



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:04 PM EDT

PDB ID : 4F4O / pdb\_00004f4o  
Title : Structure of the Haptoglobin-Haemoglobin Complex  
Authors : Andersen, C.B.F.; Torvund-Jensen, M.; Nielsen, M.J.; Oliveira, C.L.P.; Hersleth, H.P.; Andersen, N.H.; Pedersen, J.S.; Andersen, G.R.; Moestrup, S.K.  
Deposited on : 2012-05-11  
Resolution : 2.90 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:

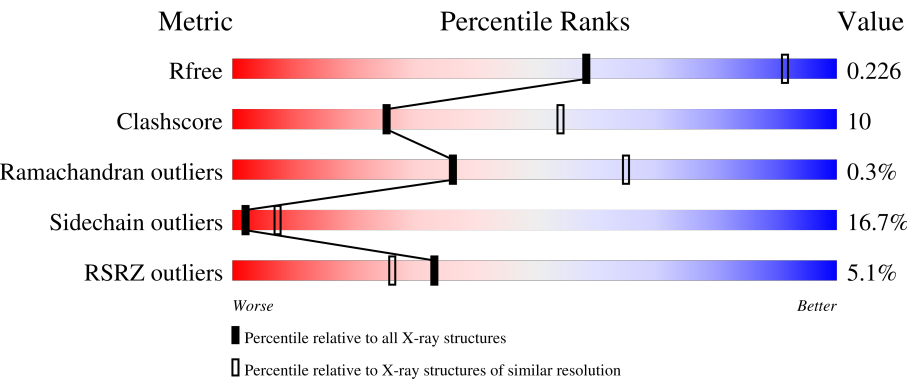
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

# 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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

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     | 141    | <div><div></div><div>80%16%..</div></div>   |
| 1   | D     | 141    | <div><div>3%</div><div>79%18%..</div></div> |
| 1   | G     | 141    | <div><div>%</div><div>80%16%..</div></div>  |
| 1   | J     | 141    | <div><div>30%</div><div>76%21%.</div></div> |
| 2   | B     | 146    | <div><div>3%</div><div>69%27%. </div></div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | E     | 146    |                  |
| 2   | H     | 146    |                  |
| 2   | K     | 146    |                  |
| 3   | C     | 347    |                  |
| 3   | F     | 347    |                  |
| 3   | I     | 347    |                  |
| 3   | L     | 347    |                  |
| 4   | M     | 2      |                  |
| 4   | O     | 2      |                  |
| 4   | Q     | 2      |                  |
| 5   | N     | 2      |                  |
| 5   | P     | 2      |                  |
| 5   | R     | 2      |                  |
| 5   | S     | 2      |                  |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19196 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 Hemoglobin subunit alpha.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 677 | 192 | 193 | 2 |         |         |       |
| 1   | D     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 677 | 192 | 193 | 2 |         |         |       |
| 1   | G     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 677 | 192 | 193 | 2 |         |         |       |
| 1   | J     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1064  | 677 | 192 | 193 | 2 |         |         |       |

- Molecule 2 is a protein called Hemoglobin subunit beta.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 146      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1144  | 731 | 205 | 206 | 2 |         |         |       |
| 2   | E     | 146      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1144  | 731 | 205 | 206 | 2 |         |         |       |
| 2   | H     | 146      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1144  | 731 | 205 | 206 | 2 |         |         |       |
| 2   | K     | 146      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1144  | 731 | 205 | 206 | 2 |         |         |       |

- Molecule 3 is a protein called Haptoglobin.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 309      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2428  | 1546 | 411 | 457 | 14 |         |         |       |
| 3   | F     | 309      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2428  | 1546 | 411 | 457 | 14 |         |         |       |
| 3   | I     | 309      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2428  | 1546 | 411 | 457 | 14 |         |         |       |
| 3   | L     | 309      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2428  | 1546 | 411 | 457 | 14 |         |         |       |

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



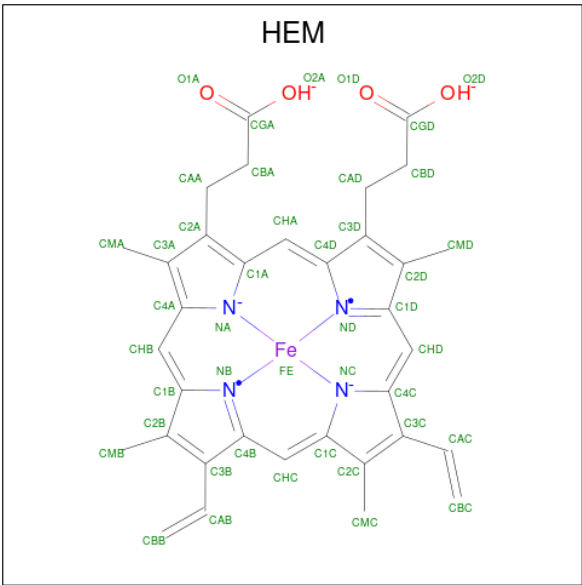
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4   | M     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 4   | O     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 4   | Q     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



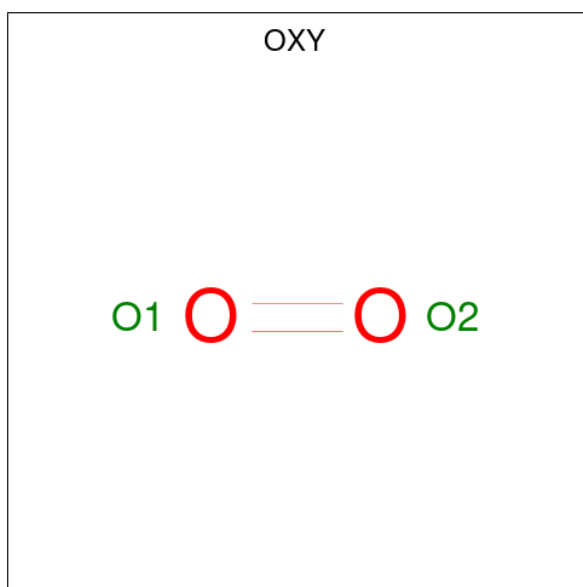
| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|---------|-------|
| 5   | N     | 2        | Total | C  | N | O | 0       | 0       | 0     |
|     |       |          | 24    | 14 | 1 | 9 |         |         |       |
| 5   | P     | 2        | Total | C  | N | O | 0       | 0       | 0     |
|     |       |          | 24    | 14 | 1 | 9 |         |         |       |
| 5   | R     | 2        | Total | C  | N | O | 0       | 0       | 0     |
|     |       |          | 24    | 14 | 1 | 9 |         |         |       |
| 5   | S     | 2        | Total | C  | N | O | 0       | 0       | 0     |
|     |       |          | 24    | 14 | 1 | 9 |         |         |       |

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



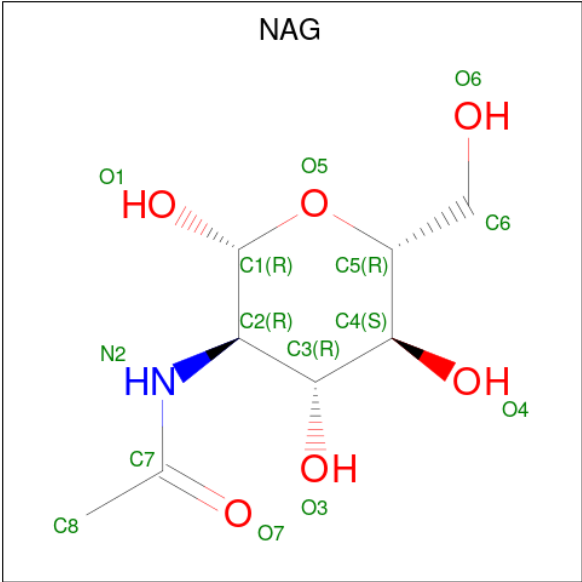
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 6   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 7 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O<sub>2</sub>).



| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 7   | A     | 1        | Total O<br>2 2 | 0       | 0       |
| 7   | B     | 1        | Total O<br>2 2 | 0       | 0       |
| 7   | D     | 1        | Total O<br>2 2 | 0       | 0       |
| 7   | E     | 1        | Total O<br>2 2 | 0       | 0       |
| 7   | G     | 1        | Total O<br>2 2 | 0       | 0       |
| 7   | H     | 1        | Total O<br>2 2 | 0       | 0       |
| 7   | J     | 1        | Total O<br>2 2 | 0       | 0       |
| 7   | K     | 1        | Total O<br>2 2 | 0       | 0       |

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 8   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | L     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | L     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

### 3 Residue-property plots

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

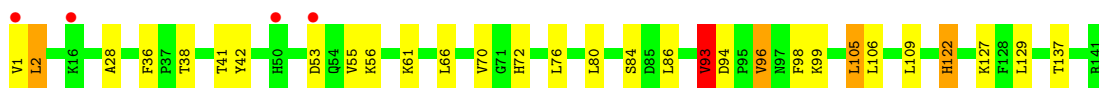
- Molecule 1: Hemoglobin subunit alpha

Chain A: 



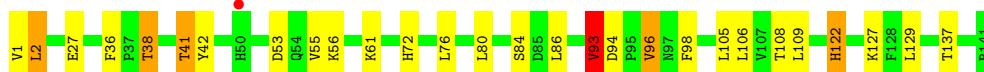
- Molecule 1: Hemoglobin subunit alpha

Chain D: 



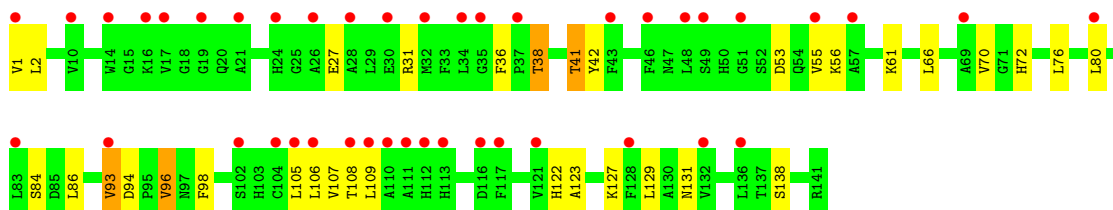
- Molecule 1: Hemoglobin subunit alpha

Chain G: 



- Molecule 1: Hemoglobin subunit alpha

Chain J: 



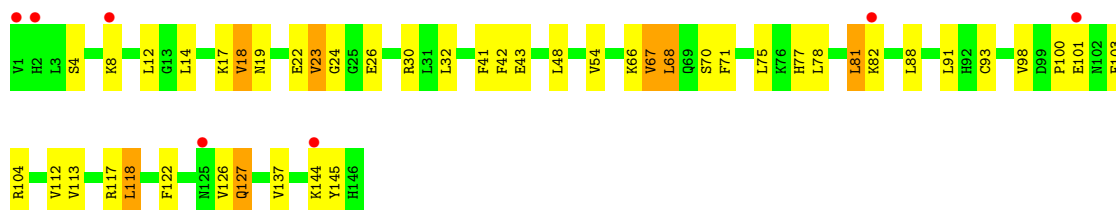
- Molecule 2: Hemoglobin subunit beta

Chain B: 

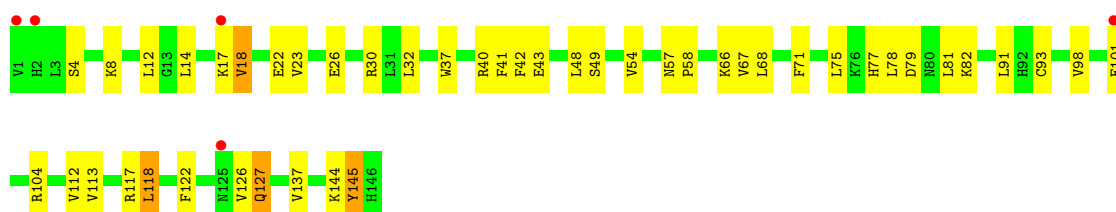




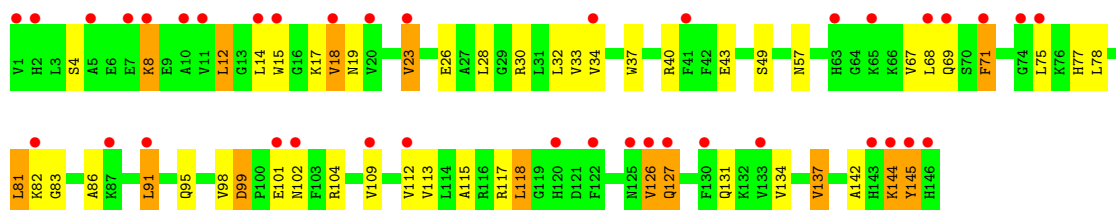
• Molecule 2: Hemoglobin subunit beta



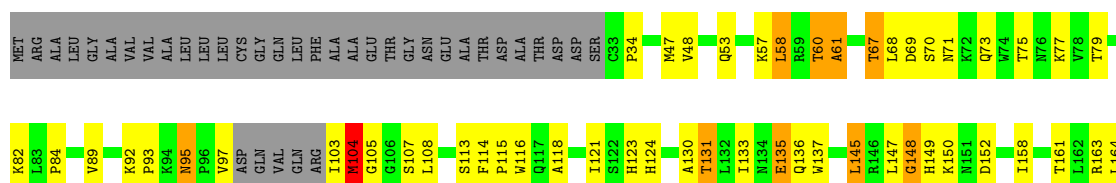
• Molecule 2: Hemoglobin subunit beta

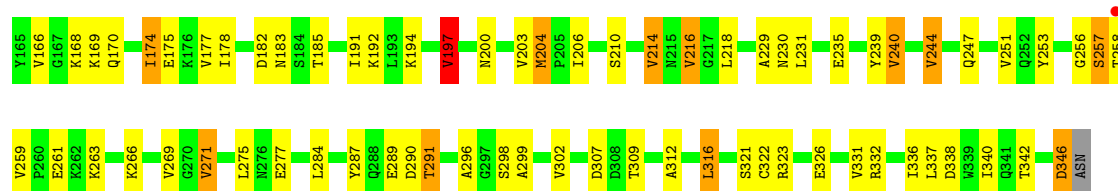


• Molecule 2: Hemoglobin subunit beta



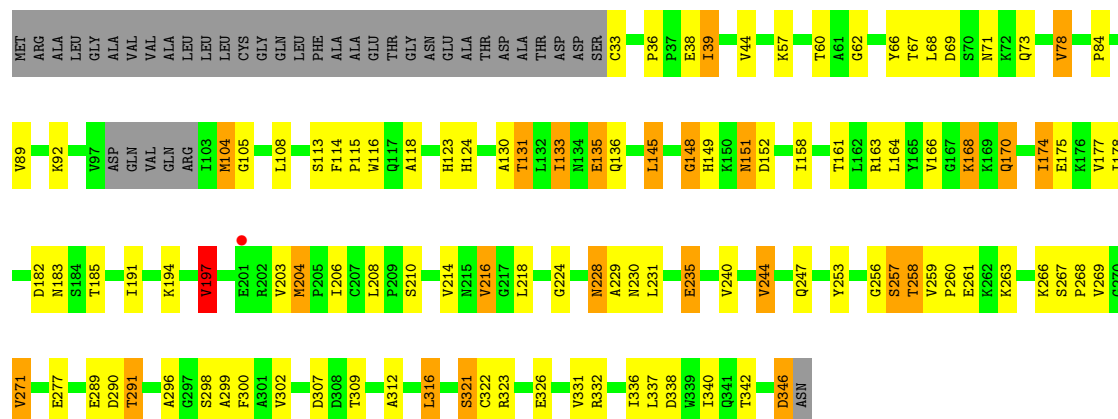
• Molecule 3: Haptoglobin





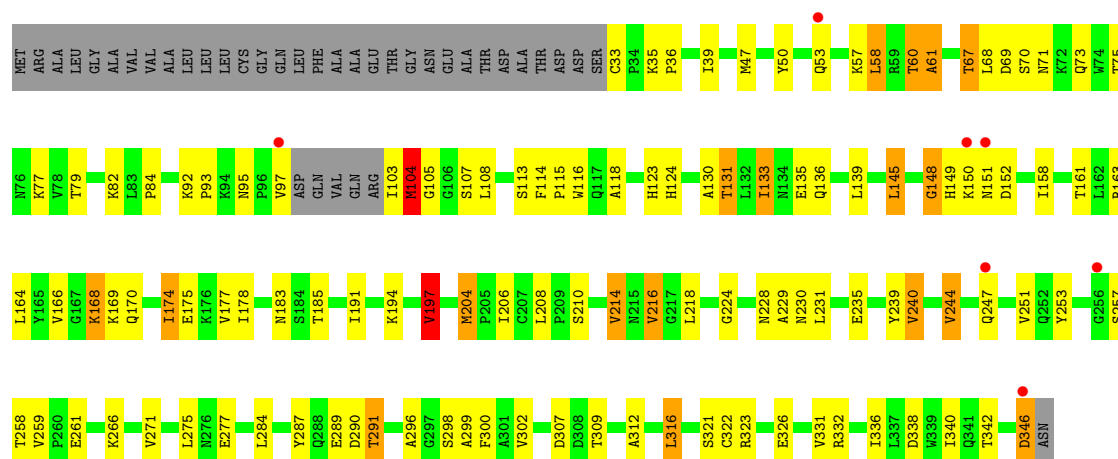
• Molecule 3: Haptoglobin

Chain F: 57% 24% 7% 11%



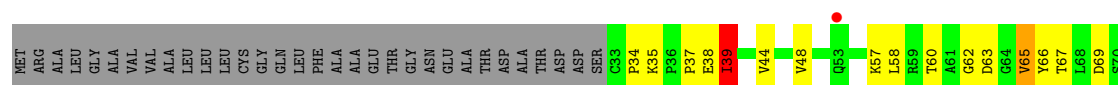
• Molecule 3: Haptoglobin

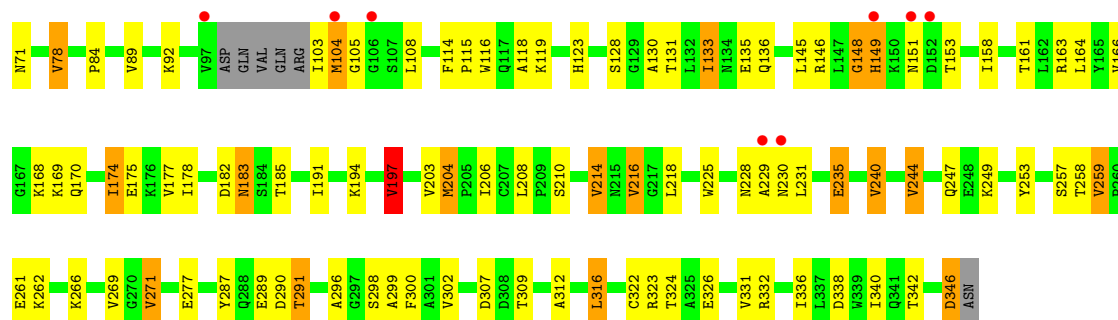
Chain I: 55% 29% 5% 11%



• Molecule 3: Haptoglobin

Chain L: 56% 27% 5% 11%





- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

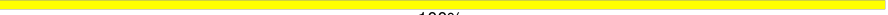
MAG1  
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%

MAG1  
MAG2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1  
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%

MAG1  
FUC2

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

MAG1  
FUC2

- Molecule 5:  $\alpha$ -L-fucopyranose-(1-6)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain S:

100%

MAG1  
FUC2

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 72.88Å 197.78Å 322.07Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.90<br>20.00 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.0 (20.00-2.90)<br>98.7 (20.00-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.09 (at 2.91Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.7.2_869)                           | Depositor        |
| R, $R_{free}$                                                           | 0.211 , 0.229<br>0.207 , 0.226                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2251 reflections (2.18%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 75.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.173                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 60.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 19196                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 93.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: HEM, FUC, OXY, NAG

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     | 0.76         | 2/1091 (0.2%)   | 1.01        | 3/1480 (0.2%)   |
| 1   | D     | 0.76         | 1/1091 (0.1%)   | 1.02        | 5/1480 (0.3%)   |
| 1   | G     | 0.73         | 1/1091 (0.1%)   | 1.01        | 5/1480 (0.3%)   |
| 1   | J     | 0.48         | 0/1091          | 0.93        | 4/1480 (0.3%)   |
| 2   | B     | 0.69         | 1/1169 (0.1%)   | 0.99        | 5/1580 (0.3%)   |
| 2   | E     | 0.59         | 0/1169          | 0.98        | 1/1580 (0.1%)   |
| 2   | H     | 0.70         | 0/1169          | 1.00        | 3/1580 (0.2%)   |
| 2   | K     | 0.61         | 1/1169 (0.1%)   | 0.98        | 6/1580 (0.4%)   |
| 3   | C     | 0.71         | 2/2487 (0.1%)   | 1.15        | 17/3377 (0.5%)  |
| 3   | F     | 0.76         | 1/2487 (0.0%)   | 1.20        | 17/3377 (0.5%)  |
| 3   | I     | 0.77         | 3/2487 (0.1%)   | 1.20        | 18/3377 (0.5%)  |
| 3   | L     | 0.66         | 2/2487 (0.1%)   | 1.11        | 13/3377 (0.4%)  |
| All | All   | 0.70         | 14/18988 (0.1%) | 1.09        | 97/25748 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | C     | 0                   | 2                   |
| 3   | F     | 0                   | 2                   |
| 3   | I     | 0                   | 2                   |
| 3   | L     | 0                   | 3                   |
| All | All   | 0                   | 9                   |

All (14) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | K     | 98  | VAL  | CA-CB | 9.27  | 1.65        | 1.54     |
| 3   | F     | 151 | ASN  | C-N   | -8.54 | 1.21        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 93  | VAL  | CA-CB | 8.07  | 1.63        | 1.54     |
| 3   | I     | 131 | THR  | N-CA  | 5.98  | 1.53        | 1.46     |
| 3   | L     | 149 | HIS  | CA-C  | -5.79 | 1.45        | 1.52     |
| 3   | C     | 214 | VAL  | CA-CB | 5.77  | 1.60        | 1.53     |
| 1   | A     | 55  | VAL  | CA-CB | 5.65  | 1.62        | 1.54     |
| 3   | L     | 214 | VAL  | CA-CB | 5.55  | 1.60        | 1.53     |
| 3   | I     | 150 | LYS  | C-N   | 5.46  | 1.41        | 1.33     |
| 3   | I     | 214 | VAL  | CA-CB | 5.41  | 1.59        | 1.53     |
| 1   | G     | 93  | VAL  | CA-CB | 5.35  | 1.60        | 1.54     |
| 1   | A     | 93  | VAL  | CA-CB | 5.24  | 1.60        | 1.54     |
| 2   | B     | 126 | VAL  | CA-CB | 5.19  | 1.61        | 1.54     |
| 3   | C     | 131 | THR  | N-CA  | 5.00  | 1.52        | 1.46     |

