |
| 3   | F     | 706 | FAD  | C7-C6-C5X   | -2.02  | 117.95      | 121.08   |
| 3   | A     | 701 | FAD  | C4-C4X-N5   | 2.00   | 120.87      | 118.68   |
| 3   | B     | 702 | FAD  | C6-C5X-C9A  | 2.01   | 121.61      | 119.00   |
| 3   | F     | 706 | FAD  | O4'-C4'-C3' | 2.05   | 114.19      | 109.09   |
| 2   | D     | 803 | SHG  | O3-C3-C4    | 2.13   | 114.99      | 110.36   |
| 3   | E     | 705 | FAD  | O2'-C2'-C1' | 2.17   | 114.80      | 109.79   |
| 3   | E     | 705 | FAD  | O2P-P-O1P   | 2.18   | 123.54      | 112.28   |
| 3   | C     | 704 | FAD  | O2A-PA-O1A  | 2.20   | 123.64      | 112.28   |
| 2   | B     | 802 | SHG  | C3-C4-C5    | 2.28   | 114.23      | 110.22   |
| 3   | D     | 703 | FAD  | C4X-N5-C5X  | 2.28   | 119.17      | 116.76   |
| 2   | H     | 807 | SHG  | O1-C1-O5    | 2.29   | 116.98      | 110.20   |
| 3   | G     | 708 | FAD  | O4'-C4'-C3' | 2.35   | 114.92      | 109.09   |
| 3   | D     | 703 | FAD  | C4X-C10-N10 | 2.39   | 122.18      | 120.52   |
| 3   | E     | 705 | FAD  | C5X-C9A-N10 | 2.44   | 119.47      | 117.66   |

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| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2   | F     | 806 | SHG  | C3-C4-C5    | 2.49 | 114.60      | 110.22   |
| 2   | C     | 804 | SHG  | O3-C3-C2    | 2.49 | 113.91      | 109.15   |
| 2   | B     | 802 | SHG  | O5-C1-C2    | 2.49 | 118.73      | 110.52   |
| 3   | A     | 701 | FAD  | C6-C5X-N5   | 2.53 | 121.93      | 118.97   |
| 2   | A     | 801 | SHG  | O5-C5-C6    | 2.54 | 112.50      | 106.41   |
| 2   | H     | 807 | SHG  | O4-C4-C5    | 2.56 | 115.74      | 109.28   |
| 2   | C     | 804 | SHG  | C6-C5-C4    | 2.60 | 119.08      | 113.00   |
| 2   | H     | 807 | SHG  | C1-O5-C5    | 2.60 | 118.09      | 113.39   |
| 3   | F     | 706 | FAD  | C6-C5X-C9A  | 2.61 | 122.39      | 119.00   |
| 2   | D     | 803 | SHG  | O5-C1-C2    | 2.62 | 119.18      | 110.52   |
| 2   | A     | 801 | SHG  | O5-C1-C2    | 2.69 | 119.40      | 110.52   |
| 3   | F     | 706 | FAD  | C4-C4X-N5   | 2.74 | 121.68      | 118.68   |
| 2   | H     | 807 | SHG  | O5-C5-C6    | 2.76 | 113.03      | 106.41   |
| 2   | H     | 807 | SHG  | O3-C3-C4    | 2.77 | 116.39      | 110.36   |
| 2   | H     | 807 | SHG  | O3-C3-C2    | 2.77 | 114.45      | 109.15   |
| 3   | A     | 701 | FAD  | C5X-C9A-N10 | 2.80 | 119.74      | 117.66   |
| 3   | C     | 704 | FAD  | C5X-C9A-N10 | 2.86 | 119.78      | 117.66   |
| 2   | A     | 801 | SHG  | O4-C4-C5    | 2.88 | 116.55      | 109.28   |
| 2   | B     | 802 | SHG  | O3-C3-C2    | 2.90 | 114.70      | 109.15   |
| 3   | C     | 704 | FAD  | C4X-N5-C5X  | 2.91 | 119.83      | 116.76   |
| 2   | H     | 807 | SHG  | C3-C4-C5    | 2.93 | 115.39      | 110.22   |
| 3   | H     | 707 | FAD  | C5X-C9A-N10 | 3.01 | 119.89      | 117.66   |
