



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:12 AM UTC

PDB ID : 6WYD / pdb\_00006wyd  
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)  
COMPLEX WITH Compound-12 (AKA; 7-benzyl-1H-[1,2,3]triazolo[4,5-b]py  
rid  
Authors : Khan, J.A.  
Deposited on : 2020-05-12  
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

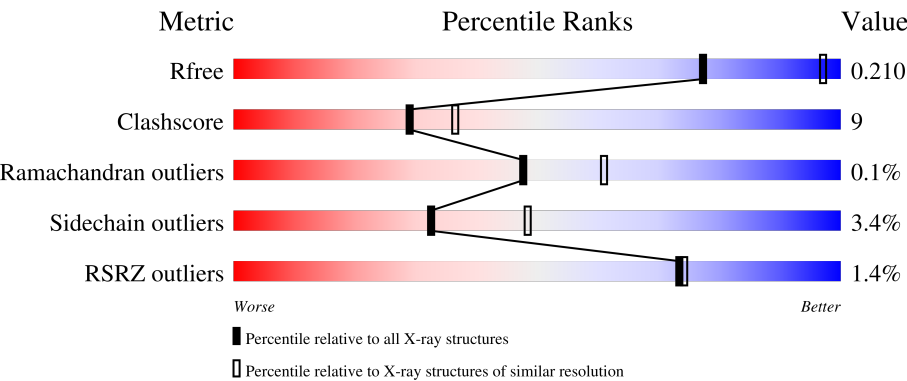
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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 <sub>free</sub>     | 180053                      | 1091 (2.54-2.54)                                      |
| Clashscore            | 190562                      | 1120 (2.54-2.54)                                      |
| Ramachandran outliers | 187476                      | 1106 (2.54-2.54)                                      |
| Sidechain outliers    | 187428                      | 1106 (2.54-2.54)                                      |
| RSRZ outliers         | 180081                      | 1091 (2.54-2.54)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                           |
|-----|-------|--------|--------------------------------------------|
| 1   | A     | 105    | <div><div></div><div>79%17%..</div></div>  |
| 1   | D     | 105    | <div><div>%</div><div>78%20%.</div></div>  |
| 1   | F     | 105    | <div><div>%</div><div>75%22%..</div></div> |
| 1   | H     | 105    | <div><div>%</div><div>84%14%. </div></div> |

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| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 2   | B     | 467    | <div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>  |
| 2   | E     | 467    | <div> <div>3%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>•</div> </div> </div> |
| 2   | G     | 467    | <div> <div>2%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>•</div> </div> </div> |
| 2   | I     | 467    | <div> <div></div> <div> <div></div> <div>83%</div> <div>16%</div> <div>•</div> </div> </div>   |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | NAG  | B     | 604 | -         | -        | X       | -                |
| 4   | NAG  | E     | 608 | -         | -        | X       | -                |
| 4   | NAG  | G     | 603 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 18734 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 Myeloperoxidase light chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 822   | 521 | 146 | 150 | 5 |         |         |       |
| 1   | D     | 103      | Total | C   | N   | O   | S | 3       | 0       | 0     |
|     |       |          | 820   | 519 | 145 | 151 | 5 |         |         |       |
| 1   | F     | 103      | Total | C   | N   | O   | S | 3       | 0       | 0     |
|     |       |          | 820   | 519 | 145 | 151 | 5 |         |         |       |
| 1   | H     | 103      | Total | C   | N   | O   | S | 3       | 0       | 0     |
|     |       |          | 813   | 516 | 144 | 148 | 5 |         |         |       |

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 465      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3630  | 2304 | 650 | 649 | 27 |         |         |       |
| 2   | E     | 465      | Total | C    | N   | O   | S  | 21      | 0       | 0     |
|     |       |          | 3603  | 2286 | 643 | 648 | 26 |         |         |       |
| 2   | G     | 465      | Total | C    | N   | O   | S  | 32      | 0       | 0     |
|     |       |          | 3639  | 2303 | 653 | 656 | 27 |         |         |       |
| 2   | I     | 465      | Total | C    | N   | O   | S  | 37      | 0       | 0     |
|     |       |          | 3637  | 2306 | 649 | 655 | 27 |         |         |       |

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

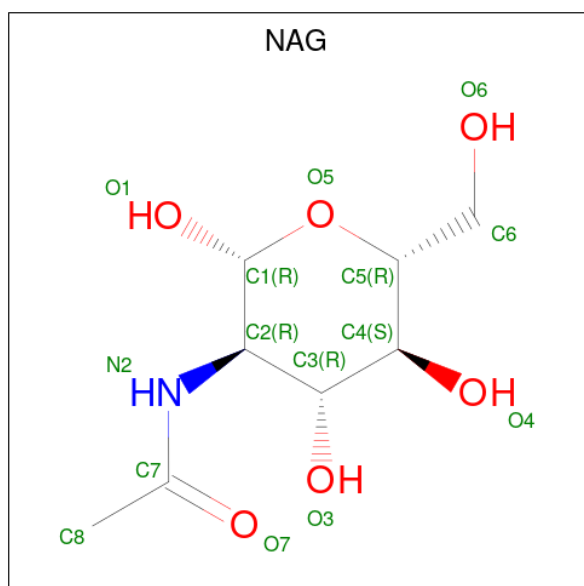
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | E     | 2        | Total | Cl | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | F     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | G     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | H     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | I     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



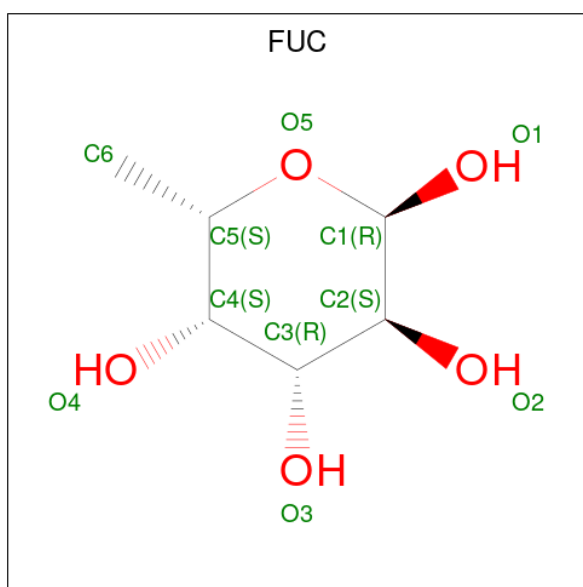
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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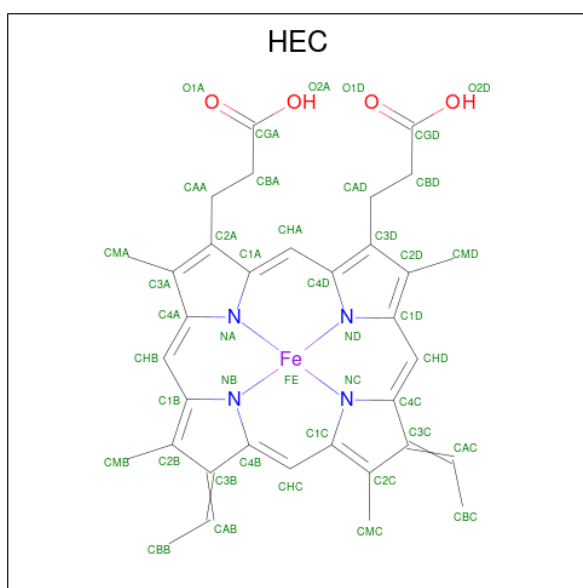
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 5 is alpha-L-fucopyranose (CCD ID: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



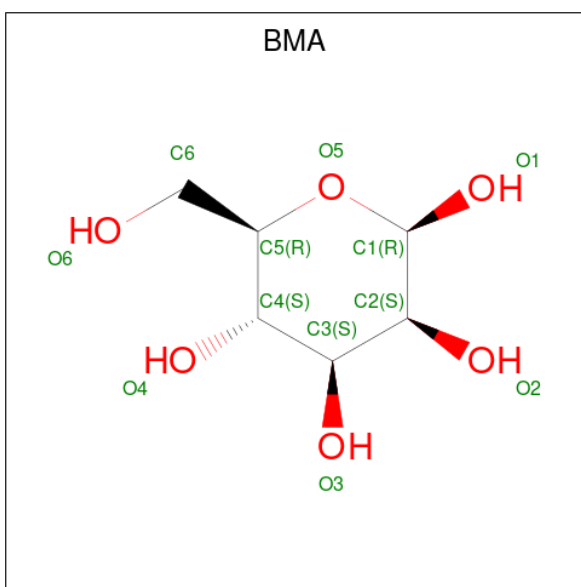
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 5   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |
| 5   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 10    | 6 | 4 |         |         |

- Molecule 6 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



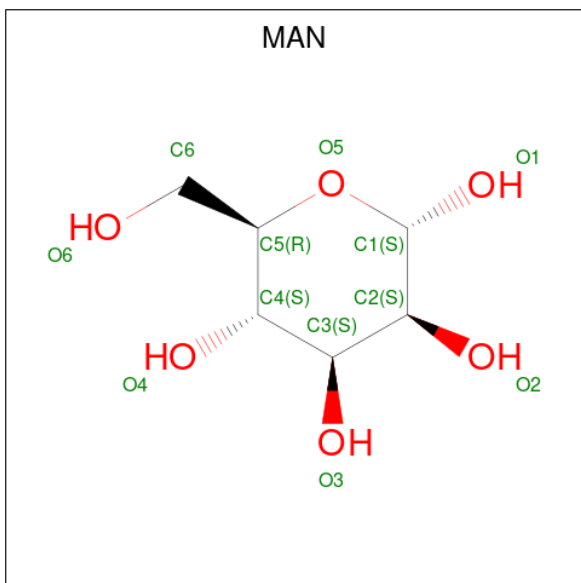
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 6   | B     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       | 0       |
| 6   | E     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       | 0       |
| 6   | G     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       | 0       |
| 6   | I     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       | 0       |

- Molecule 7 is beta-D-mannopyranose (CCD ID: BMA) (formula:  $C_6H_{12}O_6$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 7   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 7   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 7   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

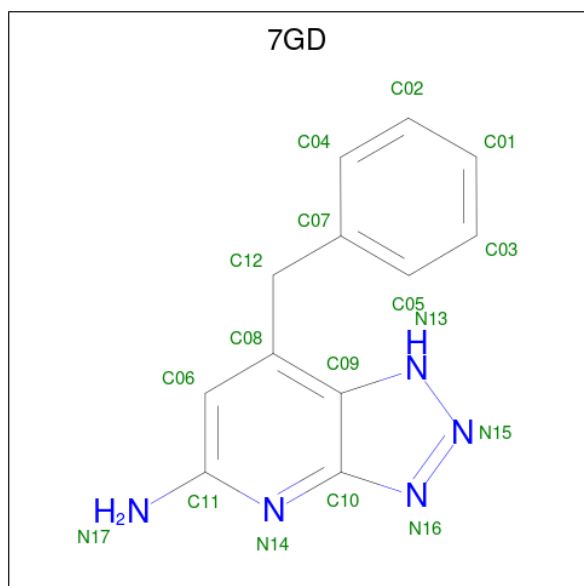
- Molecule 8 is alpha-D-mannopyranose (CCD ID: MAN) (formula:  $C_6H_{12}O_6$ ).





| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 8   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 8   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 8   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 8   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 8   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 8   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 8   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

- Molecule 9 is 7-benzyl-1H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (CCD ID: 7GD) (formula: C<sub>12</sub>H<sub>11</sub>N<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | B     | 1        | Total | C  | N | 0       | 0       |
|     |       |          | 17    | 12 | 5 |         |         |
| 9   | E     | 1        | Total | C  | N | 0       | 0       |
|     |       |          | 17    | 12 | 5 |         |         |
| 9   | G     | 1        | Total | C  | N | 0       | 0       |
|     |       |          | 17    | 12 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | H     | 1        | Total | C  | N | 0       | 0       |
|     |       |          | 17    | 12 | 5 |         |         |

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 10  | B     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 10  | E     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 10  | G     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 10  | I     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 11 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11  | A     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |
| 11  | B     | 66       | Total | O  | 0       | 0       |
|     |       |          | 66    | 66 |         |         |
| 11  | D     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 11  | E     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |
| 11  | F     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 11  | G     | 43       | Total | O  | 0       | 0       |
|     |       |          | 43    | 43 |         |         |
| 11  | H     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 11  | I     | 45       | Total | O  | 0       | 0       |
|     |       |          | 45    | 45 |         |         |

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

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

- Molecule 1: Myeloperoxidase light chain

Chain A: 



- Molecule 1: Myeloperoxidase light chain

Chain D: 



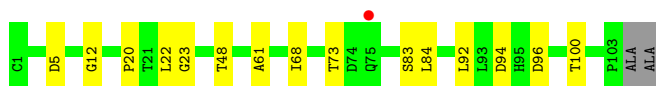
- Molecule 1: Myeloperoxidase light chain

Chain F: 



- Molecule 1: Myeloperoxidase light chain

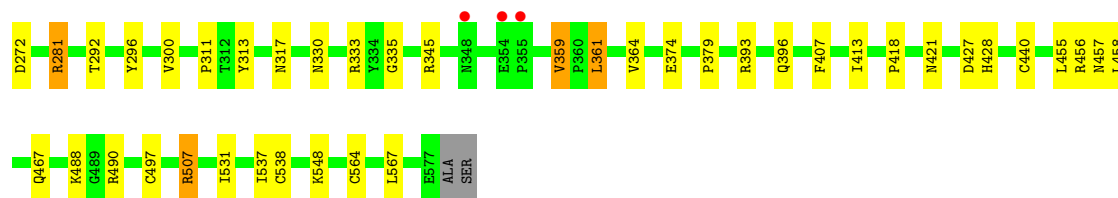
Chain H: 



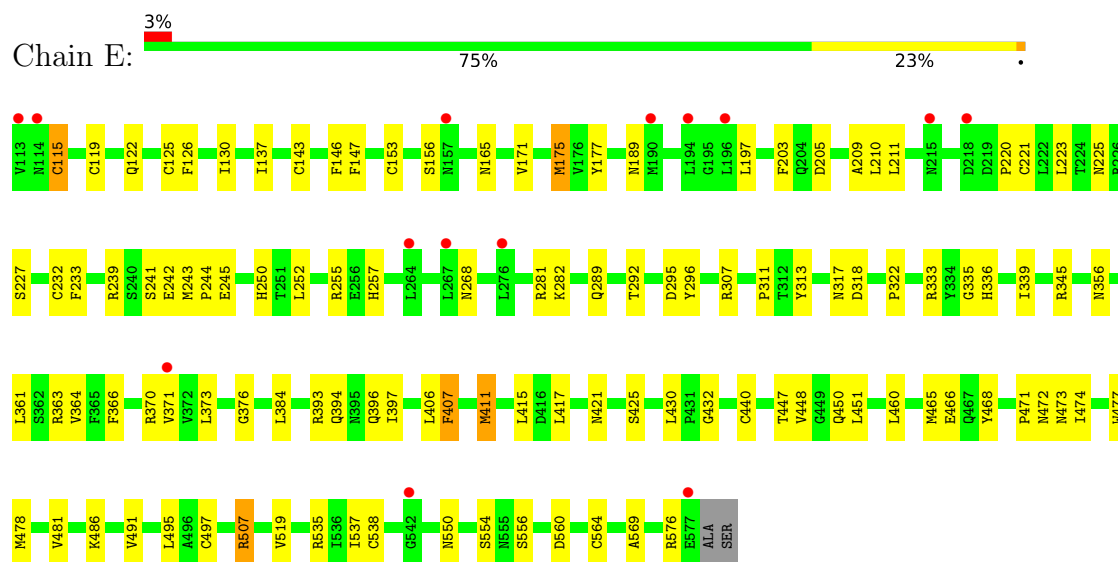
- Molecule 2: Myeloperoxidase heavy chain

Chain B: 

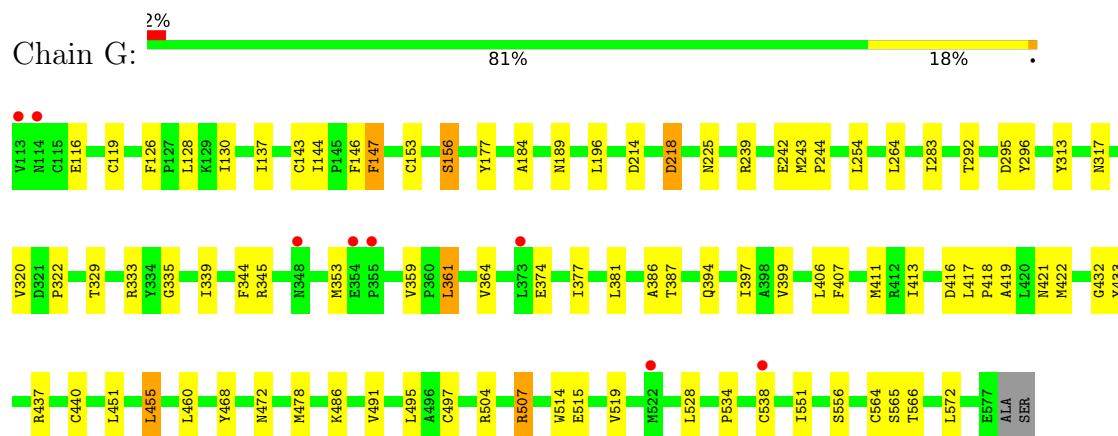




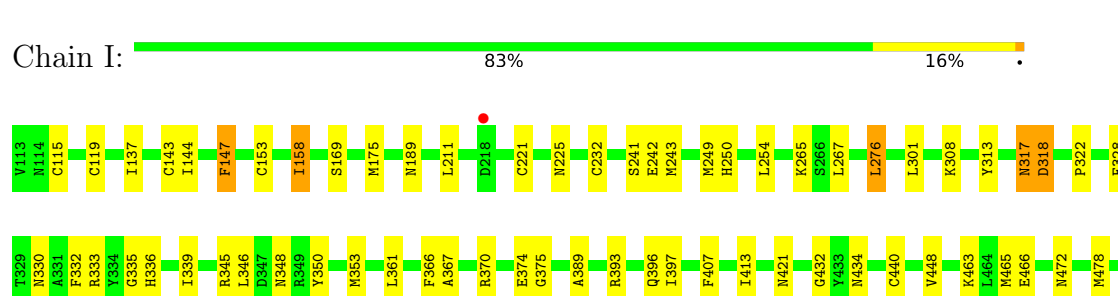
• Molecule 2: Myeloperoxidase heavy chain



• Molecule 2: Myeloperoxidase heavy chain



• Molecule 2: Myeloperoxidase heavy chain





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 143.68Å 150.65Å 231.06Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 115.53 – 2.55<br>115.53 – 2.55                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 100.0 (115.53-2.55)<br>97.8 (115.53-2.55)                   | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.31 (at 2.42Å)                                             | Xtriage          |
| Refinement program                                                      | BUSTER 2.9.6                                                | Depositor        |
| R, $R_{free}$                                                           | 0.194 , 0.254<br>0.207 , 0.210                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4654 reflections (4.85%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 52.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.174                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 55.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.017 for -k,-h,-l                                          | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 18734                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 50.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: HEC, CL, BMA, CA, NAG, MAN, 7GD, FUC

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

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | A     | 0.81         | 0/847   | 1.34        | 6/1155 (0.5%)    |
| 1   | D     | 0.84         | 0/845   | 1.38        | 10/1153 (0.9%)   |
| 1   | F     | 0.79         | 0/845   | 1.35        | 7/1153 (0.6%)    |
| 1   | H     | 0.79         | 0/838   | 1.32        | 10/1144 (0.9%)   |
| 2   | B     | 0.87         | 0/3715  | 1.36        | 22/5054 (0.4%)   |
| 2   | E     | 0.87         | 0/3688  | 1.37        | 21/5022 (0.4%)   |
| 2   | G     | 0.84         | 0/3725  | 1.34        | 14/5069 (0.3%)   |
| 2   | I     | 0.84         | 0/3722  | 1.33        | 12/5064 (0.2%)   |
| All | All   | 0.84         | 0/18225 | 1.35        | 102/24814 (0.4%) |

There are no bond length outliers.