All (97) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | I     | 197 | VAL  | CB-CA-C | -9.31 | 102.28      | 110.94   |
| 3   | C     | 197 | VAL  | CB-CA-C | -9.25 | 102.34      | 110.94   |
| 3   | F     | 136 | GLN  | N-CA-C  | 9.09  | 124.61      | 112.88   |
| 3   | L     | 136 | GLN  | N-CA-C  | 9.07  | 124.58      | 112.88   |
| 3   | C     | 136 | GLN  | N-CA-C  | 8.82  | 124.26      | 112.88   |
| 3   | I     | 136 | GLN  | N-CA-C  | 8.73  | 125.00      | 113.30   |
| 3   | F     | 322 | CYS  | CA-C-N  | -8.63 | 108.83      | 122.65   |
| 3   | F     | 322 | CYS  | C-N-CA  | -8.63 | 108.83      | 122.65   |
| 3   | C     | 322 | CYS  | CA-C-N  | -8.49 | 109.06      | 122.65   |
| 3   | C     | 322 | CYS  | C-N-CA  | -8.49 | 109.06      | 122.65   |
| 3   | I     | 61  | ALA  | N-CA-C  | 8.39  | 124.13      | 112.04   |
| 3   | I     | 322 | CYS  | CA-C-N  | -8.35 | 109.29      | 122.65   |
| 3   | I     | 322 | CYS  | C-N-CA  | -8.35 | 109.29      | 122.65   |
| 3   | F     | 197 | VAL  | CB-CA-C | -8.18 | 103.33      | 110.94   |
| 3   | L     | 197 | VAL  | CB-CA-C | -8.04 | 103.46      | 110.94   |
| 3   | F     | 33  | CYS  | CA-C-N  | 8.04  | 128.10      | 119.90   |
| 3   | F     | 33  | CYS  | C-N-CA  | 8.04  | 128.10      | 119.90   |
| 3   | I     | 35  | LYS  | CA-C-N  | 8.03  | 125.44      | 119.66   |
| 3   | I     | 35  | LYS  | C-N-CA  | 8.03  | 125.44      | 119.66   |
| 3   | F     | 78  | VAL  | N-CA-C  | 7.82  | 119.87      | 111.58   |
| 3   | L     | 148 | GLY  | N-CA-C  | 7.74  | 122.00      | 112.64   |
| 3   | L     | 78  | VAL  | N-CA-C  | 7.34  | 119.00      | 111.00   |
| 3   | L     | 322 | CYS  | CA-C-N  | -7.30 | 110.98      | 122.65   |
| 3   | L     | 322 | CYS  | C-N-CA  | -7.30 | 110.98      | 122.65   |
| 2   | B     | 42  | PHE  | N-CA-C  | 7.00  | 120.70      | 112.72   |
| 2   | H     | 145 | TYR  | CB-CA-C | -7.00 | 101.71      | 112.07   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | C     | 149 | HIS  | N-CA-C  | 6.99  | 119.75      | 109.69   |
| 3   | C     | 61  | ALA  | N-CA-C  | 6.76  | 121.78      | 112.04   |
| 1   | G     | 72  | HIS  | N-CA-C  | 6.76  | 120.42      | 112.72   |
| 1   | A     | 72  | HIS  | N-CA-C  | 6.59  | 120.23      | 112.72   |
| 1   | G     | 96  | VAL  | CB-CA-C | -6.59 | 101.95      | 112.16   |
| 3   | F     | 114 | PHE  | CA-C-N  | 6.50  | 126.43      | 119.28   |
| 3   | F     | 114 | PHE  | C-N-CA  | 6.50  | 126.43      | 119.28   |
| 2   | E     | 42  | PHE  | N-CA-C  | 6.43  | 120.83      | 112.92   |
| 1   | J     | 72  | HIS  | N-CA-C  | 6.36  | 119.97      | 112.72   |
| 3   | L     | 65  | VAL  | N-CA-C  | 6.32  | 116.96      | 107.80   |
| 2   | H     | 49  | SER  | N-CA-C  | 6.26  | 117.80      | 110.97   |
| 2   | H     | 42  | PHE  | N-CA-C  | 6.25  | 119.84      | 112.72   |
| 1   | D     | 96  | VAL  | CB-CA-C | -6.22 | 102.97      | 112.05   |
| 3   | L     | 39  | ILE  | CA-C-N  | -6.21 | 113.55      | 119.76   |
| 3   | L     | 39  | ILE  | C-N-CA  | -6.21 | 113.55      | 119.76   |
| 3   | C     | 104 | MET  | CA-C-N  | -6.20 | 114.62      | 122.19   |
| 3   | C     | 104 | MET  | C-N-CA  | -6.20 | 114.62      | 122.19   |
| 1   | J     | 96  | VAL  | CB-CA-C | -6.09 | 102.72      | 112.16   |
| 1   | G     | 36  | PHE  | CA-C-N  | 5.93  | 125.61      | 119.56   |
| 1   | G     | 36  | PHE  | C-N-CA  | 5.93  | 125.61      | 119.56   |
| 1   | A     | 96  | VAL  | CB-CA-C | -5.89 | 103.03      | 112.16   |
| 2   | K     | 57  | ASN  | CA-C-N  | 5.82  | 125.36      | 119.19   |
| 2   | K     | 57  | ASN  | C-N-CA  | 5.82  | 125.36      | 119.19   |
| 2   | B     | 145 | TYR  | CB-CA-C | -5.79 | 102.01      | 111.68   |
| 3   | L     | 170 | GLN  | CB-CA-C | -5.76 | 102.05      | 110.06   |
| 2   | K     | 99  | ASP  | CA-C-N  | 5.76  | 127.04      | 119.84   |
| 2   | K     | 99  | ASP  | C-N-CA  | 5.76  | 127.04      | 119.84   |
| 3   | F     | 224 | GLY  | N-CA-C  | 5.75  | 119.72      | 110.87   |
| 3   | I     | 61  | ALA  | CA-C-N  | 5.74  | 132.04      | 121.70   |
| 3   | I     | 61  | ALA  | C-N-CA  | 5.74  | 132.04      | 121.70   |
| 3   | L     | 114 | PHE  | CA-C-N  | 5.74  | 125.41      | 119.56   |
| 3   | L     | 114 | PHE  | C-N-CA  | 5.74  | 125.41      | 119.56   |
| 3   | L     | 300 | PHE  | N-CA-C  | -5.73 | 99.19       | 108.41   |
| 2   | K     | 49  | SER  | N-CA-C  | 5.64  | 118.16      | 111.33   |
| 3   | I     | 131 | THR  | N-CA-C  | 5.63  | 122.78      | 110.80   |
| 3   | C     | 114 | PHE  | CA-C-N  | 5.62  | 125.46      | 119.28   |
| 3   | C     | 114 | PHE  | C-N-CA  | 5.62  | 125.46      | 119.28   |
| 3   | F     | 170 | GLN  | CB-CA-C | -5.62 | 102.25      | 110.06   |
| 3   | C     | 150 | LYS  | CA-C-O  | -5.61 | 115.45      | 121.56   |
| 3   | C     | 170 | GLN  | CB-CA-C | -5.55 | 102.34      | 110.06   |
| 1   | D     | 72  | HIS  | N-CA-C  | 5.54  | 119.04      | 112.72   |
| 2   | B     | 35  | TYR  | CA-C-N  | 5.47  | 125.14      | 119.56   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 35  | TYR  | C-N-CA  | 5.47  | 125.14      | 119.56   |
| 3   | C     | 95  | ASN  | CA-C-N  | 5.42  | 125.72      | 119.92   |
| 3   | C     | 95  | ASN  | C-N-CA  | 5.42  | 125.72      | 119.92   |
| 3   | F     | 39  | ILE  | CA-C-N  | -5.40 | 114.36      | 119.76   |
| 3   | F     | 39  | ILE  | C-N-CA  | -5.40 | 114.36      | 119.76   |
| 3   | I     | 114 | PHE  | CA-C-N  | 5.39  | 125.21      | 119.28   |
| 3   | I     | 114 | PHE  | C-N-CA  | 5.39  | 125.21      | 119.28   |
| 2   | K     | 33  | VAL  | N-CA-C  | 5.36  | 116.02      | 110.82   |
| 3   | F     | 131 | THR  | N-CA-C  | 5.27  | 122.03      | 110.80   |
| 1   | D     | 137 | THR  | N-CA-C  | 5.26  | 119.86      | 113.38   |
| 1   | D     | 36  | PHE  | CA-C-N  | 5.26  | 124.92      | 119.56   |
| 1   | D     | 36  | PHE  | C-N-CA  | 5.26  | 124.92      | 119.56   |
| 3   | C     | 131 | THR  | N-CA-C  | 5.25  | 121.99      | 110.80   |
| 3   | I     | 300 | PHE  | N-CA-C  | -5.24 | 98.77       | 107.99   |
| 3   | F     | 135 | GLU  | N-CA-C  | 5.23  | 116.98      | 111.28   |
| 3   | I     | 104 | MET  | CA-C-N  | -5.22 | 114.52      | 122.04   |
| 3   | I     | 104 | MET  | C-N-CA  | -5.22 | 114.52      | 122.04   |
| 3   | I     | 170 | GLN  | CB-CA-C | -5.20 | 102.83      | 110.06   |
| 3   | F     | 300 | PHE  | N-CA-C  | -5.18 | 100.07      | 108.41   |
| 3   | I     | 39  | ILE  | N-CA-C  | 5.16  | 113.51      | 107.89   |
| 3   | C     | 135 | GLU  | N-CA-C  | 5.13  | 116.87      | 111.28   |
| 1   | A     | 73  | LEU  | N-CA-C  | 5.12  | 118.31      | 111.75   |
| 3   | I     | 224 | GLY  | N-CA-C  | 5.12  | 118.76      | 110.87   |
| 1   | J     | 36  | PHE  | CA-C-N  | 5.10  | 126.22      | 119.84   |
| 1   | J     | 36  | PHE  | C-N-CA  | 5.10  | 126.22      | 119.84   |
| 1   | G     | 137 | THR  | N-CA-C  | 5.10  | 119.65      | 113.38   |
| 2   | B     | 49  | SER  | N-CA-C  | 5.04  | 117.17      | 111.02   |
| 3   | C     | 121 | ILE  | N-CA-C  | 5.03  | 115.09      | 107.75   |
| 3   | F     | 228 | ASN  | N-CA-C  | 5.01  | 117.81      | 109.94   |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | C     | 148 | GLY  | Peptide |
| 3   | C     | 257 | SER  | Peptide |
| 3   | F     | 148 | GLY  | Peptide |
| 3   | F     | 257 | SER  | Peptide |
| 3   | I     | 148 | GLY  | Peptide |
| 3   | I     | 257 | SER  | Peptide |
| 3   | L     | 148 | GLY  | Peptide |
| 3   | L     | 257 | SER  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | L     | 34  | PRO  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1064  | 0        | 1060     | 11      | 0            |
| 1   | D     | 1064  | 0        | 1060     | 12      | 0            |
| 1   | G     | 1064  | 0        | 1060     | 11      | 0            |
| 1   | J     | 1064  | 0        | 1060     | 16      | 0            |
| 2   | B     | 1144  | 0        | 1141     | 21      | 0            |
| 2   | E     | 1144  | 0        | 1141     | 23      | 0            |
| 2   | H     | 1144  | 0        | 1141     | 22      | 0            |
| 2   | K     | 1144  | 0        | 1141     | 35      | 0            |
| 3   | C     | 2428  | 0        | 2396     | 61      | 0            |
| 3   | F     | 2428  | 0        | 2395     | 57      | 0            |
| 3   | I     | 2428  | 0        | 2395     | 58      | 0            |
| 3   | L     | 2428  | 0        | 2397     | 64      | 0            |
| 4   | M     | 28    | 0        | 25       | 1       | 0            |
| 4   | O     | 28    | 0        | 25       | 1       | 0            |
| 4   | Q     | 28    | 0        | 25       | 1       | 0            |
| 5   | N     | 24    | 0        | 22       | 0       | 0            |
| 5   | P     | 24    | 0        | 22       | 2       | 0            |
| 5   | R     | 24    | 0        | 22       | 0       | 0            |
| 5   | S     | 24    | 0        | 22       | 5       | 0            |
| 6   | A     | 43    | 0        | 30       | 1       | 0            |
| 6   | B     | 43    | 0        | 30       | 4       | 0            |
| 6   | D     | 43    | 0        | 30       | 0       | 0            |
| 6   | E     | 43    | 0        | 30       | 5       | 0            |
| 6   | G     | 43    | 0        | 30       | 0       | 0            |
| 6   | H     | 43    | 0        | 30       | 4       | 0            |
| 6   | J     | 43    | 0        | 30       | 0       | 0            |
| 6   | K     | 43    | 0        | 30       | 2       | 0            |
| 7   | A     | 2     | 0        | 0        | 0       | 0            |
| 7   | B     | 2     | 0        | 0        | 0       | 0            |
| 7   | D     | 2     | 0        | 0        | 0       | 0            |
| 7   | E     | 2     | 0        | 0        | 0       | 0            |
| 7   | G     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | H     | 2     | 0        | 0        | 0       | 0            |
| 7   | J     | 2     | 0        | 0        | 0       | 0            |
| 7   | K     | 2     | 0        | 0        | 0       | 0            |
| 8   | C     | 28    | 0        | 26       | 1       | 0            |
| 8   | F     | 28    | 0        | 26       | 0       | 0            |
| 8   | I     | 28    | 0        | 26       | 0       | 0            |
| 8   | L     | 28    | 0        | 26       | 1       | 0            |
| All | All   | 19196 | 0        | 18894    | 364     | 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 10.