| 2   | F     | 806 | SHG  | O5-C5-C6    | 3.07 | 113.78      | 106.41   |
| 2   | G     | 808 | SHG  | C3-C4-C5    | 3.08 | 115.64      | 110.22   |
| 2   | G     | 808 | SHG  | O5-C1-C2    | 3.08 | 120.68      | 110.52   |
| 2   | C     | 804 | SHG  | O3-C3-C4    | 3.16 | 117.23      | 110.36   |
| 2   | B     | 802 | SHG  | O3-C3-C4    | 3.17 | 117.25      | 110.36   |
| 2   | H     | 807 | SHG  | O5-C1-C2    | 3.18 | 121.00      | 110.52   |
| 2   | E     | 805 | SHG  | O5-C1-C2    | 3.22 | 121.14      | 110.52   |
| 2   | A     | 801 | SHG  | O3-C3-C2    | 3.32 | 115.49      | 109.15   |
| 3   | F     | 706 | FAD  | C5X-C9A-N10 | 3.37 | 120.16      | 117.66   |
| 3   | B     | 702 | FAD  | C4-C4X-N5   | 3.38 | 122.38      | 118.68   |
| 3   | A     | 701 | FAD  | C4X-N5-C5X  | 3.39 | 120.34      | 116.76   |
| 2   | E     | 805 | SHG  | O5-C5-C6    | 3.45 | 114.68      | 106.41   |
| 2   | F     | 806 | SHG  | O5-C1-C2    | 3.49 | 122.05      | 110.52   |
| 3   | D     | 703 | FAD  | O4'-C4'-C3' | 3.64 | 118.13      | 109.09   |
| 2   | E     | 805 | SHG  | C1-O5-C5    | 3.66 | 120.00      | 113.39   |
| 2   | C     | 804 | SHG  | C1-O5-C5    | 3.69 | 120.05      | 113.39   |
| 2   | G     | 808 | SHG  | O3-C3-C4    | 3.72 | 118.46      | 110.36   |
| 2   | G     | 808 | SHG  | O3-C3-C2    | 3.73 | 116.28      | 109.15   |
| 2   | C     | 804 | SHG  | O5-C1-C2    | 3.75 | 122.89      | 110.52   |
| 2   | E     | 805 | SHG  | C3-C4-C5    | 3.79 | 116.89      | 110.22   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 803 | SHG  | C1-O5-C5    | 3.80  | 120.25      | 113.39   |
| 2   | F     | 806 | SHG  | C1-O5-C5    | 3.81  | 120.27      | 113.39   |
| 2   | D     | 803 | SHG  | O3-C3-C2    | 3.84  | 116.50      | 109.15   |
| 3   | C     | 704 | FAD  | C1'-N10-C9A | 3.85  | 121.88      | 118.35   |
| 2   | A     | 801 | SHG  | C3-C4-C5    | 3.91  | 117.11      | 110.22   |
| 3   | G     | 708 | FAD  | C4X-N5-C5X  | 4.02  | 121.00      | 116.76   |
| 2   | F     | 806 | SHG  | O3-C3-C2    | 4.12  | 117.02      | 109.15   |
| 2   | B     | 802 | SHG  | C1-O5-C5    | 4.16  | 120.90      | 113.39   |
| 2   | D     | 803 | SHG  | C3-C4-C5    | 4.18  | 117.58      | 110.22   |
| 2   | G     | 808 | SHG  | C1-O5-C5    | 4.25  | 121.06      | 113.39   |
| 3   | F     | 706 | FAD  | C4X-N5-C5X  | 4.38  | 121.39      | 116.76   |
| 3   | H     | 707 | FAD  | C4X-N5-C5X  | 4.39  | 121.40      | 116.76   |
| 3   | D     | 703 | FAD  | C1'-N10-C9A | 4.55  | 122.51      | 118.35   |
| 2   | C     | 804 | SHG  | C3-C4-C5    | 4.64  | 118.40      | 110.22   |
| 3   | B     | 702 | FAD  | C4X-N5-C5X  | 4.66  | 121.68      | 116.76   |
| 2   | A     | 801 | SHG  | O5-C5-C4    | 4.85  | 118.59      | 109.66   |