All (102) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | G     | 519 | VAL  | N-CA-C   | -7.90 | 103.55      | 110.74   |
| 2   | B     | 427 | ASP  | CA-CB-CG | 7.57  | 120.17      | 112.60   |
| 2   | I     | 550 | ASN  | CA-CB-CG | 7.00  | 119.60      | 112.60   |
| 2   | G     | 130 | ILE  | N-CA-C   | 6.83  | 114.66      | 107.76   |
| 2   | E     | 550 | ASN  | CA-CB-CG | 6.80  | 119.40      | 112.60   |
| 1   | F     | 37  | TYR  | CA-C-N   | 6.68  | 129.54      | 120.38   |
| 1   | F     | 37  | TYR  | C-N-CA   | 6.68  | 129.54      | 120.38   |
| 2   | B     | 157 | ASN  | CA-CB-CG | 6.61  | 119.21      | 112.60   |
| 2   | B     | 457 | ASN  | CA-CB-CG | 6.61  | 119.21      | 112.60   |
| 2   | B     | 158 | ILE  | CA-C-N   | 6.47  | 130.02      | 120.90   |
| 2   | B     | 158 | ILE  | C-N-CA   | 6.47  | 130.02      | 120.90   |
| 2   | E     | 177 | TYR  | N-CA-C   | 6.43  | 119.28      | 111.82   |
| 1   | D     | 12  | GLY  | CA-C-N   | 6.42  | 129.95      | 120.90   |
| 1   | D     | 12  | GLY  | C-N-CA   | 6.42  | 129.95      | 120.90   |
| 2   | I     | 375 | GLY  | N-CA-C   | 6.42  | 125.19      | 115.63   |
| 2   | E     | 407 | PHE  | CA-CB-CG | 6.41  | 120.21      | 113.80   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | B     | 281 | ARG  | CA-C-N   | 6.39  | 128.84      | 120.28   |
| 2   | B     | 281 | ARG  | C-N-CA   | 6.39  | 128.84      | 120.28   |
| 2   | I     | 397 | ILE  | N-CA-C   | 6.37  | 116.48      | 110.30   |
| 2   | E     | 203 | PHE  | N-CA-C   | 6.32  | 118.68      | 109.07   |
| 1   | F     | 54  | ASN  | CA-CB-CG | 6.16  | 118.75      | 112.60   |
| 1   | D     | 96  | ASP  | CA-CB-CG | 6.14  | 118.74      | 112.60   |
| 1   | A     | 20  | PRO  | N-CA-C   | 6.13  | 121.89      | 113.98   |
| 1   | A     | 69  | VAL  | N-CA-C   | 6.09  | 116.25      | 110.53   |
| 1   | H     | 48  | THR  | CB-CA-C  | 6.08  | 116.78      | 109.85   |
| 1   | A     | 43  | LEU  | N-CA-C   | 6.07  | 117.30      | 109.65   |
| 2   | B     | 177 | TYR  | N-CA-C   | 5.97  | 120.85      | 113.50   |
| 1   | H     | 96  | ASP  | CA-CB-CG | 5.96  | 118.56      | 112.60   |
| 2   | E     | 397 | ILE  | N-CA-C   | 5.92  | 115.98      | 110.42   |
| 2   | B     | 374 | GLU  | N-CA-C   | 5.89  | 119.99      | 113.21   |
| 1   | A     | 9   | THR  | N-CA-C   | -5.86 | 102.64      | 110.55   |
| 1   | D     | 9   | THR  | N-CA-C   | -5.83 | 103.01      | 110.53   |
| 1   | D     | 15  | ASN  | N-CA-C   | -5.77 | 104.91      | 111.14   |
| 2   | B     | 300 | VAL  | N-CA-C   | -5.77 | 106.08      | 111.45   |
| 2   | E     | 407 | PHE  | CA-C-N   | 5.76  | 128.00      | 120.28   |
| 2   | E     | 407 | PHE  | C-N-CA   | 5.76  | 128.00      | 120.28   |
| 2   | I     | 147 | PHE  | CA-CB-CG | 5.76  | 119.56      | 113.80   |
| 2   | G     | 407 | PHE  | CA-C-N   | 5.75  | 127.98      | 120.28   |
| 2   | G     | 407 | PHE  | C-N-CA   | 5.75  | 127.98      | 120.28   |
| 2   | I     | 407 | PHE  | CA-C-N   | 5.72  | 128.74      | 120.79   |
| 2   | I     | 407 | PHE  | C-N-CA   | 5.72  | 128.74      | 120.79   |
| 2   | G     | 218 | ASP  | CA-CB-CG | 5.65  | 118.25      | 112.60   |
| 2   | B     | 144 | ILE  | N-CA-C   | -5.63 | 102.07      | 107.76   |
| 1   | D     | 96  | ASP  | N-CA-C   | -5.58 | 106.64      | 113.50   |
| 1   | H     | 84  | LEU  | CA-C-N   | 5.58  | 128.32      | 120.28   |
| 1   | H     | 84  | LEU  | C-N-CA   | 5.58  | 128.32      | 120.28   |
| 2   | I     | 318 | ASP  | CA-CB-CG | 5.54  | 118.14      | 112.60   |
| 2   | G     | 556 | SER  | N-CA-C   | 5.54  | 117.55      | 108.52   |
| 2   | E     | 205 | ASP  | CA-CB-CG | 5.50  | 118.10      | 112.60   |
| 1   | H     | 5   | ASP  | CA-CB-CG | 5.49  | 118.09      | 112.60   |
| 2   | B     | 548 | LYS  | N-CA-C   | -5.46 | 102.79      | 110.50   |
| 2   | I     | 144 | ILE  | N-CA-C   | -5.45 | 102.25      | 107.76   |
| 2   | B     | 567 | LEU  | N-CA-C   | 5.44  | 117.49      | 109.50   |
| 1   | F     | 30  | VAL  | N-CA-C   | -5.38 | 104.18      | 110.05   |
| 2   | G     | 397 | ILE  | N-CA-C   | 5.35  | 115.45      | 110.42   |
| 1   | H     | 20  | PRO  | N-CA-C   | 5.35  | 120.62      | 114.20   |
| 1   | H     | 12  | GLY  | CA-C-N   | 5.34  | 128.81      | 120.75   |
| 1   | H     | 12  | GLY  | C-N-CA   | 5.34  | 128.81      | 120.75   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | E     | 318 | ASP  | CA-CB-CG | 5.33  | 117.93      | 112.60   |
| 2   | G     | 386 | ALA  | N-CA-C   | 5.32  | 119.88      | 113.17   |
| 1   | D     | 88  | GLN  | N-CA-C   | 5.30  | 117.06      | 111.28   |
| 2   | E     | 373 | LEU  | N-CA-C   | 5.30  | 119.38      | 113.02   |
| 1   | F     | 9   | THR  | N-CA-C   | -5.30 | 102.90      | 110.59   |
| 2   | I     | 158 | ILE  | N-CA-C   | -5.30 | 107.67      | 112.12   |
| 2   | G     | 177 | TYR  | N-CA-C   | 5.30  | 118.90      | 112.23   |
| 2   | E     | 468 | TYR  | N-CA-C   | 5.29  | 119.80      | 112.45   |
| 2   | E     | 147 | PHE  | CA-CB-CG | 5.26  | 119.06      | 113.80   |
| 2   | B     | 272 | ASP  | CA-C-N   | 5.26  | 125.78      | 119.94   |
| 2   | B     | 272 | ASP  | C-N-CA   | 5.26  | 125.78      | 119.94   |
| 2   | E     | 466 | GLU  | CA-C-N   | 5.26  | 127.60      | 120.65   |
| 2   | E     | 466 | GLU  | C-N-CA   | 5.26  | 127.60      | 120.65   |
| 2   | B     | 359 | VAL  | CB-CA-C  | 5.25  | 116.33      | 110.71   |
| 2   | I     | 432 | GLY  | CA-C-N   | 5.25  | 128.70      | 120.82   |
| 2   | I     | 432 | GLY  | C-N-CA   | 5.25  | 128.70      | 120.82   |
| 1   | F     | 5   | ASP  | CA-CB-CG | 5.23  | 117.83      | 112.60   |
| 2   | G     | 374 | GLU  | N-CA-C   | 5.18  | 118.70      | 111.56   |
| 2   | G     | 468 | TYR  | N-CA-C   | 5.17  | 118.74      | 112.23   |
| 2   | E     | 473 | ASN  | CA-CB-CG | 5.14  | 117.74      | 112.60   |
| 2   | B     | 147 | PHE  | CA-CB-CG | 5.11  | 118.91      | 113.80   |
| 2   | B     | 184 | ALA  | CA-C-N   | 5.11  | 127.08      | 120.44   |
| 2   | B     | 184 | ALA  | C-N-CA   | 5.11  | 127.08      | 120.44   |
| 2   | I     | 317 | ASN  | CA-CB-CG | 5.10  | 117.70      | 112.60   |
| 1   | A     | 10  | ILE  | CA-C-N   | 5.10  | 129.34      | 120.68   |
| 1   | A     | 10  | ILE  | C-N-CA   | 5.10  | 129.34      | 120.68   |
| 2   | E     | 451 | LEU  | CA-C-N   | 5.09  | 125.75      | 119.99   |
| 2   | E     | 451 | LEU  | C-N-CA   | 5.09  | 125.75      | 119.99   |
| 2   | B     | 407 | PHE  | CA-C-N   | 5.09  | 128.46      | 120.82   |
| 2   | B     | 407 | PHE  | C-N-CA   | 5.09  | 128.46      | 120.82   |
| 2   | G     | 147 | PHE  | CA-CB-CG | 5.09  | 118.89      | 113.80   |
| 2   | E     | 250 | HIS  | CA-C-N   | 5.08  | 127.09      | 120.28   |
| 2   | E     | 250 | HIS  | C-N-CA   | 5.08  | 127.09      | 120.28   |
| 2   | E     | 307 | ARG  | CA-C-N   | 5.08  | 127.54      | 120.63   |
| 2   | E     | 307 | ARG  | C-N-CA   | 5.08  | 127.54      | 120.63   |
| 2   | G     | 399 | VAL  | N-CA-C   | 5.07  | 116.54      | 109.80   |
| 2   | G     | 214 | ASP  | CA-CB-CG | 5.06  | 117.66      | 112.60   |
| 2   | B     | 359 | VAL  | N-CA-CB  | 5.06  | 117.45      | 111.08   |
| 1   | H     | 61  | ALA  | CA-C-N   | 5.05  | 127.05      | 120.28   |
| 1   | H     | 61  | ALA  | C-N-CA   | 5.05  | 127.05      | 120.28   |
| 1   | D     | 98  | ASP  | N-CA-C   | 5.04  | 117.36      | 108.75   |
| 1   | D     | 37  | TYR  | CA-C-N   | 5.02  | 127.25      | 120.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 37  | TYR  | C-N-CA | 5.02  | 127.25      | 120.38   |
| 1   | F     | 15  | ASN  | N-CA-C | -5.01 | 105.72      | 111.14   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 822   | 0        | 780      | 16      | 0            |
| 1   | D     | 820   | 0        | 774      | 14      | 0            |
| 1   | F     | 820   | 0        | 774      | 13      | 0            |
| 1   | H     | 813   | 0        | 766      | 7       | 0            |
| 2   | B     | 3630  | 0        | 3570     | 59      | 0            |
| 2   | E     | 3603  | 0        | 3515     | 73      | 0            |
| 2   | G     | 3639  | 0        | 3571     | 58      | 0            |
| 2   | I     | 3637  | 0        | 3579     | 54      | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 2     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 70    | 0        | 65       | 15      | 0            |
| 4   | E     | 70    | 0        | 65       | 15      | 0            |
| 4   | G     | 56    | 0        | 52       | 16      | 0            |
| 4   | I     | 70    | 0        | 65       | 14      | 0            |
| 5   | B     | 10    | 0        | 10       | 1       | 0            |
| 5   | E     | 10    | 0        | 10       | 2       | 0            |
| 5   | G     | 10    | 0        | 10       | 1       | 0            |
| 5   | I     | 10    | 0        | 10       | 2       | 0            |
| 6   | B     | 43    | 0        | 32       | 17      | 0            |
| 6   | E     | 43    | 0        | 32       | 15      | 0            |
| 6   | G     | 43    | 0        | 32       | 14      | 0            |
| 6   | I     | 43    | 0        | 32       | 15      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | B     | 11    | 0        | 9        | 4       | 0            |
| 7   | E     | 11    | 0        | 10       | 2       | 0            |
| 7   | G     | 11    | 0        | 10       | 4       | 0            |
| 7   | I     | 11    | 0        | 10       | 3       | 0            |
| 8   | B     | 22    | 0        | 20       | 2       | 0            |
| 8   | E     | 22    | 0        | 20       | 1       | 0            |
| 8   | G     | 22    | 0        | 20       | 2       | 0            |
| 8   | I     | 22    | 0        | 20       | 2       | 0            |
| 9   | B     | 17    | 0        | 0        | 0       | 0            |
| 9   | E     | 17    | 0        | 0        | 2       | 0            |
| 9   | G     | 17    | 0        | 0        | 1       | 0            |
| 9   | H     | 17    | 0        | 0        | 0       | 0            |
| 10  | B     | 1     | 0        | 0        | 0       | 0            |
| 10  | E     | 1     | 0        | 0        | 0       | 0            |
| 10  | G     | 1     | 0        | 0        | 0       | 0            |
| 10  | I     | 1     | 0        | 0        | 0       | 0            |
| 11  | A     | 20    | 0        | 0        | 0       | 0            |
| 11  | B     | 66    | 0        | 0        | 0       | 0            |
| 11  | D     | 10    | 0        | 0        | 0       | 0            |
| 11  | E     | 42    | 0        | 0        | 0       | 0            |
| 11  | F     | 18    | 0        | 0        | 0       | 0            |
| 11  | G     | 43    | 0        | 0        | 0       | 0            |
| 11  | H     | 16    | 0        | 0        | 0       | 0            |
| 11  | I     | 45    | 0        | 0        | 0       | 0            |
| All | All   | 18734 | 0        | 17863    | 295     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (295) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:317:ASN:HD21 | 4:B:604:NAG:C1   | 1.50                     | 1.22              |
| 1:F:94:ASP:OD2   | 6:G:605:HEC:HMD3 | 1.38                     | 1.20              |
| 2:I:242:GLU:OE2  | 6:I:610:HEC:HMB3 | 1.46                     | 1.15              |
| 2:B:225:ASN:HD21 | 4:B:602:NAG:C1   | 1.62                     | 1.11              |
| 1:H:94:ASP:OD2   | 6:I:610:HEC:HMD3 | 1.53                     | 1.07              |
| 2:G:242:GLU:OE2  | 6:G:605:HEC:HMB3 | 1.57                     | 1.01              |
| 2:E:317:ASN:HD21 | 4:E:608:NAG:C1   | 1.73                     | 1.01              |
| 2:E:242:GLU:OE2  | 6:E:610:HEC:HMB3 | 1.63                     | 0.97              |
| 1:A:94:ASP:OD2   | 6:B:606:HEC:HMD2 | 1.65                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:B:604:NAG:O4   | 4:E:601:NAG:C1   | 2.13                     | 0.96              |
| 2:B:317:ASN:ND2  | 4:B:604:NAG:C1   | 2.30                     | 0.95              |
| 4:G:606:NAG:C1   | 4:I:608:NAG:O4   | 2.17                     | 0.93              |
| 2:E:115:CYS:HG   | 2:E:125:CYS:HG   | 0.98                     | 0.93              |
| 2:I:317:ASN:HD21 | 4:I:608:NAG:C1   | 1.82                     | 0.93              |
| 1:A:94:ASP:OD2   | 6:B:606:HEC:CMD  | 2.17                     | 0.92              |
| 2:E:119:CYS:HG   | 2:E:143:CYS:HG   | 0.94                     | 0.91              |
| 1:F:94:ASP:OD2   | 6:G:605:HEC:CMD  | 2.19                     | 0.91              |
| 2:I:242:GLU:OE2  | 6:I:610:HEC:CMB  | 2.18                     | 0.91              |
| 2:G:242:GLU:OE2  | 6:G:605:HEC:CMB  | 2.19                     | 0.89              |
| 2:G:440:CYS:HG   | 2:G:497:CYS:HG   | 1.03                     | 0.87              |
| 2:G:153:CYS:HG   | 2:I:153:CYS:HG   | 1.16                     | 0.87              |
| 2:B:243:MET:CE   | 6:B:606:HEC:HBB1 | 2.05                     | 0.86              |
| 1:D:94:ASP:OD2   | 6:E:610:HEC:HMD2 | 1.76                     | 0.86              |
| 2:I:538:CYS:HG   | 2:I:564:CYS:HG   | 0.91                     | 0.86              |
| 1:H:94:ASP:OD2   | 6:I:610:HEC:CMD  | 2.25                     | 0.85              |
| 2:G:225:ASN:HD21 | 4:G:602:NAG:C1   | 1.89                     | 0.84              |
| 4:G:603:NAG:O4   | 4:I:601:NAG:C1   | 2.26                     | 0.84              |
| 2:G:317:ASN:HD21 | 4:G:603:NAG:C1   | 1.91                     | 0.83              |
| 2:B:242:GLU:OE2  | 6:B:606:HEC:HMB3 | 1.78                     | 0.83              |
| 2:B:153:CYS:HG   | 2:E:153:CYS:HG   | 0.94                     | 0.81              |
| 2:G:538:CYS:HG   | 2:G:564:CYS:HG   | 1.28                     | 0.81              |
| 2:E:317:ASN:ND2  | 4:E:608:NAG:C1   | 2.43                     | 0.80              |
| 2:B:242:GLU:OE2  | 6:B:606:HEC:CMB  | 2.30                     | 0.80              |
| 2:B:538:CYS:HG   | 2:B:564:CYS:HG   | 0.85                     | 0.79              |
| 2:B:115:CYS:HG   | 2:B:125:CYS:HG   | 0.84                     | 0.78              |
| 2:E:242:GLU:OE2  | 6:E:610:HEC:CMB  | 2.31                     | 0.78              |
| 1:D:94:ASP:OD2   | 6:E:610:HEC:CMD  | 2.31                     | 0.78              |
| 2:B:335:GLY:HA3  | 6:B:606:HEC:HBC2 | 1.63                     | 0.77              |
| 2:I:221:CYS:HG   | 2:I:232:CYS:HG   | 0.77                     | 0.77              |
| 2:B:119:CYS:HG   | 2:B:143:CYS:HG   | 0.81                     | 0.77              |
| 2:E:313:TYR:HD1  | 2:E:507:ARG:HD3  | 1.50                     | 0.76              |
| 4:B:607:NAG:C1   | 4:E:608:NAG:O4   | 2.34                     | 0.76              |
| 2:E:440:CYS:HG   | 2:E:497:CYS:HG   | 1.19                     | 0.75              |
| 2:B:225:ASN:ND2  | 4:B:602:NAG:C1   | 2.46                     | 0.75              |
| 2:I:339:ILE:HD13 | 6:I:610:HEC:HBB2 | 1.69                     | 0.74              |
| 2:G:339:ILE:HD13 | 6:G:605:HEC:HBB2 | 1.69                     | 0.74              |
| 2:G:153:CYS:SG   | 2:G:156:SER:HB2  | 2.28                     | 0.73              |
| 1:F:19:SER:HB3   | 1:F:22:LEU:HG    | 1.71                     | 0.73              |
| 2:G:313:TYR:HD1  | 2:G:507:ARG:HD3  | 1.54                     | 0.73              |
| 2:I:317:ASN:ND2  | 4:I:608:NAG:C1   | 2.52                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:B:606:HEC:HBB3 | 6:B:606:HEC:HMB1 | 1.71                     | 0.72              |
| 2:B:153:CYS:HG   | 2:E:153:CYS:CB   | 2.03                     | 0.71              |
| 2:G:189:ASN:HD21 | 4:G:601:NAG:C1   | 2.03                     | 0.71              |
| 4:G:606:NAG:O4   | 7:G:607:BMA:C1   | 2.40                     | 0.70              |
| 2:G:119:CYS:HG   | 2:G:143:CYS:HG   | 0.71                     | 0.69              |
| 2:B:243:MET:SD   | 6:B:606:HEC:HBB1 | 2.33                     | 0.69              |
| 7:G:607:BMA:O3   | 8:G:608:MAN:H2   | 1.93                     | 0.69              |
| 7:I:602:BMA:O6   | 8:I:604:MAN:C1   | 2.41                     | 0.69              |
| 4:E:601:NAG:O4   | 7:E:602:BMA:C1   | 2.41                     | 0.68              |
| 2:I:335:GLY:HA3  | 6:I:610:HEC:HBC2 | 1.75                     | 0.67              |
| 2:E:313:TYR:CD1  | 2:E:507:ARG:HD3  | 2.30                     | 0.67              |
| 4:B:607:NAG:O4   | 7:B:608:BMA:C1   | 2.44                     | 0.66              |
| 2:B:333:ARG:HH11 | 2:B:421:ASN:HD22 | 1.44                     | 0.65              |
| 2:I:243:MET:HE1  | 6:I:610:HEC:HBB1 | 1.79                     | 0.65              |
| 2:E:209:ALA:HB3  | 2:E:255:ARG:HG2  | 1.79                     | 0.65              |
| 2:I:313:TYR:HD1  | 2:I:507:ARG:HD3  | 1.61                     | 0.65              |
| 2:B:333:ARG:HH21 | 6:B:606:HEC:HAD1 | 1.61                     | 0.65              |
| 2:E:336:HIS:HA   | 2:E:339:ILE:HD12 | 1.78                     | 0.64              |
| 2:G:335:GLY:HA3  | 6:G:605:HEC:HBC2 | 1.78                     | 0.64              |
| 2:I:225:ASN:HD21 | 4:I:606:NAG:C1   | 2.10                     | 0.64              |
| 4:B:604:NAG:C4   | 4:E:601:NAG:C1   | 2.76                     | 0.64              |
| 2:G:243:MET:SD   | 6:G:605:HEC:HAB  | 2.38                     | 0.64              |
| 2:E:317:ASN:HD21 | 4:E:608:NAG:C2   | 2.11                     | 0.63              |
| 6:B:606:HEC:HMB1 | 6:B:606:HEC:CBB  | 2.30                     | 0.62              |
| 4:I:601:NAG:O4   | 7:I:602:BMA:C1   | 2.47                     | 0.62              |
| 4:G:606:NAG:C1   | 4:I:608:NAG:C4   | 2.77                     | 0.62              |
| 2:I:333:ARG:HH21 | 6:I:610:HEC:HAD1 | 1.65                     | 0.61              |
| 2:E:244:PRO:HD3  | 2:E:364:VAL:O    | 2.00                     | 0.61              |
| 4:E:608:NAG:O6   | 5:E:609:FUC:O5   | 2.18                     | 0.61              |
| 2:E:225:ASN:HD21 | 4:E:606:NAG:C1   | 2.14                     | 0.60              |
| 2:E:407:PHE:HB2  | 2:E:411:MET:CE   | 2.31                     | 0.60              |
| 2:G:313:TYR:CD1  | 2:G:507:ARG:HD3  | 2.37                     | 0.60              |
| 2:I:119:CYS:HG   | 2:I:143:CYS:HG   | 1.47                     | 0.59              |
| 2:G:243:MET:CE   | 6:G:605:HEC:HBB1 | 2.32                     | 0.59              |
| 2:G:317:ASN:ND2  | 4:G:603:NAG:C1   | 2.63                     | 0.59              |
| 2:B:317:ASN:HD21 | 4:B:604:NAG:C2   | 2.15                     | 0.59              |
| 2:B:313:TYR:CD1  | 2:B:507:ARG:HD3  | 2.38                     | 0.59              |
| 2:B:333:ARG:HH11 | 2:B:421:ASN:ND2  | 2.01                     | 0.59              |
| 2:B:221:CYS:HG   | 2:B:232:CYS:HG   | 0.65                     | 0.59              |
| 2:B:440:CYS:HG   | 2:B:497:CYS:CB   | 2.13                     | 0.59              |
| 4:I:608:NAG:O6   | 5:I:609:FUC:C1   | 2.51                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:241:SER:O    | 2:I:366:PHE:HA   | 2.02                     | 0.58              |
| 2:I:243:MET:SD   | 6:I:610:HEC:CAB  | 2.91                     | 0.58              |
| 2:B:313:TYR:HD1  | 2:B:507:ARG:HD3  | 1.68                     | 0.58              |
| 2:E:225:ASN:HD21 | 4:E:606:NAG:C2   | 2.17                     | 0.57              |
| 2:E:335:GLY:HA3  | 6:E:610:HEC:HBC2 | 1.85                     | 0.57              |
| 2:I:339:ILE:CD1  | 6:I:610:HEC:HBB2 | 2.34                     | 0.57              |
| 2:E:407:PHE:HB2  | 2:E:411:MET:HE1  | 1.87                     | 0.57              |
| 2:E:241:SER:O    | 2:E:366:PHE:HA   | 2.05                     | 0.56              |
| 2:E:333:ARG:HH11 | 2:E:421:ASN:HD22 | 1.53                     | 0.56              |
| 2:B:242:GLU:OE2  | 6:B:606:HEC:HMB1 | 2.06                     | 0.56              |
| 4:B:607:NAG:C1   | 4:E:608:NAG:C4   | 2.83                     | 0.56              |
| 2:B:333:ARG:NH1  | 2:B:421:ASN:HD22 | 2.03                     | 0.56              |
| 1:A:19:SER:HB3   | 1:A:22:LEU:HD22  | 1.87                     | 0.56              |
| 2:E:394:GLN:HB3  | 2:E:460:LEU:HD22 | 1.88                     | 0.56              |
| 2:G:243:MET:HE1  | 6:G:605:HEC:HBB1 | 1.88                     | 0.55              |
| 1:D:8:ARG:HB2    | 2:E:281:ARG:HH12 | 1.71                     | 0.55              |
| 2:E:243:MET:CE   | 6:E:610:HEC:HBB1 | 2.36                     | 0.55              |
| 4:G:603:NAG:C4   | 4:I:601:NAG:C1   | 2.85                     | 0.55              |
| 7:B:608:BMA:O6   | 8:B:610:MAN:C1   | 2.55                     | 0.55              |
| 2:E:211:LEU:HB2  | 2:E:233:PHE:CD1  | 2.42                     | 0.55              |
| 1:H:22:LEU:HB3   | 2:I:322:PRO:HD2  | 1.89                     | 0.55              |
| 2:E:243:MET:SD   | 6:E:610:HEC:HBB1 | 2.46                     | 0.55              |
| 1:A:69:VAL:HG11  | 2:B:418:PRO:HG2  | 1.89                     | 0.54              |
| 2:B:243:MET:SD   | 6:B:606:HEC:CBB  | 2.95                     | 0.54              |
| 2:E:252:LEU:HD11 | 2:E:537:ILE:HA   | 1.89                     | 0.54              |
| 2:I:333:ARG:NH2  | 6:I:610:HEC:HAD1 | 2.22                     | 0.54              |
| 1:A:11:THR:HG22  | 1:A:13:MET:H     | 1.72                     | 0.54              |
| 2:G:333:ARG:HH11 | 2:G:421:ASN:HD22 | 1.55                     | 0.54              |
| 2:I:333:ARG:HH11 | 2:I:421:ASN:HD22 | 1.56                     | 0.53              |
| 2:I:313:TYR:CD1  | 2:I:507:ARG:HD3  | 2.42                     | 0.53              |
| 2:E:243:MET:HE1  | 6:E:610:HEC:HBB1 | 1.91                     | 0.53              |
| 6:B:606:HEC:CMB  | 6:B:606:HEC:CBB  | 2.86                     | 0.53              |
| 2:I:491:VAL:HB   | 2:I:495:LEU:HB2  | 1.90                     | 0.53              |
| 2:I:367:ALA:HB1  | 2:I:370:ARG:HG3  | 1.91                     | 0.53              |
| 6:E:610:HEC:HBB3 | 6:E:610:HEC:HMB1 | 1.91                     | 0.53              |
| 4:I:601:NAG:C4   | 7:I:602:BMA:C1   | 2.87                     | 0.52              |
| 2:G:244:PRO:HD3  | 2:G:364:VAL:O    | 2.09                     | 0.52              |
| 4:G:606:NAG:HO4  | 7:G:607:BMA:C1   | 2.21                     | 0.52              |
| 2:I:243:MET:SD   | 6:I:610:HEC:HAB  | 2.50                     | 0.52              |
| 2:I:225:ASN:ND2  | 4:I:606:NAG:C1   | 2.71                     | 0.52              |
| 2:I:317:ASN:ND2  | 4:I:608:NAG:O5   | 2.35                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:189:ASN:HD21 | 2:B:192:ASN:HD21 | 1.57                     | 0.52              |
| 1:D:29:PHE:CE1   | 2:E:165:ASN:HB2  | 2.45                     | 0.52              |
| 2:I:265:LYS:HD3  | 2:I:276:LEU:HD21 | 1.91                     | 0.52              |
| 2:E:371:VAL:O    | 2:E:376:GLY:HA2  | 2.10                     | 0.51              |
| 4:B:607:NAG:C4   | 7:B:608:BMA:C1   | 2.88                     | 0.51              |
| 1:D:92:LEU:HG    | 2:E:175:MET:HE2  | 1.92                     | 0.51              |
| 2:E:119:CYS:HG   | 2:E:143:CYS:CB   | 2.23                     | 0.50              |
| 2:G:514:TRP:CE2  | 2:G:515:GLU:HG3  | 2.46                     | 0.50              |
| 2:E:220:PRO:HA   | 2:E:223:LEU:HD12 | 1.92                     | 0.50              |
| 1:A:94:ASP:CG    | 6:B:606:HEC:HMD2 | 2.34                     | 0.50              |
| 2:E:317:ASN:CG   | 4:E:608:NAG:C1   | 2.84                     | 0.50              |
| 2:E:393:ARG:HB2  | 2:E:396:GLN:HB2  | 1.92                     | 0.50              |
| 2:E:440:CYS:HG   | 2:E:497:CYS:CB   | 2.24                     | 0.50              |
| 2:G:320:VAL:HG22 | 4:G:603:NAG:H62  | 1.93                     | 0.50              |
| 2:G:416:ASP:OD1  | 2:G:418:PRO:HD2  | 2.12                     | 0.50              |
| 2:E:317:ASN:OD1  | 4:E:608:NAG:C1   | 2.60                     | 0.50              |
| 2:I:434:ASN:HB2  | 2:I:472:ASN:HA   | 1.93                     | 0.50              |
| 2:B:333:ARG:NH2  | 6:B:606:HEC:HAD1 | 2.25                     | 0.50              |
| 2:E:411:MET:HE3  | 2:E:415:LEU:HG   | 1.92                     | 0.50              |
| 2:I:440:CYS:CB   | 2:I:497:CYS:HG   | 2.23                     | 0.49              |
| 1:D:83:SER:HB3   | 2:E:554:SER:O    | 2.11                     | 0.49              |
| 2:G:394:GLN:HB3  | 2:G:460:LEU:HD22 | 1.94                     | 0.49              |
| 2:E:292:THR:HA   | 2:E:296:TYR:HB3  | 1.95                     | 0.49              |
| 1:A:59:ALA:HB2   | 2:B:467:GLN:O    | 2.12                     | 0.49              |
| 2:B:243:MET:HE1  | 6:B:606:HEC:HBB1 | 1.91                     | 0.49              |
| 2:E:535:ARG:HD3  | 2:E:569:ALA:HA   | 1.95                     | 0.49              |
| 2:B:137:ILE:HG12 | 2:B:413:ILE:HD11 | 1.93                     | 0.49              |
| 2:E:333:ARG:HH11 | 2:E:421:ASN:ND2  | 2.10                     | 0.48              |
| 2:E:339:ILE:HD13 | 6:E:610:HEC:HBB2 | 1.95                     | 0.48              |
| 2:G:225:ASN:ND2  | 4:G:602:NAG:C1   | 2.69                     | 0.48              |
| 2:G:440:CYS:HG   | 2:G:497:CYS:CB   | 2.26                     | 0.48              |
| 4:G:603:NAG:O4   | 4:I:601:NAG:C2   | 2.61                     | 0.48              |
| 2:G:128:LEU:HB2  | 2:G:144:ILE:HB   | 1.95                     | 0.48              |
| 2:I:345:ARG:NH2  | 2:I:374:GLU:HB2  | 2.29                     | 0.48              |
| 2:E:425:SER:HA   | 2:E:430:LEU:HD12 | 1.96                     | 0.48              |
| 2:G:242:GLU:OE2  | 6:G:605:HEC:HMB1 | 2.12                     | 0.48              |
| 2:E:471:PRO:HA   | 2:E:474:ILE:HG13 | 1.94                     | 0.48              |
| 1:D:94:ASP:CG    | 6:E:610:HEC:HMD2 | 2.38                     | 0.47              |
| 2:B:239:ARG:O    | 2:B:242:GLU:HB2  | 2.13                     | 0.47              |
| 2:B:317:ASN:CG   | 4:B:604:NAG:C1   | 2.87                     | 0.47              |
| 1:F:1:CYS:HG     | 1:F:14:CYS:CB    | 2.27                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:225:ASN:HD21 | 4:B:602:NAG:C2   | 2.24                     | 0.47              |
| 2:I:393:ARG:HB2  | 2:I:396:GLN:HB2  | 1.96                     | 0.47              |
| 2:E:478:MET:HE3  | 2:E:478:MET:HA   | 1.97                     | 0.47              |
| 2:B:317:ASN:ND2  | 4:B:604:NAG:O5   | 2.40                     | 0.47              |
| 2:E:221:CYS:SG   | 2:E:232:CYS:SG   | 3.02                     | 0.47              |
| 1:H:92:LEU:HD22  | 2:I:249:MET:HB3  | 1.96                     | 0.47              |
| 7:G:607:BMA:H62  | 8:G:609:MAN:C1   | 2.44                     | 0.47              |
| 2:B:393:ARG:HB2  | 2:B:396:GLN:HB2  | 1.96                     | 0.47              |
| 2:E:239:ARG:HD2  | 9:E:611:7GD:C10  | 2.45                     | 0.47              |
| 1:F:11:THR:O     | 1:F:24:ALA:HA    | 2.15                     | 0.46              |
| 2:B:177:TYR:OH   | 2:B:281:ARG:HA   | 2.16                     | 0.46              |
| 4:B:604:NAG:O6   | 5:B:605:FUC:C1   | 2.63                     | 0.46              |
| 1:F:103:PRO:HD2  | 2:G:147:PHE:HB3  | 1.97                     | 0.46              |
| 2:I:189:ASN:HD21 | 4:I:605:NAG:C1   | 2.28                     | 0.46              |
| 2:I:448:VAL:HB   | 2:I:465:MET:HG3  | 1.97                     | 0.46              |
| 1:D:22:LEU:HB3   | 2:E:322:PRO:HD2  | 1.97                     | 0.46              |
| 2:E:363:ARG:O    | 2:E:370:ARG:NH1  | 2.48                     | 0.46              |
| 1:F:31:ARG:CZ    | 1:F:35:ALA:HB2   | 2.45                     | 0.46              |
| 2:G:491:VAL:HB   | 2:G:495:LEU:HB2  | 1.97                     | 0.46              |
| 2:I:328:PHE:CG   | 2:I:502:GLN:HG2  | 2.51                     | 0.46              |
| 2:I:523:GLN:HB3  | 2:I:574:SER:HB3  | 1.98                     | 0.46              |
| 1:A:44:PRO:HD3   | 2:B:148:ARG:CZ   | 2.46                     | 0.46              |
| 2:G:243:MET:SD   | 6:G:605:HEC:HBB1 | 2.56                     | 0.46              |
| 1:F:22:LEU:HB3   | 2:G:322:PRO:HD2  | 1.98                     | 0.46              |
| 2:G:239:ARG:HA   | 9:G:610:7GD:C03  | 2.46                     | 0.46              |
| 2:G:406:LEU:HD22 | 2:G:417:LEU:HB2  | 1.98                     | 0.46              |
| 2:I:333:ARG:HH11 | 2:I:421:ASN:ND2  | 2.13                     | 0.46              |
| 2:E:197:LEU:HG   | 2:E:257:HIS:CD2  | 2.51                     | 0.45              |
| 2:E:448:VAL:HB   | 2:E:465:MET:HG3  | 1.97                     | 0.45              |
| 1:A:48:THR:HG22  | 1:A:51:VAL:HG23  | 1.98                     | 0.45              |
| 2:B:243:MET:HE3  | 6:B:606:HEC:HBB1 | 1.96                     | 0.45              |
| 2:E:243:MET:SD   | 6:E:610:HEC:CBB  | 3.04                     | 0.45              |
| 1:F:38:GLU:HG3   | 1:F:51:VAL:HG11  | 1.98                     | 0.45              |
| 1:A:36:GLU:OE2   | 1:D:18:ARG:NH1   | 2.48                     | 0.45              |
| 2:G:317:ASN:OD1  | 4:G:603:NAG:C1   | 2.65                     | 0.45              |
| 4:G:603:NAG:O6   | 5:G:604:FUC:C1   | 2.65                     | 0.45              |
| 1:D:84:LEU:HB3   | 2:E:384:LEU:HD23 | 1.98                     | 0.45              |
| 2:E:242:GLU:HG3  | 9:E:611:7GD:N13  | 2.32                     | 0.45              |
| 2:E:282:LYS:NZ   | 2:E:519:VAL:O    | 2.46                     | 0.45              |
| 2:I:308:LYS:HE3  | 8:I:603:MAN:C1   | 2.47                     | 0.45              |
| 2:G:137:ILE:HG12 | 2:G:413:ILE:HD11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:538:CYS:SG   | 2:E:564:CYS:SG   | 3.10                     | 0.44              |
| 2:G:361:LEU:HA   | 2:G:364:VAL:HG22 | 1.99                     | 0.44              |
| 2:I:243:MET:SD   | 6:I:610:HEC:CBB  | 3.06                     | 0.44              |
| 2:E:432:GLY:HA3  | 2:E:472:ASN:O    | 2.17                     | 0.44              |
| 1:A:61:ALA:HB3   | 2:B:128:LEU:HD23 | 2.00                     | 0.44              |
| 2:B:115:CYS:CB   | 2:B:125:CYS:HG   | 2.26                     | 0.44              |
| 1:H:23:GLY:HA2   | 2:I:169:SER:OG   | 2.17                     | 0.44              |
| 2:B:243:MET:HE2  | 2:B:245:GLU:OE1  | 2.17                     | 0.44              |
| 2:B:311:PRO:O    | 2:B:507:ARG:NH2  | 2.38                     | 0.43              |
| 2:G:419:ALA:HA   | 2:G:422:MET:HE3  | 2.00                     | 0.43              |
| 1:A:81:GLU:HB2   | 2:B:490:ARG:NH2  | 2.33                     | 0.43              |
| 2:G:451:LEU:HG   | 2:G:455:LEU:HD22 | 2.00                     | 0.43              |
| 2:B:456:ARG:HG2  | 2:G:119:CYS:SG   | 2.59                     | 0.43              |
| 7:E:602:BMA:O6   | 8:E:604:MAN:H3   | 2.18                     | 0.43              |
| 4:E:608:NAG:O6   | 5:E:609:FUC:C1   | 2.66                     | 0.43              |
| 1:F:10:ILE:HG21  | 2:G:184:ALA:HB2  | 2.00                     | 0.43              |
| 2:E:311:PRO:O    | 2:E:507:ARG:NH2  | 2.50                     | 0.43              |
| 2:B:153:CYS:SG   | 2:E:153:CYS:CB   | 3.06                     | 0.43              |
| 2:I:332:PHE:HD1  | 2:I:499:ILE:HG12 | 1.83                     | 0.43              |
| 2:B:252:LEU:HD11 | 2:B:537:ILE:HA   | 2.01                     | 0.43              |
| 2:I:211:LEU:HD11 | 2:I:250:HIS:HB3  | 2.00                     | 0.43              |
| 2:I:221:CYS:CB   | 2:I:232:CYS:HG   | 2.28                     | 0.43              |
| 2:B:177:TYR:CZ   | 2:B:281:ARG:HA   | 2.54                     | 0.43              |
| 2:E:268:ASN:HD21 | 2:E:576:ARG:HA   | 1.82                     | 0.43              |
| 2:E:411:MET:HB2  | 2:E:411:MET:HE2  | 1.77                     | 0.43              |
| 2:I:243:MET:CE   | 6:I:610:HEC:HBB1 | 2.47                     | 0.43              |
| 2:B:292:THR:HA   | 2:B:296:TYR:HB3  | 2.01                     | 0.43              |
| 2:G:534:PRO:HG3  | 2:G:551:ILE:HD12 | 2.01                     | 0.42              |
| 2:E:406:LEU:HD22 | 2:E:417:LEU:HB2  | 2.01                     | 0.42              |
| 2:B:361:LEU:O    | 2:B:364:VAL:HG22 | 2.20                     | 0.42              |
| 2:G:126:PHE:HB3  | 2:G:146:PHE:HD1  | 1.84                     | 0.42              |
| 2:G:417:LEU:HD13 | 6:G:605:HEC:HMA2 | 2.00                     | 0.42              |
| 2:E:126:PHE:HB3  | 2:E:146:PHE:HD1  | 1.84                     | 0.42              |
| 1:F:83:SER:O     | 1:F:86:PHE:HB3   | 2.19                     | 0.42              |
| 2:G:333:ARG:HH11 | 2:G:421:ASN:ND2  | 2.15                     | 0.42              |
| 2:E:171:VAL:HB   | 2:E:289:GLN:HG2  | 2.01                     | 0.42              |
| 2:G:153:CYS:CB   | 2:I:153:CYS:HG   | 2.30                     | 0.42              |
| 2:G:377:ILE:HD12 | 2:G:381:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:100:THR:HG21 | 2:B:428:HIS:CE1  | 2.54                     | 0.42              |
| 2:G:243:MET:SD   | 6:G:605:HEC:CAB  | 3.05                     | 0.42              |
| 2:G:478:MET:HE3  | 2:G:478:MET:HA   | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:115:CYS:HB2  | 2:I:147:PHE:CZ   | 2.55                     | 0.42              |
| 6:I:610:HEC:CMB  | 6:I:610:HEC:HBB3 | 2.50                     | 0.42              |
| 2:B:214:ASP:OD2  | 2:B:216:LEU:HG   | 2.19                     | 0.42              |
| 2:E:189:ASN:HD21 | 4:E:605:NAG:H2   | 1.85                     | 0.42              |
| 2:G:292:THR:HA   | 2:G:296:TYR:HB3  | 2.01                     | 0.42              |
| 2:I:330:ASN:HA   | 2:I:333:ARG:HD2  | 2.00                     | 0.42              |
| 2:I:346:LEU:HB3  | 2:I:350:TYR:HA   | 2.02                     | 0.42              |
| 2:E:126:PHE:HB3  | 2:E:146:PHE:CD1  | 2.55                     | 0.42              |
| 2:B:345:ARG:HA   | 2:B:379:PRO:O    | 2.20                     | 0.42              |
| 2:E:491:VAL:HB   | 2:E:495:LEU:HB2  | 2.01                     | 0.41              |
| 1:A:100:THR:HG22 | 2:B:149:SER:HB3  | 2.02                     | 0.41              |
| 1:D:90:GLY:C     | 6:E:610:HEC:HBC3 | 2.46                     | 0.41              |
| 2:G:317:ASN:ND2  | 4:G:603:NAG:O5   | 2.53                     | 0.41              |
| 2:G:264:LEU:HD21 | 2:G:572:LEU:HD22 | 2.03                     | 0.41              |
| 2:G:283:ILE:HG23 | 2:G:528:LEU:HD21 | 2.02                     | 0.41              |
| 1:H:68:ILE:CD1   | 2:I:463:LYS:HB3  | 2.50                     | 0.41              |
| 2:I:478:MET:HE3  | 2:I:478:MET:HA   | 2.02                     | 0.41              |
| 1:A:47:TRP:O     | 2:B:121:GLN:OE1  | 2.39                     | 0.41              |
| 1:D:90:GLY:HA3   | 6:E:610:HEC:HBC3 | 2.02                     | 0.41              |
| 2:G:344:PHE:CD1  | 2:G:387:THR:HG21 | 2.55                     | 0.41              |
| 1:D:16:ASN:O     | 1:D:20:PRO:HA    | 2.20                     | 0.41              |
| 1:A:35:ALA:HB3   | 2:B:160:ILE:HG21 | 2.02                     | 0.41              |
| 2:B:157:ASN:HD22 | 2:B:157:ASN:H    | 1.69                     | 0.41              |
| 1:D:11:THR:O     | 1:D:24:ALA:HA    | 2.21                     | 0.41              |
| 1:F:29:PHE:CZ    | 2:G:329:THR:HG21 | 2.56                     | 0.41              |
| 1:H:83:SER:O     | 2:I:389:ALA:HB2  | 2.21                     | 0.41              |
| 2:I:504:ARG:HD3  | 5:I:609:FUC:H62  | 2.03                     | 0.41              |
| 2:E:477:TRP:O    | 2:E:481:VAL:HG22 | 2.20                     | 0.41              |
| 1:F:16:ASN:O     | 1:F:20:PRO:HA    | 2.21                     | 0.41              |
| 2:E:130:ILE:HD12 | 2:E:137:ILE:HD13 | 2.04                     | 0.40              |
| 2:G:333:ARG:NH2  | 6:G:605:HEC:HAD1 | 2.37                     | 0.40              |
| 2:I:137:ILE:HG12 | 2:I:413:ILE:HD11 | 2.03                     | 0.40              |
| 2:B:115:CYS:HB2  | 2:B:147:PHE:CZ   | 2.56                     | 0.40              |
| 6:E:610:HEC:CMB  | 6:E:610:HEC:HBB3 | 2.51                     | 0.40              |
| 2:G:432:GLY:HA3  | 2:G:472:ASN:O    | 2.21                     | 0.40              |
| 2:G:433:TYR:CZ   | 2:G:437:ARG:HD3  | 2.56                     | 0.40              |
| 7:B:608:BMA:O6   | 8:B:610:MAN:O5   | 2.39                     | 0.40              |
| 2:E:243:MET:HE2  | 2:E:245:GLU:CD   | 2.47                     | 0.40              |
| 2:I:336:HIS:HA   | 2:I:339:ILE:HD12 | 2.03                     | 0.40              |
| 2:B:153:CYS:SG   | 2:E:153:CYS:HB2  | 2.62                     | 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     | 101/105 (96%)   | 97 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 1   | D     | 101/105 (96%)   | 96 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 1   | F     | 101/105 (96%)   | 97 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 1   | H     | 101/105 (96%)   | 100 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 2   | B     | 463/467 (99%)   | 442 (96%)  | 20 (4%)  | 1 (0%)   | 43          | 56  |
| 2   | E     | 463/467 (99%)   | 442 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 2   | G     | 463/467 (99%)   | 437 (94%)  | 26 (6%)  | 0        | 100         | 100 |
| 2   | I     | 463/467 (99%)   | 442 (96%)  | 20 (4%)  | 1 (0%)   | 43          | 56  |
| All | All   | 2256/2288 (99%) | 2153 (95%) | 101 (4%) | 2 (0%)   | 48          | 61  |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 348 | ASN  |
| 2   | B     | 158 | ILE  |