All (364) 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:K:101[B]:GLU:HG3 | 3:L:230:ASN:HD22 | 1.12                     | 1.12              |
| 2:E:101[B]:GLU:HG3 | 3:F:230:ASN:HD22 | 1.08                     | 1.11              |
| 2:H:101[B]:GLU:HG3 | 3:I:230:ASN:HD22 | 1.10                     | 1.08              |
| 2:B:101[B]:GLU:HG3 | 3:C:230:ASN:HD22 | 1.12                     | 1.07              |
| 2:H:101[B]:GLU:HG3 | 3:I:230:ASN:ND2  | 1.86                     | 0.91              |
| 3:F:118:ALA:HB3    | 3:F:130:ALA:HB3  | 1.54                     | 0.89              |
| 2:E:101[B]:GLU:HG3 | 3:F:230:ASN:ND2  | 1.86                     | 0.88              |
| 3:L:118:ALA:HB3    | 3:L:130:ALA:HB3  | 1.56                     | 0.88              |
| 2:B:101[B]:GLU:HG3 | 3:C:230:ASN:ND2  | 1.90                     | 0.88              |
| 3:C:118:ALA:HB3    | 3:C:130:ALA:HB3  | 1.56                     | 0.87              |
| 2:H:22:GLU:OE1     | 2:H:117:ARG:NH2  | 2.09                     | 0.86              |
| 3:L:235:GLU:HB2    | 5:S:2:FUC:H61    | 1.57                     | 0.86              |
| 3:C:123:HIS:HB3    | 3:C:161:THR:HG23 | 1.61                     | 0.83              |
| 3:I:118:ALA:HB3    | 3:I:130:ALA:HB3  | 1.61                     | 0.82              |
| 3:I:60:THR:HG22    | 3:I:84:PRO:HB3   | 1.62                     | 0.81              |
| 3:I:123:HIS:HB3    | 3:I:161:THR:HG23 | 1.62                     | 0.81              |
| 3:L:123:HIS:HB3    | 3:L:161:THR:HG23 | 1.63                     | 0.80              |
| 3:F:123:HIS:HB3    | 3:F:161:THR:HG23 | 1.62                     | 0.80              |
| 1:G:122:HIS:HD2    | 2:H:30:ARG:HD3   | 1.48                     | 0.78              |
| 3:C:60:THR:HG22    | 3:C:84:PRO:HB3   | 1.66                     | 0.78              |
| 3:C:61:ALA:HB3     | 3:C:79:THR:HG22  | 1.66                     | 0.77              |
| 1:J:122:HIS:HD2    | 2:K:30:ARG:HD3   | 1.49                     | 0.77              |
| 3:I:104:MET:HE2    | 3:I:323:ARG:HG3  | 1.67                     | 0.77              |
| 1:A:122:HIS:HD2    | 2:B:30:ARG:HD3   | 1.50                     | 0.77              |
| 3:F:104:MET:HE2    | 3:F:323:ARG:HG3  | 1.68                     | 0.76              |
| 2:K:101[B]:GLU:HG3 | 3:L:230:ASN:ND2  | 1.94                     | 0.76              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 3:F:92:LYS:H      | 3:F:204:MET:HE2  | 1.50                     | 0.75              |
| 2:K:26:GLU:OE2    | 2:K:117:ARG:NH1  | 2.19                     | 0.74              |
| 3:I:92:LYS:H      | 3:I:204:MET:HE2  | 1.52                     | 0.74              |
| 3:C:104:MET:HE2   | 3:C:323:ARG:HG3  | 1.71                     | 0.73              |
| 3:I:61:ALA:HB3    | 3:I:79:THR:HG22  | 1.71                     | 0.71              |
| 3:L:104:MET:HE2   | 3:L:323:ARG:HG3  | 1.72                     | 0.71              |
| 3:L:92:LYS:H      | 3:L:204:MET:HE2  | 1.56                     | 0.71              |
| 3:F:216:VAL:HA    | 3:F:244:VAL:HG22 | 1.73                     | 0.70              |
| 3:F:151:ASN:OD1   | 3:F:152:ASP:N    | 2.25                     | 0.70              |
| 3:L:216:VAL:HA    | 3:L:244:VAL:HG22 | 1.74                     | 0.70              |
| 3:C:152:ASP:HB3   | 8:C:1003:NAG:H82 | 1.74                     | 0.69              |
| 3:C:346:ASP:OD1   | 3:C:346:ASP:N    | 2.26                     | 0.69              |
| 3:C:92:LYS:H      | 3:C:204:MET:HE2  | 1.56                     | 0.69              |
| 2:B:22:GLU:OE1    | 2:B:117:ARG:NH2  | 2.25                     | 0.69              |
| 2:E:101[B]:GLU:CG | 3:F:230:ASN:HD22 | 1.97                     | 0.69              |
| 2:H:98:VAL:O      | 2:H:145:TYR:OH   | 2.07                     | 0.68              |
| 3:I:346:ASP:OD1   | 3:I:346:ASP:N    | 2.27                     | 0.68              |
| 3:C:216:VAL:HA    | 3:C:244:VAL:HG22 | 1.76                     | 0.68              |
| 3:F:105:GLY:HA3   | 3:F:289:GLU:HG2  | 1.76                     | 0.68              |
| 3:F:131:THR:HG21  | 3:F:299:ALA:N    | 2.08                     | 0.68              |
| 2:B:98:VAL:O      | 2:B:145:TYR:OH   | 2.10                     | 0.67              |
| 3:C:158:ILE:O     | 3:C:161:THR:HB   | 1.95                     | 0.67              |
| 3:F:346:ASP:OD1   | 3:F:346:ASP:N    | 2.27                     | 0.67              |
| 1:D:122:HIS:HD2   | 2:E:30:ARG:HD3   | 1.60                     | 0.66              |
| 3:L:158:ILE:O     | 3:L:161:THR:HB   | 1.95                     | 0.66              |
| 3:L:346:ASP:N     | 3:L:346:ASP:OD1  | 2.29                     | 0.66              |
| 3:I:158:ILE:O     | 3:I:161:THR:HB   | 1.96                     | 0.66              |
| 2:H:101[B]:GLU:CG | 3:I:230:ASN:HD22 | 1.98                     | 0.65              |
| 3:C:174:ILE:HD12  | 3:C:191:ILE:HG23 | 1.79                     | 0.65              |
| 3:F:131:THR:HG21  | 3:F:299:ALA:H    | 1.61                     | 0.65              |
| 3:C:131:THR:HG21  | 3:C:299:ALA:N    | 2.11                     | 0.65              |
| 2:E:22:GLU:OE1    | 2:E:117:ARG:NH2  | 2.30                     | 0.65              |
| 3:I:216:VAL:HA    | 3:I:244:VAL:HG22 | 1.79                     | 0.65              |
| 3:C:307:ASP:HB3   | 3:C:309:THR:HG23 | 1.78                     | 0.64              |
| 3:I:131:THR:HG21  | 3:I:299:ALA:N    | 2.13                     | 0.64              |
| 3:F:158:ILE:O     | 3:F:161:THR:HB   | 1.96                     | 0.64              |
| 2:E:26:GLU:OE2    | 2:E:117:ARG:NH1  | 2.31                     | 0.64              |
| 3:L:69:ASP:HB3    | 3:L:71:ASN:H     | 1.63                     | 0.64              |
| 3:L:105:GLY:HA3   | 3:L:289:GLU:HG2  | 1.78                     | 0.64              |
| 2:E:82:LYS:H      | 2:E:82:LYS:HD2   | 1.64                     | 0.63              |
| 2:H:82:LYS:H      | 2:H:82:LYS:HD2   | 1.63                     | 0.63              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:82:LYS:H      | 2:B:82:LYS:HD2   | 1.64                     | 0.62              |
| 2:B:101[B]:GLU:CG | 3:C:230:ASN:HD22 | 2.01                     | 0.62              |
| 3:C:105:GLY:HA3   | 3:C:289:GLU:HG2  | 1.82                     | 0.62              |
| 6:K:201:HEM:HMC2  | 6:K:201:HEM:HBC2 | 1.82                     | 0.62              |
| 1:J:94:ASP:OD1    | 1:J:96:VAL:HG22  | 2.00                     | 0.61              |
| 3:C:34:PRO:HD2    | 3:F:68:LEU:HD21  | 1.82                     | 0.61              |
| 3:L:307:ASP:HB3   | 3:L:309:THR:HG23 | 1.83                     | 0.61              |
| 3:L:163:ARG:HG3   | 3:L:163:ARG:HH11 | 1.66                     | 0.61              |
| 3:L:131:THR:HG21  | 3:L:299:ALA:N    | 2.16                     | 0.60              |
| 3:F:174:ILE:HD12  | 3:F:191:ILE:HG23 | 1.83                     | 0.60              |
| 3:I:105:GLY:HA3   | 3:I:289:GLU:HG2  | 1.84                     | 0.60              |
| 3:I:174:ILE:HD12  | 3:I:191:ILE:HG23 | 1.83                     | 0.60              |
| 3:I:307:ASP:HB3   | 3:I:309:THR:HG23 | 1.84                     | 0.60              |
| 3:C:290:ASP:CG    | 3:C:291:THR:H    | 2.10                     | 0.59              |
| 1:D:94:ASP:OD1    | 1:D:96:VAL:HG22  | 2.02                     | 0.59              |
| 3:L:174:ILE:HD12  | 3:L:191:ILE:HG23 | 1.84                     | 0.59              |
| 3:F:253:TYR:CE1   | 3:F:326:GLU:HG3  | 2.38                     | 0.59              |
| 2:K:18:VAL:HG12   | 2:K:118:LEU:HD11 | 1.85                     | 0.59              |
| 2:K:14:LEU:HD22   | 2:K:126:VAL:HG21 | 1.85                     | 0.59              |
| 3:F:69:ASP:HB3    | 3:F:71:ASN:H     | 1.68                     | 0.59              |
| 3:C:69:ASP:HB3    | 3:C:71:ASN:H     | 1.67                     | 0.58              |
| 1:G:94:ASP:OD1    | 1:G:96:VAL:HG22  | 2.02                     | 0.58              |
| 3:C:257:SER:OG    | 3:C:263:LYS:NZ   | 2.25                     | 0.58              |
| 3:C:296:ALA:HA    | 3:C:316:LEU:HB3  | 1.86                     | 0.58              |
| 3:I:290:ASP:CG    | 3:I:291:THR:H    | 2.11                     | 0.58              |
| 3:L:104:MET:HE3   | 3:L:229:ALA:HA   | 1.86                     | 0.58              |
| 1:A:94:ASP:OD1    | 1:A:96:VAL:HG22  | 2.03                     | 0.58              |
| 3:F:163:ARG:HG3   | 3:F:163:ARG:HH11 | 1.68                     | 0.58              |
| 6:B:201:HEM:HMC2  | 6:B:201:HEM:HBC2 | 1.86                     | 0.58              |
| 3:F:290:ASP:CG    | 3:F:291:THR:H    | 2.13                     | 0.57              |
| 3:I:36:PRO:HG3    | 3:L:48:VAL:HG11  | 1.85                     | 0.57              |
| 3:C:163:ARG:HG3   | 3:C:163:ARG:HH11 | 1.68                     | 0.57              |
| 3:I:69:ASP:HB3    | 3:I:71:ASN:H     | 1.69                     | 0.57              |
| 3:I:163:ARG:HG3   | 3:I:163:ARG:HH11 | 1.70                     | 0.57              |
| 3:L:253:TYR:CE1   | 3:L:326:GLU:HG3  | 2.39                     | 0.57              |
| 3:I:296:ALA:HA    | 3:I:316:LEU:HB3  | 1.86                     | 0.57              |
| 6:E:201:HEM:HMC2  | 6:E:201:HEM:HBC2 | 1.88                     | 0.56              |
| 3:F:124:HIS:CE1   | 3:F:148:GLY:HA2  | 2.40                     | 0.56              |
| 1:J:123:ALA:HA    | 2:K:34:VAL:HG22  | 1.86                     | 0.56              |
| 2:K:82:LYS:H      | 2:K:82:LYS:HD2   | 1.70                     | 0.56              |
| 3:L:235:GLU:HB2   | 5:S:2:FUC:C6     | 2.32                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:F:307:ASP:HB3    | 3:F:309:THR:HG23   | 1.86                     | 0.56              |
| 2:K:101[B]:GLU:HG2 | 3:L:228:ASN:CG     | 2.31                     | 0.56              |
| 2:K:37:TRP:HA      | 3:L:287:TYR:HB3    | 1.88                     | 0.55              |
| 2:B:26:GLU:OE2     | 2:B:117:ARG:NH1    | 2.39                     | 0.55              |
| 2:B:93:CYS:HB2     | 2:B:145:TYR:CE1    | 2.41                     | 0.55              |
| 3:C:47:MET:HG2     | 3:C:67:THR:HB      | 1.89                     | 0.55              |
| 3:F:296:ALA:HA     | 3:F:316:LEU:HB3    | 1.89                     | 0.55              |
| 3:L:183:ASN:CG     | 8:L:1002:NAG:O7    | 2.50                     | 0.55              |
| 6:H:201:HEM:HBC2   | 6:H:201:HEM:HMC2   | 1.88                     | 0.55              |
| 3:L:290:ASP:CG     | 3:L:291:THR:H      | 2.13                     | 0.55              |
| 3:I:131:THR:HG21   | 3:I:299:ALA:H      | 1.71                     | 0.55              |
| 3:I:253:TYR:CE1    | 3:I:326:GLU:HG3    | 2.41                     | 0.55              |
| 6:K:201:HEM:HMB1   | 6:K:201:HEM:HBB2   | 1.88                     | 0.54              |
| 4:M:1:NAG:O3       | 4:M:2:NAG:N2       | 2.40                     | 0.54              |
| 3:C:253:TYR:CE1    | 3:C:326:GLU:HG3    | 2.43                     | 0.54              |
| 3:F:131:THR:HG23   | 3:F:298:SER:HA     | 1.89                     | 0.54              |
| 3:I:131:THR:HG23   | 3:I:298:SER:HA     | 1.88                     | 0.54              |
| 3:L:296:ALA:HA     | 3:L:316:LEU:HB3    | 1.90                     | 0.53              |
| 6:B:201:HEM:HMB1   | 6:B:201:HEM:HBB2   | 1.91                     | 0.53              |
| 2:B:37:TRP:HA      | 3:C:287:TYR:HB3    | 1.91                     | 0.53              |
| 3:C:104:MET:HE3    | 3:C:229:ALA:HA     | 1.90                     | 0.53              |
| 3:F:89:VAL:O       | 3:F:204:MET:HE3    | 2.09                     | 0.53              |
| 2:K:101[A]:GLU:HG3 | 2:K:102:ASN:N      | 2.24                     | 0.52              |
| 6:E:201:HEM:HMB1   | 6:E:201:HEM:HBB2   | 1.90                     | 0.52              |
| 3:C:131:THR:HG23   | 3:C:298:SER:HA     | 1.90                     | 0.52              |
| 2:K:99:ASP:OD1     | 2:K:101[A]:GLU:HG2 | 2.09                     | 0.52              |
| 2:H:41:PHE:HB3     | 6:H:201:HEM:HMD2   | 1.92                     | 0.51              |
| 6:H:201:HEM:HMB1   | 6:H:201:HEM:HBB2   | 1.93                     | 0.51              |
| 3:I:118:ALA:HB2    | 3:I:166:VAL:HG12   | 1.91                     | 0.51              |
| 2:K:91:LEU:O       | 2:K:95:GLN:HB3     | 2.10                     | 0.51              |
| 2:K:101[B]:GLU:HG2 | 3:L:228:ASN:OD1    | 2.11                     | 0.51              |
| 2:K:101[B]:GLU:OE2 | 5:S:1:NAG:O7       | 2.29                     | 0.51              |
| 1:A:1:VAL:N        | 1:A:127:LYS:HD3    | 2.26                     | 0.50              |
| 3:C:131:THR:HG21   | 3:C:299:ALA:H      | 1.75                     | 0.50              |
| 1:D:53:ASP:HA      | 1:D:56:LYS:HB3     | 1.93                     | 0.50              |
| 2:E:48:LEU:HD22    | 2:E:54:VAL:HG22    | 1.94                     | 0.50              |
| 2:H:37:TRP:HA      | 3:I:287:TYR:HB3    | 1.93                     | 0.50              |
| 2:H:93:CYS:HB2     | 2:H:145:TYR:CE1    | 2.47                     | 0.50              |
| 3:I:47:MET:HG2     | 3:I:67:THR:HB      | 1.93                     | 0.50              |
| 3:F:104:MET:HE3    | 3:F:229:ALA:HA     | 1.94                     | 0.50              |
| 2:K:40:ARG:HH22    | 3:L:289:GLU:CD     | 2.19                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:104:MET:HE3  | 3:I:229:ALA:HA   | 1.93                     | 0.50              |
| 1:G:122:HIS:CD2  | 2:H:30:ARG:HD3   | 2.38                     | 0.49              |
| 3:C:69:ASP:HB2   | 3:C:73:GLN:H     | 1.78                     | 0.49              |
| 2:H:26:GLU:OE2   | 2:H:117:ARG:NH1  | 2.44                     | 0.49              |
| 3:F:92:LYS:H     | 3:F:204:MET:CE   | 2.24                     | 0.49              |
| 1:G:93:VAL:HG22  | 1:G:98:PHE:CE2   | 2.47                     | 0.49              |
| 2:B:48:LEU:HD22  | 2:B:54:VAL:HG22  | 1.94                     | 0.49              |
| 1:A:122:HIS:CD2  | 2:B:30:ARG:HD3   | 2.40                     | 0.48              |
| 3:C:118:ALA:HB2  | 3:C:166:VAL:HG12 | 1.95                     | 0.48              |
| 1:J:53:ASP:HA    | 1:J:56:LYS:HB3   | 1.95                     | 0.48              |
| 2:E:93:CYS:HB2   | 2:E:145:TYR:CE1  | 2.48                     | 0.48              |
| 1:J:122:HIS:CD2  | 2:K:30:ARG:HD3   | 2.39                     | 0.48              |
| 2:B:41:PHE:HB3   | 6:B:201:HEM:HMD2 | 1.95                     | 0.48              |
| 2:H:122:PHE:CE2  | 2:H:127:GLN:HB2  | 2.48                     | 0.48              |
| 1:D:93:VAL:HG22  | 1:D:98:PHE:CE2   | 2.49                     | 0.48              |
| 2:H:48:LEU:HD22  | 2:H:54:VAL:HG22  | 1.96                     | 0.48              |
| 2:K:109:VAL:O    | 2:K:113:VAL:HG13 | 2.13                     | 0.48              |
| 3:C:92:LYS:NZ    | 3:C:309:THR:HG22 | 2.28                     | 0.48              |
| 3:C:107:SER:HB2  | 3:C:239:TYR:O    | 2.14                     | 0.48              |
| 2:E:66:LYS:HE3   | 6:E:201:HEM:HAA1 | 1.96                     | 0.48              |
| 3:F:149:HIS:NE2  | 3:F:161:THR:HG21 | 2.29                     | 0.48              |
| 2:K:8:LYS:O      | 2:K:12:LEU:HB2   | 2.14                     | 0.48              |
| 2:E:122:PHE:CE2  | 2:E:127:GLN:HB2  | 2.49                     | 0.47              |
| 3:I:69:ASP:HB2   | 3:I:73:GLN:H     | 1.79                     | 0.47              |
| 3:L:131:THR:HG23 | 3:L:298:SER:HA   | 1.95                     | 0.47              |
| 3:F:235:GLU:HB2  | 5:P:2:FUC:H61    | 1.96                     | 0.47              |
| 3:L:135:GLU:O    | 3:L:197:VAL:HG23 | 2.14                     | 0.47              |
| 3:C:60:THR:CG2   | 3:C:84:PRO:HB3   | 2.42                     | 0.47              |
| 2:H:66:LYS:HE3   | 6:H:201:HEM:HAA1 | 1.97                     | 0.47              |
| 3:I:103:ILE:HD13 | 3:I:240:VAL:HG22 | 1.96                     | 0.47              |
| 2:B:79:ASP:OD1   | 2:B:79:ASP:N     | 2.46                     | 0.47              |
| 1:J:1:VAL:N      | 1:J:127:LYS:HD3  | 2.30                     | 0.47              |
| 1:G:42:TYR:CE2   | 1:G:93:VAL:HA    | 2.50                     | 0.47              |
| 1:A:93:VAL:HG22  | 1:A:98:PHE:CE2   | 2.49                     | 0.47              |
| 2:B:66:LYS:HE3   | 6:B:201:HEM:HAA1 | 1.96                     | 0.47              |
| 3:F:235:GLU:HA   | 5:P:2:FUC:H61    | 1.97                     | 0.47              |
| 3:F:336:ILE:HD12 | 3:F:340:ILE:HD11 | 1.97                     | 0.47              |
| 1:J:31:ARG:HD3   | 2:K:127:GLN:OE1  | 2.14                     | 0.47              |
| 2:E:41:PHE:HB3   | 6:E:201:HEM:HMD2 | 1.96                     | 0.47              |
| 3:F:116:TRP:O    | 3:F:131:THR:HA   | 2.15                     | 0.47              |
| 2:B:14:LEU:HD21  | 2:B:118:LEU:HD23 | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:93:VAL:HG22  | 1:J:98:PHE:CE2   | 2.50                     | 0.47              |
| 3:F:69:ASP:HB2   | 3:F:73:GLN:H     | 1.80                     | 0.46              |
| 3:L:69:ASP:HB3   | 3:L:71:ASN:N     | 2.29                     | 0.46              |
| 3:C:93:PRO:HG3   | 3:C:116:TRP:CZ3  | 2.51                     | 0.46              |
| 3:I:336:ILE:HD12 | 3:I:340:ILE:HD11 | 1.97                     | 0.46              |
| 2:K:142:ALA:O    | 2:K:145:TYR:HB2  | 2.15                     | 0.46              |
| 3:F:135:GLU:O    | 3:F:197:VAL:HG23 | 2.16                     | 0.46              |
| 2:K:14:LEU:O     | 2:K:18:VAL:HG13  | 2.15                     | 0.46              |
| 3:L:131:THR:HG21 | 3:L:299:ALA:H    | 1.80                     | 0.46              |
| 3:L:118:ALA:HB2  | 3:L:166:VAL:HG12 | 1.97                     | 0.46              |
| 3:C:135:GLU:O    | 3:C:197:VAL:HG23 | 2.16                     | 0.46              |
| 3:I:206:ILE:HG21 | 3:I:312:ALA:HB2  | 1.97                     | 0.46              |
| 3:F:133:ILE:CG1  | 3:F:208:LEU:HD21 | 2.46                     | 0.46              |
| 1:J:138:SER:HB2  | 3:L:271:VAL:HG13 | 1.98                     | 0.46              |
| 2:H:40:ARG:HH22  | 3:I:289:GLU:CD   | 2.23                     | 0.46              |
| 1:J:107:VAL:HG13 | 2:K:115:ALA:HB2  | 1.98                     | 0.46              |
| 2:E:67:VAL:O     | 2:E:70:SER:HB3   | 2.16                     | 0.46              |
| 3:L:175:GLU:HB2  | 3:L:194:LYS:HA   | 1.98                     | 0.46              |
| 1:D:76:LEU:HD23  | 1:D:76:LEU:HA    | 1.69                     | 0.46              |
| 2:H:14:LEU:HD21  | 2:H:118:LEU:HD23 | 1.97                     | 0.46              |
| 3:I:57:LYS:HB2   | 3:I:57:LYS:HE3   | 1.66                     | 0.46              |
| 3:C:89:VAL:O     | 3:C:204:MET:HE3  | 2.16                     | 0.46              |
| 3:L:103:ILE:HD13 | 3:L:240:VAL:HG22 | 1.97                     | 0.46              |
| 3:I:92:LYS:NZ    | 3:I:309:THR:HG22 | 2.31                     | 0.45              |
| 2:H:79:ASP:OD1   | 2:H:79:ASP:N     | 2.49                     | 0.45              |
| 1:G:1:VAL:N      | 1:G:127:LYS:HD3  | 2.30                     | 0.45              |
| 3:I:284:LEU:HD22 | 3:I:290:ASP:HB2  | 1.97                     | 0.45              |
| 4:Q:1:NAG:O3     | 4:Q:2:NAG:N2     | 2.50                     | 0.45              |
| 3:L:163:ARG:HG3  | 3:L:163:ARG:NH1  | 2.30                     | 0.45              |
| 2:B:40:ARG:HH22  | 3:C:289:GLU:CD   | 2.24                     | 0.45              |
| 3:I:135:GLU:O    | 3:I:197:VAL:HG23 | 2.16                     | 0.45              |
| 2:K:131:GLN:HA   | 2:K:134:VAL:HG22 | 1.97                     | 0.45              |
| 2:B:122:PHE:CE2  | 2:B:127:GLN:HB2  | 2.51                     | 0.45              |
| 3:F:145:LEU:HD12 | 3:F:145:LEU:HA   | 1.86                     | 0.45              |
| 3:C:48:VAL:HG11  | 3:F:36:PRO:HG3   | 1.99                     | 0.45              |
| 3:C:57:LYS:HB2   | 3:C:57:LYS:HE3   | 1.63                     | 0.45              |
| 3:C:337:LEU:HD23 | 3:C:337:LEU:HA   | 1.81                     | 0.45              |
| 4:O:1:NAG:O3     | 4:O:2:NAG:N2     | 2.49                     | 0.45              |
| 3:C:58:LEU:HD23  | 3:C:58:LEU:HA    | 1.85                     | 0.45              |
| 1:G:53:ASP:HA    | 1:G:56:LYS:HB3   | 1.98                     | 0.45              |
| 1:A:42:TYR:CE2   | 1:A:93:VAL:HA    | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:18:VAL:CG1   | 2:B:118:LEU:HD21 | 2.47                     | 0.44              |
| 3:C:206:ILE:HG21 | 3:C:312:ALA:HB2  | 2.00                     | 0.44              |
| 2:E:98:VAL:O     | 2:E:145:TYR:OH   | 2.20                     | 0.44              |
| 2:K:28:LEU:O     | 2:K:32:LEU:HD13  | 2.17                     | 0.44              |
| 3:F:118:ALA:HB2  | 3:F:166:VAL:HG12 | 2.00                     | 0.44              |
| 3:L:92:LYS:H     | 3:L:204:MET:CE   | 2.27                     | 0.44              |
| 3:C:197:VAL:HG11 | 3:C:203:VAL:HG11 | 1.98                     | 0.44              |
| 2:H:57:ASN:HA    | 2:H:58:PRO:HD3   | 1.90                     | 0.44              |
| 2:K:71:PHE:CZ    | 2:K:137:VAL:HG21 | 2.53                     | 0.44              |
| 2:K:127:GLN:O    | 2:K:131:GLN:HG2  | 2.17                     | 0.44              |
| 3:L:336:ILE:HD12 | 3:L:340:ILE:HD11 | 2.00                     | 0.44              |
| 3:C:269:VAL:HG23 | 3:C:271:VAL:H    | 1.82                     | 0.44              |
| 3:L:115:PRO:HB2  | 3:L:204:MET:HG2  | 2.00                     | 0.44              |
| 3:F:163:ARG:HG3  | 3:F:163:ARG:NH1  | 2.32                     | 0.44              |
| 3:F:290:ASP:OD2  | 3:F:321:SER:HB2  | 2.18                     | 0.44              |
| 2:K:81:LEU:HD12  | 2:K:81:LEU:HA    | 1.80                     | 0.44              |
| 3:C:92:LYS:CE    | 3:C:309:THR:HG22 | 2.47                     | 0.44              |
| 3:F:175:GLU:HB2  | 3:F:194:LYS:HA   | 1.99                     | 0.44              |
| 3:F:206:ILE:HG21 | 3:F:312:ALA:HB2  | 2.00                     | 0.44              |
| 3:I:107:SER:HB2  | 3:I:239:TYR:O    | 2.17                     | 0.44              |
| 3:L:63:ASP:OD2   | 3:L:65:VAL:HB    | 2.17                     | 0.44              |
| 1:D:1:VAL:N      | 1:D:127:LYS:HD3  | 2.33                     | 0.44              |
| 2:K:144:LYS:HD3  | 2:K:144:LYS:HA   | 1.81                     | 0.44              |
| 3:C:163:ARG:HG3  | 3:C:163:ARG:NH1  | 2.32                     | 0.44              |
| 3:I:175:GLU:HB2  | 3:I:194:LYS:HA   | 1.99                     | 0.44              |
| 1:A:66:LEU:O     | 1:A:70:VAL:HG23  | 2.17                     | 0.43              |
| 2:E:19:ASN:O     | 2:E:23:VAL:HG13  | 2.18                     | 0.43              |
| 2:E:81:LEU:HD12  | 2:E:81:LEU:HA    | 1.88                     | 0.43              |
| 1:G:2:LEU:HD12   | 1:G:2:LEU:HA     | 1.81                     | 0.43              |
| 1:G:38:THR:O     | 1:G:41:THR:HB    | 2.18                     | 0.43              |
| 3:C:145:LEU:HD12 | 3:C:145:LEU:HA   | 1.90                     | 0.43              |
| 3:F:337:LEU:HD23 | 3:F:337:LEU:HA   | 1.83                     | 0.43              |
| 1:J:66:LEU:O     | 1:J:70:VAL:HG23  | 2.17                     | 0.43              |
| 3:L:116:TRP:O    | 3:L:131:THR:HA   | 2.17                     | 0.43              |
| 3:F:197:VAL:HG11 | 3:F:203:VAL:HG11 | 2.00                     | 0.43              |
| 2:B:18:VAL:HG12  | 2:B:118:LEU:HD21 | 2.00                     | 0.43              |
| 3:I:92:LYS:H     | 3:I:204:MET:CE   | 2.27                     | 0.43              |
| 3:L:89:VAL:O     | 3:L:204:MET:HE3  | 2.18                     | 0.43              |
| 1:A:53:ASP:HA    | 1:A:56:LYS:HB3   | 2.01                     | 0.43              |
| 1:J:42:TYR:CE2   | 1:J:93:VAL:HA    | 2.53                     | 0.43              |
| 3:C:284:LEU:HD22 | 3:C:290:ASP:HB2  | 2.01                     | 0.43              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 2:E:18:VAL:HG12    | 2:E:118:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:38:THR:O       | 1:A:41:THR:HB    | 2.19                     | 0.43              |
| 3:C:175:GLU:HB2    | 3:C:194:LYS:HA   | 1.99                     | 0.43              |
| 1:G:76:LEU:HA      | 1:G:76:LEU:HD23  | 1.76                     | 0.43              |
| 2:H:101[B]:GLU:HG2 | 3:I:228:ASN:CG   | 2.44                     | 0.43              |
| 3:I:113:SER:C      | 3:I:115:PRO:HD3  | 2.44                     | 0.43              |
| 3:I:194:LYS:HE3    | 3:I:194:LYS:HB2  | 1.79                     | 0.43              |
| 3:C:137:TRP:CZ2    | 3:C:192:LYS:HD2  | 2.54                     | 0.43              |
| 3:I:58:LEU:HD23    | 3:I:58:LEU:HA    | 1.86                     | 0.43              |
| 3:C:92:LYS:HB2     | 3:C:204:MET:HE1  | 2.01                     | 0.42              |
| 3:C:104:MET:HE3    | 3:C:104:MET:HB3  | 1.90                     | 0.42              |
| 1:J:76:LEU:HD23    | 1:J:76:LEU:HA    | 1.73                     | 0.42              |
| 3:F:194:LYS:HE3    | 3:F:194:LYS:HB2  | 1.84                     | 0.42              |
| 3:C:103:ILE:HD13   | 3:C:240:VAL:HG22 | 2.01                     | 0.42              |
| 3:C:116:TRP:O      | 3:C:131:THR:HA   | 2.19                     | 0.42              |
| 3:C:336:ILE:HD12   | 3:C:340:ILE:HD11 | 2.02                     | 0.42              |
| 3:F:256:GLY:HA3    | 3:F:257:SER:HA   | 1.94                     | 0.42              |
| 2:K:101[B]:GLU:HG2 | 3:L:228:ASN:ND2  | 2.34                     | 0.42              |
| 2:B:24:GLY:HA2     | 2:B:68:LEU:HD23  | 2.02                     | 0.42              |
| 3:I:149:HIS:NE2    | 3:I:161:THR:HG21 | 2.35                     | 0.42              |
| 3:F:269:VAL:HG23   | 3:F:271:VAL:H    | 1.83                     | 0.42              |
| 2:H:18:VAL:CG1     | 2:H:118:LEU:HD21 | 2.50                     | 0.42              |
| 3:L:133:ILE:CG1    | 3:L:208:LEU:HD21 | 2.50                     | 0.42              |
| 3:L:119:LYS:HB2    | 3:L:225:TRP:CD1  | 2.54                     | 0.42              |
| 3:L:269:VAL:HG23   | 3:L:271:VAL:H    | 1.83                     | 0.42              |
| 3:I:251:VAL:HG22   | 3:I:275:LEU:HD13 | 2.02                     | 0.42              |
| 6:A:201:HEM:CMB    | 6:A:201:HEM:HBB2 | 2.50                     | 0.42              |
| 1:D:28:ALA:CB      | 1:D:105:LEU:HD13 | 2.50                     | 0.42              |
| 3:L:307:ASP:O      | 3:L:309:THR:HG23 | 2.20                     | 0.42              |
| 1:D:2:LEU:HA       | 1:D:2:LEU:HD12   | 1.82                     | 0.42              |
| 3:I:163:ARG:HG3    | 3:I:163:ARG:NH1  | 2.33                     | 0.42              |
| 3:C:256:GLY:HA3    | 3:C:257:SER:HA   | 1.95                     | 0.42              |
| 3:F:257:SER:OG     | 3:F:258:THR:HA   | 2.20                     | 0.42              |
| 3:I:130:ALA:O      | 3:I:139:LEU:O    | 2.37                     | 0.42              |
| 3:I:50:TYR:OH      | 3:L:37:PRO:HG2   | 2.20                     | 0.41              |
| 3:I:151:ASN:OD1    | 3:I:152:ASP:N    | 2.53                     | 0.41              |
| 2:K:83:GLY:HA2     | 2:K:86:ALA:HB2   | 2.02                     | 0.41              |
| 1:D:28:ALA:HB2     | 1:D:105:LEU:HD13 | 2.03                     | 0.41              |
| 1:D:66:LEU:O       | 1:D:70:VAL:HG23  | 2.20                     | 0.41              |
| 3:F:60:THR:HG23    | 3:F:62:GLY:O     | 2.20                     | 0.41              |
| 3:F:168:LYS:O      | 3:F:170:GLN:N    | 2.53                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 3:F:267:SER:HA     | 3:F:268:PRO:HD2  | 1.86                     | 0.41              |
| 3:I:145:LEU:HD12   | 3:I:145:LEU:HA   | 1.80                     | 0.41              |
| 3:L:235:GLU:HA     | 5:S:2:FUC:H63    | 2.03                     | 0.41              |
| 1:D:99:LYS:HD3     | 3:F:229:ALA:O    | 2.20                     | 0.41              |
| 3:L:146:ARG:HD3    | 3:L:151:ASN:HA   | 2.03                     | 0.41              |
| 3:I:133:ILE:CG1    | 3:I:208:LEU:HD21 | 2.50                     | 0.41              |
| 3:L:58:LEU:HD22    | 3:L:84:PRO:HB2   | 2.03                     | 0.41              |
| 3:L:249:LYS:HB3    | 3:L:249:LYS:HE2  | 1.90                     | 0.41              |
| 1:A:76:LEU:HA      | 1:A:76:LEU:HD23  | 1.73                     | 0.41              |
| 2:E:100:PRO:HA     | 2:E:103:PHE:CD2  | 2.56                     | 0.41              |
| 3:I:124:HIS:CE1    | 3:I:148:GLY:HA2  | 2.55                     | 0.41              |
| 1:J:27:GLU:CD      | 1:J:108:THR:HG23 | 2.46                     | 0.41              |
| 3:L:66:TYR:CZ      | 3:L:84:PRO:HD3   | 2.55                     | 0.41              |
| 2:E:101[B]:GLU:HG2 | 3:F:228:ASN:CG   | 2.46                     | 0.41              |
| 2:K:19:ASN:O       | 2:K:23:VAL:HG13  | 2.20                     | 0.41              |
| 3:L:235:GLU:CB     | 5:S:2:FUC:H61    | 2.38                     | 0.41              |
| 1:A:52:SER:HB3     | 1:A:55:VAL:HG13  | 2.02                     | 0.41              |
| 2:E:88:LEU:HD11    | 6:E:201:HEM:HMA1 | 2.03                     | 0.41              |
| 2:H:18:VAL:HG12    | 2:H:118:LEU:HD21 | 2.02                     | 0.41              |
| 1:J:38:THR:O       | 1:J:41:THR:HB    | 2.21                     | 0.41              |
| 2:K:15:TRP:O       | 2:K:18:VAL:HG22  | 2.21                     | 0.41              |
| 3:L:149:HIS:HB3    | 3:L:153:THR:OG1  | 2.21                     | 0.41              |
| 3:C:113:SER:C      | 3:C:115:PRO:HD3  | 2.45                     | 0.41              |
| 3:C:147:LEU:HD23   | 3:C:147:LEU:HA   | 1.91                     | 0.41              |
| 3:C:251:VAL:HG22   | 3:C:275:LEU:HD13 | 2.02                     | 0.41              |
| 1:D:42:TYR:CE2     | 1:D:93:VAL:HA    | 2.56                     | 0.41              |
| 2:E:18:VAL:CG1     | 2:E:118:LEU:HD21 | 2.50                     | 0.41              |
| 3:I:93:PRO:HG3     | 3:I:116:TRP:CZ3  | 2.56                     | 0.41              |
| 2:K:26:GLU:OE1     | 2:K:30:ARG:NH2   | 2.42                     | 0.41              |
| 3:I:92:LYS:HB2     | 3:I:204:MET:HE1  | 2.03                     | 0.41              |
| 2:E:14:LEU:HD21    | 2:E:118:LEU:HD23 | 2.04                     | 0.40              |
| 3:L:194:LYS:HB2    | 3:L:194:LYS:HE3  | 1.82                     | 0.40              |
| 3:L:206:ILE:HD13   | 3:L:312:ALA:HB2  | 2.03                     | 0.40              |
| 3:F:151:ASN:OD1    | 3:F:152:ASP:OD1  | 2.40                     | 0.40              |
| 3:F:260:PRO:HA     | 3:F:263:LYS:HE2  | 2.03                     | 0.40              |
| 1:J:131:ASN:CG     | 3:L:324:THR:HG23 | 2.47                     | 0.40              |
| 3:L:39:ILE:HG21    | 3:L:39:ILE:HD13  | 1.69                     | 0.40              |
| 3:C:124:HIS:CE1    | 3:C:148:GLY:HA2  | 2.57                     | 0.40              |
| 3:I:60:THR:CG2     | 3:I:84:PRO:HB3   | 2.40                     | 0.40              |
| 3:I:92:LYS:CE      | 3:I:309:THR:HG22 | 2.51                     | 0.40              |
| 3:L:58:LEU:HD23    | 3:L:58:LEU:HA    | 1.80                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:113:SER:C    | 3:F:115:PRO:HD3  | 2.45                     | 0.40              |
| 3:I:206:ILE:HD13 | 3:I:312:ALA:HB2  | 2.02                     | 0.40              |
| 3:L:60:THR:HG23  | 3:L:62:GLY:O     | 2.22                     | 0.40              |
| 3:L:197:VAL:HG11 | 3:L:203:VAL:HG11 | 2.02                     | 0.40              |
| 3:L:259:VAL:HG11 | 3:L:262:LYS:HD2  | 2.03                     | 0.40              |
| 2:E:24:GLY:HA2   | 2:E:68:LEU:HD23  | 2.03                     | 0.40              |
| 3:F:66:TYR:CZ    | 3:F:84:PRO:HD3   | 2.57                     | 0.40              |
| 1:G:27:GLU:CD    | 1:G:108:THR:HG23 | 2.47                     | 0.40              |
| 2:K:18:VAL:CG1   | 2:K:118:LEU:HD21 | 2.51                     | 0.40              |
| 3:L:66:TYR:CE1   | 3:L:84:PRO:HD3   | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 139/141 (99%) | 134 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 1   | D     | 139/141 (99%) | 135 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | G     | 139/141 (99%) | 133 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | J     | 139/141 (99%) | 134 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 2   | B     | 145/146 (99%) | 143 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 2   | E     | 145/146 (99%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 2   | H     | 145/146 (99%) | 143 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 2   | K     | 145/146 (99%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 3   | C     | 305/347 (88%) | 288 (94%) | 15 (5%) | 2 (1%)   | 18          | 48  |
| 3   | F     | 305/347 (88%) | 284 (93%) | 20 (7%) | 1 (0%)   | 36          | 65  |
| 3   | I     | 305/347 (88%) | 287 (94%) | 15 (5%) | 3 (1%)   | 12          | 39  |
| 3   | L     | 305/347 (88%) | 285 (93%) | 18 (6%) | 2 (1%)   | 18          | 48  |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| All | All   | 2356/2536 (93%) | 2250 (96%) | 98 (4%) | 8 (0%)   | 36          | 65 |