| 2   | C     | 804 | SHG  | O5-C5-C4    | 4.87  | 118.62      | 109.66   |
| 2   | A     | 801 | SHG  | C1-O5-C5    | 4.98  | 122.37      | 113.39   |
| 2   | E     | 805 | SHG  | O3-C3-C2    | 5.22  | 119.13      | 109.15   |
| 2   | F     | 806 | SHG  | O5-C5-C4    | 5.32  | 119.46      | 109.66   |
| 3   | B     | 702 | FAD  | C1'-N10-C9A | 5.44  | 123.33      | 118.35   |
| 2   | E     | 805 | SHG  | O5-C5-C4    | 5.52  | 119.82      | 109.66   |
| 2   | G     | 808 | SHG  | O5-C5-C4    | 5.73  | 120.21      | 109.66   |
| 3   | H     | 707 | FAD  | C1'-N10-C9A | 5.77  | 123.63      | 118.35   |
| 3   | D     | 703 | FAD  | C4-N3-C2    | 5.91  | 120.33      | 115.16   |
| 3   | F     | 706 | FAD  | C1'-N10-C9A | 6.03  | 123.87      | 118.35   |
| 2   | B     | 802 | SHG  | O5-C5-C4    | 6.11  | 120.91      | 109.66   |
| 2   | D     | 803 | SHG  | O5-C5-C4    | 6.17  | 121.02      | 109.66   |
| 2   | H     | 807 | SHG  | O5-C5-C4    | 6.24  | 121.15      | 109.66   |
| 3   | H     | 707 | FAD  | C4-N3-C2    | 6.58  | 120.92      | 115.16   |
| 3   | E     | 705 | FAD  | C1'-N10-C9A | 7.71  | 125.41      | 118.35   |
| 3   | B     | 702 | FAD  | C4-N3-C2    | 8.09  | 122.23      | 115.16   |
| 3   | F     | 706 | FAD  | C4-N3-C2    | 8.09  | 122.23      | 115.16   |
| 3   | G     | 708 | FAD  | C4-N3-C2    | 9.16  | 123.17      | 115.16   |
| 2   | D     | 803 | SHG  | F2-C2-C3    | 9.22  | 115.24      | 108.49   |
| 3   | C     | 704 | FAD  | C4-N3-C2    | 9.70  | 123.65      | 115.16   |
| 2   | B     | 802 | SHG  | F2-C2-C3    | 9.73  | 115.62      | 108.49   |
| 3   | E     | 705 | FAD  | C4-N3-C2    | 11.22 | 124.97      | 115.16   |
| 2   | H     | 807 | SHG  | F2-C2-C3    | 11.35 | 116.80      | 108.49   |
| 3   | A     | 701 | FAD  | C4-N3-C2    | 11.84 | 125.51      | 115.16   |
| 2   | F     | 806 | SHG  | F2-C2-C3    | 12.92 | 117.96      | 108.49   |
| 2   | A     | 801 | SHG  | F2-C2-C3    | 13.88 | 118.66      | 108.49   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | E     | 805 | SHG  | F2-C2-C3 | 14.10 | 118.82      | 108.49   |
| 2   | G     | 808 | SHG  | F2-C2-C3 | 16.90 | 120.87      | 108.49   |
| 2   | C     | 804 | SHG  | F2-C2-C3 | 17.19 | 121.08      | 108.49   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 31 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 701 | FAD  | 4       | 0            |
| 2   | A     | 801 | SHG  | 4       | 0            |
| 3   | B     | 702 | FAD  | 4       | 0            |
| 2   | B     | 802 | SHG  | 1       | 0            |
| 3   | C     | 704 | FAD  | 1       | 0            |
| 2   | C     | 804 | SHG  | 5       | 0            |
| 3   | D     | 703 | FAD  | 2       | 0            |
| 2   | D     | 803 | SHG  | 3       | 0            |
| 3   | E     | 705 | FAD  | 1       | 0            |