### 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     | 87/90 (97%) | 86 (99%)  | 1 (1%)   | 65          | 79 |
| 1   | D     | 87/90 (97%) | 86 (99%)  | 1 (1%)   | 65          | 79 |
| 1   | F     | 87/90 (97%) | 86 (99%)  | 1 (1%)   | 65          | 79 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | H     | 85/90 (94%)     | 83 (98%)   | 2 (2%)   | 43          | 61 |
| 2   | B     | 385/412 (93%)   | 372 (97%)  | 13 (3%)  | 32          | 48 |
| 2   | E     | 380/412 (92%)   | 363 (96%)  | 17 (4%)  | 24          | 38 |
| 2   | G     | 390/412 (95%)   | 373 (96%)  | 17 (4%)  | 25          | 38 |
| 2   | I     | 390/412 (95%)   | 378 (97%)  | 12 (3%)  | 35          | 53 |
| All | All   | 1891/2008 (94%) | 1827 (97%) | 64 (3%)  | 32          | 48 |

All (64) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | THR  |
| 2   | B     | 156 | SER  |
| 2   | B     | 157 | ASN  |
| 2   | B     | 159 | THR  |
| 2   | B     | 175 | MET  |
| 2   | B     | 227 | SER  |
| 2   | B     | 330 | ASN  |
| 2   | B     | 359 | VAL  |
| 2   | B     | 361 | LEU  |
| 2   | B     | 455 | LEU  |
| 2   | B     | 458 | LEU  |
| 2   | B     | 488 | LYS  |
| 2   | B     | 507 | ARG  |
| 2   | B     | 531 | ILE  |
| 1   | D     | 73  | THR  |
| 2   | E     | 115 | CYS  |
| 2   | E     | 122 | GLN  |
| 2   | E     | 156 | SER  |
| 2   | E     | 175 | MET  |
| 2   | E     | 210 | LEU  |
| 2   | E     | 227 | SER  |
| 2   | E     | 295 | ASP  |
| 2   | E     | 345 | ARG  |
| 2   | E     | 356 | ASN  |
| 2   | E     | 361 | LEU  |
| 2   | E     | 411 | MET  |
| 2   | E     | 447 | THR  |
| 2   | E     | 450 | GLN  |
| 2   | E     | 486 | LYS  |
| 2   | E     | 507 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 556 | SER  |
| 2   | E     | 560 | ASP  |
| 1   | F     | 19  | SER  |
| 2   | G     | 116 | GLU  |
| 2   | G     | 156 | SER  |
| 2   | G     | 196 | LEU  |
| 2   | G     | 218 | ASP  |
| 2   | G     | 254 | LEU  |
| 2   | G     | 295 | ASP  |
| 2   | G     | 345 | ARG  |
| 2   | G     | 353 | MET  |
| 2   | G     | 359 | VAL  |
| 2   | G     | 361 | LEU  |
| 2   | G     | 411 | MET  |
| 2   | G     | 455 | LEU  |
| 2   | G     | 486 | LYS  |
| 2   | G     | 504 | ARG  |
| 2   | G     | 507 | ARG  |
| 2   | G     | 565 | SER  |
| 2   | G     | 566 | THR  |
| 1   | H     | 73  | THR  |
| 1   | H     | 100 | THR  |
| 2   | I     | 158 | ILE  |
| 2   | I     | 175 | MET  |
| 2   | I     | 254 | LEU  |
| 2   | I     | 267 | LEU  |
| 2   | I     | 276 | LEU  |
| 2   | I     | 301 | LEU  |
| 2   | I     | 318 | ASP  |
| 2   | I     | 353 | MET  |
| 2   | I     | 361 | LEU  |
| 2   | I     | 466 | GLU  |
| 2   | I     | 486 | LYS  |
| 2   | I     | 531 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 114 | ASN  |
| 2   | B     | 121 | GLN  |
| 2   | B     | 157 | ASN  |
| 2   | B     | 189 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 225 | ASN  |
| 2   | B     | 396 | GLN  |
| 2   | B     | 409 | GLN  |
| 2   | B     | 467 | GLN  |
| 2   | B     | 516 | ASN  |
| 2   | B     | 563 | ASN  |
| 1   | D     | 54  | ASN  |
| 2   | E     | 200 | ASN  |
| 2   | E     | 257 | HIS  |
| 2   | E     | 317 | ASN  |
| 2   | E     | 351 | GLN  |
| 2   | E     | 396 | GLN  |
| 2   | E     | 421 | ASN  |
| 2   | E     | 516 | ASN  |
| 2   | E     | 540 | ASN  |
| 2   | E     | 549 | ASN  |
| 2   | E     | 571 | ASN  |
| 1   | F     | 75  | GLN  |
| 2   | G     | 189 | ASN  |
| 2   | G     | 225 | ASN  |
| 2   | G     | 392 | ASN  |
| 2   | G     | 409 | GLN  |
| 2   | G     | 467 | GLN  |
| 2   | G     | 516 | ASN  |
| 2   | G     | 540 | ASN  |
| 2   | G     | 549 | ASN  |
| 2   | I     | 392 | ASN  |
| 2   | I     | 396 | GLN  |
| 2   | I     | 409 | GLN  |
| 2   | I     | 540 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 12 are monoatomic - leaving 43 for Mogul analysis.