All (8) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 258 | THR  |
| 3   | L     | 169 | LYS  |
| 3   | L     | 258 | THR  |
| 3   | C     | 169 | LYS  |
| 3   | C     | 258 | THR  |
| 3   | I     | 168 | LYS  |
| 3   | I     | 169 | LYS  |
| 3   | I     | 258 | THR  |

### 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     | 111/111 (100%)  | 98 (88%)   | 13 (12%)  | 5           | 17 |
| 1   | D     | 111/111 (100%)  | 97 (87%)   | 14 (13%)  | 4           | 14 |
| 1   | G     | 111/111 (100%)  | 97 (87%)   | 14 (13%)  | 4           | 14 |
| 1   | J     | 111/111 (100%)  | 98 (88%)   | 13 (12%)  | 5           | 17 |
| 2   | B     | 120/119 (101%)  | 97 (81%)   | 23 (19%)  | 1           | 5  |
| 2   | E     | 120/119 (101%)  | 96 (80%)   | 24 (20%)  | 1           | 4  |
| 2   | H     | 120/119 (101%)  | 96 (80%)   | 24 (20%)  | 1           | 4  |
| 2   | K     | 120/119 (101%)  | 96 (80%)   | 24 (20%)  | 1           | 4  |
| 3   | C     | 268/296 (90%)   | 219 (82%)  | 49 (18%)  | 2           | 6  |
| 3   | F     | 268/296 (90%)   | 225 (84%)  | 43 (16%)  | 2           | 8  |
| 3   | I     | 268/296 (90%)   | 220 (82%)  | 48 (18%)  | 2           | 6  |
| 3   | L     | 268/296 (90%)   | 224 (84%)  | 44 (16%)  | 2           | 8  |
| All | All   | 1996/2104 (95%) | 1663 (83%) | 333 (17%) | 2           | 7  |

All (333) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 2   | LEU  |
| 1   | A     | 38  | THR  |
| 1   | A     | 41  | THR  |
| 1   | A     | 55  | VAL  |
| 1   | A     | 61  | LYS  |
| 1   | A     | 80  | LEU  |
| 1   | A     | 84  | SER  |
| 1   | A     | 86  | LEU  |
| 1   | A     | 93  | VAL  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 106 | LEU  |
| 1   | A     | 109 | LEU  |
| 1   | A     | 129 | LEU  |
| 2   | B     | 4   | SER  |
| 2   | B     | 8   | LYS  |
| 2   | B     | 12  | LEU  |
| 2   | B     | 17  | LYS  |
| 2   | B     | 18  | VAL  |
| 2   | B     | 23  | VAL  |
| 2   | B     | 32  | LEU  |
| 2   | B     | 43  | GLU  |
| 2   | B     | 67  | VAL  |
| 2   | B     | 68  | LEU  |
| 2   | B     | 71  | PHE  |
| 2   | B     | 75  | LEU  |
| 2   | B     | 77  | HIS  |
| 2   | B     | 78  | LEU  |
| 2   | B     | 81  | LEU  |
| 2   | B     | 91  | LEU  |
| 2   | B     | 112 | VAL  |
| 2   | B     | 113 | VAL  |
| 2   | B     | 118 | LEU  |
| 2   | B     | 126 | VAL  |
| 2   | B     | 127 | GLN  |
| 2   | B     | 137 | VAL  |
| 2   | B     | 144 | LYS  |
| 3   | C     | 53  | GLN  |
| 3   | C     | 58  | LEU  |
| 3   | C     | 60  | THR  |
| 3   | C     | 67  | THR  |
| 3   | C     | 68  | LEU  |
| 3   | C     | 70  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 75  | THR  |
| 3   | C     | 77  | LYS  |
| 3   | C     | 82  | LYS  |
| 3   | C     | 95  | ASN  |
| 3   | C     | 97  | VAL  |
| 3   | C     | 104 | MET  |
| 3   | C     | 108 | LEU  |
| 3   | C     | 133 | ILE  |
| 3   | C     | 145 | LEU  |
| 3   | C     | 164 | LEU  |
| 3   | C     | 168 | LYS  |
| 3   | C     | 174 | ILE  |
| 3   | C     | 177 | VAL  |
| 3   | C     | 178 | ILE  |
| 3   | C     | 182 | ASP  |
| 3   | C     | 183 | ASN  |
| 3   | C     | 185 | THR  |
| 3   | C     | 197 | VAL  |
| 3   | C     | 200 | ASN  |
| 3   | C     | 204 | MET  |
| 3   | C     | 210 | SER  |
| 3   | C     | 214 | VAL  |
| 3   | C     | 216 | VAL  |
| 3   | C     | 218 | LEU  |
| 3   | C     | 231 | LEU  |
| 3   | C     | 235 | GLU  |
| 3   | C     | 240 | VAL  |
| 3   | C     | 244 | VAL  |
| 3   | C     | 247 | GLN  |
| 3   | C     | 259 | VAL  |
| 3   | C     | 261 | GLU  |
| 3   | C     | 266 | LYS  |
| 3   | C     | 271 | VAL  |
| 3   | C     | 277 | GLU  |
| 3   | C     | 291 | THR  |
| 3   | C     | 302 | VAL  |
| 3   | C     | 316 | LEU  |
| 3   | C     | 321 | SER  |
| 3   | C     | 331 | VAL  |
| 3   | C     | 332 | ARG  |
| 3   | C     | 338 | ASP  |
| 3   | C     | 342 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 346 | ASP  |
| 1   | D     | 2   | LEU  |
| 1   | D     | 38  | THR  |
| 1   | D     | 41  | THR  |
| 1   | D     | 55  | VAL  |
| 1   | D     | 61  | LYS  |
| 1   | D     | 80  | LEU  |
| 1   | D     | 84  | SER  |
| 1   | D     | 86  | LEU  |
| 1   | D     | 93  | VAL  |
| 1   | D     | 105 | LEU  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 109 | LEU  |
| 1   | D     | 122 | HIS  |
| 1   | D     | 129 | LEU  |
| 2   | E     | 4   | SER  |
| 2   | E     | 8   | LYS  |
| 2   | E     | 12  | LEU  |
| 2   | E     | 17  | LYS  |
| 2   | E     | 18  | VAL  |
| 2   | E     | 23  | VAL  |
| 2   | E     | 32  | LEU  |
| 2   | E     | 43  | GLU  |
| 2   | E     | 67  | VAL  |
| 2   | E     | 68  | LEU  |
| 2   | E     | 71  | PHE  |
| 2   | E     | 75  | LEU  |
| 2   | E     | 77  | HIS  |
| 2   | E     | 78  | LEU  |
| 2   | E     | 81  | LEU  |
| 2   | E     | 91  | LEU  |
| 2   | E     | 104 | ARG  |
| 2   | E     | 112 | VAL  |
| 2   | E     | 113 | VAL  |
| 2   | E     | 118 | LEU  |
| 2   | E     | 126 | VAL  |
| 2   | E     | 127 | GLN  |
| 2   | E     | 137 | VAL  |
| 2   | E     | 144 | LYS  |
| 3   | F     | 38  | GLU  |
| 3   | F     | 39  | ILE  |
| 3   | F     | 44  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | F     | 57  | LYS  |
| 3   | F     | 67  | THR  |
| 3   | F     | 78  | VAL  |
| 3   | F     | 104 | MET  |
| 3   | F     | 108 | LEU  |
| 3   | F     | 133 | ILE  |
| 3   | F     | 145 | LEU  |
| 3   | F     | 164 | LEU  |
| 3   | F     | 168 | LYS  |
| 3   | F     | 174 | ILE  |
| 3   | F     | 177 | VAL  |
| 3   | F     | 178 | ILE  |
| 3   | F     | 182 | ASP  |
| 3   | F     | 183 | ASN  |
| 3   | F     | 185 | THR  |
| 3   | F     | 197 | VAL  |
| 3   | F     | 204 | MET  |
| 3   | F     | 210 | SER  |
| 3   | F     | 214 | VAL  |
| 3   | F     | 216 | VAL  |
| 3   | F     | 218 | LEU  |
| 3   | F     | 231 | LEU  |
| 3   | F     | 235 | GLU  |
| 3   | F     | 240 | VAL  |
| 3   | F     | 244 | VAL  |
| 3   | F     | 247 | GLN  |
| 3   | F     | 259 | VAL  |
| 3   | F     | 261 | GLU  |
| 3   | F     | 266 | LYS  |
| 3   | F     | 271 | VAL  |
| 3   | F     | 277 | GLU  |
| 3   | F     | 291 | THR  |
| 3   | F     | 302 | VAL  |
| 3   | F     | 316 | LEU  |
| 3   | F     | 321 | SER  |
| 3   | F     | 331 | VAL  |
| 3   | F     | 332 | ARG  |
| 3   | F     | 338 | ASP  |
| 3   | F     | 342 | THR  |
| 3   | F     | 346 | ASP  |
| 1   | G     | 2   | LEU  |
| 1   | G     | 38  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 41  | THR  |
| 1   | G     | 55  | VAL  |
| 1   | G     | 61  | LYS  |
| 1   | G     | 80  | LEU  |
| 1   | G     | 84  | SER  |
| 1   | G     | 86  | LEU  |
| 1   | G     | 93  | VAL  |
| 1   | G     | 105 | LEU  |
| 1   | G     | 106 | LEU  |
| 1   | G     | 109 | LEU  |
| 1   | G     | 122 | HIS  |
| 1   | G     | 129 | LEU  |
| 2   | H     | 4   | SER  |
| 2   | H     | 8   | LYS  |
| 2   | H     | 12  | LEU  |
| 2   | H     | 17  | LYS  |
| 2   | H     | 18  | VAL  |
| 2   | H     | 23  | VAL  |
| 2   | H     | 32  | LEU  |
| 2   | H     | 43  | GLU  |
| 2   | H     | 67  | VAL  |
| 2   | H     | 68  | LEU  |
| 2   | H     | 71  | PHE  |
| 2   | H     | 75  | LEU  |
| 2   | H     | 77  | HIS  |
| 2   | H     | 78  | LEU  |
| 2   | H     | 81  | LEU  |
| 2   | H     | 91  | LEU  |
| 2   | H     | 104 | ARG  |
| 2   | H     | 112 | VAL  |
| 2   | H     | 113 | VAL  |
| 2   | H     | 118 | LEU  |
| 2   | H     | 126 | VAL  |
| 2   | H     | 127 | GLN  |
| 2   | H     | 137 | VAL  |
| 2   | H     | 144 | LYS  |
| 3   | I     | 33  | CYS  |
| 3   | I     | 53  | GLN  |
| 3   | I     | 58  | LEU  |
| 3   | I     | 60  | THR  |
| 3   | I     | 67  | THR  |
| 3   | I     | 68  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 70  | SER  |
| 3   | I     | 75  | THR  |
| 3   | I     | 77  | LYS  |
| 3   | I     | 82  | LYS  |
| 3   | I     | 95  | ASN  |
| 3   | I     | 97  | VAL  |
| 3   | I     | 104 | MET  |
| 3   | I     | 108 | LEU  |
| 3   | I     | 133 | ILE  |
| 3   | I     | 145 | LEU  |
| 3   | I     | 164 | LEU  |
| 3   | I     | 168 | LYS  |
| 3   | I     | 174 | ILE  |
| 3   | I     | 177 | VAL  |
| 3   | I     | 178 | ILE  |
| 3   | I     | 183 | ASN  |
| 3   | I     | 185 | THR  |
| 3   | I     | 197 | VAL  |
| 3   | I     | 204 | MET  |
| 3   | I     | 210 | SER  |
| 3   | I     | 214 | VAL  |
| 3   | I     | 216 | VAL  |
| 3   | I     | 218 | LEU  |
| 3   | I     | 231 | LEU  |
| 3   | I     | 235 | GLU  |
| 3   | I     | 240 | VAL  |
| 3   | I     | 244 | VAL  |
| 3   | I     | 247 | GLN  |
| 3   | I     | 259 | VAL  |
| 3   | I     | 261 | GLU  |
| 3   | I     | 266 | LYS  |
| 3   | I     | 271 | VAL  |
| 3   | I     | 277 | GLU  |
| 3   | I     | 291 | THR  |
| 3   | I     | 302 | VAL  |
| 3   | I     | 316 | LEU  |
| 3   | I     | 321 | SER  |
| 3   | I     | 331 | VAL  |
| 3   | I     | 332 | ARG  |
| 3   | I     | 338 | ASP  |
| 3   | I     | 342 | THR  |
| 3   | I     | 346 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 2   | LEU  |
| 1   | J     | 38  | THR  |
| 1   | J     | 41  | THR  |
| 1   | J     | 55  | VAL  |
| 1   | J     | 61  | LYS  |
| 1   | J     | 80  | LEU  |
| 1   | J     | 84  | SER  |
| 1   | J     | 86  | LEU  |
| 1   | J     | 93  | VAL  |
| 1   | J     | 105 | LEU  |
| 1   | J     | 106 | LEU  |
| 1   | J     | 109 | LEU  |
| 1   | J     | 129 | LEU  |
| 2   | K     | 4   | SER  |
| 2   | K     | 8   | LYS  |
| 2   | K     | 12  | LEU  |
| 2   | K     | 17  | LYS  |
| 2   | K     | 18  | VAL  |
| 2   | K     | 23  | VAL  |
| 2   | K     | 43  | GLU  |
| 2   | K     | 67  | VAL  |
| 2   | K     | 68  | LEU  |
| 2   | K     | 69  | GLN  |
| 2   | K     | 71  | PHE  |
| 2   | K     | 75  | LEU  |
| 2   | K     | 77  | HIS  |
| 2   | K     | 78  | LEU  |
| 2   | K     | 81  | LEU  |
| 2   | K     | 91  | LEU  |
| 2   | K     | 104 | ARG  |
| 2   | K     | 112 | VAL  |
| 2   | K     | 118 | LEU  |
| 2   | K     | 126 | VAL  |
| 2   | K     | 127 | GLN  |
| 2   | K     | 137 | VAL  |
| 2   | K     | 144 | LYS  |
| 2   | K     | 145 | TYR  |
| 3   | L     | 35  | LYS  |
| 3   | L     | 38  | GLU  |
| 3   | L     | 39  | ILE  |
| 3   | L     | 44  | VAL  |
| 3   | L     | 57  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L     | 67  | THR  |
| 3   | L     | 78  | VAL  |
| 3   | L     | 104 | MET  |
| 3   | L     | 108 | LEU  |
| 3   | L     | 128 | SER  |
| 3   | L     | 133 | ILE  |
| 3   | L     | 145 | LEU  |
| 3   | L     | 164 | LEU  |
| 3   | L     | 168 | LYS  |
| 3   | L     | 174 | ILE  |
| 3   | L     | 177 | VAL  |
| 3   | L     | 178 | ILE  |
| 3   | L     | 182 | ASP  |
| 3   | L     | 183 | ASN  |
| 3   | L     | 185 | THR  |
| 3   | L     | 197 | VAL  |
| 3   | L     | 204 | MET  |
| 3   | L     | 210 | SER  |
| 3   | L     | 214 | VAL  |
| 3   | L     | 216 | VAL  |
| 3   | L     | 218 | LEU  |
| 3   | L     | 231 | LEU  |
| 3   | L     | 235 | GLU  |
| 3   | L     | 240 | VAL  |
| 3   | L     | 244 | VAL  |
| 3   | L     | 247 | GLN  |
| 3   | L     | 259 | VAL  |
| 3   | L     | 261 | GLU  |
| 3   | L     | 266 | LYS  |
| 3   | L     | 271 | VAL  |
| 3   | L     | 277 | GLU  |
| 3   | L     | 291 | THR  |
| 3   | L     | 302 | VAL  |
| 3   | L     | 316 | LEU  |
| 3   | L     | 331 | VAL  |
| 3   | L     | 332 | ARG  |
| 3   | L     | 338 | ASP  |
| 3   | L     | 342 | THR  |
| 3   | L     | 346 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 122 | HIS  |
| 2   | B     | 139 | ASN  |
| 3   | C     | 73  | GLN  |
| 3   | C     | 117 | GLN  |
| 3   | C     | 136 | GLN  |
| 3   | C     | 230 | ASN  |
| 3   | C     | 247 | GLN  |
| 1   | D     | 122 | HIS  |
| 2   | E     | 50  | ASN  |
| 2   | E     | 97  | HIS  |
| 2   | E     | 139 | ASN  |
| 3   | F     | 117 | GLN  |
| 3   | F     | 230 | ASN  |
| 1   | G     | 122 | HIS  |
| 2   | H     | 139 | ASN  |
| 3   | I     | 73  | GLN  |
| 3   | I     | 117 | GLN  |
| 3   | I     | 136 | GLN  |
| 3   | I     | 230 | ASN  |
| 2   | K     | 97  | HIS  |
| 3   | L     | 117 | GLN  |
| 3   | L     | 136 | GLN  |
| 3   | L     | 230 | ASN  |
| 3   | L     | 247 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