| 2   | E     | 805 | SHG  | 4       | 0            |
| 2   | F     | 806 | SHG  | 2       | 0            |
| 3   | G     | 708 | FAD  | 2       | 0            |
| 2   | G     | 808 | SHG  | 4       | 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%)   | -0.07  | 23 (3%)  | 39 | 49 | 16, 22, 45, 69        | 0     |
| 1   | B     | 577/623 (92%)   | -0.10  | 18 (3%)  | 49 | 60 | 15, 23, 42, 67        | 0     |
| 1   | C     | 577/623 (92%)   | 0.03   | 24 (4%)  | 37 | 47 | 18, 26, 46, 71        | 0     |
| 1   | D     | 577/623 (92%)   | -0.05  | 20 (3%)  | 44 | 55 | 16, 25, 45, 72        | 0     |
| 1   | E     | 577/623 (92%)   | -0.00  | 26 (4%)  | 34 | 44 | 18, 26, 45, 72        | 0     |
| 1   | F     | 577/623 (92%)   | 0.06   | 32 (5%)  | 26 | 36 | 17, 27, 47, 71        | 0     |
| 1   | G     | 577/623 (92%)   | -0.02  | 24 (4%)  | 37 | 47 | 18, 25, 48, 67        | 0     |
| 1   | H     | 577/623 (92%)   | -0.08  | 22 (3%)  | 41 | 51 | 16, 24, 43, 71        | 0     |
| All | All   | 4616/4984 (92%) | -0.03  | 189 (4%) | 38 | 48 | 15, 25, 45, 72        | 0     |

All (189) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 619 | THR  | 13.2 |
| 1   | H     | 619 | THR  | 12.9 |
| 1   | E     | 619 | THR  | 11.0 |
| 1   | A     | 619 | THR  | 10.5 |
| 1   | D     | 619 | THR  | 9.5  |
| 1   | G     | 619 | THR  | 9.0  |
| 1   | B     | 619 | THR  | 8.9  |
| 1   | F     | 619 | THR  | 8.4  |
| 1   | F     | 44  | ASP  | 8.0  |
| 1   | F     | 343 | ALA  | 8.0  |
| 1   | D     | 45  | ILE  | 7.4  |
| 1   | G     | 343 | ALA  | 7.0  |
| 1   | D     | 343 | ALA  | 6.8  |
| 1   | B     | 343 | ALA  | 6.7  |
| 1   | C     | 389 | LEU  | 6.5  |
| 1   | G     | 45  | ILE  | 6.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 44  | ASP  | 6.3  |
| 1   | B     | 618 | PHE  | 6.3  |
| 1   | H     | 344 | ASN  | 6.3  |
| 1   | G     | 389 | LEU  | 6.0  |
| 1   | F     | 45  | ILE  | 5.9  |
| 1   | E     | 343 | ALA  | 5.9  |
| 1   | H     | 343 | ALA  | 5.9  |
| 1   | G     | 385 | THR  | 5.9  |
| 1   | H     | 45  | ILE  | 5.6  |
| 1   | C     | 383 | ARG  | 5.5  |
| 1   | A     | 389 | LEU  | 5.5  |
| 1   | A     | 343 | ALA  | 5.4  |
| 1   | F     | 344 | ASN  | 5.4  |
| 1   | F     | 388 | GLU  | 5.3  |
| 1   | C     | 618 | PHE  | 5.3  |
| 1   | A     | 390 | THR  | 5.2  |
| 1   | F     | 342 | PRO  | 5.2  |
| 1   | D     | 388 | GLU  | 5.1  |
| 1   | A     | 388 | GLU  | 5.1  |
| 1   | E     | 618 | PHE  | 5.1  |
| 1   | C     | 384 | GLY  | 4.9  |
| 1   | C     | 45  | ILE  | 4.9  |
| 1   | D     | 618 | PHE  | 4.8  |
| 1   | F     | 384 | GLY  | 4.7  |
| 1   | A     | 344 | ASN  | 4.7  |
| 1   | H     | 345 | PRO  | 4.6  |
| 1   | D     | 385 | THR  | 4.6  |
| 1   | A     | 384 | GLY  | 4.5  |
| 1   | A     | 385 | THR  | 4.5  |
| 1   | F     | 389 | LEU  | 4.5  |