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 |
| 6   | HEC  | G     | 605 | 2    | 46,50,50     | 1.96 | 13 (28%) | 58,82,82    | 1.32 | 9 (15%)  |
| 4   | NAG  | G     | 606 | -    | 14,14,15     | 1.24 | 3 (21%)  | 17,19,21    | 2.13 | 6 (35%)  |
| 8   | MAN  | G     | 609 | -    | 11,11,12     | 1.55 | 2 (18%)  | 15,15,17    | 2.34 | 6 (40%)  |
| 4   | NAG  | I     | 608 | -    | 14,14,15     | 1.59 | 3 (21%)  | 17,19,21    | 3.28 | 6 (35%)  |
| 4   | NAG  | B     | 603 | -    | 14,14,15     | 1.28 | 1 (7%)   | 17,19,21    | 2.53 | 5 (29%)  |
| 4   | NAG  | B     | 601 | -    | 14,14,15     | 1.87 | 5 (35%)  | 17,19,21    | 2.31 | 5 (29%)  |
| 4   | NAG  | I     | 606 | -    | 14,14,15     | 1.35 | 2 (14%)  | 17,19,21    | 2.63 | 9 (52%)  |
| 5   | FUC  | B     | 605 | -    | 10,10,11     | 1.48 | 2 (20%)  | 14,14,16    | 2.25 | 6 (42%)  |
| 6   | HEC  | I     | 610 | 2    | 46,50,50     | 1.68 | 9 (19%)  | 58,82,82    | 1.80 | 12 (20%) |
| 7   | BMA  | I     | 602 | -    | 11,11,12     | 0.97 | 0        | 15,15,17    | 2.93 | 4 (26%)  |
| 8   | MAN  | I     | 603 | -    | 11,11,12     | 1.21 | 1 (9%)   | 15,15,17    | 2.07 | 5 (33%)  |
| 4   | NAG  | B     | 607 | -    | 14,14,15     | 1.19 | 1 (7%)   | 17,19,21    | 2.27 | 9 (52%)  |
| 4   | NAG  | E     | 607 | -    | 14,14,15     | 1.45 | 3 (21%)  | 17,19,21    | 1.96 | 6 (35%)  |
| 4   | NAG  | B     | 604 | -    | 14,14,15     | 1.03 | 1 (7%)   | 17,19,21    | 3.59 | 9 (52%)  |
| 4   | NAG  | G     | 602 | -    | 14,14,15     | 1.37 | 3 (21%)  | 17,19,21    | 2.06 | 4 (23%)  |
| 4   | NAG  | E     | 605 | -    | 14,14,15     | 1.65 | 3 (21%)  | 17,19,21    | 2.40 | 6 (35%)  |
| 5   | FUC  | E     | 609 | -    | 10,10,11     | 1.11 | 0        | 14,14,16    | 1.89 | 5 (35%)  |
| 7   | BMA  | B     | 608 | -    | 11,11,12     | 1.13 | 0        | 15,15,17    | 2.50 | 4 (26%)  |
| 7   | BMA  | E     | 602 | -    | 11,11,12     | 1.57 | 3 (27%)  | 15,15,17    | 2.90 | 10 (66%) |
| 4   | NAG  | G     | 603 | -    | 14,14,15     | 1.42 | 2 (14%)  | 17,19,21    | 3.07 | 9 (52%)  |
| 8   | MAN  | E     | 603 | -    | 11,11,12     | 1.14 | 0        | 15,15,17    | 1.92 | 5 (33%)  |
| 4   | NAG  | E     | 608 | -    | 14,14,15     | 0.97 | 0        | 17,19,21    | 3.80 | 5 (29%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | I     | 601 | -    | 14,14,15     | 1.19 | 1 (7%)   | 17,19,21    | 1.96 | 5 (29%)  |
| 8   | MAN  | E     | 604 | -    | 11,11,12     | 1.29 | 1 (9%)   | 15,15,17    | 2.09 | 3 (20%)  |
| 6   | HEC  | B     | 606 | 2    | 46,50,50     | 1.98 | 16 (34%) | 58,82,82    | 1.64 | 12 (20%) |
| 4   | NAG  | B     | 602 | -    | 14,14,15     | 1.34 | 2 (14%)  | 17,19,21    | 3.29 | 8 (47%)  |
| 4   | NAG  | I     | 607 | -    | 14,14,15     | 1.59 | 3 (21%)  | 17,19,21    | 1.98 | 7 (41%)  |
| 8   | MAN  | B     | 610 | -    | 11,11,12     | 1.63 | 3 (27%)  | 15,15,17    | 2.49 | 5 (33%)  |
| 4   | NAG  | I     | 605 | -    | 14,14,15     | 1.40 | 3 (21%)  | 17,19,21    | 1.79 | 5 (29%)  |
| 6   | HEC  | E     | 610 | 2    | 46,50,50     | 1.71 | 14 (30%) | 58,82,82    | 1.56 | 11 (18%) |
| 8   | MAN  | G     | 608 | -    | 11,11,12     | 1.10 | 0        | 15,15,17    | 2.01 | 5 (33%)  |
| 5   | FUC  | G     | 604 | -    | 10,10,11     | 1.19 | 1 (10%)  | 14,14,16    | 2.12 | 6 (42%)  |
| 4   | NAG  | G     | 601 | -    | 14,14,15     | 1.48 | 1 (7%)   | 17,19,21    | 2.37 | 8 (47%)  |
| 7   | BMA  | G     | 607 | -    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 2.07 | 3 (20%)  |
| 9   | 7GD  | G     | 610 | -    | 19,19,19     | 4.92 | 13 (68%) | 18,26,26    | 1.48 | 3 (16%)  |
| 9   | 7GD  | E     | 611 | -    | 19,19,19     | 5.29 | 13 (68%) | 18,26,26    | 1.71 | 3 (16%)  |
| 9   | 7GD  | H     | 201 | -    | 19,19,19     | 5.11 | 13 (68%) | 18,26,26    | 1.73 | 2 (11%)  |
| 8   | MAN  | B     | 609 | -    | 11,11,12     | 1.36 | 2 (18%)  | 15,15,17    | 1.89 | 2 (13%)  |
| 5   | FUC  | I     | 609 | -    | 10,10,11     | 1.32 | 0        | 14,14,16    | 2.38 | 6 (42%)  |
| 4   | NAG  | E     | 601 | -    | 14,14,15     | 1.25 | 1 (7%)   | 17,19,21    | 2.67 | 7 (41%)  |
| 8   | MAN  | I     | 604 | -    | 11,11,12     | 1.89 | 3 (27%)  | 15,15,17    | 3.01 | 4 (26%)  |
| 9   | 7GD  | B     | 611 | -    | 19,19,19     | 5.22 | 14 (73%) | 18,26,26    | 1.50 | 2 (11%)  |
| 4   | NAG  | E     | 606 | -    | 14,14,15     | 1.09 | 1 (7%)   | 17,19,21    | 2.71 | 9 (52%)  |

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   |
|-----|------|-------|-----|------|---------|------------|---------|
| 6   | HEC  | G     | 605 | 2    | -       | 8/14/54/54 | -       |
| 4   | NAG  | G     | 606 | -    | -       | 0/6/23/26  | 0/1/1/1 |
| 8   | MAN  | G     | 609 | -    | -       | 2/2/19/22  | 0/1/1/1 |
| 4   | NAG  | I     | 608 | -    | -       | 2/6/23/26  | 0/1/1/1 |
| 4   | NAG  | B     | 603 | -    | -       | 1/6/23/26  | 0/1/1/1 |
| 4   | NAG  | B     | 601 | -    | -       | 0/6/23/26  | 0/1/1/1 |
| 4   | NAG  | I     | 606 | -    | -       | 1/6/23/26  | 0/1/1/1 |
| 7   | BMA  | I     | 602 | -    | -       | 1/2/19/22  | 0/1/1/1 |
| 6   | HEC  | I     | 610 | 2    | -       | 8/14/54/54 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | FUC  | B     | 605 | -    | -       | -          | 0/1/1/1 |
| 8   | MAN  | I     | 603 | -    | -       | 2/2/19/22  | 0/1/1/1 |
| 4   | NAG  | B     | 607 | -    | -       | 2/6/23/26  | 0/1/1/1 |
| 4   | NAG  | E     | 607 | -    | -       | 2/6/23/26  | 0/1/1/1 |
| 4   | NAG  | B     | 604 | -    | -       | 2/6/23/26  | 0/1/1/1 |
| 4   | NAG  | G     | 602 | -    | -       | 0/6/23/26  | 0/1/1/1 |
| 4   | NAG  | E     | 605 | -    | -       | 1/6/23/26  | 0/1/1/1 |
| 5   | FUC  | E     | 609 | -    | -       | -          | 0/1/1/1 |
| 7   | BMA  | B     | 608 | -    | -       | 0/2/19/22  | 0/1/1/1 |
| 7   | BMA  | E     | 602 | -    | -       | 2/2/19/22  | 0/1/1/1 |
| 4   | NAG  | G     | 603 | -    | -       | 2/6/23/26  | 0/1/1/1 |
| 8   | MAN  | E     | 603 | -    | -       | 0/2/19/22  | 0/1/1/1 |
| 4   | NAG  | E     | 608 | -    | -       | 0/6/23/26  | 0/1/1/1 |
| 4   | NAG  | I     | 601 | -    | -       | 2/6/23/26  | 0/1/1/1 |
| 8   | MAN  | E     | 604 | -    | -       | 1/2/19/22  | 1/1/1/1 |
| 6   | HEC  | B     | 606 | 2    | -       | 6/14/54/54 | -       |
| 4   | NAG  | B     | 602 | -    | -       | 1/6/23/26  | 0/1/1/1 |
| 4   | NAG  | I     | 607 | -    | -       | 2/6/23/26  | 0/1/1/1 |
| 8   | MAN  | B     | 610 | -    | -       | 0/2/19/22  | 0/1/1/1 |
| 4   | NAG  | I     | 605 | -    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | HEC  | E     | 610 | 2    | -       | 6/14/54/54 | -       |
| 8   | MAN  | G     | 608 | -    | -       | 1/2/19/22  | 0/1/1/1 |
| 5   | FUC  | G     | 604 | -    | -       | -          | 0/1/1/1 |
| 4   | NAG  | G     | 601 | -    | -       | 1/6/23/26  | 0/1/1/1 |
| 7   | BMA  | G     | 607 | -    | -       | 2/2/19/22  | 0/1/1/1 |
| 9   | 7GD  | G     | 610 | -    | -       | 0/4/4/4    | 0/3/3/3 |
| 9   | 7GD  | E     | 611 | -    | -       | 0/4/4/4    | 0/3/3/3 |
| 9   | 7GD  | H     | 201 | -    | -       | 0/4/4/4    | 0/3/3/3 |
| 8   | MAN  | B     | 609 | -    | -       | 2/2/19/22  | 0/1/1/1 |
| 5   | FUC  | I     | 609 | -    | -       | -          | 0/1/1/1 |
| 4   | NAG  | E     | 601 | -    | -       | 0/6/23/26  | 0/1/1/1 |
| 8   | MAN  | I     | 604 | -    | -       | 1/2/19/22  | 0/1/1/1 |
| 9   | 7GD  | B     | 611 | -    | -       | 0/4/4/4    | 0/3/3/3 |
| 4   | NAG  | E     | 606 | -    | -       | 1/6/23/26  | 0/1/1/1 |

All (163) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | E     | 611 | 7GD  | C10-N14 | 12.98 | 1.52        | 1.34     |
| 9   | B     | 611 | 7GD  | C10-N14 | 12.81 | 1.52        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | H     | 201 | 7GD  | C10-N14 | 12.70 | 1.51        | 1.34     |
| 9   | G     | 610 | 7GD  | C10-N14 | 11.83 | 1.50        | 1.34     |
| 9   | B     | 611 | 7GD  | C09-C08 | 8.27  | 1.53        | 1.40     |
| 9   | E     | 611 | 7GD  | C09-C08 | 8.04  | 1.53        | 1.40     |
| 9   | H     | 201 | 7GD  | C09-C08 | 7.37  | 1.52        | 1.40     |
| 9   | E     | 611 | 7GD  | C02-C04 | 6.88  | 1.50        | 1.38     |
| 9   | G     | 610 | 7GD  | C02-C04 | 6.80  | 1.50        | 1.38     |
| 9   | G     | 610 | 7GD  | C09-C08 | 6.51  | 1.50        | 1.40     |
| 9   | E     | 611 | 7GD  | C03-C05 | 6.50  | 1.50        | 1.38     |
| 9   | E     | 611 | 7GD  | C05-C07 | 6.41  | 1.51        | 1.38     |
| 9   | G     | 610 | 7GD  | C03-C05 | 6.38  | 1.49        | 1.38     |
| 9   | B     | 611 | 7GD  | C02-C04 | 6.38  | 1.49        | 1.38     |
| 9   | H     | 201 | 7GD  | C02-C04 | 6.27  | 1.49        | 1.38     |
| 9   | H     | 201 | 7GD  | C03-C05 | 6.22  | 1.49        | 1.38     |
| 9   | B     | 611 | 7GD  | C03-C05 | 6.14  | 1.49        | 1.38     |
| 9   | B     | 611 | 7GD  | C05-C07 | 5.97  | 1.50        | 1.38     |
| 9   | G     | 610 | 7GD  | C04-C07 | 5.82  | 1.50        | 1.38     |
| 9   | E     | 611 | 7GD  | C02-C01 | 5.73  | 1.50        | 1.38     |
| 9   | B     | 611 | 7GD  | C04-C07 | 5.69  | 1.50        | 1.38     |
| 9   | H     | 201 | 7GD  | C05-C07 | 5.65  | 1.50        | 1.38     |
| 9   | E     | 611 | 7GD  | C04-C07 | 5.65  | 1.50        | 1.38     |
| 9   | G     | 610 | 7GD  | C05-C07 | 5.60  | 1.50        | 1.38     |
| 9   | E     | 611 | 7GD  | C03-C01 | 5.45  | 1.50        | 1.38     |
| 9   | H     | 201 | 7GD  | C04-C07 | 5.42  | 1.49        | 1.38     |
| 9   | H     | 201 | 7GD  | C02-C01 | 5.41  | 1.50        | 1.38     |
| 9   | B     | 611 | 7GD  | C03-C01 | 5.36  | 1.50        | 1.38     |
| 9   | H     | 201 | 7GD  | C03-C01 | 5.34  | 1.50        | 1.38     |
| 9   | G     | 610 | 7GD  | C02-C01 | 5.32  | 1.49        | 1.38     |
| 9   | B     | 611 | 7GD  | C02-C01 | 5.29  | 1.49        | 1.38     |
| 9   | G     | 610 | 7GD  | C03-C01 | 5.28  | 1.49        | 1.38     |
| 6   | G     | 605 | HEC  | CBC-CAC | -4.90 | 1.31        | 1.49     |
| 6   | B     | 606 | HEC  | CBB-CAB | -4.83 | 1.31        | 1.49     |
| 6   | B     | 606 | HEC  | CBC-CAC | -4.79 | 1.31        | 1.49     |
| 6   | G     | 605 | HEC  | CAB-C3B | 4.76  | 1.50        | 1.35     |
| 9   | H     | 201 | 7GD  | C06-C11 | 4.68  | 1.47        | 1.40     |
| 9   | B     | 611 | 7GD  | C06-C11 | 4.42  | 1.47        | 1.40     |
| 6   | I     | 610 | HEC  | CAC-C3C | 4.39  | 1.49        | 1.35     |
| 9   | E     | 611 | 7GD  | C11-N14 | 4.25  | 1.45        | 1.35     |
| 6   | I     | 610 | HEC  | CBC-CAC | -4.25 | 1.33        | 1.49     |
| 9   | G     | 610 | 7GD  | C06-C11 | 4.25  | 1.46        | 1.40     |
| 6   | B     | 606 | HEC  | CAC-C3C | 4.07  | 1.48        | 1.35     |
| 6   | I     | 610 | HEC  | CAB-C3B | 4.05  | 1.48        | 1.35     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | I     | 610 | HEC  | CBB-CAB | -4.04 | 1.34        | 1.49     |
| 9   | H     | 201 | 7GD  | C06-C08 | 4.04  | 1.45        | 1.39     |
| 9   | E     | 611 | 7GD  | C06-C11 | 4.03  | 1.46        | 1.40     |
| 4   | B     | 601 | NAG  | C4-C5   | 4.02  | 1.61        | 1.53     |
| 9   | H     | 201 | 7GD  | C11-N14 | 4.00  | 1.44        | 1.35     |
| 6   | E     | 610 | HEC  | CBC-CAC | -4.00 | 1.34        | 1.49     |
| 6   | E     | 610 | HEC  | CBB-CAB | -3.98 | 1.34        | 1.49     |
| 9   | G     | 610 | 7GD  | C06-C08 | 3.96  | 1.45        | 1.39     |
| 9   | B     | 611 | 7GD  | C11-N14 | 3.93  | 1.44        | 1.35     |
| 6   | G     | 605 | HEC  | C1B-NB  | -3.89 | 1.32        | 1.39     |
| 6   | G     | 605 | HEC  | CBB-CAB | -3.83 | 1.35        | 1.49     |
| 9   | B     | 611 | 7GD  | C06-C08 | 3.76  | 1.45        | 1.39     |
| 6   | G     | 605 | HEC  | CAC-C3C | 3.72  | 1.47        | 1.35     |
| 8   | I     | 604 | MAN  | O2-C2   | 3.65  | 1.51        | 1.43     |
| 6   | E     | 610 | HEC  | CAC-C3C | 3.63  | 1.46        | 1.35     |
| 6   | E     | 610 | HEC  | C1D-C2D | 3.60  | 1.51        | 1.43     |
| 9   | G     | 610 | 7GD  | C11-N14 | 3.60  | 1.43        | 1.35     |
| 6   | B     | 606 | HEC  | CAB-C3B | 3.52  | 1.46        | 1.35     |
| 6   | B     | 606 | HEC  | C3D-C2D | -3.49 | 1.29        | 1.38     |
| 9   | B     | 611 | 7GD  | N16-N15 | 3.48  | 1.39        | 1.31     |
| 6   | G     | 605 | HEC  | C1D-ND  | -3.46 | 1.33        | 1.39     |
| 9   | E     | 611 | 7GD  | C06-C08 | 3.43  | 1.44        | 1.39     |
| 6   | G     | 605 | HEC  | C3D-C2D | -3.36 | 1.30        | 1.38     |
| 9   | G     | 610 | 7GD  | C11-N17 | 3.29  | 1.44        | 1.35     |
| 9   | H     | 201 | 7GD  | N16-N15 | 3.27  | 1.39        | 1.31     |
| 4   | I     | 606 | NAG  | C4-C5   | 3.22  | 1.59        | 1.53     |
| 4   | G     | 601 | NAG  | C4-C5   | 3.20  | 1.59        | 1.53     |
| 6   | E     | 610 | HEC  | CAB-C3B | 3.15  | 1.45        | 1.35     |
| 9   | E     | 611 | 7GD  | N16-N15 | 3.15  | 1.39        | 1.31     |
| 4   | B     | 601 | NAG  | O4-C4   | 3.13  | 1.50        | 1.43     |
| 4   | I     | 608 | NAG  | C4-C5   | 3.09  | 1.59        | 1.53     |
| 6   | B     | 606 | HEC  | C4A-C3A | -3.08 | 1.39        | 1.45     |
| 9   | H     | 201 | 7GD  | C11-N17 | 3.07  | 1.43        | 1.35     |
| 9   | B     | 611 | 7GD  | C11-N17 | 3.07  | 1.43        | 1.35     |
| 9   | E     | 611 | 7GD  | C11-N17 | 3.00  | 1.43        | 1.35     |
| 4   | B     | 607 | NAG  | O5-C1   | -2.98 | 1.38        | 1.43     |
| 9   | G     | 610 | 7GD  | N16-N15 | 2.98  | 1.38        | 1.31     |
| 6   | B     | 606 | HEC  | C4B-NB  | -2.93 | 1.34        | 1.39     |
| 4   | E     | 601 | NAG  | C4-C3   | 2.93  | 1.60        | 1.52     |
| 6   | B     | 606 | HEC  | C1D-C2D | 2.91  | 1.50        | 1.43     |
| 8   | B     | 610 | MAN  | C2-C3   | 2.82  | 1.56        | 1.52     |
| 6   | I     | 610 | HEC  | C4B-NB  | -2.80 | 1.34        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | I     | 607 | NAG  | C1-C2   | 2.78  | 1.56        | 1.52     |
| 6   | E     | 610 | HEC  | C4B-NB  | -2.78 | 1.34        | 1.39     |
| 4   | I     | 606 | NAG  | C4-C3   | 2.77  | 1.59        | 1.52     |
| 4   | B     | 604 | NAG  | C4-C3   | 2.75  | 1.59        | 1.52     |
| 6   | E     | 610 | HEC  | C1A-C2A | -2.75 | 1.40        | 1.45     |
| 4   | I     | 608 | NAG  | O7-C7   | 2.75  | 1.29        | 1.23     |
| 8   | B     | 610 | MAN  | O2-C2   | 2.70  | 1.49        | 1.43     |
| 6   | B     | 606 | HEC  | C4D-ND  | -2.68 | 1.34        | 1.39     |
| 7   | E     | 602 | BMA  | O5-C5   | 2.67  | 1.48        | 1.43     |
| 4   | I     | 607 | NAG  | C4-C3   | 2.67  | 1.59        | 1.52     |
| 8   | B     | 609 | MAN  | O5-C1   | 2.66  | 1.48        | 1.43     |
| 6   | B     | 606 | HEC  | CHD-C1D | 2.63  | 1.45        | 1.39     |
| 4   | B     | 601 | NAG  | C4-C3   | 2.63  | 1.59        | 1.52     |
| 5   | B     | 605 | FUC  | O5-C5   | 2.63  | 1.48        | 1.43     |
| 4   | E     | 605 | NAG  | C4-C5   | 2.62  | 1.58        | 1.53     |
| 4   | E     | 605 | NAG  | O4-C4   | 2.61  | 1.49        | 1.43     |
| 4   | E     | 605 | NAG  | C1-C2   | 2.61  | 1.55        | 1.52     |
| 4   | B     | 602 | NAG  | C4-C5   | 2.58  | 1.58        | 1.53     |
| 6   | B     | 606 | HEC  | CMD-C2D | 2.57  | 1.56        | 1.50     |
| 9   | B     | 611 | 7GD  | C09-N13 | 2.56  | 1.38        | 1.36     |
| 6   | B     | 606 | HEC  | CHD-C4C | 2.53  | 1.43        | 1.38     |
| 8   | I     | 604 | MAN  | C2-C3   | 2.53  | 1.56        | 1.52     |
| 4   | I     | 607 | NAG  | C4-C5   | 2.52  | 1.58        | 1.53     |
| 4   | E     | 606 | NAG  | C4-C5   | 2.52  | 1.58        | 1.53     |
| 7   | G     | 607 | BMA  | C4-C3   | 2.51  | 1.58        | 1.52     |
| 6   | B     | 606 | HEC  | C1D-ND  | -2.51 | 1.34        | 1.39     |
| 8   | E     | 604 | MAN  | O2-C2   | 2.48  | 1.48        | 1.43     |
| 6   | G     | 605 | HEC  | C1D-C2D | 2.47  | 1.48        | 1.43     |
| 6   | G     | 605 | HEC  | C4A-C3A | -2.43 | 1.40        | 1.45     |
| 4   | B     | 601 | NAG  | C3-C2   | 2.43  | 1.57        | 1.52     |
| 6   | G     | 605 | HEC  | C3B-C2B | -2.42 | 1.33        | 1.41     |
| 4   | I     | 608 | NAG  | O5-C5   | -2.41 | 1.38        | 1.43     |
| 4   | B     | 603 | NAG  | C4-C3   | 2.38  | 1.58        | 1.52     |
| 4   | G     | 602 | NAG  | C4-C5   | 2.37  | 1.58        | 1.53     |
| 6   | I     | 610 | HEC  | C1B-NB  | -2.37 | 1.35        | 1.39     |
| 6   | I     | 610 | HEC  | C3B-C2B | -2.37 | 1.33        | 1.41     |
| 4   | G     | 602 | NAG  | C3-C2   | 2.35  | 1.57        | 1.52     |
| 4   | G     | 606 | NAG  | C4-C5   | 2.34  | 1.58        | 1.53     |
| 7   | E     | 602 | BMA  | C4-C5   | 2.34  | 1.58        | 1.53     |
| 6   | B     | 606 | HEC  | C1A-C2A | -2.33 | 1.41        | 1.45     |
| 6   | G     | 605 | HEC  | C4D-ND  | -2.33 | 1.35        | 1.39     |
| 6   | E     | 610 | HEC  | C1D-ND  | -2.30 | 1.35        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | G     | 603 | NAG  | C2-N2   | -2.30 | 1.42        | 1.46     |
| 4   | B     | 602 | NAG  | C1-C2   | 2.28  | 1.55        | 1.52     |
| 8   | G     | 609 | MAN  | O5-C5   | 2.27  | 1.47        | 1.43     |
| 4   | I     | 605 | NAG  | C4-C5   | 2.26  | 1.57        | 1.53     |
| 4   | E     | 607 | NAG  | C4-C5   | 2.25  | 1.57        | 1.53     |
| 4   | B     | 601 | NAG  | O5-C5   | 2.24  | 1.47        | 1.43     |
| 8   | I     | 604 | MAN  | O5-C5   | 2.23  | 1.47        | 1.43     |
| 5   | G     | 604 | FUC  | C1-C2   | 2.22  | 1.57        | 1.52     |
| 6   | B     | 606 | HEC  | C3B-C2B | -2.22 | 1.33        | 1.41     |
| 6   | I     | 610 | HEC  | CHA-C1A | -2.20 | 1.34        | 1.38     |
| 6   | E     | 610 | HEC  | CHC-C1C | -2.20 | 1.34        | 1.39     |
| 6   | E     | 610 | HEC  | C1B-NB  | -2.19 | 1.35        | 1.39     |
| 4   | E     | 607 | NAG  | C3-C2   | 2.18  | 1.57        | 1.52     |
| 8   | G     | 609 | MAN  | C6-C5   | 2.16  | 1.59        | 1.51     |
| 4   | I     | 601 | NAG  | O6-C6   | 2.15  | 1.51        | 1.42     |
| 7   | E     | 602 | BMA  | O2-C2   | 2.15  | 1.47        | 1.43     |
| 6   | G     | 605 | HEC  | CHA-C1A | -2.14 | 1.34        | 1.38     |
| 6   | G     | 605 | HEC  | C3B-C4B | 2.13  | 1.49        | 1.46     |
| 6   | I     | 610 | HEC  | C3D-C2D | -2.11 | 1.33        | 1.38     |
| 4   | G     | 602 | NAG  | C4-C3   | 2.10  | 1.57        | 1.52     |
| 6   | E     | 610 | HEC  | CHA-C4D | -2.09 | 1.34        | 1.39     |
| 4   | G     | 606 | NAG  | C4-C3   | 2.08  | 1.57        | 1.52     |
| 4   | G     | 606 | NAG  | C1-C2   | 2.07  | 1.55        | 1.52     |
| 8   | B     | 610 | MAN  | C1-C2   | 2.06  | 1.57        | 1.52     |
| 4   | I     | 605 | NAG  | C3-C2   | 2.06  | 1.56        | 1.52     |
| 6   | E     | 610 | HEC  | C3B-C4B | -2.05 | 1.42        | 1.46     |
| 8   | B     | 609 | MAN  | C1-C2   | 2.05  | 1.57        | 1.52     |
| 5   | B     | 605 | FUC  | O4-C4   | 2.05  | 1.48        | 1.43     |
| 6   | B     | 606 | HEC  | C1B-NB  | -2.03 | 1.35        | 1.39     |
| 6   | E     | 610 | HEC  | C3D-C2D | -2.03 | 1.33        | 1.38     |
| 4   | G     | 603 | NAG  | O7-C7   | 2.03  | 1.27        | 1.23     |
| 4   | I     | 605 | NAG  | O5-C5   | 2.03  | 1.47        | 1.43     |
| 8   | I     | 603 | MAN  | C2-C3   | 2.02  | 1.55        | 1.52     |
| 6   | E     | 610 | HEC  | C4D-ND  | -2.01 | 1.35        | 1.39     |
| 4   | E     | 607 | NAG  | C4-C3   | 2.01  | 1.57        | 1.52     |