14 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | NAG  | M     | 1   | 3,4  | 14,14,15     | 2.47 | 6 (42%)     | 17,19,21    | 3.21 | 10 (58%)    |
| 4   | NAG  | M     | 2   | 4    | 14,14,15     | 2.51 | 7 (50%)     | 17,19,21    | 1.67 | 3 (17%)     |
| 5   | NAG  | N     | 1   | 3,5  | 14,14,15     | 2.16 | 5 (35%)     | 17,19,21    | 2.41 | 6 (35%)     |
| 5   | FUC  | N     | 2   | 5    | 10,10,11     | 2.75 | 4 (40%)     | 14,14,16    | 2.54 | 3 (21%)     |
| 4   | NAG  | O     | 1   | 3,4  | 14,14,15     | 2.55 | 6 (42%)     | 17,19,21    | 3.69 | 13 (76%)    |
| 4   | NAG  | O     | 2   | 4    | 14,14,15     | 2.14 | 6 (42%)     | 17,19,21    | 1.53 | 3 (17%)     |
| 5   | NAG  | P     | 1   | 3,5  | 14,14,15     | 2.10 | 6 (42%)     | 17,19,21    | 2.37 | 6 (35%)     |
| 5   | FUC  | P     | 2   | 5    | 10,10,11     | 2.43 | 5 (50%)     | 14,14,16    | 2.20 | 3 (21%)     |
| 4   | NAG  | Q     | 1   | 3,4  | 14,14,15     | 2.23 | 6 (42%)     | 17,19,21    | 3.45 | 10 (58%)    |
| 4   | NAG  | Q     | 2   | 4    | 14,14,15     | 2.36 | 7 (50%)     | 17,19,21    | 1.65 | 2 (11%)     |
| 5   | NAG  | R     | 1   | 3,5  | 14,14,15     | 2.12 | 5 (35%)     | 17,19,21    | 2.19 | 5 (29%)     |
| 5   | FUC  | R     | 2   | 5    | 10,10,11     | 2.78 | 5 (50%)     | 14,14,16    | 2.77 | 4 (28%)     |
| 5   | NAG  | S     | 1   | 3,5  | 14,14,15     | 0.42 | 0           | 17,19,21    | 1.40 | 3 (17%)     |
| 5   | FUC  | S     | 2   | 5    | 10,10,11     | 0.47 | 0           | 14,14,16    | 0.94 | 1 (7%)      |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | M     | 1   | 3,4  | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | M     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | N     | 1   | 3,5  | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | FUC  | N     | 2   | 5    | -       | -         | 0/1/1/1 |
| 4   | NAG  | O     | 1   | 3,4  | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | O     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | P     | 1   | 3,5  | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | FUC  | P     | 2   | 5    | -       | -         | 0/1/1/1 |
| 4   | NAG  | Q     | 1   | 3,4  | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | Q     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | R     | 1   | 3,5  | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | FUC  | R     | 2   | 5    | -       | -         | 0/1/1/1 |
| 5   | NAG  | S     | 1   | 3,5  | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | FUC  | S     | 2   | 5    | -       | -         | 0/1/1/1 |

All (68) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | R     | 2   | FUC  | O5-C5 | 6.31  | 1.56        | 1.43     |
| 5   | N     | 2   | FUC  | O5-C5 | 6.15  | 1.55        | 1.43     |
| 4   | O     | 1   | NAG  | C2-N2 | 5.04  | 1.54        | 1.46     |
| 4   | O     | 1   | NAG  | C7-N2 | 4.97  | 1.50        | 1.34     |
| 5   | P     | 2   | FUC  | O5-C5 | 4.90  | 1.53        | 1.43     |
| 5   | N     | 1   | NAG  | O5-C5 | 4.87  | 1.52        | 1.43     |
| 5   | R     | 1   | NAG  | O5-C5 | 4.77  | 1.52        | 1.43     |
| 4   | M     | 2   | NAG  | O5-C5 | 4.70  | 1.52        | 1.43     |
| 4   | Q     | 2   | NAG  | O5-C5 | 4.59  | 1.52        | 1.43     |
| 4   | M     | 1   | NAG  | C7-N2 | 4.58  | 1.49        | 1.34     |
| 4   | M     | 1   | NAG  | C2-N2 | 4.56  | 1.53        | 1.46     |
| 4   | Q     | 1   | NAG  | C7-N2 | 4.45  | 1.48        | 1.34     |
| 4   | M     | 2   | NAG  | C2-N2 | 4.09  | 1.53        | 1.46     |
| 5   | R     | 2   | FUC  | C2-C3 | -4.07 | 1.46        | 1.52     |
| 4   | O     | 2   | NAG  | O5-C5 | 3.93  | 1.51        | 1.43     |
| 5   | N     | 2   | FUC  | C2-C3 | -3.89 | 1.46        | 1.52     |
| 5   | P     | 1   | NAG  | C7-N2 | 3.87  | 1.46        | 1.34     |
| 5   | P     | 1   | NAG  | O5-C5 | 3.87  | 1.51        | 1.43     |
| 5   | N     | 1   | NAG  | C7-N2 | 3.79  | 1.46        | 1.34     |
| 5   | R     | 1   | NAG  | C7-N2 | 3.78  | 1.46        | 1.34     |
| 4   | Q     | 1   | NAG  | C2-N2 | 3.74  | 1.52        | 1.46     |
| 4   | M     | 2   | NAG  | C7-N2 | 3.71  | 1.46        | 1.34     |
| 4   | Q     | 2   | NAG  | C7-N2 | 3.55  | 1.45        | 1.34     |
| 4   | O     | 2   | NAG  | C7-N2 | 3.45  | 1.45        | 1.34     |
| 5   | N     | 2   | FUC  | C4-C3 | -3.28 | 1.43        | 1.52     |
| 4   | M     | 2   | NAG  | C4-C3 | -3.22 | 1.44        | 1.52     |
| 4   | Q     | 2   | NAG  | C2-N2 | 3.18  | 1.51        | 1.46     |
| 4   | O     | 1   | NAG  | O5-C5 | 3.09  | 1.49        | 1.43     |
| 4   | M     | 2   | NAG  | C1-C2 | 3.07  | 1.56        | 1.52     |
| 5   | R     | 1   | NAG  | O4-C4 | 3.04  | 1.50        | 1.43     |
| 4   | O     | 2   | NAG  | C4-C3 | -2.98 | 1.44        | 1.52     |
| 5   | P     | 2   | FUC  | C4-C3 | -2.95 | 1.44        | 1.52     |
| 4   | M     | 1   | NAG  | O5-C5 | 2.94  | 1.49        | 1.43     |
| 5   | P     | 2   | FUC  | O3-C3 | 2.92  | 1.50        | 1.43     |
| 4   | Q     | 1   | NAG  | O4-C4 | 2.89  | 1.50        | 1.43     |
| 4   | Q     | 2   | NAG  | C4-C3 | -2.88 | 1.44        | 1.52     |
| 5   | P     | 1   | NAG  | C2-N2 | 2.87  | 1.51        | 1.46     |
| 4   | Q     | 1   | NAG  | O5-C5 | 2.86  | 1.49        | 1.43     |
| 4   | Q     | 2   | NAG  | C1-C2 | 2.84  | 1.56        | 1.52     |
| 4   | M     | 1   | NAG  | O4-C4 | 2.83  | 1.50        | 1.43     |
| 5   | N     | 1   | NAG  | O4-C4 | 2.81  | 1.49        | 1.43     |
| 5   | R     | 2   | FUC  | C4-C3 | -2.76 | 1.45        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | P     | 2   | FUC  | C2-C3 | -2.71 | 1.48        | 1.52     |
| 5   | P     | 1   | NAG  | C4-C3 | -2.71 | 1.45        | 1.52     |
| 4   | O     | 2   | NAG  | C2-N2 | 2.65  | 1.50        | 1.46     |
| 4   | M     | 1   | NAG  | C3-C2 | -2.59 | 1.47        | 1.52     |
| 4   | M     | 1   | NAG  | O5-C1 | -2.58 | 1.39        | 1.43     |
| 4   | M     | 2   | NAG  | O3-C3 | 2.54  | 1.49        | 1.43     |
| 4   | O     | 2   | NAG  | O3-C3 | 2.41  | 1.48        | 1.43     |
| 4   | O     | 1   | NAG  | C3-C2 | -2.40 | 1.47        | 1.52     |
| 5   | N     | 1   | NAG  | C4-C3 | -2.39 | 1.46        | 1.52     |
| 4   | O     | 1   | NAG  | O5-C1 | -2.38 | 1.39        | 1.43     |
| 5   | P     | 2   | FUC  | O5-C1 | -2.38 | 1.39        | 1.43     |
| 4   | O     | 1   | NAG  | O4-C4 | 2.37  | 1.48        | 1.43     |
| 4   | Q     | 2   | NAG  | O4-C4 | 2.35  | 1.48        | 1.43     |
| 5   | P     | 1   | NAG  | O3-C3 | 2.35  | 1.48        | 1.43     |
| 4   | Q     | 2   | NAG  | O3-C3 | 2.29  | 1.48        | 1.43     |
| 4   | Q     | 1   | NAG  | O5-C1 | -2.23 | 1.39        | 1.43     |
| 4   | O     | 2   | NAG  | O4-C4 | 2.22  | 1.48        | 1.43     |
| 5   | N     | 1   | NAG  | C2-N2 | 2.19  | 1.49        | 1.46     |
| 5   | R     | 2   | FUC  | O3-C3 | 2.17  | 1.48        | 1.43     |
| 5   | P     | 1   | NAG  | O4-C4 | 2.17  | 1.48        | 1.43     |
| 5   | R     | 2   | FUC  | O4-C4 | 2.15  | 1.48        | 1.43     |
| 5   | R     | 1   | NAG  | C4-C3 | -2.14 | 1.46        | 1.52     |
| 5   | N     | 2   | FUC  | O4-C4 | 2.14  | 1.48        | 1.43     |
| 4   | Q     | 1   | NAG  | O3-C3 | 2.14  | 1.48        | 1.43     |
| 4   | M     | 2   | NAG  | O4-C4 | 2.10  | 1.48        | 1.43     |
| 5   | R     | 1   | NAG  | O3-C3 | 2.01  | 1.47        | 1.43     |

All (72) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | Q     | 1   | NAG  | O5-C1-C2 | 8.71  | 124.76      | 111.29   |
| 4   | O     | 1   | NAG  | O5-C1-C2 | 8.20  | 123.98      | 111.29   |
| 5   | R     | 2   | FUC  | O5-C5-C6 | 6.62  | 121.78      | 107.40   |
| 4   | O     | 1   | NAG  | C2-N2-C7 | 6.43  | 131.52      | 122.90   |
| 5   | P     | 1   | NAG  | C2-N2-C7 | -6.35 | 114.39      | 122.90   |
| 5   | N     | 2   | FUC  | O5-C5-C6 | 6.29  | 121.05      | 107.40   |
| 4   | M     | 1   | NAG  | O5-C1-C2 | 6.25  | 120.95      | 111.29   |
| 5   | N     | 1   | NAG  | C2-N2-C7 | -6.06 | 114.77      | 122.90   |
| 5   | R     | 1   | NAG  | C2-N2-C7 | -5.68 | 115.29      | 122.90   |
| 4   | M     | 2   | NAG  | C2-N2-C7 | -5.43 | 115.62      | 122.90   |
| 5   | R     | 2   | FUC  | C1-O5-C5 | -5.39 | 100.24      | 112.97   |
| 4   | M     | 1   | NAG  | C2-N2-C7 | 5.33  | 130.04      | 122.90   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | N     | 2   | FUC  | C1-O5-C5 | -4.97 | 101.24      | 112.97   |
| 5   | P     | 2   | FUC  | C1-O5-C5 | -4.91 | 101.38      | 112.97   |
| 4   | Q     | 1   | NAG  | C8-C7-N2 | 4.87  | 124.19      | 116.12   |
| 4   | O     | 1   | NAG  | O7-C7-C8 | -4.79 | 113.53      | 122.05   |
| 4   | M     | 1   | NAG  | O3-C3-C2 | -4.74 | 99.56       | 109.40   |
| 4   | Q     | 2   | NAG  | C2-N2-C7 | -4.72 | 116.58      | 122.90   |
| 5   | N     | 1   | NAG  | C1-O5-C5 | -4.61 | 106.00      | 112.19   |
| 5   | P     | 2   | FUC  | O5-C5-C6 | 4.54  | 117.26      | 107.40   |
| 4   | M     | 1   | NAG  | O7-C7-C8 | -4.49 | 114.06      | 122.05   |
| 4   | Q     | 1   | NAG  | O7-C7-C8 | -4.45 | 114.12      | 122.05   |
| 5   | R     | 2   | FUC  | C6-C5-C4 | -4.40 | 105.04      | 113.08   |
| 5   | N     | 2   | FUC  | C6-C5-C4 | -4.30 | 105.22      | 113.08   |
| 4   | O     | 2   | NAG  | C2-N2-C7 | -4.19 | 117.29      | 122.90   |
| 4   | Q     | 1   | NAG  | O4-C4-C3 | 4.00  | 119.81      | 110.38   |
| 4   | O     | 1   | NAG  | C1-C2-N2 | 4.00  | 116.74      | 110.43   |
| 4   | O     | 1   | NAG  | O3-C3-C2 | -4.00 | 101.10      | 109.40   |
| 4   | Q     | 1   | NAG  | O5-C5-C6 | -3.92 | 100.04      | 107.66   |
| 4   | Q     | 1   | NAG  | O3-C3-C2 | -3.91 | 101.27      | 109.40   |
| 4   | Q     | 1   | NAG  | O3-C3-C4 | 3.68  | 119.06      | 110.38   |
| 5   | R     | 1   | NAG  | C1-O5-C5 | -3.62 | 107.33      | 112.19   |
| 5   | N     | 1   | NAG  | C4-C3-C2 | 3.59  | 116.29      | 111.02   |
| 4   | M     | 1   | NAG  | C4-C3-C2 | 3.59  | 116.28      | 111.02   |
| 4   | O     | 1   | NAG  | O5-C5-C6 | -3.52 | 100.81      | 107.66   |
| 4   | M     | 1   | NAG  | O4-C4-C3 | 3.51  | 118.64      | 110.38   |
| 5   | S     | 1   | NAG  | C1-O5-C5 | -3.50 | 107.49      | 112.19   |
| 5   | P     | 1   | NAG  | C1-O5-C5 | -3.39 | 107.64      | 112.19   |
| 5   | P     | 1   | NAG  | C4-C3-C2 | 3.33  | 115.90      | 111.02   |
| 5   | P     | 2   | FUC  | C6-C5-C4 | -3.32 | 107.00      | 113.08   |
| 4   | O     | 1   | NAG  | O4-C4-C3 | 3.30  | 118.17      | 110.38   |
| 4   | O     | 1   | NAG  | C1-O5-C5 | -3.22 | 107.87      | 112.19   |
| 4   | O     | 1   | NAG  | C4-C3-C2 | 3.11  | 115.58      | 111.02   |
| 4   | M     | 1   | NAG  | C8-C7-N2 | 3.10  | 121.25      | 116.12   |
| 5   | R     | 1   | NAG  | C4-C3-C2 | 3.03  | 115.47      | 111.02   |
| 4   | O     | 1   | NAG  | C8-C7-N2 | 2.82  | 120.80      | 116.12   |
| 4   | Q     | 2   | NAG  | C1-O5-C5 | -2.82 | 108.41      | 112.19   |
| 5   | P     | 1   | NAG  | C8-C7-N2 | 2.78  | 120.73      | 116.12   |
| 4   | M     | 1   | NAG  | C1-C2-N2 | 2.72  | 114.71      | 110.43   |
| 5   | N     | 1   | NAG  | O3-C3-C2 | -2.71 | 103.78      | 109.40   |
| 4   | M     | 1   | NAG  | C1-O5-C5 | -2.58 | 108.72      | 112.19   |
| 5   | R     | 2   | FUC  | O2-C2-C1 | 2.55  | 115.05      | 109.22   |
| 4   | O     | 2   | NAG  | C4-C3-C2 | 2.46  | 114.63      | 111.02   |
| 4   | O     | 1   | NAG  | O3-C3-C4 | 2.43  | 116.10      | 110.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | M     | 1   | NAG  | O3-C3-C4 | 2.42  | 116.07      | 110.38   |
| 5   | R     | 1   | NAG  | O4-C4-C5 | 2.41  | 115.25      | 109.32   |
| 4   | O     | 2   | NAG  | O7-C7-N2 | -2.39 | 117.77      | 121.98   |
| 5   | S     | 1   | NAG  | C8-C7-N2 | 2.38  | 120.06      | 116.12   |
| 4   | Q     | 1   | NAG  | C1-O5-C5 | -2.34 | 109.05      | 112.19   |
| 5   | P     | 1   | NAG  | O5-C1-C2 | 2.29  | 114.84      | 111.29   |
| 4   | Q     | 1   | NAG  | C4-C3-C2 | 2.27  | 114.34      | 111.02   |
| 5   | S     | 2   | FUC  | C1-O5-C5 | -2.25 | 107.66      | 112.97   |
| 5   | R     | 1   | NAG  | O5-C5-C4 | 2.19  | 116.16      | 110.83   |
| 5   | N     | 1   | NAG  | O4-C4-C5 | 2.18  | 114.68      | 109.32   |
| 4   | M     | 2   | NAG  | O7-C7-N2 | -2.17 | 118.15      | 121.98   |
| 4   | Q     | 1   | NAG  | C1-C2-N2 | 2.15  | 113.81      | 110.43   |
| 4   | M     | 2   | NAG  | C1-O5-C5 | -2.11 | 109.36      | 112.19   |
| 4   | O     | 1   | NAG  | O7-C7-N2 | 2.09  | 125.67      | 121.98   |
| 5   | S     | 1   | NAG  | C2-N2-C7 | -2.06 | 120.14      | 122.90   |
| 5   | N     | 1   | NAG  | O5-C5-C4 | 2.05  | 115.81      | 110.83   |
| 4   | O     | 1   | NAG  | C6-C5-C4 | 2.04  | 118.02      | 113.02   |
| 5   | P     | 1   | NAG  | O6-C6-C5 | 2.03  | 118.24      | 111.33   |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | M     | 1   | NAG  | C3-C2-N2-C7 |
| 4   | O     | 1   | NAG  | C3-C2-N2-C7 |
| 4   | Q     | 1   | NAG  | C3-C2-N2-C7 |
| 4   | O     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | Q     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | M     | 1   | NAG  | O5-C5-C6-O6 |
| 4   | O     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | Q     | 1   | NAG  | C4-C5-C6-O6 |
| 4   | M     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | R     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | P     | 1   | NAG  | C4-C5-C6-O6 |

There are no ring outliers.