| 1   | C     | 385 | THR  | 4.5  |
| 1   | C     | 345 | PRO  | 4.5  |
| 1   | F     | 385 | THR  | 4.5  |
| 1   | C     | 343 | ALA  | 4.4  |
| 1   | H     | 44  | ASP  | 4.4  |
| 1   | D     | 344 | ASN  | 4.3  |
| 1   | H     | 43  | MET  | 4.3  |
| 1   | E     | 345 | PRO  | 4.3  |
| 1   | G     | 344 | ASN  | 4.2  |
| 1   | E     | 44  | ASP  | 4.2  |
| 1   | C     | 390 | THR  | 4.1  |
| 1   | G     | 618 | PHE  | 4.0  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | D            | 345        | PRO         | 4.0         |
| 1          | G            | 342        | PRO         | 4.0         |
| 1          | C            | 617        | PRO         | 4.0         |
| 1          | G            | 390        | THR         | 4.0         |
| 1          | A            | 43         | MET         | 3.9         |
| 1          | F            | 345        | PRO         | 3.9         |
| 1          | F            | 390        | THR         | 3.9         |
| 1          | E            | 388        | GLU         | 3.9         |
| 1          | H            | 618        | PHE         | 3.9         |
| 1          | A            | 459        | VAL         | 3.9         |
| 1          | G            | 186        | ASP         | 3.9         |
| 1          | C            | 341        | ASN         | 3.8         |
| 1          | E            | 385        | THR         | 3.8         |
| 1          | A            | 383        | ARG         | 3.8         |
| 1          | C            | 388        | GLU         | 3.8         |
| 1          | G            | 44         | ASP         | 3.7         |
| 1          | A            | 345        | PRO         | 3.7         |
| 1          | G            | 401        | THR         | 3.6         |
| 1          | E            | 384        | GLY         | 3.6         |
| 1          | D            | 617        | PRO         | 3.6         |
| 1          | B            | 345        | PRO         | 3.5         |
| 1          | C            | 344        | ASN         | 3.5         |
| 1          | E            | 342        | PRO         | 3.5         |
| 1          | H            | 459        | VAL         | 3.5         |
| 1          | H            | 617        | PRO         | 3.5         |
| 1          | G            | 345        | PRO         | 3.5         |
| 1          | E            | 344        | ASN         | 3.4         |
| 1          | B            | 341        | ASN         | 3.3         |
| 1          | G            | 43         | MET         | 3.3         |
| 1          | B            | 389        | LEU         | 3.3         |
| 1          | D            | 186        | ASP         | 3.2         |
| 1          | F            | 618        | PHE         | 3.2         |
| 1          | F            | 43         | MET         | 3.2         |