All (261) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 4   | E     | 608 | NAG  | C1-O5-C5 | -11.27 | 97.08       | 112.19   |
| 4   | I     | 608 | NAG  | C1-O5-C5 | -10.38 | 98.27       | 112.19   |
| 4   | B     | 602 | NAG  | C1-O5-C5 | -9.91  | 98.91       | 112.19   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 604 | NAG  | C1-O5-C5    | -9.77 | 99.09       | 112.19   |
| 8   | I     | 604 | MAN  | C1-O5-C5    | 8.79  | 123.97      | 112.19   |
| 7   | I     | 602 | BMA  | C1-C2-C3    | -7.73 | 98.39       | 109.64   |
| 8   | B     | 610 | MAN  | C1-O5-C5    | 6.77  | 121.26      | 112.19   |
| 7   | E     | 602 | BMA  | C1-O5-C5    | -6.57 | 103.38      | 112.19   |
| 4   | E     | 608 | NAG  | O4-C4-C3    | -6.43 | 95.21       | 110.38   |
| 4   | G     | 603 | NAG  | C1-O5-C5    | -6.38 | 103.63      | 112.19   |
| 7   | B     | 608 | BMA  | C1-O5-C5    | -6.35 | 103.68      | 112.19   |
| 8   | B     | 609 | MAN  | C1-O5-C5    | 6.29  | 120.62      | 112.19   |
| 4   | G     | 603 | NAG  | O4-C4-C5    | -6.21 | 94.03       | 109.32   |
| 4   | E     | 605 | NAG  | C1-C2-N2    | 6.09  | 120.03      | 110.43   |
| 4   | E     | 608 | NAG  | O4-C4-C5    | -5.99 | 94.58       | 109.32   |
| 9   | H     | 201 | 7GD  | C09-C10-N14 | -5.89 | 119.04      | 124.22   |
| 7   | B     | 608 | BMA  | C1-C2-C3    | -5.79 | 101.21      | 109.64   |
| 4   | G     | 606 | NAG  | C1-O5-C5    | -5.78 | 104.44      | 112.19   |
| 4   | B     | 603 | NAG  | C1-O5-C5    | 5.68  | 119.79      | 112.19   |
| 6   | B     | 606 | HEC  | CMD-C2D-C1D | 5.65  | 134.02      | 125.42   |
| 8   | I     | 603 | MAN  | C1-O5-C5    | 5.62  | 119.72      | 112.19   |
| 8   | I     | 604 | MAN  | O2-C2-C3    | 5.55  | 121.65      | 110.15   |
| 4   | B     | 604 | NAG  | O4-C4-C5    | -5.50 | 95.79       | 109.32   |
| 9   | E     | 611 | 7GD  | C09-C10-N14 | -5.47 | 119.41      | 124.22   |
| 4   | E     | 601 | NAG  | C2-N2-C7    | 5.45  | 130.21      | 122.90   |
| 4   | B     | 603 | NAG  | C1-C2-N2    | 5.43  | 118.99      | 110.43   |
| 8   | G     | 608 | MAN  | C1-O5-C5    | 5.40  | 119.42      | 112.19   |
| 4   | E     | 601 | NAG  | C1-C2-N2    | -5.35 | 102.00      | 110.43   |
| 4   | E     | 606 | NAG  | C1-O5-C5    | -5.32 | 105.05      | 112.19   |
| 9   | B     | 611 | 7GD  | C09-C10-N14 | -5.18 | 119.66      | 124.22   |
| 4   | I     | 605 | NAG  | O5-C1-C2    | -5.16 | 103.31      | 111.29   |
| 4   | E     | 606 | NAG  | O5-C1-C2    | -5.15 | 103.33      | 111.29   |
| 4   | G     | 602 | NAG  | C4-C3-C2    | 5.07  | 118.45      | 111.02   |
| 8   | G     | 609 | MAN  | C1-O5-C5    | 5.03  | 118.93      | 112.19   |
| 8   | E     | 604 | MAN  | C1-O5-C5    | 4.99  | 118.88      | 112.19   |
| 4   | I     | 606 | NAG  | O5-C1-C2    | -4.97 | 103.61      | 111.29   |
| 7   | I     | 602 | BMA  | C2-C3-C4    | 4.96  | 119.58      | 110.86   |
| 4   | G     | 601 | NAG  | C1-C2-N2    | 4.88  | 118.12      | 110.43   |
| 7   | G     | 607 | BMA  | C1-O5-C5    | -4.78 | 105.78      | 112.19   |
| 4   | B     | 604 | NAG  | C1-C2-N2    | -4.73 | 102.97      | 110.43   |
| 4   | B     | 602 | NAG  | O4-C4-C3    | -4.73 | 99.23       | 110.38   |
| 6   | I     | 610 | HEC  | CBD-CAD-C3D | -4.73 | 99.47       | 112.53   |
| 9   | G     | 610 | 7GD  | C09-C10-N14 | -4.71 | 120.07      | 124.22   |
| 7   | G     | 607 | BMA  | C1-C2-C3    | -4.69 | 102.81      | 109.64   |
| 4   | I     | 601 | NAG  | C3-C4-C5    | 4.65  | 118.67      | 110.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 601 | NAG  | C1-O5-C5    | -4.62 | 105.99      | 112.19   |
| 4   | B     | 603 | NAG  | O5-C1-C2    | -4.61 | 104.16      | 111.29   |
| 5   | I     | 609 | FUC  | C1-C2-C3    | 4.56  | 116.28      | 109.64   |
| 4   | E     | 606 | NAG  | O4-C4-C3    | -4.55 | 99.65       | 110.38   |
| 7   | I     | 602 | BMA  | O5-C5-C6    | 4.54  | 116.50      | 107.66   |
| 4   | G     | 603 | NAG  | O4-C4-C3    | -4.50 | 99.77       | 110.38   |
| 7   | E     | 602 | BMA  | C1-C2-C3    | -4.49 | 103.11      | 109.64   |
| 6   | E     | 610 | HEC  | CBB-CAB-C3B | -4.41 | 118.62      | 127.43   |
| 4   | E     | 605 | NAG  | C1-O5-C5    | 4.39  | 118.07      | 112.19   |
| 8   | G     | 609 | MAN  | O2-C2-C3    | 4.38  | 119.23      | 110.15   |
| 4   | B     | 601 | NAG  | C6-C5-C4    | 4.36  | 123.73      | 113.02   |
| 6   | E     | 610 | HEC  | CMD-C2D-C1D | 4.36  | 132.06      | 125.42   |
| 4   | B     | 601 | NAG  | O4-C4-C5    | 4.33  | 120.00      | 109.32   |
| 4   | G     | 601 | NAG  | O5-C1-C2    | -4.31 | 104.62      | 111.29   |
| 6   | B     | 606 | HEC  | CBB-CAB-C3B | -4.30 | 118.83      | 127.43   |
| 6   | I     | 610 | HEC  | CMD-C2D-C1D | 4.29  | 131.96      | 125.42   |
| 4   | E     | 607 | NAG  | C1-O5-C5    | 4.23  | 117.86      | 112.19   |
| 4   | I     | 606 | NAG  | C6-C5-C4    | 4.22  | 123.38      | 113.02   |
| 4   | E     | 601 | NAG  | C8-C7-N2    | -4.18 | 109.18      | 116.12   |
| 7   | I     | 602 | BMA  | C1-O5-C5    | -4.18 | 106.59      | 112.19   |
| 4   | I     | 607 | NAG  | C2-N2-C7    | 4.15  | 128.47      | 122.90   |
| 5   | I     | 609 | FUC  | O5-C5-C4    | 4.10  | 116.93      | 109.55   |
| 8   | E     | 604 | MAN  | O2-C2-C3    | 4.08  | 118.60      | 110.15   |
| 4   | I     | 608 | NAG  | C3-C4-C5    | 4.03  | 117.54      | 110.23   |
| 4   | B     | 604 | NAG  | O5-C5-C6    | 4.02  | 115.50      | 107.66   |
| 4   | I     | 606 | NAG  | C1-O5-C5    | -4.02 | 106.80      | 112.19   |
| 4   | E     | 605 | NAG  | O4-C4-C5    | 3.99  | 119.15      | 109.32   |
| 6   | I     | 610 | HEC  | CBB-CAB-C3B | -3.98 | 119.48      | 127.43   |
| 6   | I     | 610 | HEC  | CHC-C4B-NB  | 3.95  | 128.76      | 124.45   |
| 8   | E     | 603 | MAN  | C1-O5-C5    | 3.94  | 117.47      | 112.19   |
| 5   | B     | 605 | FUC  | C1-C2-C3    | 3.94  | 115.38      | 109.64   |
| 4   | I     | 601 | NAG  | C2-N2-C7    | 3.87  | 128.08      | 122.90   |
| 4   | G     | 603 | NAG  | C8-C7-N2    | -3.86 | 109.71      | 116.12   |
| 4   | G     | 601 | NAG  | O4-C4-C5    | 3.84  | 118.77      | 109.32   |
| 4   | B     | 607 | NAG  | C8-C7-N2    | -3.82 | 109.78      | 116.12   |
| 8   | B     | 610 | MAN  | O2-C2-C1    | -3.81 | 100.50      | 109.22   |
| 6   | I     | 610 | HEC  | CBA-CAA-C2A | -3.79 | 102.07      | 112.53   |
| 6   | I     | 610 | HEC  | CMB-C2B-C1B | 3.77  | 131.15      | 125.42   |
| 4   | G     | 602 | NAG  | C1-O5-C5    | -3.76 | 107.15      | 112.19   |
| 4   | I     | 607 | NAG  | O5-C1-C2    | -3.74 | 105.50      | 111.29   |
| 4   | I     | 608 | NAG  | C8-C7-N2    | -3.72 | 109.95      | 116.12   |
| 4   | E     | 607 | NAG  | O5-C1-C2    | -3.64 | 105.66      | 111.29   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 606 | HEC  | CBD-CAD-C3D | -3.60 | 102.57      | 112.53   |
| 7   | E     | 602 | BMA  | C2-C3-C4    | 3.57  | 117.14      | 110.86   |
| 4   | B     | 601 | NAG  | O5-C1-C2    | -3.54 | 105.81      | 111.29   |
| 5   | G     | 604 | FUC  | C1-O5-C5    | 3.51  | 121.25      | 112.97   |
| 4   | B     | 602 | NAG  | C2-N2-C7    | 3.48  | 127.56      | 122.90   |
| 4   | I     | 606 | NAG  | C2-N2-C7    | 3.47  | 127.55      | 122.90   |
| 8   | I     | 604 | MAN  | O3-C3-C2    | 3.44  | 117.07      | 110.05   |
| 8   | G     | 609 | MAN  | O5-C5-C6    | 3.43  | 114.33      | 107.66   |
| 4   | B     | 604 | NAG  | C8-C7-N2    | -3.43 | 110.44      | 116.12   |
| 4   | E     | 608 | NAG  | O5-C5-C6    | 3.42  | 114.31      | 107.66   |
| 5   | B     | 605 | FUC  | O3-C3-C2    | -3.36 | 103.20      | 110.05   |
| 4   | E     | 606 | NAG  | C3-C4-C5    | 3.32  | 116.26      | 110.23   |
| 6   | E     | 610 | HEC  | CBD-CAD-C3D | -3.28 | 103.47      | 112.53   |
| 4   | G     | 606 | NAG  | O3-C3-C4    | 3.27  | 118.08      | 110.38   |
| 5   | E     | 609 | FUC  | O5-C5-C4    | 3.26  | 115.42      | 109.55   |
| 4   | E     | 601 | NAG  | O4-C4-C5    | -3.26 | 101.30      | 109.32   |
| 4   | B     | 607 | NAG  | O3-C3-C2    | 3.25  | 116.15      | 109.40   |
| 4   | G     | 603 | NAG  | C4-C3-C2    | -3.24 | 106.27      | 111.02   |
| 8   | G     | 609 | MAN  | C2-C3-C4    | 3.24  | 116.55      | 110.86   |
| 7   | E     | 602 | BMA  | O5-C5-C6    | 3.22  | 113.93      | 107.66   |
| 5   | I     | 609 | FUC  | O3-C3-C2    | -3.22 | 103.48      | 110.05   |
| 5   | G     | 604 | FUC  | C1-C2-C3    | 3.21  | 114.31      | 109.64   |
| 4   | I     | 601 | NAG  | O4-C4-C3    | -3.21 | 102.82      | 110.38   |
| 5   | G     | 604 | FUC  | O5-C5-C4    | 3.19  | 115.30      | 109.55   |
| 4   | B     | 604 | NAG  | C3-C4-C5    | 3.19  | 116.01      | 110.23   |
| 5   | B     | 605 | FUC  | O2-C2-C1    | 3.10  | 116.33      | 109.22   |
| 4   | B     | 602 | NAG  | C6-C5-C4    | 3.10  | 120.64      | 113.02   |
| 5   | I     | 609 | FUC  | C1-O5-C5    | 3.10  | 120.28      | 112.97   |
| 4   | B     | 607 | NAG  | O4-C4-C5    | -3.10 | 101.69      | 109.32   |
| 4   | B     | 607 | NAG  | C6-C5-C4    | -3.10 | 105.42      | 113.02   |
| 8   | E     | 604 | MAN  | O3-C3-C2    | 3.09  | 116.36      | 110.05   |
| 6   | B     | 606 | HEC  | CHA-C4D-C3D | -3.09 | 118.54      | 125.30   |
| 4   | E     | 608 | NAG  | C6-C5-C4    | 3.03  | 120.46      | 113.02   |
| 6   | B     | 606 | HEC  | C4A-NA-C1A  | -3.03 | 100.89      | 105.82   |
| 5   | E     | 609 | FUC  | C2-C3-C4    | 3.02  | 116.18      | 110.86   |
| 4   | G     | 601 | NAG  | C3-C4-C5    | 3.02  | 115.71      | 110.23   |
| 6   | G     | 605 | HEC  | CHA-C4D-C3D | -3.02 | 118.69      | 125.30   |
| 4   | B     | 602 | NAG  | O5-C1-C2    | -3.01 | 106.64      | 111.29   |
| 4   | B     | 604 | NAG  | O6-C6-C5    | -2.98 | 101.18      | 111.33   |
| 4   | B     | 603 | NAG  | O5-C5-C4    | 2.98  | 118.08      | 110.83   |
| 5   | B     | 605 | FUC  | O4-C4-C5    | 2.98  | 116.31      | 109.74   |
| 4   | I     | 606 | NAG  | O3-C3-C4    | 2.98  | 117.39      | 110.38   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | E     | 603 | MAN  | O2-C2-C3    | 2.97  | 116.29      | 110.15   |
| 6   | B     | 606 | HEC  | CMD-C2D-C3D | -2.94 | 119.39      | 125.62   |
| 4   | G     | 602 | NAG  | C6-C5-C4    | 2.93  | 120.22      | 113.02   |
| 6   | G     | 605 | HEC  | CMD-C2D-C1D | 2.93  | 129.88      | 125.42   |
| 4   | I     | 606 | NAG  | O4-C4-C3    | -2.93 | 103.48      | 110.38   |
| 4   | B     | 604 | NAG  | O5-C1-C2    | -2.92 | 106.77      | 111.29   |
| 6   | I     | 610 | HEC  | C2A-C1A-NA  | 2.90  | 113.13      | 110.32   |
| 6   | E     | 610 | HEC  | CHA-C4D-C3D | -2.90 | 118.95      | 125.30   |
| 4   | E     | 607 | NAG  | O5-C5-C4    | 2.89  | 117.85      | 110.83   |
| 8   | G     | 608 | MAN  | O2-C2-C1    | 2.89  | 115.83      | 109.22   |
| 5   | E     | 609 | FUC  | C1-C2-C3    | 2.88  | 113.83      | 109.64   |
| 4   | E     | 601 | NAG  | C4-C3-C2    | -2.87 | 106.81      | 111.02   |
| 8   | I     | 603 | MAN  | O5-C1-C2    | 2.87  | 117.63      | 110.79   |
| 6   | E     | 610 | HEC  | CBA-CAA-C2A | -2.87 | 104.61      | 112.53   |
| 4   | B     | 602 | NAG  | O3-C3-C2    | 2.85  | 115.32      | 109.40   |
| 4   | I     | 606 | NAG  | O4-C4-C5    | -2.85 | 102.31      | 109.32   |
| 4   | B     | 601 | NAG  | C4-C3-C2    | 2.83  | 115.16      | 111.02   |
| 4   | I     | 606 | NAG  | C4-C3-C2    | 2.83  | 115.16      | 111.02   |
| 6   | I     | 610 | HEC  | CHC-C4B-C3B | -2.83 | 120.44      | 125.21   |
| 5   | B     | 605 | FUC  | O5-C5-C4    | 2.81  | 114.61      | 109.55   |
| 4   | B     | 602 | NAG  | C1-C2-N2    | -2.80 | 106.02      | 110.43   |
| 9   | E     | 611 | 7GD  | N17-C11-N14 | 2.78  | 121.07      | 116.59   |
| 4   | E     | 607 | NAG  | C1-C2-N2    | 2.78  | 114.82      | 110.43   |
| 8   | E     | 603 | MAN  | O5-C1-C2    | 2.78  | 117.42      | 110.79   |
| 4   | I     | 608 | NAG  | O4-C4-C3    | -2.78 | 103.83      | 110.38   |
| 4   | I     | 608 | NAG  | O4-C4-C5    | -2.77 | 102.49      | 109.32   |
| 4   | G     | 606 | NAG  | C8-C7-N2    | -2.75 | 111.56      | 116.12   |
| 7   | E     | 602 | BMA  | O3-C3-C4    | 2.74  | 116.83      | 110.38   |
| 4   | E     | 606 | NAG  | C8-C7-N2    | -2.71 | 111.62      | 116.12   |
| 5   | I     | 609 | FUC  | O5-C1-C2    | 2.71  | 117.25      | 110.79   |
| 8   | E     | 603 | MAN  | C2-C3-C4    | 2.69  | 115.59      | 110.86   |
| 5   | E     | 609 | FUC  | C1-O5-C5    | 2.69  | 119.31      | 112.97   |
| 7   | E     | 602 | BMA  | C3-C4-C5    | 2.69  | 115.11      | 110.23   |
| 4   | G     | 603 | NAG  | O5-C1-C2    | -2.69 | 107.14      | 111.29   |
| 4   | G     | 601 | NAG  | C8-C7-N2    | -2.68 | 111.67      | 116.12   |
| 7   | B     | 608 | BMA  | O3-C3-C2    | -2.68 | 104.59      | 110.05   |
| 8   | I     | 604 | MAN  | O5-C1-C2    | 2.67  | 117.17      | 110.79   |
| 4   | E     | 607 | NAG  | C4-C3-C2    | 2.66  | 114.92      | 111.02   |
| 8   | B     | 610 | MAN  | O2-C2-C3    | 2.65  | 115.64      | 110.15   |
| 4   | G     | 606 | NAG  | C4-C3-C2    | -2.65 | 107.14      | 111.02   |
| 4   | G     | 603 | NAG  | O7-C7-C8    | 2.64  | 126.75      | 122.05   |
| 6   | I     | 610 | HEC  | C4A-NA-C1A  | -2.64 | 101.52      | 105.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | E     | 606 | NAG  | C2-N2-C7    | 2.64  | 126.43      | 122.90   |
| 4   | I     | 608 | NAG  | O3-C3-C2    | -2.63 | 103.95      | 109.40   |
| 6   | G     | 605 | HEC  | C4A-NA-C1A  | -2.63 | 101.54      | 105.82   |
| 6   | B     | 606 | HEC  | CHC-C4B-NB  | 2.62  | 127.31      | 124.45   |
| 4   | B     | 603 | NAG  | C3-C4-C5    | 2.57  | 114.89      | 110.23   |
| 5   | B     | 605 | FUC  | O5-C1-C2    | 2.57  | 116.92      | 110.79   |
| 6   | G     | 605 | HEC  | CBD-CAD-C3D | -2.57 | 105.43      | 112.53   |
| 4   | E     | 601 | NAG  | C1-O5-C5    | -2.54 | 108.79      | 112.19   |
| 4   | I     | 605 | NAG  | C2-N2-C7    | 2.53  | 126.29      | 122.90   |
| 7   | E     | 602 | BMA  | O4-C4-C5    | -2.50 | 103.16      | 109.32   |
| 9   | H     | 201 | 7GD  | N17-C11-N14 | 2.48  | 120.58      | 116.59   |
| 6   | B     | 606 | HEC  | CHB-C1B-C2B | -2.47 | 120.25      | 127.43   |
| 8   | I     | 603 | MAN  | O5-C5-C4    | 2.47  | 116.84      | 110.83   |
| 4   | I     | 607 | NAG  | O5-C5-C4    | 2.46  | 116.81      | 110.83   |
| 4   | I     | 607 | NAG  | C3-C4-C5    | 2.44  | 114.66      | 110.23   |
| 7   | G     | 607 | BMA  | C3-C4-C5    | 2.43  | 114.63      | 110.23   |
| 4   | E     | 601 | NAG  | O7-C7-N2    | 2.42  | 126.27      | 121.98   |
| 4   | B     | 607 | NAG  | C3-C4-C5    | 2.42  | 114.61      | 110.23   |
| 6   | I     | 610 | HEC  | CHA-C4D-ND  | 2.41  | 128.24      | 123.86   |
| 4   | G     | 606 | NAG  | C2-N2-C7    | 2.41  | 126.13      | 122.90   |
| 5   | G     | 604 | FUC  | O3-C3-C2    | -2.41 | 105.14      | 110.05   |
| 8   | G     | 608 | MAN  | O2-C2-C3    | 2.39  | 115.11      | 110.15   |
| 4   | E     | 606 | NAG  | O7-C7-N2    | 2.39  | 126.21      | 121.98   |
| 4   | I     | 607 | NAG  | C1-O5-C5    | 2.39  | 115.39      | 112.19   |
| 4   | E     | 607 | NAG  | C3-C4-C5    | 2.39  | 114.56      | 110.23   |
| 6   | I     | 610 | HEC  | CHA-C4D-C3D | -2.39 | 120.08      | 125.30   |
| 9   | G     | 610 | 7GD  | C08-C12-C07 | -2.38 | 108.96      | 114.21   |
| 4   | B     | 607 | NAG  | C1-O5-C5    | -2.37 | 109.01      | 112.19   |
| 7   | B     | 608 | BMA  | C2-C3-C4    | 2.35  | 115.00      | 110.86   |
| 4   | E     | 606 | NAG  | C6-C5-C4    | 2.35  | 118.78      | 113.02   |
| 4   | E     | 605 | NAG  | C3-C4-C5    | 2.34  | 114.47      | 110.23   |
| 5   | G     | 604 | FUC  | O5-C1-C2    | 2.34  | 116.37      | 110.79   |
| 4   | B     | 607 | NAG  | O5-C1-C2    | -2.33 | 107.69      | 111.29   |
| 6   | G     | 605 | HEC  | C3D-C4D-ND  | 2.33  | 112.73      | 110.15   |
| 4   | E     | 606 | NAG  | C4-C3-C2    | 2.32  | 114.42      | 111.02   |
| 8   | I     | 603 | MAN  | O3-C3-C4    | 2.32  | 115.83      | 110.38   |
| 5   | E     | 609 | FUC  | O4-C4-C5    | 2.31  | 114.84      | 109.74   |
| 6   | B     | 606 | HEC  | CHB-C1B-NB  | 2.31  | 128.06      | 123.86   |
| 9   | G     | 610 | 7GD  | N17-C11-N14 | 2.31  | 120.30      | 116.59   |
| 4   | I     | 605 | NAG  | O5-C5-C4    | 2.30  | 116.42      | 110.83   |
| 6   | E     | 610 | HEC  | C2A-C1A-NA  | 2.30  | 112.54      | 110.32   |
| 8   | I     | 603 | MAN  | O3-C3-C2    | 2.30  | 114.74      | 110.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 7   | E     | 602 | BMA  | O5-C5-C4    | 2.29  | 116.40      | 110.83   |
| 4   | B     | 604 | NAG  | O7-C7-C8    | 2.29  | 126.13      | 122.05   |
| 5   | G     | 604 | FUC  | O3-C3-C4    | -2.27 | 105.02      | 110.38   |
| 6   | E     | 610 | HEC  | C4A-NA-C1A  | -2.27 | 102.13      | 105.82   |
| 4   | B     | 607 | NAG  | O5-C5-C6    | 2.25  | 112.03      | 107.66   |
| 8   | G     | 609 | MAN  | O3-C3-C4    | 2.25  | 115.67      | 110.38   |
| 6   | I     | 610 | HEC  | O2D-CGD-CBD | 2.24  | 121.08      | 114.00   |
| 4   | G     | 602 | NAG  | C2-N2-C7    | 2.24  | 125.90      | 122.90   |
| 4   | G     | 601 | NAG  | C1-O5-C5    | 2.24  | 115.19      | 112.19   |
| 4   | E     | 605 | NAG  | O6-C6-C5    | 2.23  | 118.91      | 111.33   |
| 4   | I     | 601 | NAG  | O3-C3-C4    | 2.20  | 115.56      | 110.38   |
| 6   | E     | 610 | HEC  | O2A-CGA-CBA | 2.19  | 120.93      | 114.00   |
| 8   | G     | 608 | MAN  | C3-C4-C5    | 2.19  | 114.20      | 110.23   |
| 9   | B     | 611 | 7GD  | N17-C11-N14 | 2.19  | 120.11      | 116.59   |
| 6   | G     | 605 | HEC  | C3A-C4A-NA  | 2.18  | 113.67      | 109.64   |
| 6   | G     | 605 | HEC  | O2A-CGA-CBA | 2.18  | 120.89      | 114.00   |
| 8   | E     | 603 | MAN  | C1-C2-C3    | 2.18  | 112.81      | 109.64   |
| 7   | E     | 602 | BMA  | O3-C3-C2    | -2.17 | 105.62      | 110.05   |
| 6   | B     | 606 | HEC  | CHA-C4D-ND  | 2.17  | 127.79      | 123.86   |
| 4   | B     | 602 | NAG  | C8-C7-N2    | -2.16 | 112.53      | 116.12   |
| 4   | B     | 607 | NAG  | O5-C5-C4    | -2.16 | 105.57      | 110.83   |
| 8   | G     | 608 | MAN  | C1-C2-C3    | 2.15  | 112.77      | 109.64   |
| 6   | E     | 610 | HEC  | C3D-C4D-ND  | 2.15  | 112.53      | 110.15   |
| 4   | G     | 603 | NAG  | O3-C3-C2    | 2.13  | 113.83      | 109.40   |
| 8   | B     | 610 | MAN  | O5-C1-C2    | 2.13  | 115.86      | 110.79   |
| 8   | B     | 610 | MAN  | O3-C3-C2    | 2.12  | 114.38      | 110.05   |
| 5   | I     | 609 | FUC  | C6-C5-C4    | 2.12  | 116.96      | 113.08   |
| 4   | I     | 606 | NAG  | C1-C2-N2    | -2.10 | 107.13      | 110.43   |
| 4   | E     | 605 | NAG  | O5-C5-C6    | -2.09 | 103.59      | 107.66   |
| 6   | E     | 610 | HEC  | CHC-C4B-C3B | -2.09 | 121.68      | 125.21   |
| 8   | B     | 609 | MAN  | C1-C2-C3    | 2.09  | 112.68      | 109.64   |
| 6   | G     | 605 | HEC  | CHB-C1B-C2B | -2.08 | 121.39      | 127.43   |
| 4   | I     | 607 | NAG  | C8-C7-N2    | -2.07 | 112.68      | 116.12   |
| 8   | G     | 609 | MAN  | O4-C4-C3    | 2.07  | 115.24      | 110.38   |
| 4   | I     | 605 | NAG  | C3-C4-C5    | 2.06  | 113.97      | 110.23   |
| 4   | I     | 605 | NAG  | C4-C3-C2    | 2.06  | 114.03      | 111.02   |
| 4   | G     | 601 | NAG  | O5-C5-C6    | -2.05 | 103.68      | 107.66   |
| 6   | E     | 610 | HEC  | CHC-C4B-NB  | 2.04  | 126.67      | 124.45   |
| 6   | G     | 605 | HEC  | CBA-CAA-C2A | -2.03 | 106.91      | 112.53   |
| 6   | B     | 606 | HEC  | C3A-C4A-NA  | 2.03  | 113.40      | 109.64   |
| 6   | B     | 606 | HEC  | C3D-C4D-ND  | 2.03  | 112.41      | 110.15   |
| 4   | G     | 603 | NAG  | O6-C6-C5    | -2.03 | 104.44      | 111.33   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | I     | 607 | NAG  | O7-C7-N2    | 2.02  | 125.56      | 121.98   |
| 4   | G     | 601 | NAG  | O5-C5-C4    | 2.02  | 115.74      | 110.83   |
| 4   | I     | 601 | NAG  | C8-C7-N2    | -2.01 | 112.78      | 116.12   |
| 7   | E     | 602 | BMA  | O4-C4-C3    | -2.01 | 105.65      | 110.38   |
| 4   | G     | 606 | NAG  | O4-C4-C5    | -2.00 | 104.39      | 109.32   |
| 9   | E     | 611 | 7GD  | C08-C12-C07 | -2.00 | 109.80      | 114.21   |