9 monomers are involved in 10 short contacts:

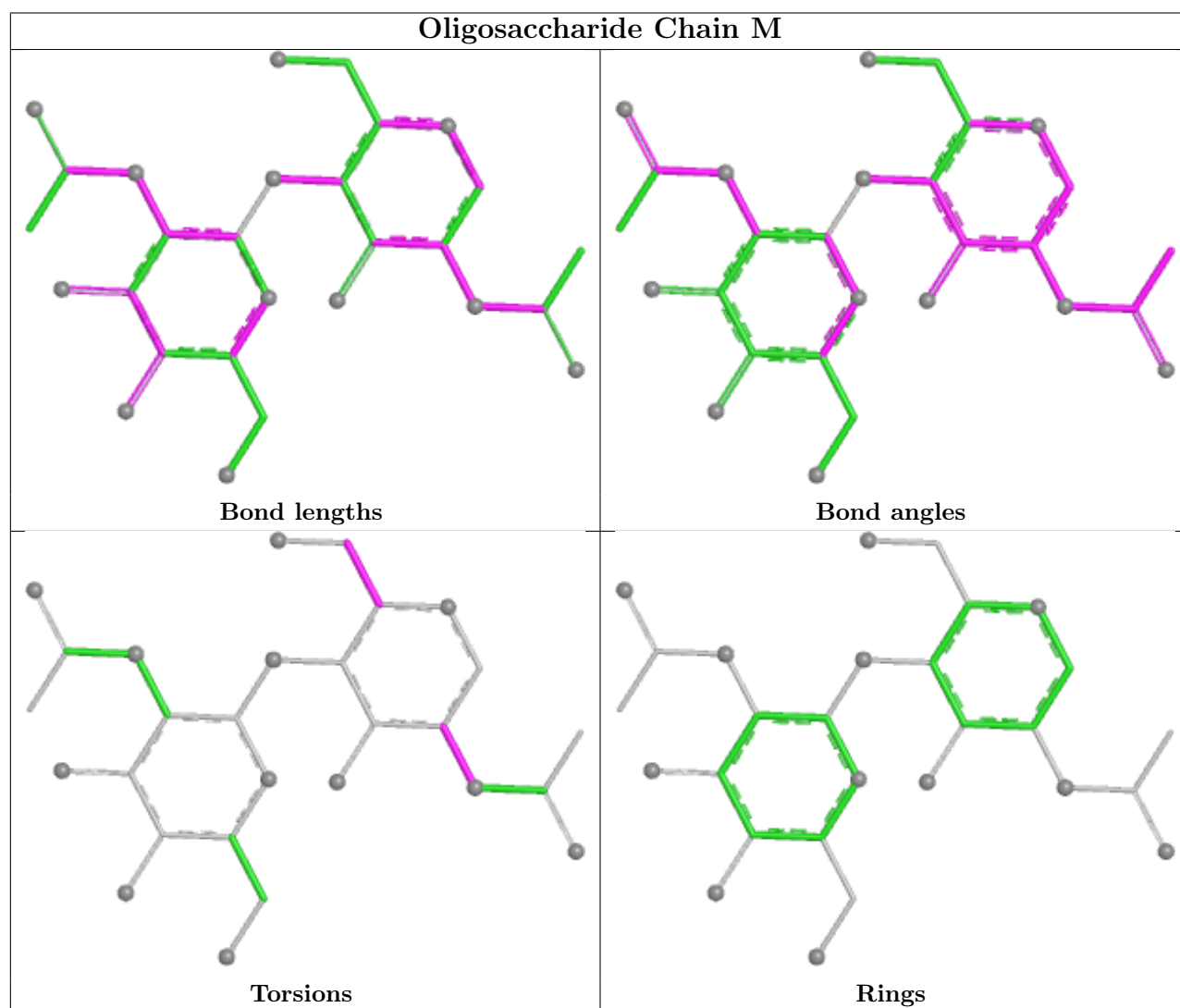
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | M     | 1   | NAG  | 1       | 0            |
| 4   | Q     | 2   | NAG  | 1       | 0            |

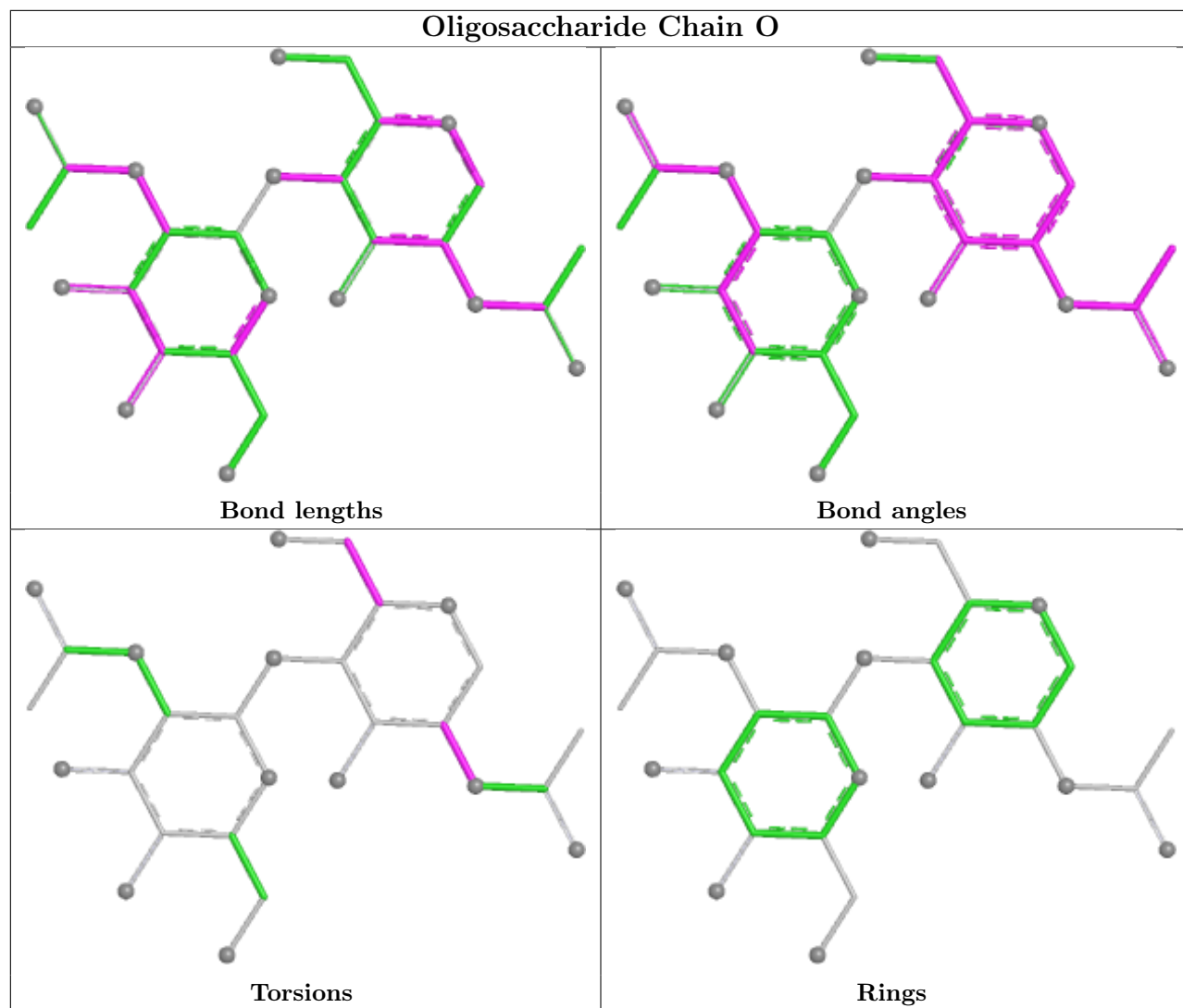
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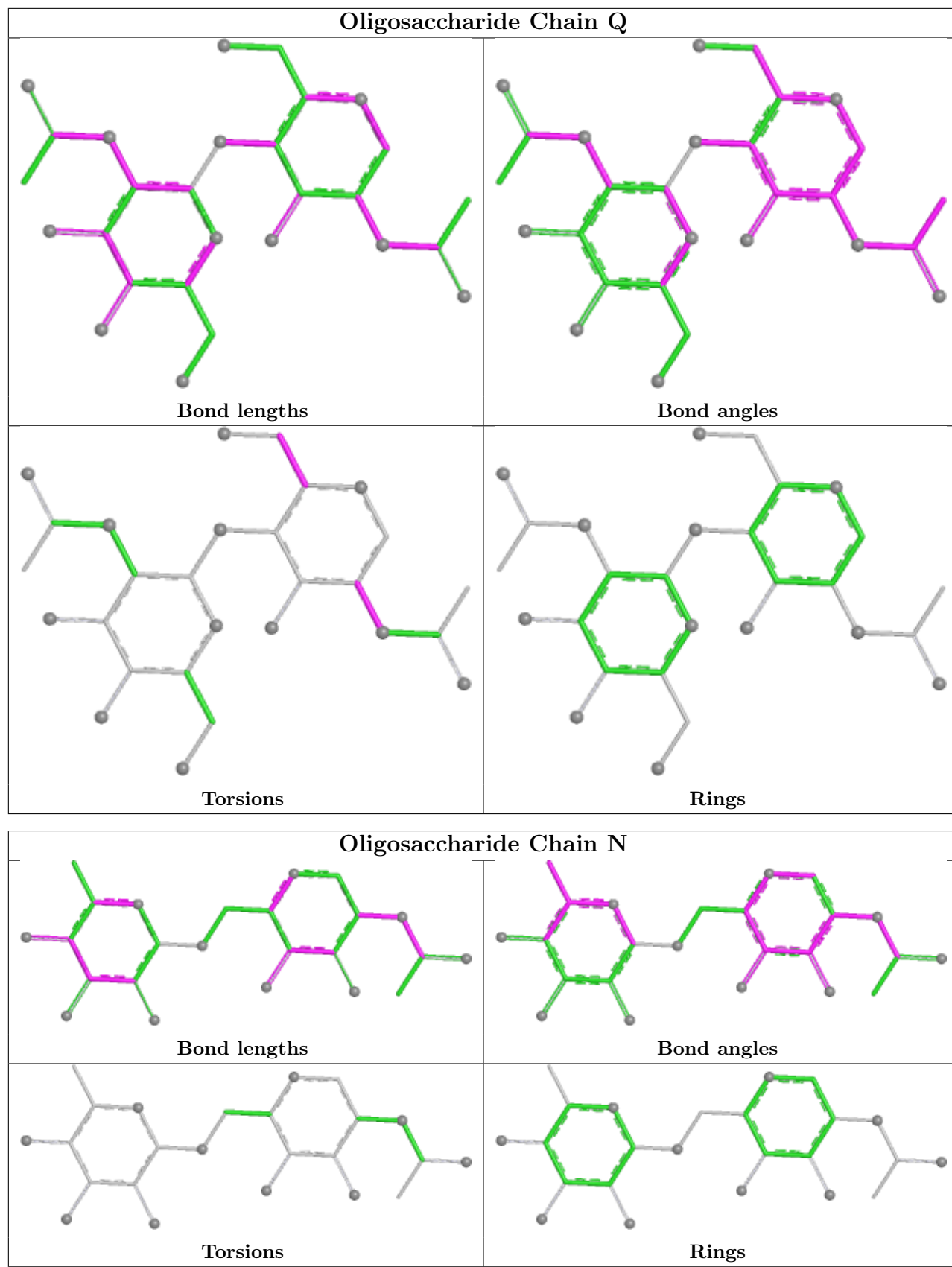
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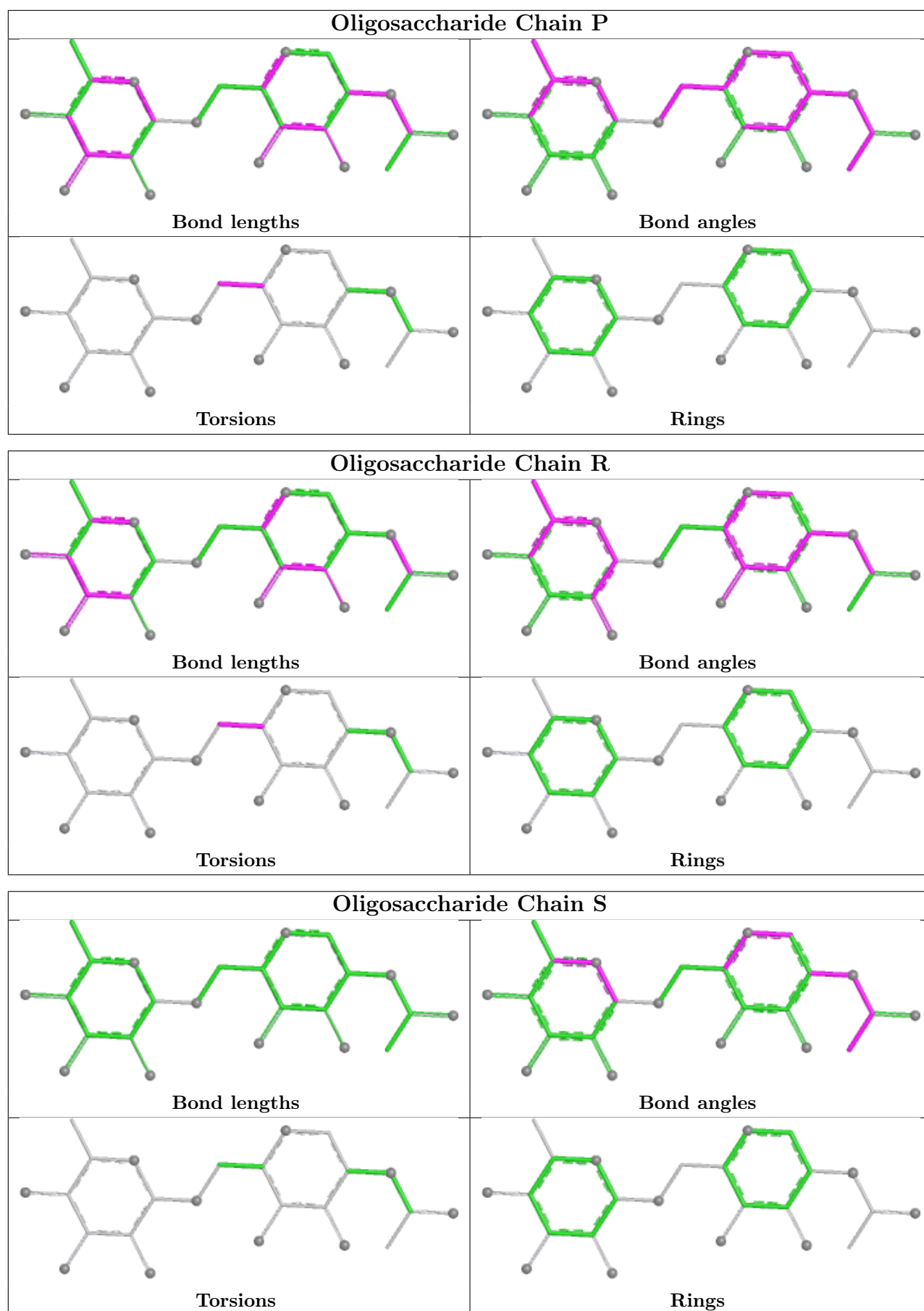
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | S     | 1   | NAG  | 1       | 0            |
| 4   | Q     | 1   | NAG  | 1       | 0            |
| 4   | O     | 2   | NAG  | 1       | 0            |
| 5   | S     | 2   | FUC  | 4       | 0            |
| 4   | M     | 2   | NAG  | 1       | 0            |
| 5   | P     | 2   | FUC  | 2       | 0            |
| 4   | O     | 1   | NAG  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry

24 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | OXY  | H     | 202  | 6    | 1,1,1        | 0.14 | 0        | -           |      |          |
| 7   | OXY  | K     | 202  | 6    | 1,1,1        | 0.13 | 0        | -           |      |          |
| 6   | HEM  | B     | 201  | 7,2  | 50,50,50     | 2.03 | 10 (20%) | 67,82,82    | 1.42 | 9 (13%)  |
| 8   | NAG  | F     | 1003 | 3    | 14,14,15     | 2.36 | 6 (42%)  | 17,19,21    | 2.21 | 4 (23%)  |
| 6   | HEM  | H     | 201  | 7,2  | 50,50,50     | 2.01 | 7 (14%)  | 67,82,82    | 1.47 | 7 (10%)  |
| 8   | NAG  | L     | 1002 | 3    | 14,14,15     | 0.43 | 0        | 17,19,21    | 1.38 | 3 (17%)  |
| 8   | NAG  | C     | 1004 | 3    | 14,14,15     | 2.53 | 7 (50%)  | 17,19,21    | 2.55 | 9 (52%)  |
| 7   | OXY  | J     | 202  | 6    | 1,1,1        | 0.17 | 0        | -           |      |          |
| 7   | OXY  | B     | 202  | 6    | 1,1,1        | 0.17 | 0        | -           |      |          |
| 6   | HEM  | G     | 201  | 1,7  | 50,50,50     | 1.84 | 11 (22%) | 67,82,82    | 1.44 | 7 (10%)  |
| 8   | NAG  | L     | 1001 | 3    | 14,14,15     | 2.52 | 7 (50%)  | 17,19,21    | 2.18 | 5 (29%)  |
| 6   | HEM  | A     | 201  | 1,7  | 50,50,50     | 2.07 | 10 (20%) | 67,82,82    | 1.44 | 7 (10%)  |
| 8   | NAG  | I     | 1004 | 3    | 14,14,15     | 1.88 | 5 (35%)  | 17,19,21    | 1.98 | 4 (23%)  |
| 8   | NAG  | I     | 1003 | 3    | 14,14,15     | 2.15 | 5 (35%)  | 17,19,21    | 1.59 | 3 (17%)  |
| 6   | HEM  | K     | 201  | 7,2  | 50,50,50     | 2.11 | 10 (20%) | 67,82,82    | 1.47 | 8 (11%)  |
| 8   | NAG  | C     | 1003 | 3    | 14,14,15     | 2.24 | 5 (35%)  | 17,19,21    | 2.17 | 7 (41%)  |
| 7   | OXY  | E     | 202  | 6    | 1,1,1        | 0.17 | 0        | -           |      |          |
| 6   | HEM  | E     | 201  | 7,2  | 50,50,50     | 1.96 | 8 (16%)  | 67,82,82    | 1.43 | 6 (8%)   |
| 7   | OXY  | D     | 202  | 6    | 1,1,1        | 0.20 | 0        | -           |      |          |
| 8   | NAG  | F     | 1004 | 3    | 14,14,15     | 1.81 | 6 (42%)  | 17,19,21    | 1.66 | 2 (11%)  |
| 6   | HEM  | J     | 201  | 1,7  | 50,50,50     | 1.89 | 9 (18%)  | 67,82,82    | 1.38 | 6 (8%)   |
| 7   | OXY  | G     | 202  | 6    | 1,1,1        | 0.19 | 0        | -           |      |          |
| 7   | OXY  | A     | 202  | 6    | 1,1,1        | 0.18 | 0        | -           |      |          |
| 6   | HEM  | D     | 201  | 1,7  | 50,50,50     | 1.88 | 11 (22%) | 67,82,82    | 1.28 | 7 (10%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 8   | NAG  | F     | 1004 | 3    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | HEM  | J     | 201  | 1,7  | -       | 1/14/54/54 | -       |
| 8   | NAG  | I     | 1003 | 3    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | HEM  | B     | 201  | 7,2  | -       | 6/14/54/54 | -       |
| 8   | NAG  | F     | 1003 | 3    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | HEM  | K     | 201  | 7,2  | -       | 3/14/54/54 | -       |
| 8   | NAG  | C     | 1003 | 3    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | HEM  | H     | 201  | 7,2  | -       | 6/14/54/54 | -       |
| 6   | HEM  | G     | 201  | 1,7  | -       | 2/14/54/54 | -       |
| 8   | NAG  | C     | 1004 | 3    | -       | 3/6/23/26  | 0/1/1/1 |
| 8   | NAG  | L     | 1001 | 3    | -       | 3/6/23/26  | 0/1/1/1 |
| 6   | HEM  | A     | 201  | 1,7  | -       | 1/14/54/54 | -       |
| 8   | NAG  | L     | 1002 | 3    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | HEM  | D     | 201  | 1,7  | -       | 2/14/54/54 | -       |
| 8   | NAG  | I     | 1004 | 3    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | HEM  | E     | 201  | 7,2  | -       | 6/14/54/54 | -       |