| 1          | B            | 385        | THR         | 3.2         |
| 1          | H            | 341        | ASN         | 3.2         |
| 1          | B            | 186        | ASP         | 3.2         |
| 1          | B            | 45         | ILE         | 3.2         |
| 1          | E            | 45         | ILE         | 3.2         |
| 1          | F            | 186        | ASP         | 3.1         |
| 1          | A            | 618        | PHE         | 3.1         |
| 1          | E            | 341        | ASN         | 3.1         |
| 1          | F            | 383        | ARG         | 3.0         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 341 | ASN  | 3.0  |
| 1   | E     | 561 | GLU  | 3.0  |
| 1   | H     | 458 | ALA  | 3.0  |
| 1   | F     | 341 | ASN  | 3.0  |
| 1   | C     | 392 | SER  | 3.0  |
| 1   | B     | 344 | ASN  | 3.0  |
| 1   | D     | 44  | ASP  | 2.9  |
| 1   | F     | 272 | GLU  | 2.9  |
| 1   | H     | 186 | ASP  | 2.9  |
| 1   | C     | 43  | MET  | 2.9  |
| 1   | D     | 389 | LEU  | 2.9  |
| 1   | D     | 342 | PRO  | 2.9  |
| 1   | F     | 187 | ASP  | 2.9  |
| 1   | F     | 347 | GLU  | 2.8  |
| 1   | C     | 186 | ASP  | 2.8  |
| 1   | G     | 82  | SER  | 2.8  |
| 1   | D     | 43  | MET  | 2.8  |
| 1   | D     | 269 | ASP  | 2.7  |
| 1   | A     | 381 | THR  | 2.7  |
| 1   | A     | 400 | SER  | 2.7  |
| 1   | G     | 269 | ASP  | 2.7  |
| 1   | D     | 272 | GLU  | 2.7  |
| 1   | A     | 458 | ALA  | 2.6  |
| 1   | G     | 458 | ALA  | 2.6  |
| 1   | G     | 384 | GLY  | 2.6  |
| 1   | A     | 382 | ILE  | 2.6  |
| 1   | F     | 290 | ALA  | 2.6  |
| 1   | H     | 232 | GLY  | 2.6  |
| 1   | B     | 44  | ASP  | 2.6  |
| 1   | B     | 388 | GLU  | 2.6  |
| 1   | A     | 401 | THR  | 2.6  |
| 1   | E     | 269 | ASP  | 2.6  |
| 1   | F     | 391 | TYR  | 2.6  |
| 1   | H     | 389 | LEU  | 2.6  |
| 1   | F     | 81  | ASP  | 2.5  |
| 1   | C     | 396 | THR  | 2.5  |
| 1   | E     | 458 | ALA  | 2.5  |
| 1   | F     | 188 | ALA  | 2.5  |
| 1   | G     | 388 | GLU  | 2.5  |
| 1   | H     | 342 | PRO  | 2.5  |
| 1   | F     | 268 | THR  | 2.5  |
| 1   | A     | 342 | PRO  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 617 | PRO  | 2.5  |
| 1   | E     | 43  | MET  | 2.5  |
| 1   | C     | 305 | SER  | 2.5  |
| 1   | B     | 390 | THR  | 2.4  |
| 1   | D     | 390 | THR  | 2.4  |
| 1   | A     | 133 | ALA  | 2.4  |
| 1   | E     | 347 | GLU  | 2.4  |
| 1   | E     | 389 | LEU  | 2.4  |
| 1   | E     | 232 | GLY  | 2.4  |
| 1   | D     | 341 | ASN  | 2.4  |
| 1   | H     | 385 | THR  | 2.4  |
| 1   | E     | 307 | ASP  | 2.4  |
| 1   | G     | 400 | SER  | 2.4  |
| 1   | F     | 561 | GLU  | 2.4  |
| 1   | H     | 190 | ALA  | 2.4  |
| 1   | E     | 400 | SER  | 2.3  |