There are no chirality outliers.

All (62) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | B     | 606 | HEC  | C2C-C3C-CAC-CBC |
| 6   | B     | 606 | HEC  | C4C-C3C-CAC-CBC |
| 6   | E     | 610 | HEC  | C2B-C3B-CAB-CBB |
| 6   | E     | 610 | HEC  | C4B-C3B-CAB-CBB |
| 6   | G     | 605 | HEC  | C2B-C3B-CAB-CBB |
| 6   | G     | 605 | HEC  | C4B-C3B-CAB-CBB |
| 6   | I     | 610 | HEC  | C2B-C3B-CAB-CBB |
| 6   | I     | 610 | HEC  | C4B-C3B-CAB-CBB |
| 6   | I     | 610 | HEC  | C2C-C3C-CAC-CBC |
| 6   | I     | 610 | HEC  | C4C-C3C-CAC-CBC |
| 7   | G     | 607 | BMA  | C4-C5-C6-O6     |
| 7   | E     | 602 | BMA  | O5-C5-C6-O6     |
| 8   | B     | 609 | MAN  | O5-C5-C6-O6     |
| 4   | G     | 603 | NAG  | O5-C5-C6-O6     |
| 4   | G     | 603 | NAG  | C4-C5-C6-O6     |
| 4   | B     | 607 | NAG  | O5-C5-C6-O6     |
| 8   | B     | 609 | MAN  | C4-C5-C6-O6     |
| 7   | G     | 607 | BMA  | O5-C5-C6-O6     |
| 7   | E     | 602 | BMA  | C4-C5-C6-O6     |
| 8   | G     | 609 | MAN  | C4-C5-C6-O6     |
| 4   | I     | 607 | NAG  | C4-C5-C6-O6     |
| 4   | I     | 601 | NAG  | O5-C5-C6-O6     |
| 4   | I     | 607 | NAG  | O5-C5-C6-O6     |
| 4   | I     | 601 | NAG  | C4-C5-C6-O6     |
| 4   | B     | 604 | NAG  | O5-C5-C6-O6     |
| 4   | B     | 607 | NAG  | C4-C5-C6-O6     |
| 4   | E     | 607 | NAG  | C4-C5-C6-O6     |
| 8   | G     | 609 | MAN  | O5-C5-C6-O6     |
| 8   | I     | 603 | MAN  | C4-C5-C6-O6     |
| 4   | G     | 601 | NAG  | O5-C5-C6-O6     |
| 4   | I     | 608 | NAG  | C4-C5-C6-O6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | B     | 603 | NAG  | C4-C5-C6-O6     |
| 4   | B     | 602 | NAG  | C4-C5-C6-O6     |
| 7   | I     | 602 | BMA  | O5-C5-C6-O6     |
| 8   | G     | 608 | MAN  | O5-C5-C6-O6     |
| 4   | I     | 608 | NAG  | O5-C5-C6-O6     |
| 4   | E     | 605 | NAG  | O5-C5-C6-O6     |
| 8   | E     | 604 | MAN  | C4-C5-C6-O6     |
| 6   | G     | 605 | HEC  | C3A-C2A-CAA-CBA |
| 6   | G     | 605 | HEC  | C1A-C2A-CAA-CBA |
| 4   | B     | 604 | NAG  | C4-C5-C6-O6     |
| 8   | I     | 603 | MAN  | O5-C5-C6-O6     |
| 6   | E     | 610 | HEC  | CAD-CBD-CGD-O2D |
| 4   | I     | 606 | NAG  | C4-C5-C6-O6     |
| 6   | G     | 605 | HEC  | CAA-CBA-CGA-O1A |
| 6   | B     | 606 | HEC  | CAA-CBA-CGA-O1A |
| 6   | I     | 610 | HEC  | CAD-CBD-CGD-O2D |
| 6   | E     | 610 | HEC  | CAD-CBD-CGD-O1D |
| 6   | G     | 605 | HEC  | CAD-CBD-CGD-O1D |
| 6   | G     | 605 | HEC  | CAA-CBA-CGA-O2A |
| 6   | I     | 610 | HEC  | CAA-CBA-CGA-O2A |
| 6   | G     | 605 | HEC  | CAD-CBD-CGD-O2D |
| 6   | I     | 610 | HEC  | CAA-CBA-CGA-O1A |
| 6   | B     | 606 | HEC  | CAA-CBA-CGA-O2A |
| 6   | E     | 610 | HEC  | CAA-CBA-CGA-O1A |
| 4   | E     | 606 | NAG  | C4-C5-C6-O6     |
| 6   | I     | 610 | HEC  | CAD-CBD-CGD-O1D |
| 6   | E     | 610 | HEC  | CAA-CBA-CGA-O2A |
| 8   | I     | 604 | MAN  | C4-C5-C6-O6     |
| 6   | B     | 606 | HEC  | CAD-CBD-CGD-O2D |
| 6   | B     | 606 | HEC  | CAD-CBD-CGD-O1D |
| 4   | E     | 607 | NAG  | O5-C5-C6-O6     |

All (1) ring outliers are listed below:

| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 8   | E     | 604 | MAN  | C1-C2-C3-C4-C5-O5 |

35 monomers are involved in 123 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | G     | 605 | HEC  | 14      | 0            |
| 4   | G     | 606 | NAG  | 4       | 0            |

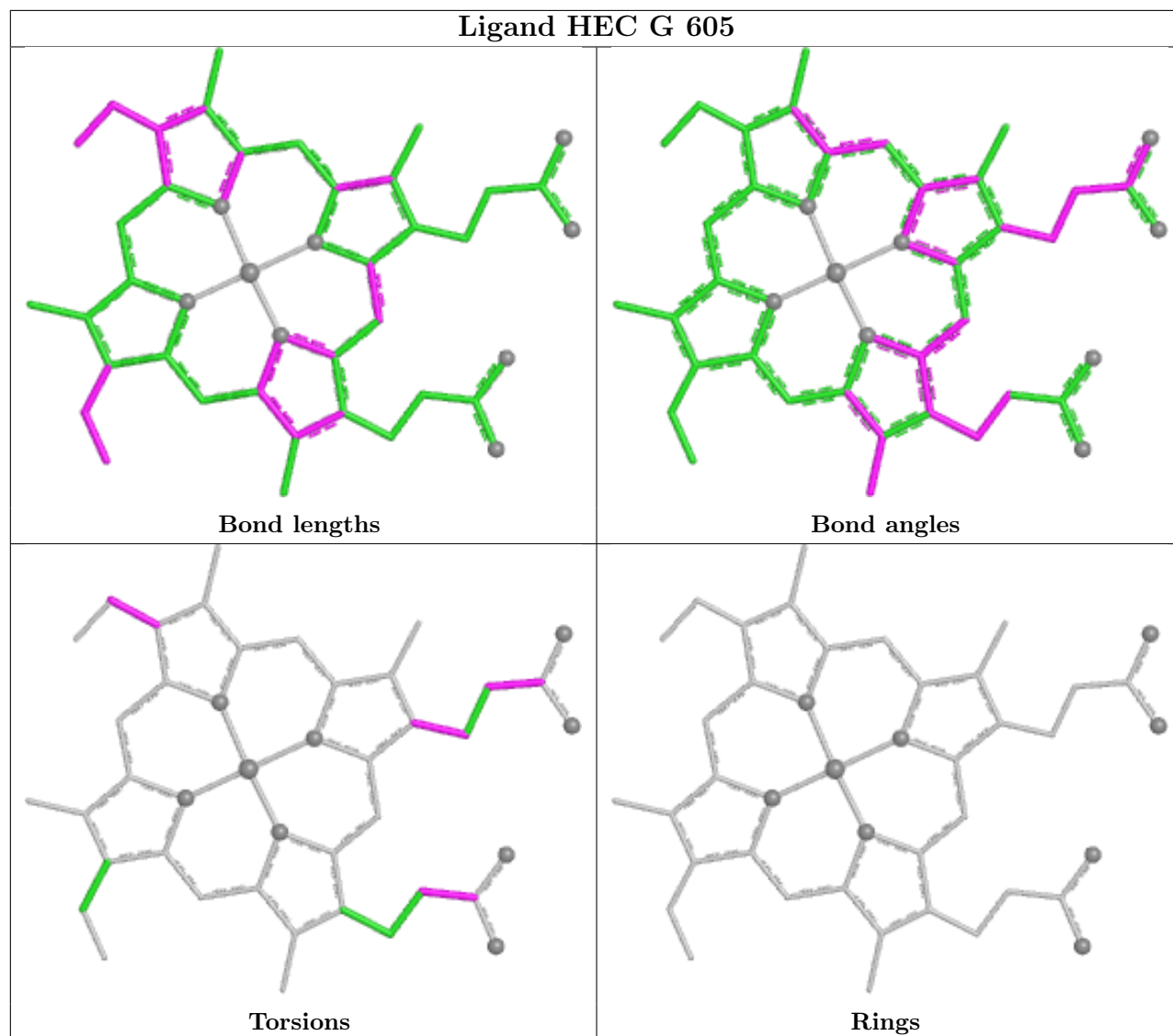
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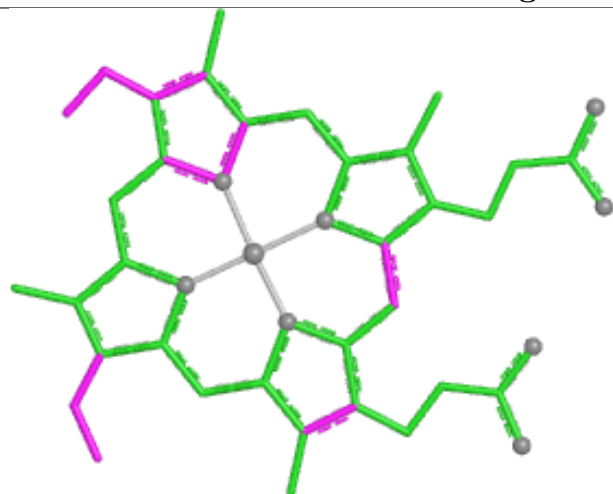
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 8   | G     | 609 | MAN  | 1       | 0            |
| 4   | I     | 608 | NAG  | 6       | 0            |
| 4   | I     | 606 | NAG  | 2       | 0            |
| 5   | B     | 605 | FUC  | 1       | 0            |
| 6   | I     | 610 | HEC  | 15      | 0            |
| 7   | I     | 602 | BMA  | 3       | 0            |
| 8   | I     | 603 | MAN  | 1       | 0            |
| 4   | B     | 607 | NAG  | 4       | 0            |
| 4   | B     | 604 | NAG  | 8       | 0            |
| 4   | G     | 602 | NAG  | 2       | 0            |
| 4   | E     | 605 | NAG  | 1       | 0            |
| 5   | E     | 609 | FUC  | 2       | 0            |
| 7   | B     | 608 | BMA  | 4       | 0            |
| 7   | E     | 602 | BMA  | 2       | 0            |
| 4   | G     | 603 | NAG  | 9       | 0            |
| 4   | E     | 608 | NAG  | 9       | 0            |
| 4   | I     | 601 | NAG  | 5       | 0            |
| 8   | E     | 604 | MAN  | 1       | 0            |
| 6   | B     | 606 | HEC  | 17      | 0            |
| 4   | B     | 602 | NAG  | 3       | 0            |
| 8   | B     | 610 | MAN  | 2       | 0            |
| 4   | I     | 605 | NAG  | 1       | 0            |
| 6   | E     | 610 | HEC  | 15      | 0            |
| 8   | G     | 608 | MAN  | 1       | 0            |
| 5   | G     | 604 | FUC  | 1       | 0            |
| 4   | G     | 601 | NAG  | 1       | 0            |
| 7   | G     | 607 | BMA  | 4       | 0            |
| 9   | G     | 610 | 7GD  | 1       | 0            |
| 9   | E     | 611 | 7GD  | 2       | 0            |
| 5   | I     | 609 | FUC  | 2       | 0            |
| 4   | E     | 601 | NAG  | 3       | 0            |
| 8   | I     | 604 | MAN  | 1       | 0            |
| 4   | E     | 606 | NAG  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

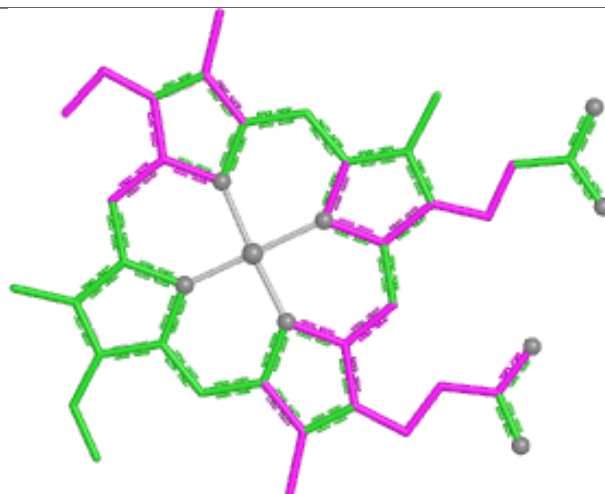
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