All (117) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 6   | K     | 201  | HEM  | C3D-C2D | 8.29 | 1.54        | 1.36     |
| 6   | B     | 201  | HEM  | C3D-C2D | 7.88 | 1.53        | 1.36     |
| 6   | A     | 201  | HEM  | C3D-C2D | 7.81 | 1.53        | 1.36     |
| 6   | H     | 201  | HEM  | C3D-C2D | 7.67 | 1.53        | 1.36     |
| 6   | J     | 201  | HEM  | C3D-C2D | 7.63 | 1.53        | 1.36     |
| 6   | E     | 201  | HEM  | C3D-C2D | 7.51 | 1.53        | 1.36     |
| 6   | D     | 201  | HEM  | C3D-C2D | 7.38 | 1.52        | 1.36     |
| 6   | G     | 201  | HEM  | C3D-C2D | 7.31 | 1.52        | 1.36     |
| 6   | A     | 201  | HEM  | FE-NC   | 7.08 | 2.18        | 1.95     |
| 6   | K     | 201  | HEM  | FE-NC   | 6.06 | 2.15        | 1.95     |
| 6   | H     | 201  | HEM  | FE-ND   | 5.98 | 2.13        | 1.94     |
| 6   | E     | 201  | HEM  | FE-ND   | 5.97 | 2.13        | 1.94     |
| 6   | K     | 201  | HEM  | FE-NB   | 5.67 | 2.12        | 1.94     |
| 6   | A     | 201  | HEM  | FE-ND   | 5.61 | 2.12        | 1.94     |
| 6   | D     | 201  | HEM  | FE-ND   | 5.52 | 2.11        | 1.94     |
| 6   | B     | 201  | HEM  | FE-NC   | 5.20 | 2.12        | 1.95     |
| 8   | C     | 1004 | NAG  | O5-C5   | 5.01 | 1.53        | 1.43     |
| 6   | B     | 201  | HEM  | FE-NB   | 4.94 | 2.10        | 1.94     |
| 6   | J     | 201  | HEM  | FE-NB   | 4.90 | 2.10        | 1.94     |
| 6   | G     | 201  | HEM  | FE-ND   | 4.80 | 2.09        | 1.94     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | L     | 1001 | NAG  | C7-N2   | 4.69  | 1.49        | 1.34     |
| 8   | C     | 1003 | NAG  | O5-C5   | 4.63  | 1.52        | 1.43     |
| 6   | D     | 201  | HEM  | FE-NC   | 4.62  | 2.10        | 1.95     |
| 8   | I     | 1003 | NAG  | O5-C5   | 4.62  | 1.52        | 1.43     |
| 6   | J     | 201  | HEM  | FE-NC   | 4.61  | 2.10        | 1.95     |
| 8   | F     | 1003 | NAG  | O5-C5   | 4.57  | 1.52        | 1.43     |
| 6   | G     | 201  | HEM  | FE-NB   | 4.55  | 2.08        | 1.94     |
| 6   | E     | 201  | HEM  | FE-NC   | 4.41  | 2.09        | 1.95     |
| 8   | C     | 1004 | NAG  | C7-N2   | 4.38  | 1.48        | 1.34     |
| 6   | H     | 201  | HEM  | FE-NA   | 4.37  | 2.09        | 1.95     |
| 6   | K     | 201  | HEM  | FE-ND   | 4.31  | 2.08        | 1.94     |
| 6   | B     | 201  | HEM  | FE-ND   | 4.29  | 2.08        | 1.94     |
| 6   | J     | 201  | HEM  | FE-ND   | 4.27  | 2.08        | 1.94     |
| 8   | C     | 1003 | NAG  | C7-N2   | 4.20  | 1.47        | 1.34     |
| 6   | E     | 201  | HEM  | FE-NA   | 4.17  | 2.08        | 1.95     |
| 6   | H     | 201  | HEM  | FE-NC   | 4.13  | 2.08        | 1.95     |
| 8   | L     | 1001 | NAG  | O5-C5   | 3.97  | 1.51        | 1.43     |
| 8   | F     | 1003 | NAG  | C7-N2   | 3.94  | 1.47        | 1.34     |
| 8   | L     | 1001 | NAG  | C2-N2   | 3.88  | 1.52        | 1.46     |
| 8   | I     | 1003 | NAG  | C7-N2   | 3.87  | 1.46        | 1.34     |
| 6   | H     | 201  | HEM  | FE-NB   | 3.74  | 2.06        | 1.94     |
| 8   | F     | 1003 | NAG  | C1-C2   | 3.56  | 1.57        | 1.52     |
| 6   | B     | 201  | HEM  | CAC-C3C | 3.53  | 1.56        | 1.47     |
| 8   | I     | 1004 | NAG  | C7-N2   | 3.39  | 1.45        | 1.34     |
| 6   | H     | 201  | HEM  | CAC-C3C | 3.36  | 1.56        | 1.47     |
| 8   | C     | 1004 | NAG  | O4-C4   | 3.34  | 1.51        | 1.43     |
| 6   | K     | 201  | HEM  | CAB-C3B | 3.31  | 1.56        | 1.47     |
| 6   | E     | 201  | HEM  | CAC-C3C | 3.26  | 1.56        | 1.47     |
| 8   | I     | 1004 | NAG  | C4-C3   | -3.24 | 1.43        | 1.52     |
| 6   | B     | 201  | HEM  | FE-NA   | 3.18  | 2.05        | 1.95     |
| 6   | A     | 201  | HEM  | FE-NB   | 3.18  | 2.04        | 1.94     |
| 6   | K     | 201  | HEM  | CAC-C3C | 3.15  | 1.55        | 1.47     |
| 8   | C     | 1003 | NAG  | C2-N2   | 3.15  | 1.51        | 1.46     |
| 6   | B     | 201  | HEM  | CAB-C3B | 3.13  | 1.55        | 1.47     |
| 8   | I     | 1003 | NAG  | C2-N2   | 3.09  | 1.51        | 1.46     |
| 8   | F     | 1004 | NAG  | O5-C5   | 3.09  | 1.49        | 1.43     |
| 8   | I     | 1004 | NAG  | O5-C1   | -3.07 | 1.38        | 1.43     |
| 6   | D     | 201  | HEM  | FE-NB   | 3.04  | 2.04        | 1.94     |
| 6   | H     | 201  | HEM  | CAB-C3B | 3.03  | 1.55        | 1.47     |
| 6   | E     | 201  | HEM  | CAB-C3B | 2.99  | 1.55        | 1.47     |
| 6   | J     | 201  | HEM  | CAC-C3C | 2.99  | 1.55        | 1.47     |
| 6   | A     | 201  | HEM  | CAC-C3C | 2.99  | 1.55        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | G     | 201  | HEM  | CMC-C2C | 2.98  | 1.56        | 1.50     |
| 8   | L     | 1001 | NAG  | C4-C3   | -2.98 | 1.44        | 1.52     |
| 6   | K     | 201  | HEM  | FE-NA   | 2.90  | 2.04        | 1.95     |
| 6   | D     | 201  | HEM  | CAC-C3C | 2.90  | 1.55        | 1.47     |
| 6   | G     | 201  | HEM  | CAC-C3C | 2.89  | 1.55        | 1.47     |
| 8   | F     | 1004 | NAG  | O5-C1   | -2.83 | 1.38        | 1.43     |
| 8   | C     | 1004 | NAG  | C4-C3   | -2.81 | 1.45        | 1.52     |
| 6   | G     | 201  | HEM  | FE-NC   | 2.80  | 2.04        | 1.95     |
| 6   | A     | 201  | HEM  | CMC-C2C | 2.80  | 1.56        | 1.50     |
| 6   | J     | 201  | HEM  | CAB-C3B | 2.80  | 1.54        | 1.47     |
| 6   | G     | 201  | HEM  | FE-NA   | 2.76  | 2.04        | 1.95     |
| 8   | F     | 1003 | NAG  | C4-C3   | -2.66 | 1.45        | 1.52     |
| 6   | D     | 201  | HEM  | CMC-C2C | 2.65  | 1.56        | 1.50     |
| 6   | E     | 201  | HEM  | FE-NB   | 2.65  | 2.03        | 1.94     |
| 8   | C     | 1004 | NAG  | O3-C3   | 2.60  | 1.49        | 1.43     |
| 8   | F     | 1004 | NAG  | C7-N2   | 2.59  | 1.42        | 1.34     |
| 6   | D     | 201  | HEM  | O1A-CGA | 2.58  | 1.30        | 1.22     |
| 6   | G     | 201  | HEM  | CAB-C3B | 2.55  | 1.54        | 1.47     |
| 8   | F     | 1003 | NAG  | C2-N2   | 2.54  | 1.50        | 1.46     |
| 8   | C     | 1003 | NAG  | C4-C3   | -2.53 | 1.45        | 1.52     |
| 6   | A     | 201  | HEM  | O1A-CGA | 2.51  | 1.30        | 1.22     |
| 8   | L     | 1001 | NAG  | O4-C4   | 2.50  | 1.49        | 1.43     |
| 8   | I     | 1003 | NAG  | O3-C3   | 2.48  | 1.49        | 1.43     |
| 8   | I     | 1004 | NAG  | O5-C5   | 2.46  | 1.48        | 1.43     |
| 6   | D     | 201  | HEM  | CAB-C3B | 2.45  | 1.53        | 1.47     |
| 6   | K     | 201  | HEM  | CMB-C2B | 2.41  | 1.55        | 1.50     |
| 8   | C     | 1004 | NAG  | C3-C2   | -2.38 | 1.47        | 1.52     |
| 8   | L     | 1001 | NAG  | C3-C2   | -2.36 | 1.47        | 1.52     |
| 6   | A     | 201  | HEM  | CAB-C3B | 2.34  | 1.53        | 1.47     |
| 6   | B     | 201  | HEM  | CMC-C2C | 2.32  | 1.55        | 1.50     |
| 8   | F     | 1003 | NAG  | O3-C3   | 2.31  | 1.48        | 1.43     |
| 6   | G     | 201  | HEM  | C2A-C3A | -2.30 | 1.32        | 1.38     |
| 6   | E     | 201  | HEM  | CMB-C2B | 2.27  | 1.55        | 1.50     |
| 8   | I     | 1003 | NAG  | C4-C3   | -2.24 | 1.46        | 1.52     |
| 6   | G     | 201  | HEM  | CMB-C2B | 2.22  | 1.55        | 1.50     |
| 8   | F     | 1004 | NAG  | C4-C3   | -2.17 | 1.46        | 1.52     |
| 6   | D     | 201  | HEM  | CMB-C2B | 2.17  | 1.55        | 1.50     |
| 6   | D     | 201  | HEM  | C2A-C3A | -2.17 | 1.33        | 1.38     |
| 6   | D     | 201  | HEM  | O1D-CGD | 2.16  | 1.29        | 1.22     |
| 6   | A     | 201  | HEM  | CMA-C3A | 2.16  | 1.55        | 1.50     |
| 8   | L     | 1001 | NAG  | O3-C3   | 2.16  | 1.48        | 1.43     |
| 6   | G     | 201  | HEM  | O1A-CGA | 2.14  | 1.29        | 1.22     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | F     | 1004 | NAG  | O4-C4   | 2.13  | 1.48        | 1.43     |
| 6   | K     | 201  | HEM  | CMC-C2C | 2.13  | 1.55        | 1.50     |
| 6   | J     | 201  | HEM  | CMB-C2B | 2.12  | 1.55        | 1.50     |
| 6   | A     | 201  | HEM  | CMB-C2B | 2.11  | 1.55        | 1.50     |
| 8   | C     | 1003 | NAG  | O3-C3   | 2.09  | 1.48        | 1.43     |
| 8   | I     | 1004 | NAG  | O4-C4   | 2.09  | 1.48        | 1.43     |
| 6   | J     | 201  | HEM  | CMC-C2C | 2.08  | 1.55        | 1.50     |
| 6   | B     | 201  | HEM  | CMD-C2D | 2.07  | 1.55        | 1.50     |
| 6   | B     | 201  | HEM  | CMB-C2B | 2.05  | 1.55        | 1.50     |
| 6   | K     | 201  | HEM  | CMA-C3A | 2.05  | 1.55        | 1.50     |
| 8   | C     | 1004 | NAG  | C1-C2   | -2.04 | 1.49        | 1.52     |
| 6   | J     | 201  | HEM  | C2A-C3A | -2.03 | 1.33        | 1.38     |
| 8   | F     | 1004 | NAG  | C1-C2   | -2.01 | 1.49        | 1.52     |

All (94) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | F     | 1003 | NAG  | O5-C1-C2    | -7.18 | 100.17      | 111.29   |
| 6   | K     | 201  | HEM  | C4D-ND-C1D  | 6.43  | 112.82      | 105.21   |
| 8   | C     | 1003 | NAG  | C2-N2-C7    | -5.74 | 115.21      | 122.90   |
| 6   | H     | 201  | HEM  | C4D-ND-C1D  | 5.73  | 111.99      | 105.21   |
| 6   | B     | 201  | HEM  | C4D-ND-C1D  | 5.51  | 111.73      | 105.21   |
| 6   | E     | 201  | HEM  | C4D-ND-C1D  | 5.44  | 111.66      | 105.21   |
| 6   | A     | 201  | HEM  | C4D-ND-C1D  | 5.39  | 111.59      | 105.21   |
| 6   | J     | 201  | HEM  | C4D-ND-C1D  | 5.37  | 111.56      | 105.21   |
| 8   | L     | 1001 | NAG  | C1-O5-C5    | -5.32 | 105.06      | 112.19   |
| 6   | G     | 201  | HEM  | C4D-ND-C1D  | 5.19  | 111.35      | 105.21   |
| 6   | D     | 201  | HEM  | C4D-ND-C1D  | 5.10  | 111.25      | 105.21   |
| 8   | C     | 1004 | NAG  | C2-N2-C7    | 4.95  | 129.53      | 122.90   |
| 8   | I     | 1004 | NAG  | C8-C7-N2    | 4.72  | 123.95      | 116.12   |
| 8   | L     | 1001 | NAG  | C2-N2-C7    | 4.33  | 128.71      | 122.90   |
| 8   | I     | 1003 | NAG  | C2-N2-C7    | -4.28 | 117.16      | 122.90   |
| 8   | C     | 1004 | NAG  | O5-C5-C6    | 4.20  | 115.84      | 107.66   |
| 8   | C     | 1004 | NAG  | C4-C3-C2    | 4.07  | 116.98      | 111.02   |
| 8   | F     | 1004 | NAG  | C1-C2-N2    | -4.07 | 104.03      | 110.43   |
| 8   | L     | 1001 | NAG  | O7-C7-C8    | -3.75 | 115.37      | 122.05   |
| 6   | A     | 201  | HEM  | CBD-CAD-C3D | -3.55 | 102.71      | 112.53   |
| 8   | F     | 1003 | NAG  | C2-N2-C7    | -3.51 | 118.20      | 122.90   |
| 8   | L     | 1002 | NAG  | C1-O5-C5    | -3.39 | 107.64      | 112.19   |
| 6   | G     | 201  | HEM  | C3B-C4B-NB  | -3.39 | 107.03      | 109.47   |
| 8   | I     | 1004 | NAG  | O7-C7-C8    | -3.36 | 116.06      | 122.05   |
| 8   | I     | 1004 | NAG  | O6-C6-C5    | 3.29  | 122.53      | 111.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | G     | 201  | HEM  | CBD-CAD-C3D | -3.26 | 103.53      | 112.53   |
| 8   | I     | 1004 | NAG  | C1-C2-N2    | -3.22 | 105.36      | 110.43   |
| 6   | A     | 201  | HEM  | CAA-CBA-CGA | -3.22 | 105.14      | 113.67   |
| 8   | C     | 1004 | NAG  | O7-C7-C8    | -3.21 | 116.34      | 122.05   |
| 6   | K     | 201  | HEM  | C2A-C1A-NA  | -3.18 | 106.62      | 110.15   |
| 8   | C     | 1003 | NAG  | O5-C1-C2    | 3.17  | 116.19      | 111.29   |
| 8   | F     | 1004 | NAG  | C8-C7-N2    | 3.15  | 121.35      | 116.12   |
| 6   | J     | 201  | HEM  | CBD-CAD-C3D | -3.12 | 103.91      | 112.53   |
| 6   | H     | 201  | HEM  | C3B-C4B-NB  | -3.04 | 107.29      | 109.47   |
| 6   | E     | 201  | HEM  | CHC-C4B-NB  | 3.02  | 127.67      | 124.42   |
| 6   | H     | 201  | HEM  | CHC-C4B-NB  | 3.01  | 127.67      | 124.42   |
| 6   | A     | 201  | HEM  | C2A-C1A-NA  | -3.01 | 106.81      | 110.15   |
| 6   | D     | 201  | HEM  | CBD-CAD-C3D | -3.00 | 104.23      | 112.53   |
| 6   | H     | 201  | HEM  | C1B-NB-C4B  | 2.92  | 108.67      | 105.21   |
| 8   | C     | 1004 | NAG  | O7-C7-N2    | 2.81  | 126.94      | 121.98   |
| 6   | G     | 201  | HEM  | CAA-CBA-CGA | -2.79 | 106.26      | 113.67   |
| 6   | B     | 201  | HEM  | CHC-C4B-NB  | 2.71  | 127.34      | 124.42   |
| 8   | C     | 1004 | NAG  | C6-C5-C4    | -2.71 | 106.37      | 113.02   |
| 6   | G     | 201  | HEM  | C1B-NB-C4B  | 2.70  | 108.40      | 105.21   |
| 6   | J     | 201  | HEM  | CAA-CBA-CGA | -2.70 | 106.52      | 113.67   |
| 8   | C     | 1004 | NAG  | O6-C6-C5    | 2.68  | 120.45      | 111.33   |
| 8   | C     | 1004 | NAG  | O4-C4-C5    | 2.68  | 115.91      | 109.32   |
| 6   | A     | 201  | HEM  | C3B-C4B-NB  | -2.65 | 107.57      | 109.47   |
| 6   | J     | 201  | HEM  | C3B-C4B-NB  | -2.63 | 107.58      | 109.47   |
| 6   | D     | 201  | HEM  | CAA-CBA-CGA | -2.63 | 106.70      | 113.67   |
| 6   | E     | 201  | HEM  | C1B-NB-C4B  | 2.59  | 108.27      | 105.21   |
| 6   | K     | 201  | HEM  | C1B-NB-C4B  | 2.56  | 108.23      | 105.21   |
| 6   | J     | 201  | HEM  | C2A-C1A-NA  | -2.55 | 107.32      | 110.15   |
| 8   | C     | 1003 | NAG  | C8-C7-N2    | 2.55  | 120.35      | 116.12   |
| 8   | I     | 1003 | NAG  | C1-O5-C5    | -2.54 | 108.78      | 112.19   |
| 6   | B     | 201  | HEM  | C2A-C1A-NA  | -2.53 | 107.34      | 110.15   |
| 6   | B     | 201  | HEM  | C1B-NB-C4B  | 2.50  | 108.17      | 105.21   |
| 6   | B     | 201  | HEM  | C3B-C4B-NB  | -2.50 | 107.67      | 109.47   |
| 8   | I     | 1003 | NAG  | O3-C3-C4    | 2.50  | 116.27      | 110.38   |
| 6   | E     | 201  | HEM  | CAD-C3D-C4D | 2.47  | 129.01      | 124.70   |
| 6   | B     | 201  | HEM  | C4A-C3A-C2A | 2.46  | 109.64      | 106.82   |
| 8   | C     | 1003 | NAG  | O3-C3-C2    | -2.44 | 104.33      | 109.40   |
| 6   | E     | 201  | HEM  | C2A-C1A-NA  | -2.44 | 107.45      | 110.15   |
| 6   | G     | 201  | HEM  | C2A-C1A-NA  | -2.43 | 107.45      | 110.15   |
| 8   | C     | 1003 | NAG  | C4-C3-C2    | 2.42  | 114.56      | 111.02   |
| 6   | H     | 201  | HEM  | C2A-C1A-NA  | -2.42 | 107.47      | 110.15   |
| 6   | D     | 201  | HEM  | C2A-C1A-NA  | -2.39 | 107.50      | 110.15   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 8   | L     | 1002 | NAG  | C8-C7-N2    | 2.38  | 120.07      | 116.12   |
| 6   | J     | 201  | HEM  | C1B-NB-C4B  | 2.36  | 108.00      | 105.21   |
| 8   | C     | 1004 | NAG  | C1-C2-N2    | -2.34 | 106.75      | 110.43   |
| 8   | F     | 1003 | NAG  | O5-C5-C6    | 2.31  | 112.17      | 107.66   |
| 6   | G     | 201  | HEM  | CHD-C4C-NC  | 2.27  | 126.92      | 124.45   |
| 6   | K     | 201  | HEM  | CHA-C4D-ND  | 2.24  | 127.14      | 124.37   |
| 6   | K     | 201  | HEM  | CAD-CBD-CGD | -2.23 | 107.75      | 113.67   |
| 6   | B     | 201  | HEM  | CAD-C3D-C4D | 2.20  | 128.54      | 124.70   |
| 6   | K     | 201  | HEM  | CHD-C1D-ND  | 2.19  | 126.78      | 124.42   |
| 6   | H     | 201  | HEM  | CAD-C3D-C4D | 2.17  | 128.47      | 124.70   |
| 6   | A     | 201  | HEM  | CHC-C4B-NB  | 2.15  | 126.74      | 124.42   |
| 6   | D     | 201  | HEM  | C1D-C2D-C3D | -2.15 | 104.72      | 106.98   |
| 6   | E     | 201  | HEM  | C3B-C4B-NB  | -2.13 | 107.94      | 109.47   |
| 8   | C     | 1003 | NAG  | C1-O5-C5    | -2.13 | 109.34      | 112.19   |
| 8   | L     | 1002 | NAG  | C2-N2-C7    | -2.12 | 120.06      | 122.90   |
| 6   | K     | 201  | HEM  | C4A-NA-C1A  | 2.12  | 109.27      | 105.82   |
| 6   | D     | 201  | HEM  | O1A-CGA-CBA | -2.10 | 116.42      | 123.09   |
| 6   | B     | 201  | HEM  | O2A-CGA-CBA | 2.09  | 120.61      | 114.00   |
| 6   | K     | 201  | HEM  | C3D-C4D-ND  | -2.09 | 107.88      | 110.17   |
| 8   | L     | 1001 | NAG  | O7-C7-N2    | 2.05  | 125.60      | 121.98   |
| 6   | B     | 201  | HEM  | O2D-CGD-CBD | 2.05  | 120.47      | 114.00   |
| 8   | F     | 1003 | NAG  | C1-C2-N2    | -2.04 | 107.22      | 110.43   |
| 8   | C     | 1003 | NAG  | O3-C3-C4    | 2.03  | 115.17      | 110.38   |
| 8   | L     | 1001 | NAG  | O5-C1-C2    | 2.03  | 114.43      | 111.29   |
| 6   | A     | 201  | HEM  | CAD-C3D-C4D | 2.02  | 128.22      | 124.70   |
| 6   | D     | 201  | HEM  | CMD-C2D-C1D | 2.02  | 128.19      | 125.03   |
| 6   | H     | 201  | HEM  | C4A-C3A-C2A | 2.01  | 109.11      | 106.82   |

There are no chirality outliers.

All (33) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | B     | 201  | HEM  | C1A-C2A-CAA-CBA |
| 6   | E     | 201  | HEM  | C1A-C2A-CAA-CBA |
| 6   | H     | 201  | HEM  | C1A-C2A-CAA-CBA |
| 8   | C     | 1004 | NAG  | C3-C2-N2-C7     |
| 8   | L     | 1001 | NAG  | C3-C2-N2-C7     |
| 8   | L     | 1001 | NAG  | O5-C5-C6-O6     |
| 6   | K     | 201  | HEM  | C3D-CAD-CBD-CGD |
| 6   | B     | 201  | HEM  | C3A-C2A-CAA-CBA |
| 6   | E     | 201  | HEM  | C3A-C2A-CAA-CBA |
| 6   | H     | 201  | HEM  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 8   | C     | 1004 | NAG  | O5-C5-C6-O6     |
| 8   | L     | 1001 | NAG  | C4-C5-C6-O6     |
| 6   | B     | 201  | HEM  | C3D-CAD-CBD-CGD |
| 6   | E     | 201  | HEM  | C3D-CAD-CBD-CGD |
| 6   | H     | 201  | HEM  | C3D-CAD-CBD-CGD |
| 6   | K     | 201  | HEM  | C1A-C2A-CAA-CBA |
| 6   | E     | 201  | HEM  | C2A-CAA-CBA-CGA |
| 6   | H     | 201  | HEM  | C2A-CAA-CBA-CGA |
| 8   | C     | 1004 | NAG  | C4-C5-C6-O6     |
| 6   | B     | 201  | HEM  | C2A-CAA-CBA-CGA |
| 6   | B     | 201  | HEM  | CAD-CBD-CGD-O2D |
| 6   | H     | 201  | HEM  | CAD-CBD-CGD-O1D |
| 6   | B     | 201  | HEM  | CAD-CBD-CGD-O1D |
| 6   | H     | 201  | HEM  | CAD-CBD-CGD-O2D |
| 6   | E     | 201  | HEM  | CAD-CBD-CGD-O1D |
| 6   | E     | 201  | HEM  | CAD-CBD-CGD-O2D |
| 6   | D     | 201  | HEM  | CAD-CBD-CGD-O2D |
| 6   | G     | 201  | HEM  | CAD-CBD-CGD-O1D |
| 6   | G     | 201  | HEM  | CAD-CBD-CGD-O2D |
| 6   | D     | 201  | HEM  | CAD-CBD-CGD-O1D |
| 6   | J     | 201  | HEM  | CAD-CBD-CGD-O1D |
| 6   | A     | 201  | HEM  | CAD-CBD-CGD-O1D |
| 6   | K     | 201  | HEM  | CAD-CBD-CGD-O1D |

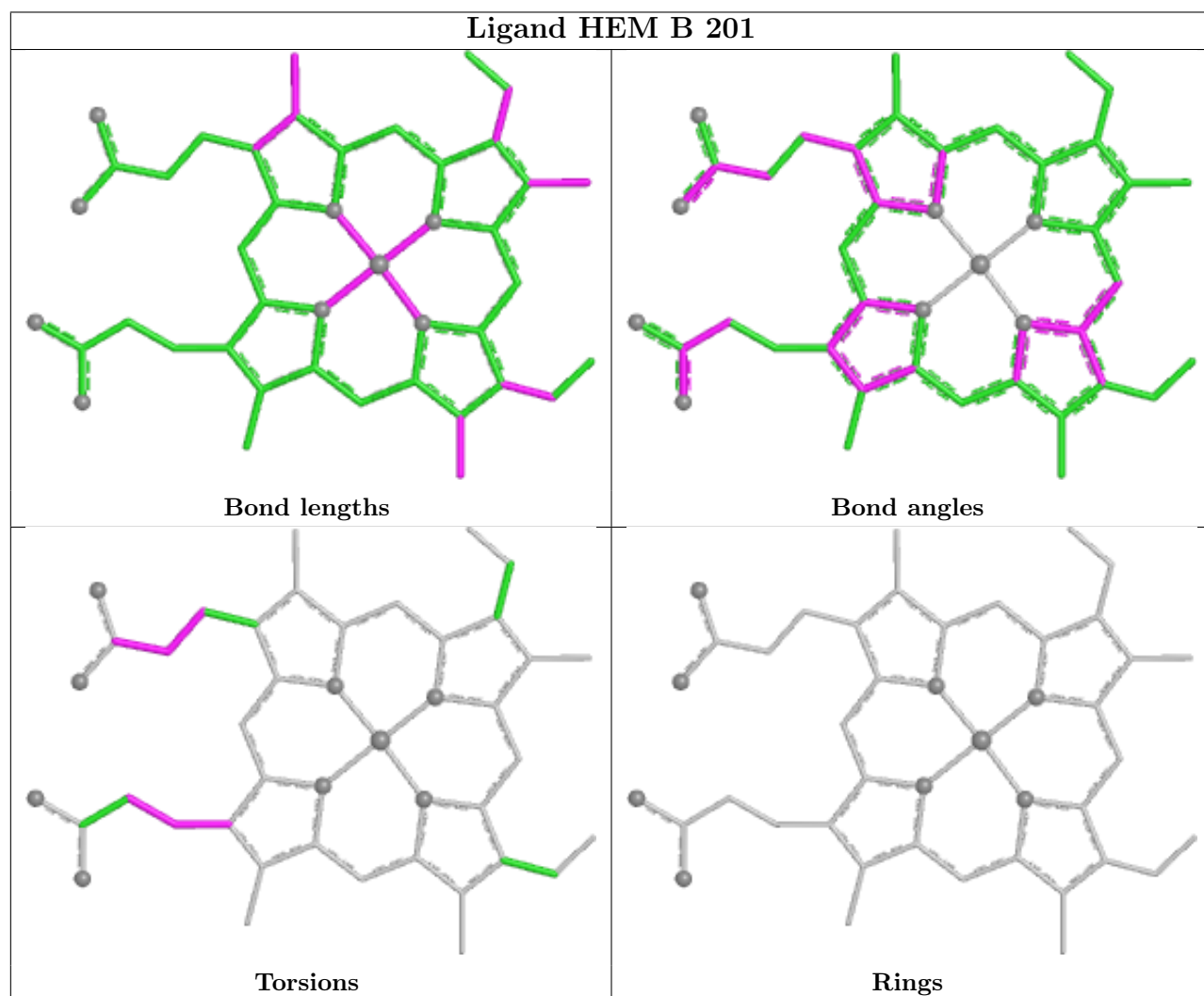
There are no ring outliers.