| 1   | E     | 459 | VAL  | 2.3  |
| 1   | F     | 387 | GLY  | 2.3  |
| 1   | E     | 186 | ASP  | 2.3  |
| 1   | C     | 418 | GLN  | 2.3  |
| 1   | C     | 272 | GLU  | 2.3  |
| 1   | C     | 342 | PRO  | 2.3  |
| 1   | D     | 309 | PHE  | 2.3  |
| 1   | H     | 268 | THR  | 2.3  |
| 1   | F     | 421 | GLU  | 2.3  |
| 1   | F     | 269 | ASP  | 2.3  |
| 1   | H     | 133 | ALA  | 2.3  |
| 1   | F     | 271 | PRO  | 2.2  |
| 1   | D     | 459 | VAL  | 2.2  |
| 1   | A     | 44  | ASP  | 2.2  |
| 1   | F     | 309 | PHE  | 2.2  |
| 1   | H     | 189 | ASP  | 2.2  |
| 1   | H     | 272 | GLU  | 2.2  |
| 1   | E     | 617 | PRO  | 2.2  |
| 1   | B     | 458 | ALA  | 2.2  |
| 1   | E     | 382 | ILE  | 2.1  |
| 1   | B     | 383 | ARG  | 2.1  |
| 1   | G     | 341 | ASN  | 2.1  |
| 1   | B     | 459 | VAL  | 2.1  |
| 1   | F     | 185 | LYS  | 2.1  |
| 1   | G     | 382 | ILE  | 2.1  |
| 1   | G     | 383 | ARG  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 561 | GLU  | 2.0  |
| 1   | A     | 186 | ASP  | 2.0  |
| 1   | B     | 418 | GLN  | 2.0  |
| 1   | B     | 561 | GLU  | 2.0  |
| 1   | E     | 272 | GLU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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   | FAD  | D     | 703 | 53/53 | 0.88 | 0.22 | 5.08  | 16,20,105,106              | 0     |
| 3   | FAD  | C     | 704 | 53/53 | 0.86 | 0.21 | 4.94  | 16,23,113,114              | 0     |
| 3   | FAD  | E     | 705 | 53/53 | 0.89 | 0.22 | 4.47  | 15,21,119,120              | 0     |
| 3   | FAD  | G     | 708 | 53/53 | 0.88 | 0.21 | 4.39  | 16,21,101,103              | 0     |
| 3   | FAD  | B     | 702 | 53/53 | 0.89 | 0.21 | 4.35  | 14,19,107,107              | 0     |
| 3   | FAD  | H     | 707 | 53/53 | 0.89 | 0.22 | 4.25  | 15,21,119,120              | 0     |
| 3   | FAD  | F     | 706 | 53/53 | 0.89 | 0.20 | 4.23  | 16,21,115,116              | 0     |
| 3   | FAD  | A     | 701 | 53/53 | 0.88 | 0.21 | 3.69  | 12,18,94,95                | 0     |
| 2   | SHG  | G     | 808 | 12/12 | 0.89 | 0.16 | 2.46  | 27,35,39,42                | 0     |
| 2   | SHG  | C     | 804 | 12/12 | 0.89 | 0.12 | 0.38  | 29,37,41,41                | 0     |
| 2   | SHG  | E     | 805 | 12/12 | 0.91 | 0.11 | 0.06  | 31,37,40,41                | 0     |
| 2   | SHG  | H     | 807 | 12/12 | 0.94 | 0.10 | -0.04 | 28,35,38,41                | 0     |
| 2   | SHG  | D     | 803 | 12/12 | 0.93 | 0.12 | -0.18 | 30,35,40,41                | 0     |
| 2   | SHG  | A     | 801 | 12/12 | 0.94 | 0.10 | -0.24 | 24,35,41,44                | 0     |
| 2   | SHG  | F     | 806 | 12/12 | 0.94 | 0.11 | -0.35 | 31,34,40,42                | 0     |
| 2   | SHG  | B     | 802 | 12/12 | 0.96 | 0.07 | -1.90 | 24,29,35,39                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.