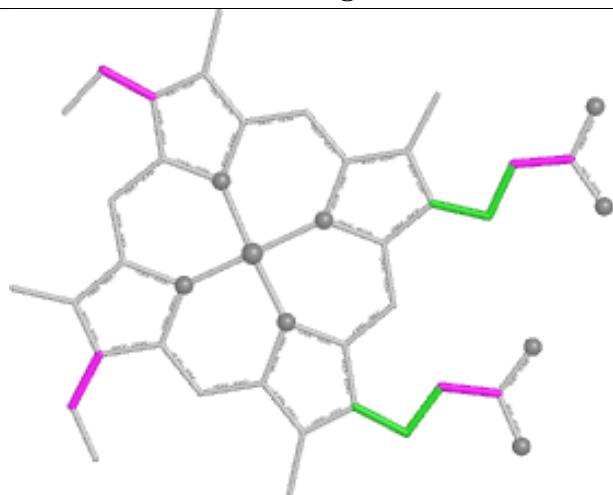
## Ligand HEC I 610



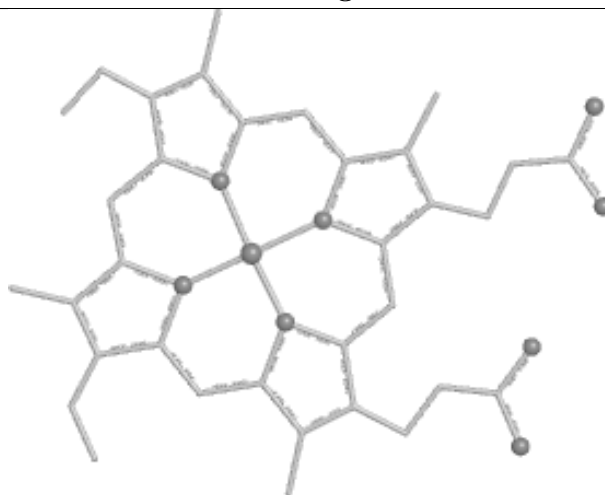
Bond lengths



Bond angles



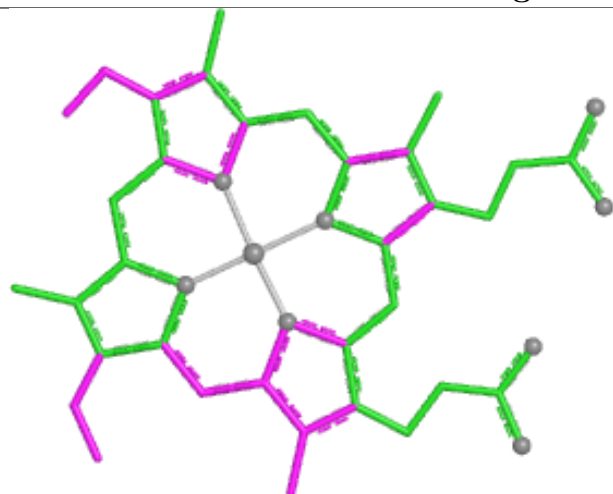
Torsions



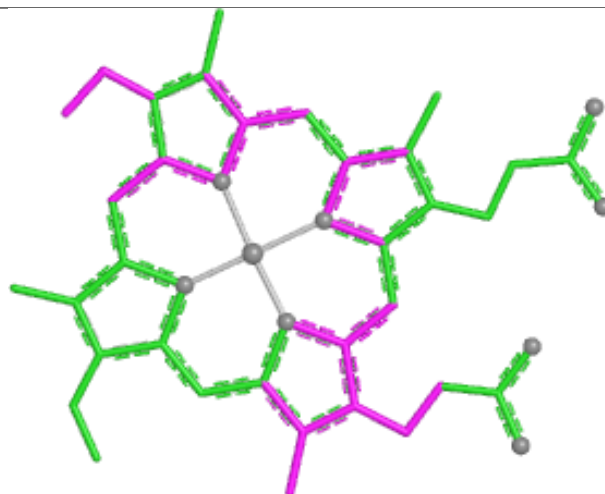
Rings



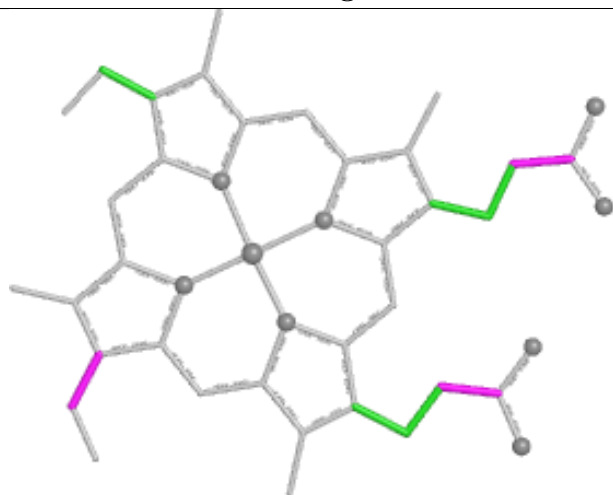
## Ligand HEC B 606



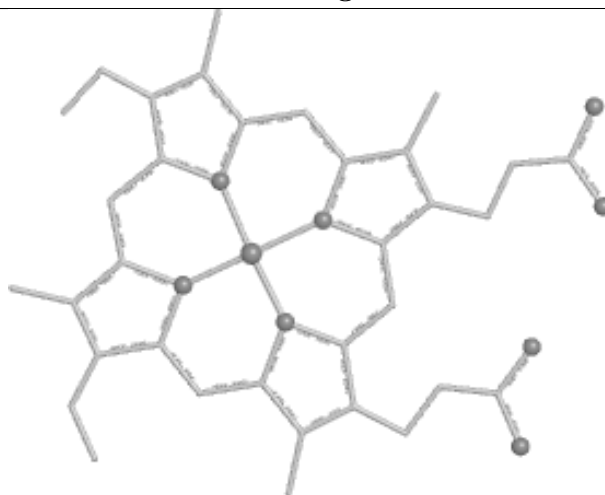
Bond lengths



Bond angles

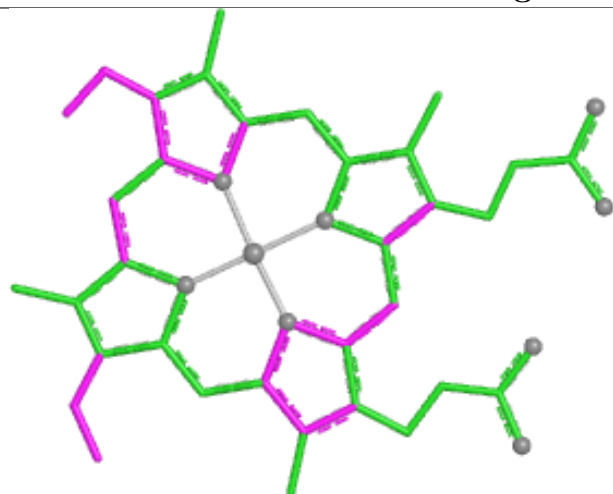


Torsions

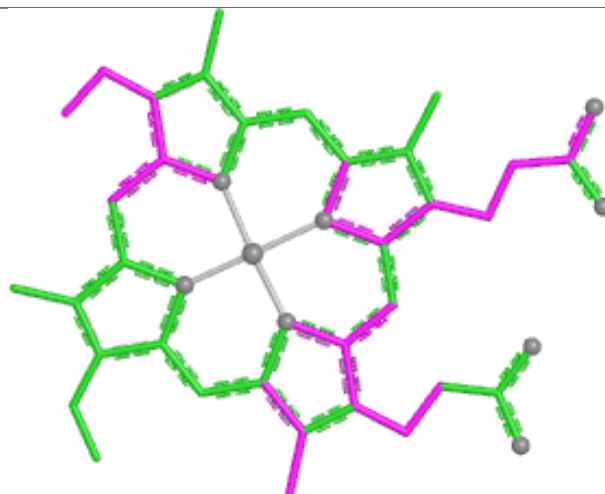


Rings

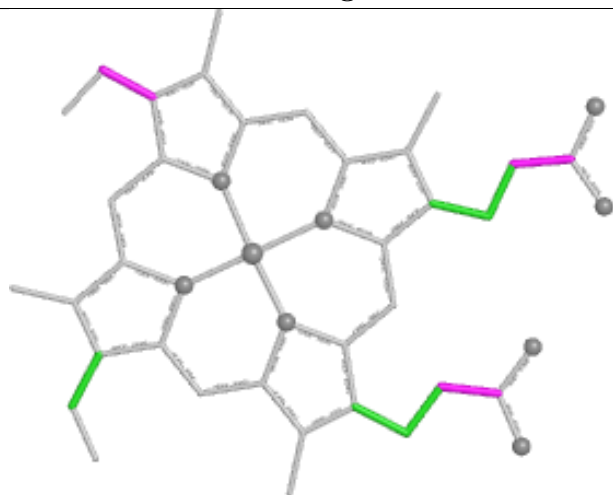
## Ligand HEC E 610



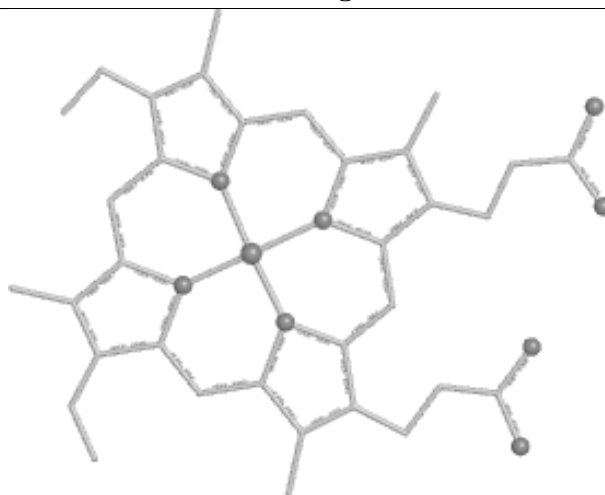
Bond lengths



Bond angles

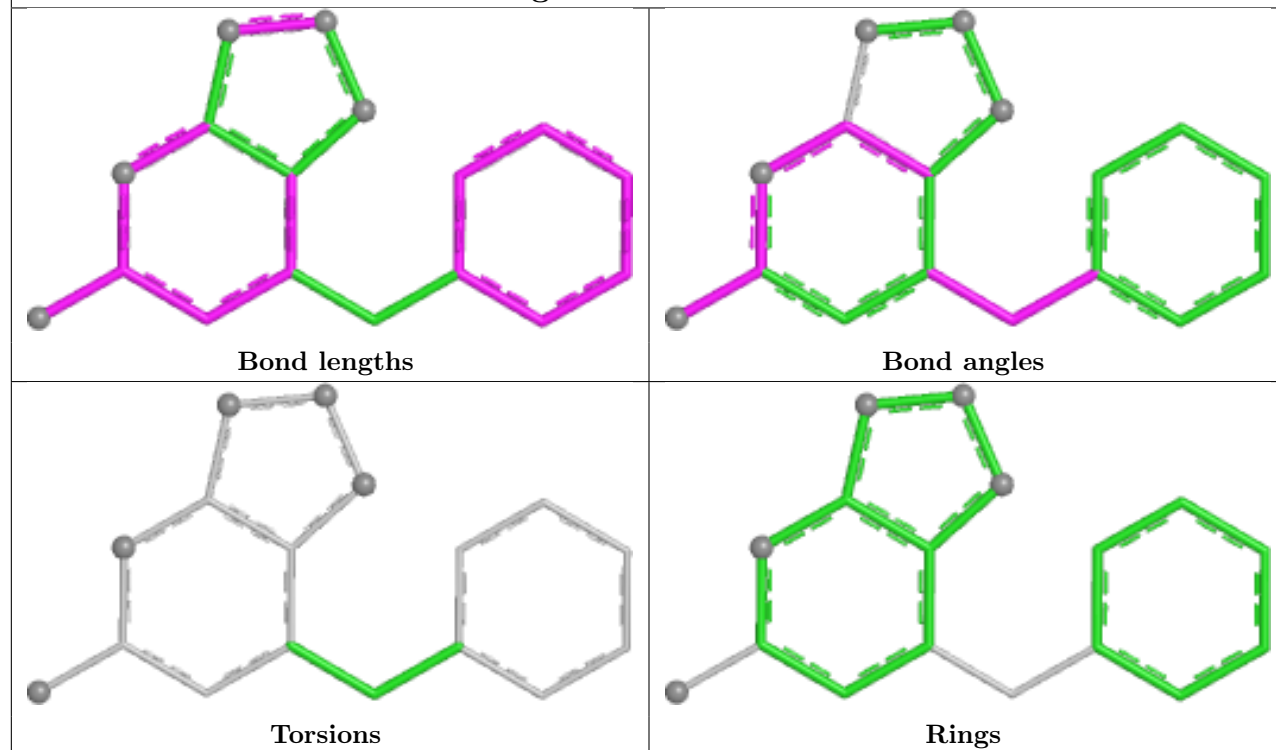


Torsions

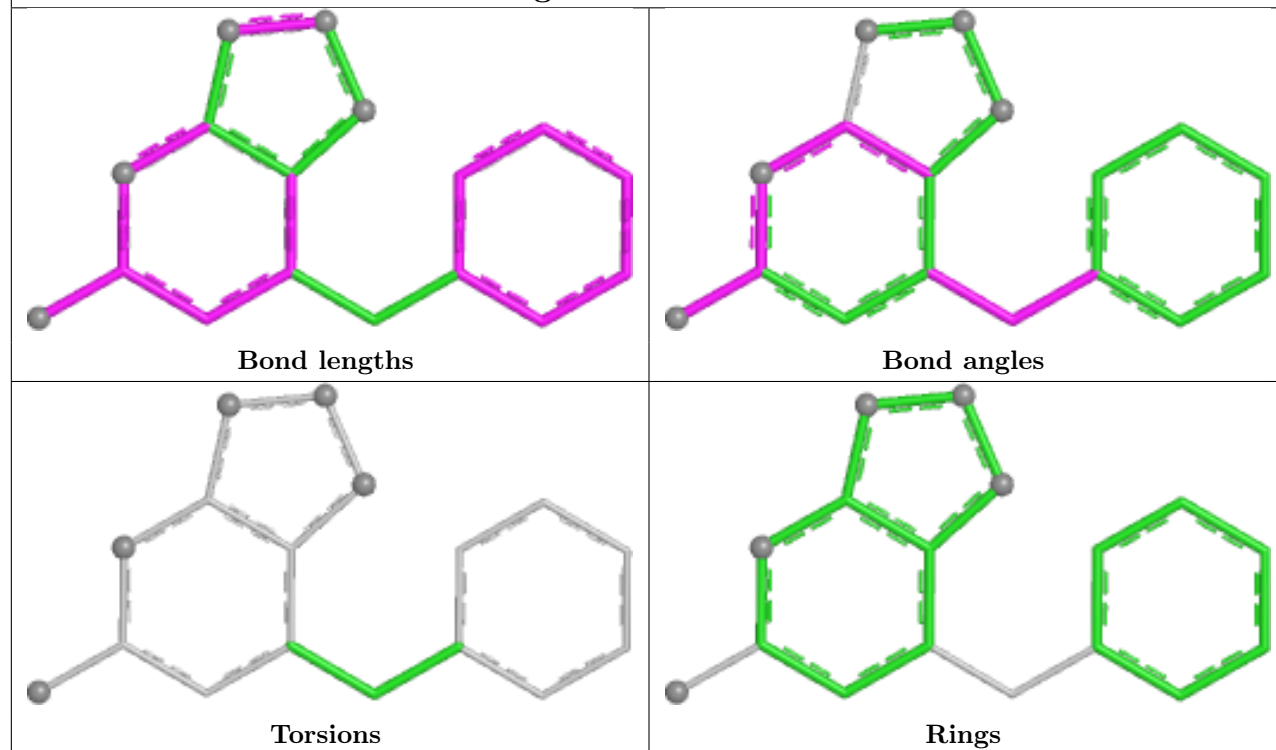


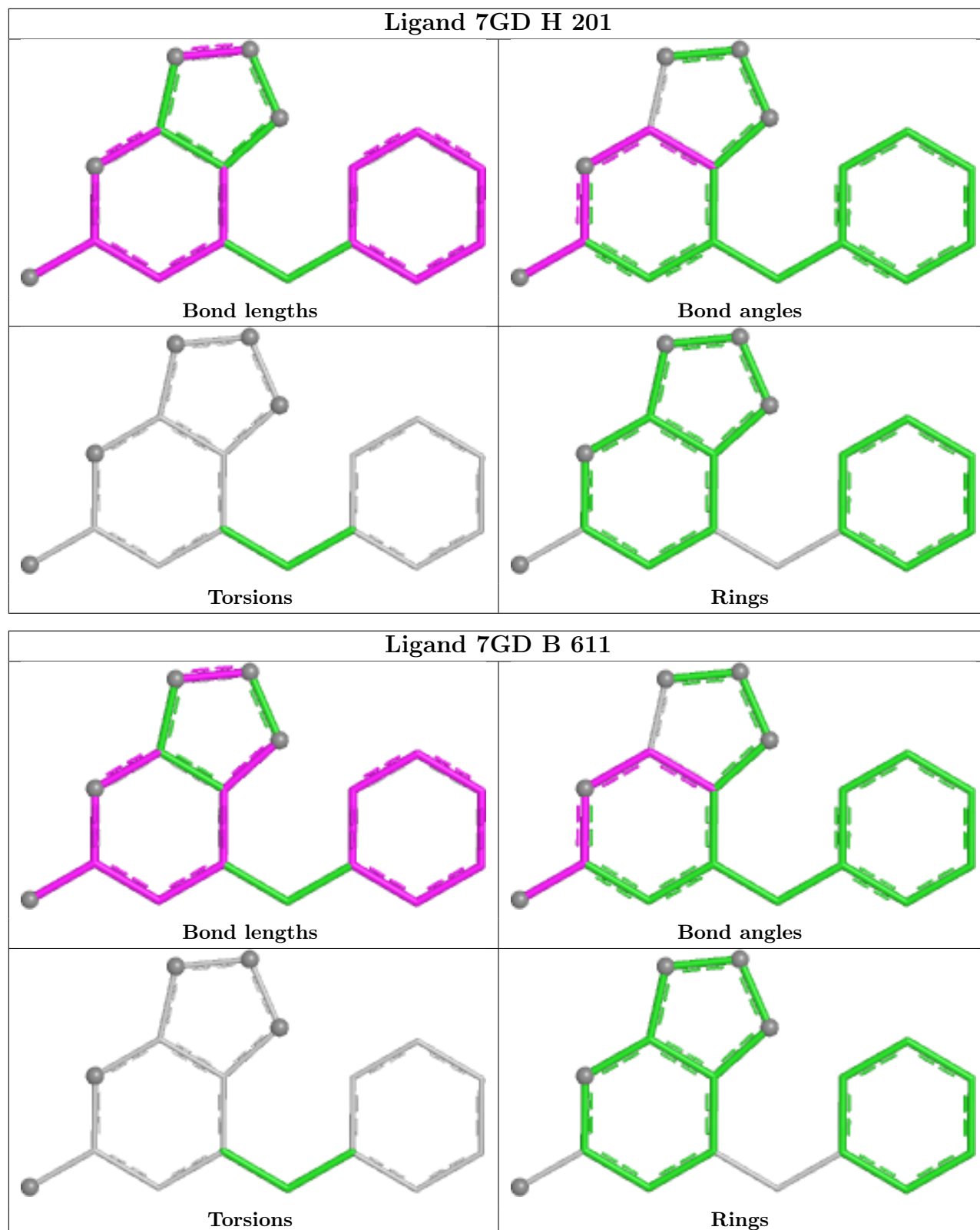
Rings

## Ligand 7GD G 610



## Ligand 7GD E 611





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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     | 103/105 (98%)   | -0.02  | 0 100 100     | 28, 43, 62, 84        | 0       |
| 1   | D     | 103/105 (98%)   | -0.01  | 1 (0%) 79 80  | 28, 46, 65, 88        | 1 (0%)  |
| 1   | F     | 103/105 (98%)   | -0.02  | 1 (0%) 79 80  | 28, 44, 66, 77        | 1 (0%)  |
| 1   | H     | 103/105 (98%)   | 0.09   | 1 (0%) 79 80  | 32, 47, 70, 83        | 1 (0%)  |
| 2   | B     | 465/467 (99%)   | 0.02   | 5 (1%) 78 79  | 27, 45, 68, 92        | 6 (1%)  |
| 2   | E     | 465/467 (99%)   | 0.42   | 14 (3%) 52 54 | 27, 52, 80, 102       | 7 (1%)  |
| 2   | G     | 465/467 (99%)   | 0.24   | 8 (1%) 69 69  | 23, 51, 73, 104       | 9 (1%)  |
| 2   | I     | 465/467 (99%)   | 0.17   | 2 (0%) 88 90  | 26, 51, 72, 82        | 12 (2%) |
| All | All   | 2272/2288 (99%) | 0.18   | 32 (1%) 73 74 | 23, 49, 73, 104       | 37 (1%) |

All (32) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 577 | GLU  | 4.1  |
| 2   | G     | 113 | VAL  | 3.6  |
| 2   | E     | 113 | VAL  | 3.4  |
| 2   | E     | 194 | LEU  | 3.3  |
| 2   | G     | 354 | GLU  | 3.3  |
| 2   | E     | 114 | ASN  | 3.3  |
| 2   | E     | 218 | ASP  | 3.3  |
| 2   | B     | 113 | VAL  | 3.0  |
| 2   | I     | 218 | ASP  | 2.8  |
| 2   | E     | 371 | VAL  | 2.7  |
| 2   | E     | 267 | LEU  | 2.7  |
| 2   | G     | 355 | PRO  | 2.6  |
| 2   | G     | 373 | LEU  | 2.5  |
| 2   | E     | 157 | ASN  | 2.5  |
| 2   | G     | 114 | ASN  | 2.5  |
| 2   | E     | 190 | MET  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 215 | ASN  | 2.5  |
| 1   | H     | 75  | GLN  | 2.4  |
| 2   | G     | 522 | MET  | 2.4  |
| 2   | E     | 276 | LEU  | 2.4  |
| 2   | B     | 355 | PRO  | 2.3  |
| 2   | E     | 264 | LEU  | 2.2  |
| 2   | B     | 159 | THR  | 2.2  |
| 2   | G     | 538 | CYS  | 2.2  |
| 2   | B     | 348 | ASN  | 2.1  |
| 2   | G     | 348 | ASN  | 2.1  |
| 1   | D     | 1   | CYS  | 2.1  |
| 1   | F     | 1   | CYS  | 2.1  |
| 2   | E     | 196 | LEU  | 2.1  |
| 2   | I     | 538 | CYS  | 2.1  |
| 2   | E     | 542 | GLY  | 2.1  |
| 2   | B     | 354 | 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | NAG  | B     | 603 | 14/15 | 0.47 | 0.18 | 106,110,113,113            | 0     |
| 4   | NAG  | E     | 607 | 14/15 | 0.68 | 0.16 | 96,99,102,102              | 0     |
| 4   | NAG  | I     | 607 | 14/15 | 0.70 | 0.15 | 82,85,88,88                | 0     |
| 8   | MAN  | G     | 608 | 11/12 | 0.71 | 0.15 | 75,77,80,81                | 0     |
| 8   | MAN  | B     | 609 | 11/12 | 0.76 | 0.17 | 79,81,84,85                | 0     |
| 4   | NAG  | G     | 602 | 14/15 | 0.76 | 0.18 | 101,105,107,107            | 0     |
| 4   | NAG  | E     | 605 | 14/15 | 0.79 | 0.13 | 63,67,69,69                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 8   | MAN  | I     | 603 | 11/12 | 0.81 | 0.15 | 75,77,79,81                 | 0     |
| 4   | NAG  | I     | 605 | 14/15 | 0.82 | 0.14 | 78,81,84,84                 | 0     |
| 4   | NAG  | E     | 606 | 14/15 | 0.83 | 0.16 | 91,95,98,98                 | 0     |
| 8   | MAN  | E     | 603 | 11/12 | 0.84 | 0.13 | 77,79,82,83                 | 0     |
| 4   | NAG  | I     | 606 | 14/15 | 0.85 | 0.12 | 67,71,73,74                 | 0     |
| 4   | NAG  | B     | 601 | 14/15 | 0.85 | 0.11 | 55,58,60,61                 | 0     |
| 4   | NAG  | G     | 601 | 14/15 | 0.85 | 0.13 | 70,74,77,77                 | 0     |
| 7   | BMA  | E     | 602 | 11/12 | 0.88 | 0.12 | 53,55,56,56                 | 0     |
| 7   | BMA  | G     | 607 | 11/12 | 0.88 | 0.12 | 49,52,53,54                 | 0     |
| 9   | 7GD  | E     | 611 | 17/17 | 0.88 | 0.11 | 42,45,48,51                 | 0     |
| 5   | FUC  | G     | 604 | 10/11 | 0.89 | 0.11 | 50,50,51,52                 | 0     |
| 3   | CL   | E     | 613 | 1/1   | 0.89 | 0.22 | 62,62,62,62                 | 0     |
| 9   | 7GD  | G     | 610 | 17/17 | 0.89 | 0.11 | 40,43,46,49                 | 0     |
| 8   | MAN  | E     | 604 | 11/12 | 0.90 | 0.11 | 48,50,52,53                 | 0     |
| 7   | BMA  | I     | 602 | 11/12 | 0.90 | 0.11 | 44,47,48,49                 | 0     |
| 8   | MAN  | G     | 609 | 11/12 | 0.90 | 0.12 | 41,43,45,46                 | 0     |
| 4   | NAG  | I     | 601 | 14/15 | 0.91 | 0.10 | 32,36,38,40                 | 0     |
| 7   | BMA  | B     | 608 | 11/12 | 0.91 | 0.09 | 34,37,39,39                 | 0     |
| 8   | MAN  | B     | 610 | 11/12 | 0.91 | 0.10 | 41,43,45,46                 | 0     |
| 8   | MAN  | I     | 604 | 11/12 | 0.91 | 0.08 | 40,42,44,46                 | 0     |
| 4   | NAG  | B     | 602 | 14/15 | 0.91 | 0.11 | 67,71,73,74                 | 0     |
| 5   | FUC  | E     | 609 | 10/11 | 0.91 | 0.12 | 55,56,57,57                 | 0     |
| 9   | 7GD  | H     | 201 | 17/17 | 0.91 | 0.10 | 42,44,47,48                 | 0     |
| 3   | CL   | I     | 612 | 1/1   | 0.92 | 0.21 | 57,57,57,57                 | 0     |
| 4   | NAG  | G     | 603 | 14/15 | 0.92 | 0.09 | 42,46,48,49                 | 0     |
| 4   | NAG  | I     | 608 | 14/15 | 0.92 | 0.09 | 38,42,44,45                 | 0     |
| 4   | NAG  | E     | 608 | 14/15 | 0.92 | 0.09 | 37,41,43,45                 | 0     |
| 4   | NAG  | B     | 604 | 14/15 | 0.92 | 0.08 | 37,41,43,44                 | 0     |
| 4   | NAG  | B     | 607 | 14/15 | 0.93 | 0.09 | 35,39,42,43                 | 0     |
| 5   | FUC  | B     | 605 | 10/11 | 0.93 | 0.10 | 44,44,45,45                 | 0     |
| 9   | 7GD  | B     | 611 | 17/17 | 0.93 | 0.08 | 36,40,44,46                 | 0     |
| 4   | NAG  | E     | 601 | 14/15 | 0.94 | 0.07 | 31,34,37,38                 | 0     |
| 5   | FUC  | I     | 609 | 10/11 | 0.95 | 0.08 | 39,40,41,41                 | 0     |
| 4   | NAG  | G     | 606 | 14/15 | 0.96 | 0.06 | 29,32,35,36                 | 0     |
| 3   | CL   | G     | 612 | 1/1   | 0.96 | 0.25 | 54,54,54,54                 | 0     |
| 6   | HEC  | B     | 606 | 43/43 | 0.96 | 0.08 | 38,39,43,47                 | 0     |
| 6   | HEC  | G     | 605 | 43/43 | 0.96 | 0.09 | 40,41,43,48                 | 0     |
| 6   | HEC  | I     | 610 | 43/43 | 0.96 | 0.09 | 44,45,49,58                 | 0     |
| 3   | CL   | B     | 613 | 1/1   | 0.96 | 0.22 | 51,51,51,51                 | 0     |
| 3   | CL   | E     | 614 | 1/1   | 0.96 | 0.09 | 37,37,37,37                 | 0     |
| 6   | HEC  | E     | 610 | 43/43 | 0.97 | 0.08 | 39,40,44,51                 | 0     |
| 3   | CL   | H     | 202 | 1/1   | 0.98 | 0.14 | 36,36,36,36                 | 0     |

*Continued on next page...*



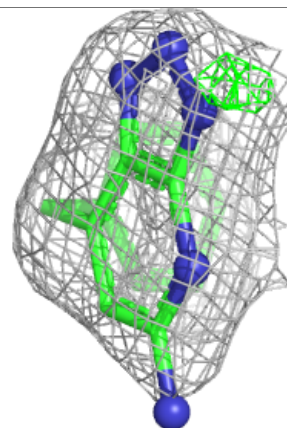
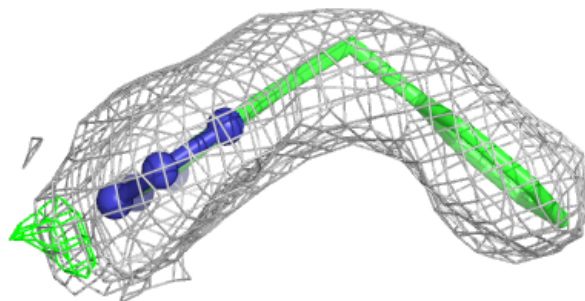
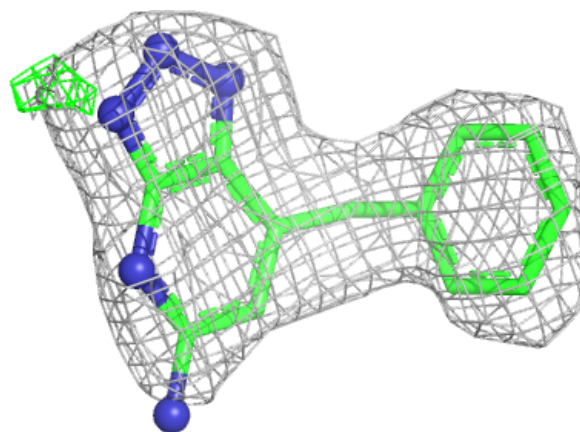
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | CL   | A     | 201 | 1/1   | 0.99 | 0.07 | 35,35,35,35                 | 0     |
| 3   | CL   | F     | 201 | 1/1   | 0.99 | 0.04 | 35,35,35,35                 | 0     |
| 10  | CA   | E     | 612 | 1/1   | 0.99 | 0.02 | 41,41,41,41                 | 0     |
| 10  | CA   | G     | 611 | 1/1   | 0.99 | 0.03 | 39,39,39,39                 | 0     |
| 10  | CA   | B     | 612 | 1/1   | 1.00 | 0.02 | 32,32,32,32                 | 0     |
| 10  | CA   | I     | 611 | 1/1   | 1.00 | 0.04 | 39,39,39,39                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

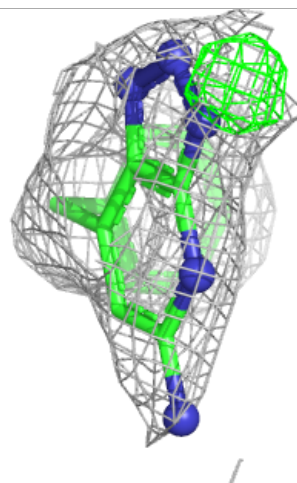
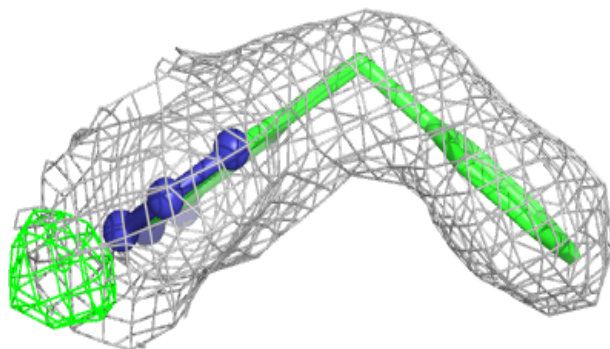
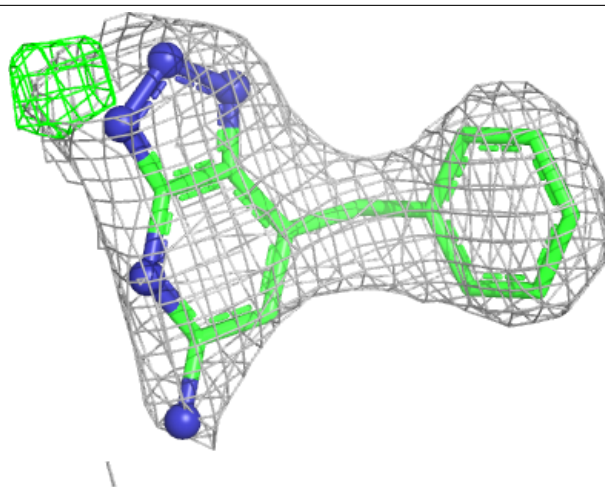
**Electron density around 7GD E 611:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
 and green (positive)



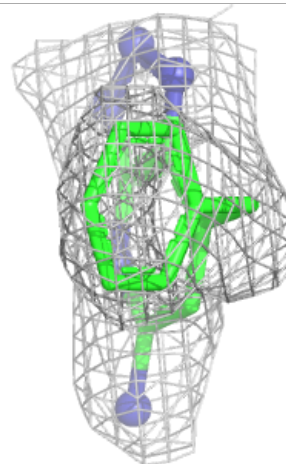
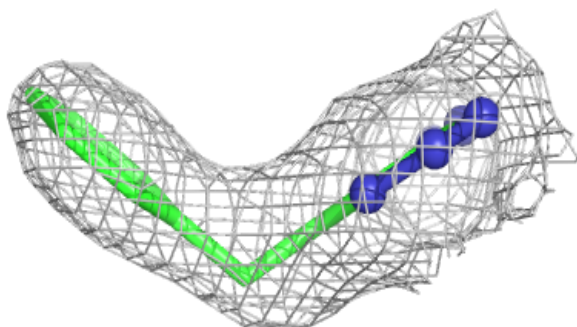
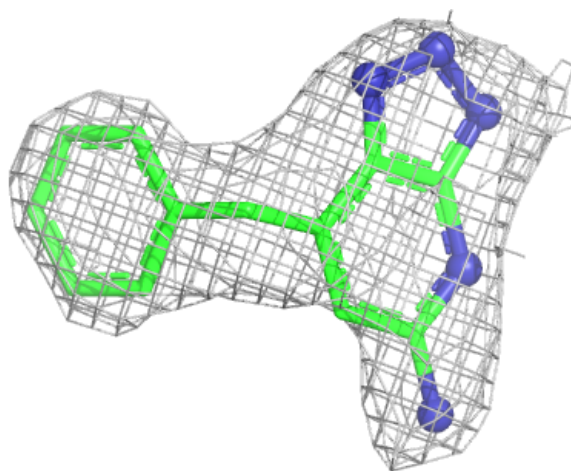
**Electron density around 7GD G 610:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



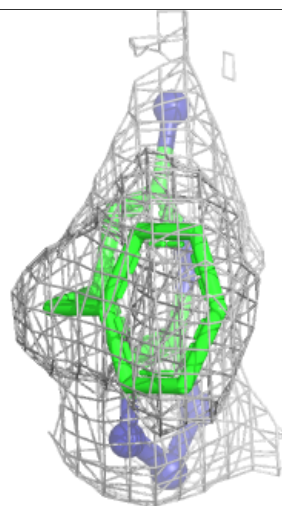
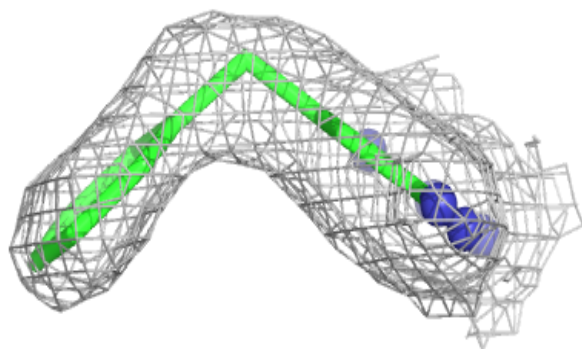
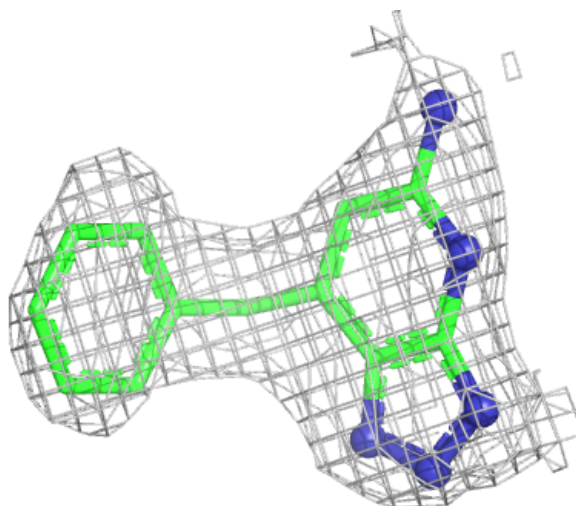
**Electron density around 7GD H 201:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



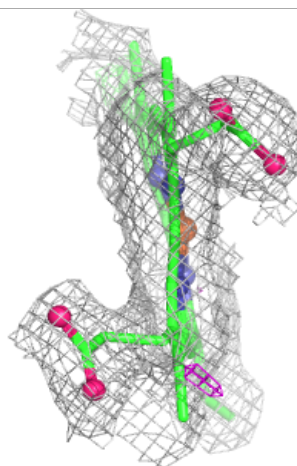
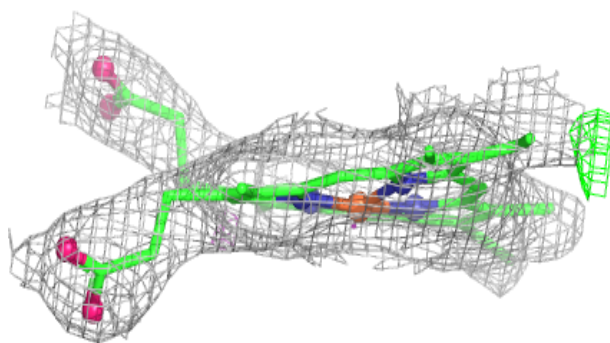
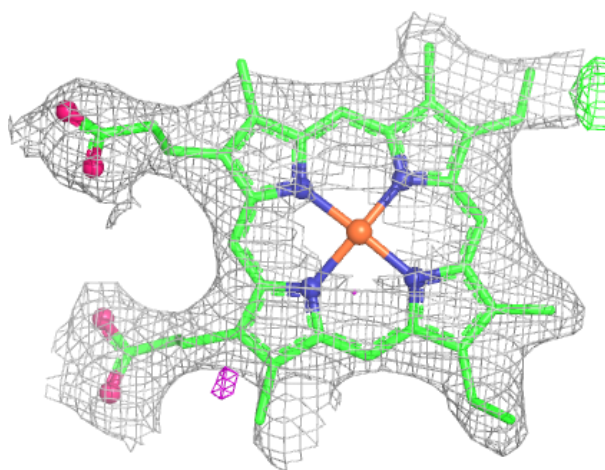
**Electron density around 7GD B 611:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



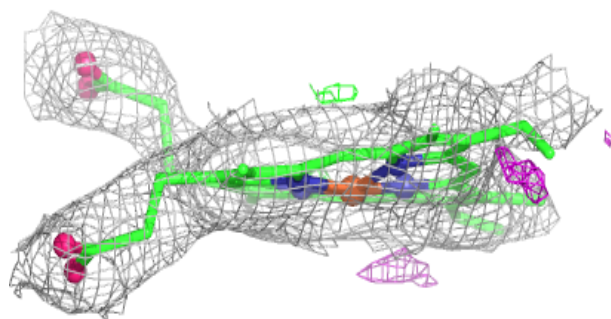
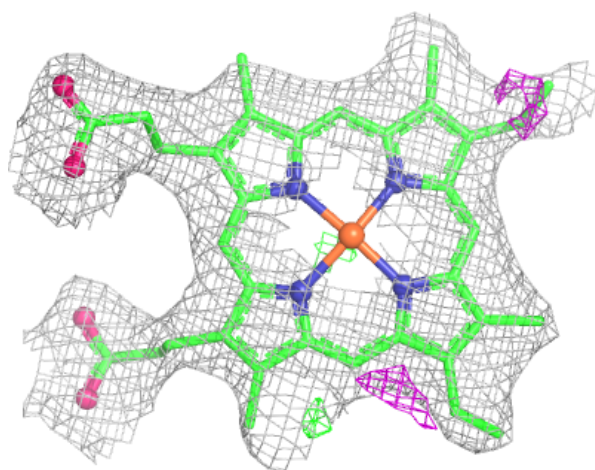
**Electron density around HEC B 606:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC G 605:**

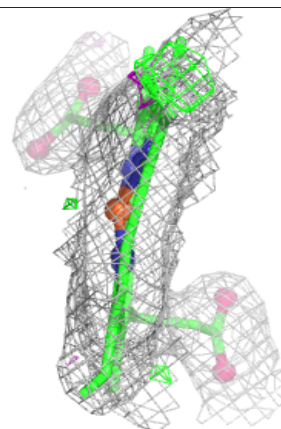
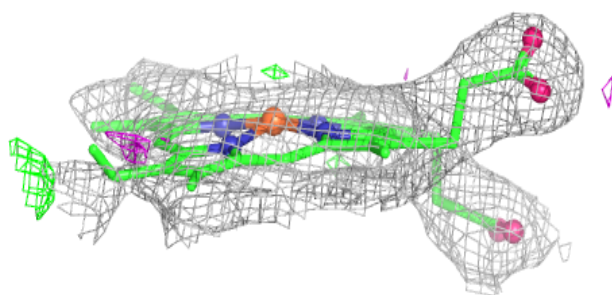
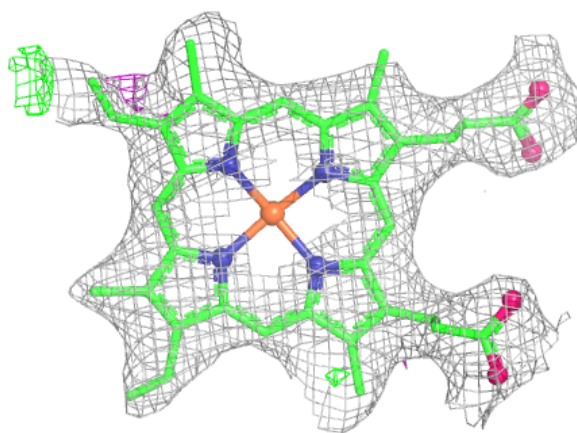
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

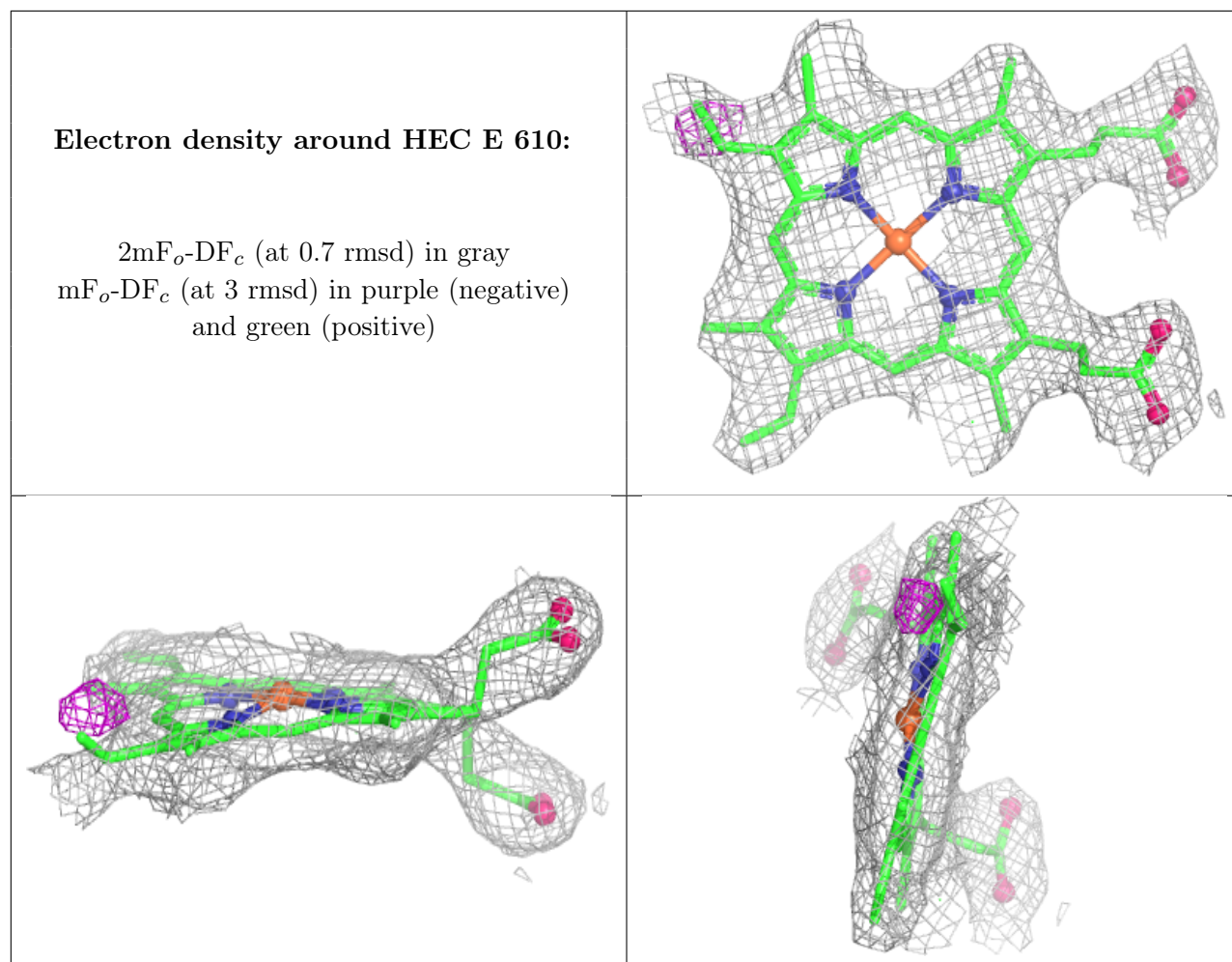




**Electron density around HEC I 610:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.