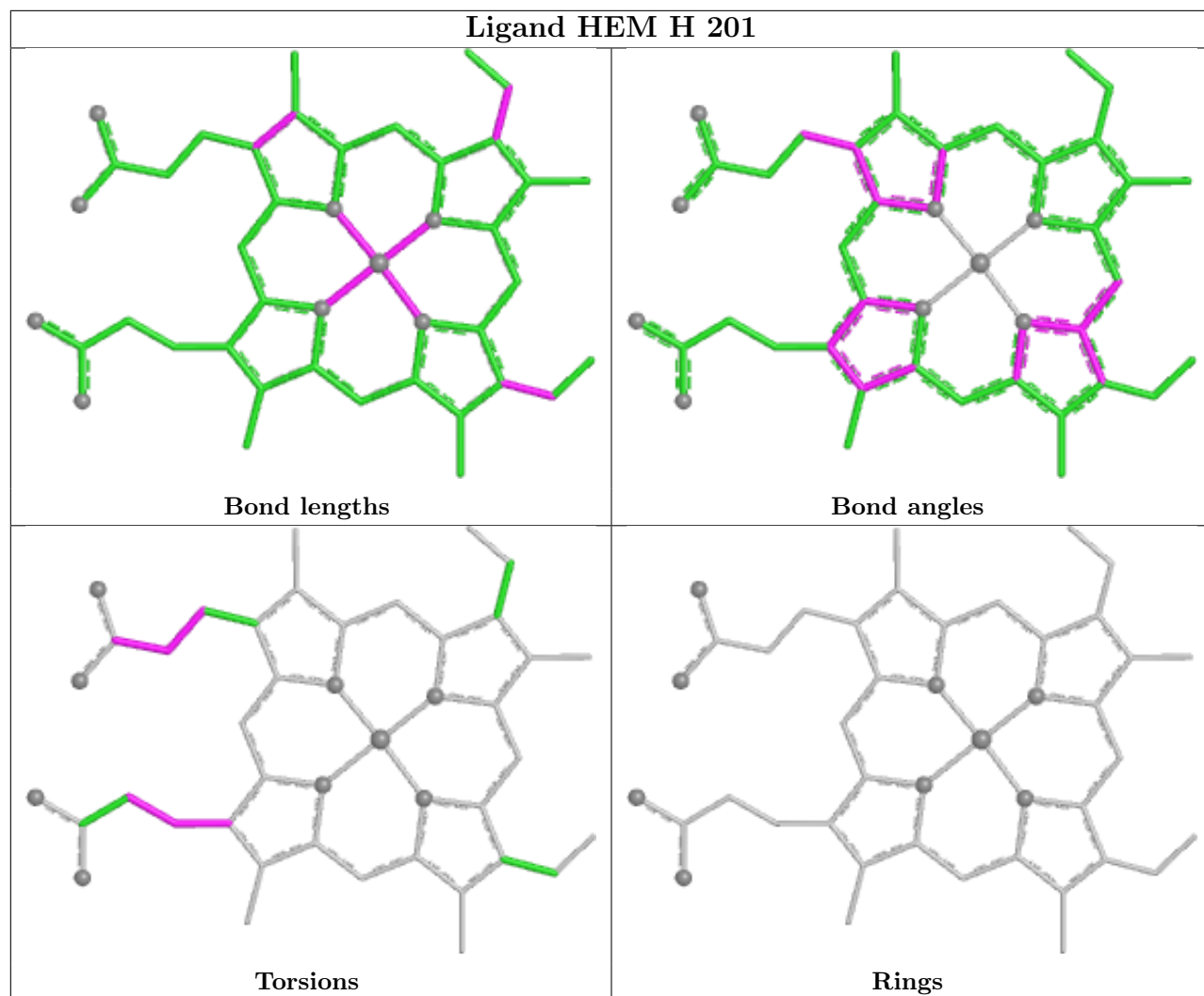
7 monomers are involved in 18 short contacts:

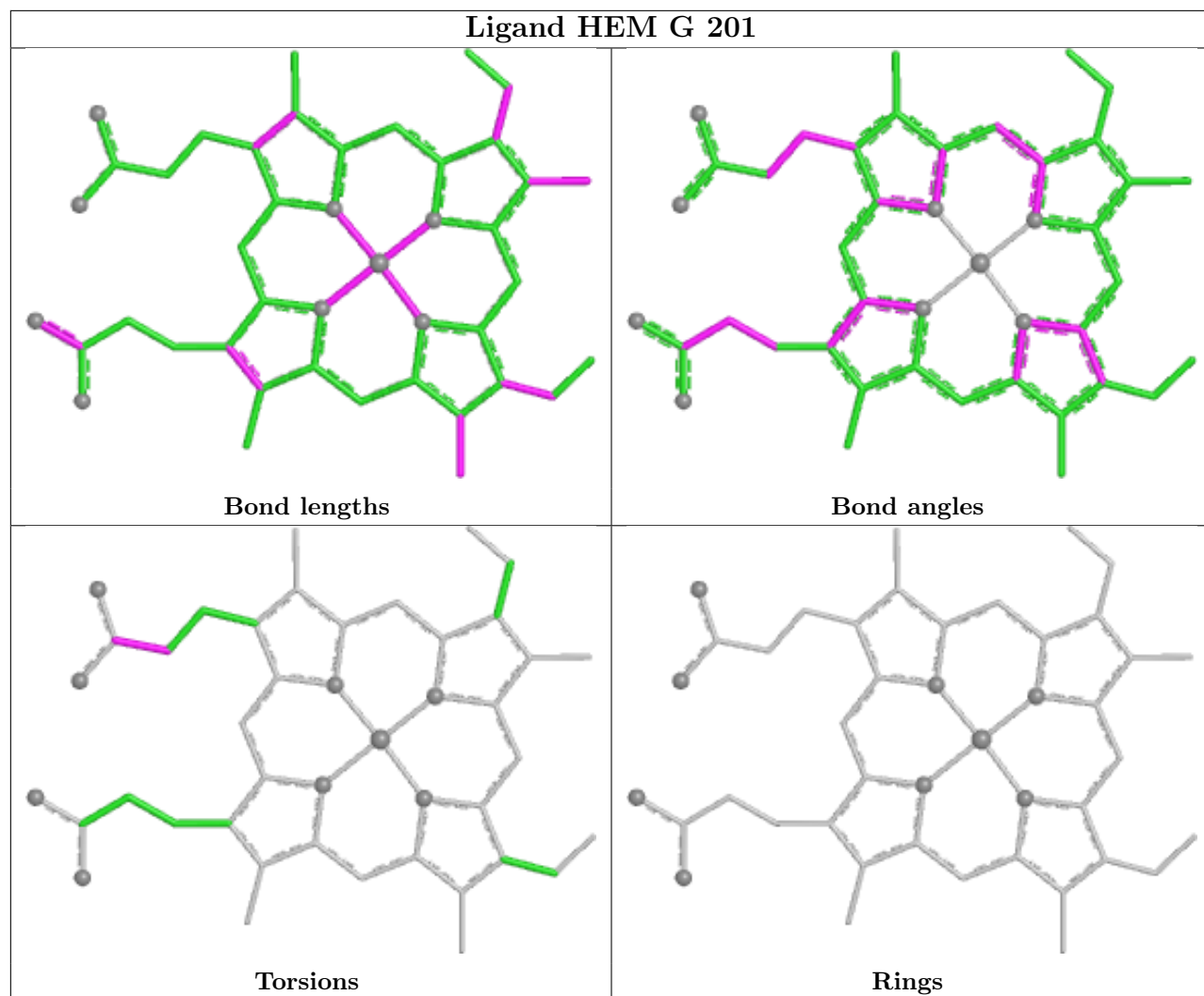
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | B     | 201  | HEM  | 4       | 0            |
| 6   | H     | 201  | HEM  | 4       | 0            |
| 8   | L     | 1002 | NAG  | 1       | 0            |
| 6   | A     | 201  | HEM  | 1       | 0            |
| 6   | K     | 201  | HEM  | 2       | 0            |
| 8   | C     | 1003 | NAG  | 1       | 0            |
| 6   | E     | 201  | HEM  | 5       | 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

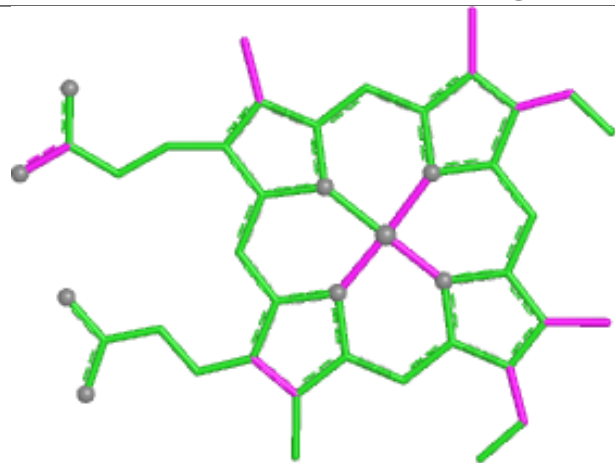
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



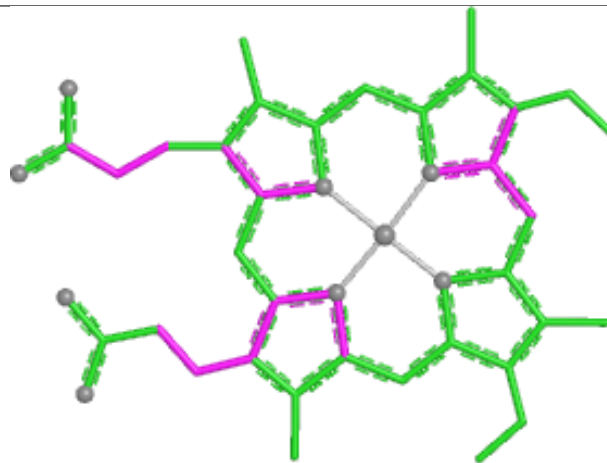




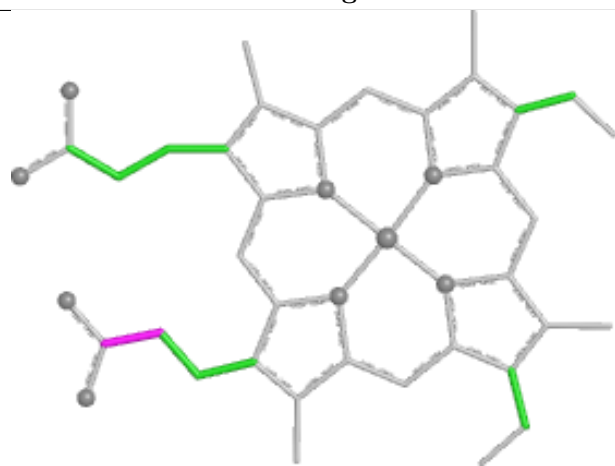
## Ligand HEM A 201



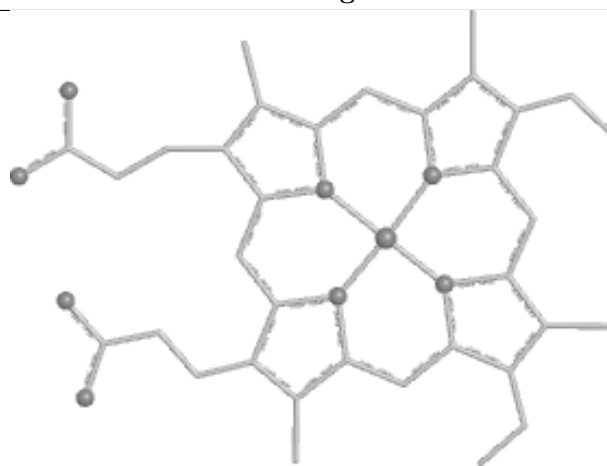
Bond lengths



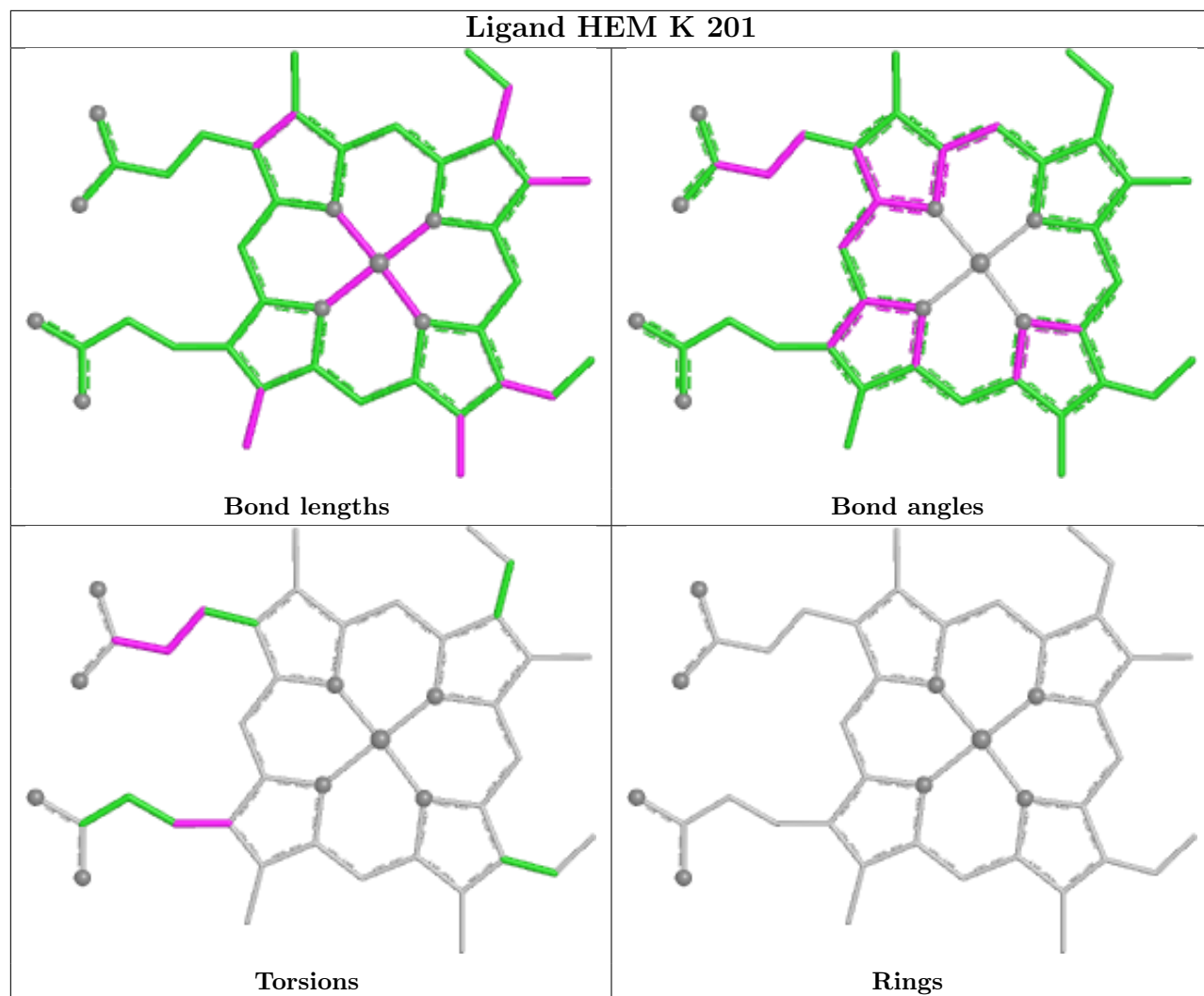
Bond angles

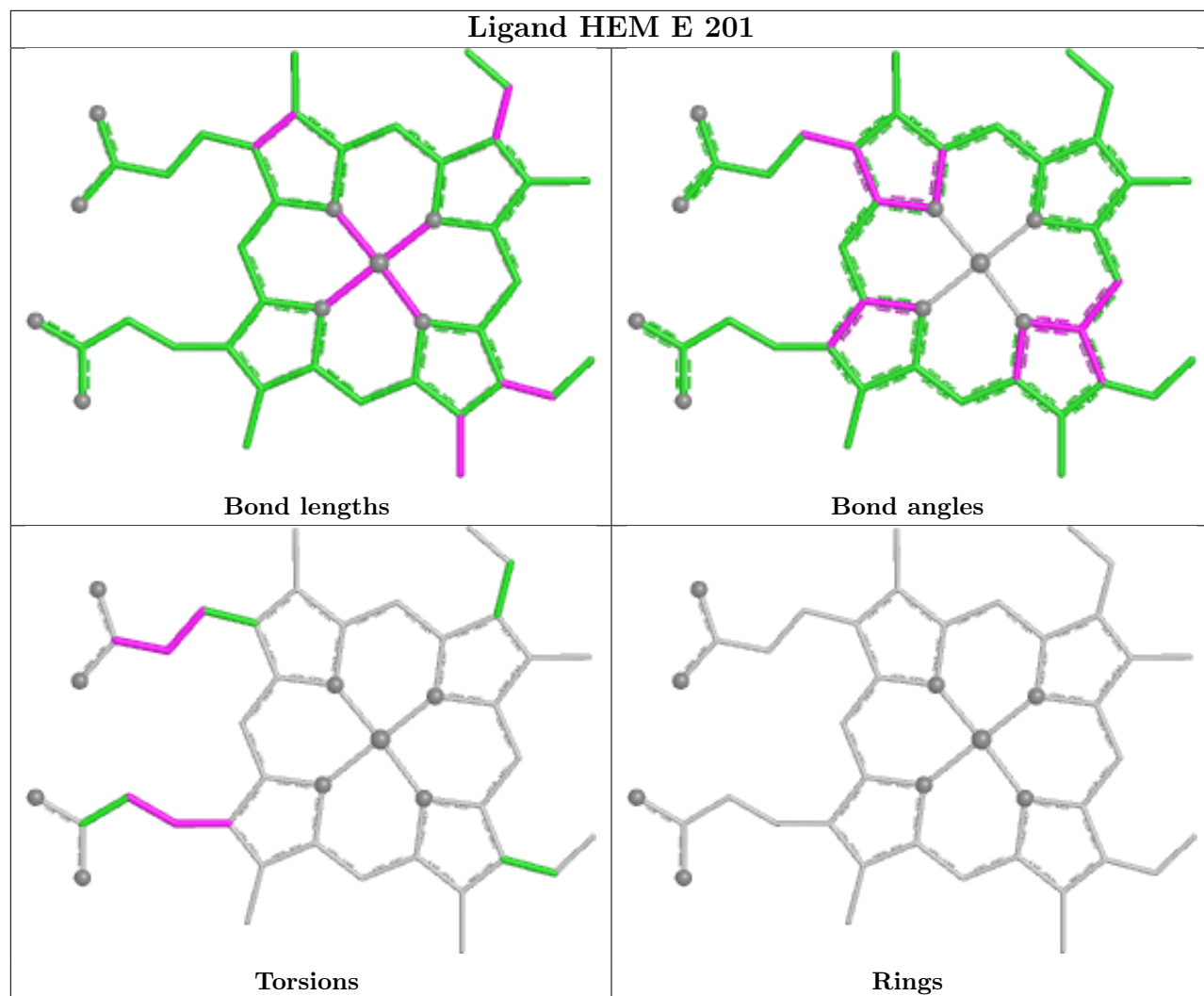


Torsions

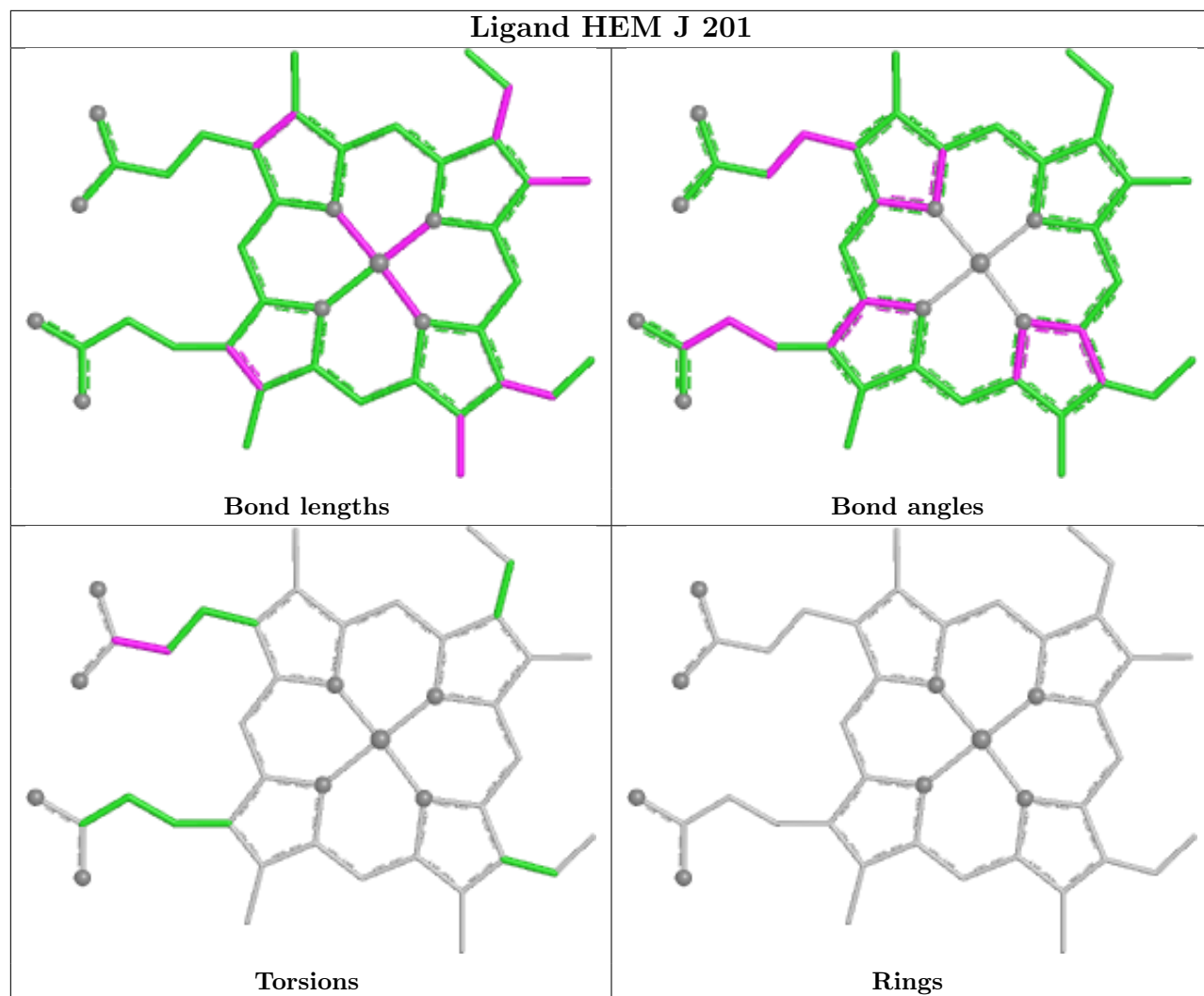


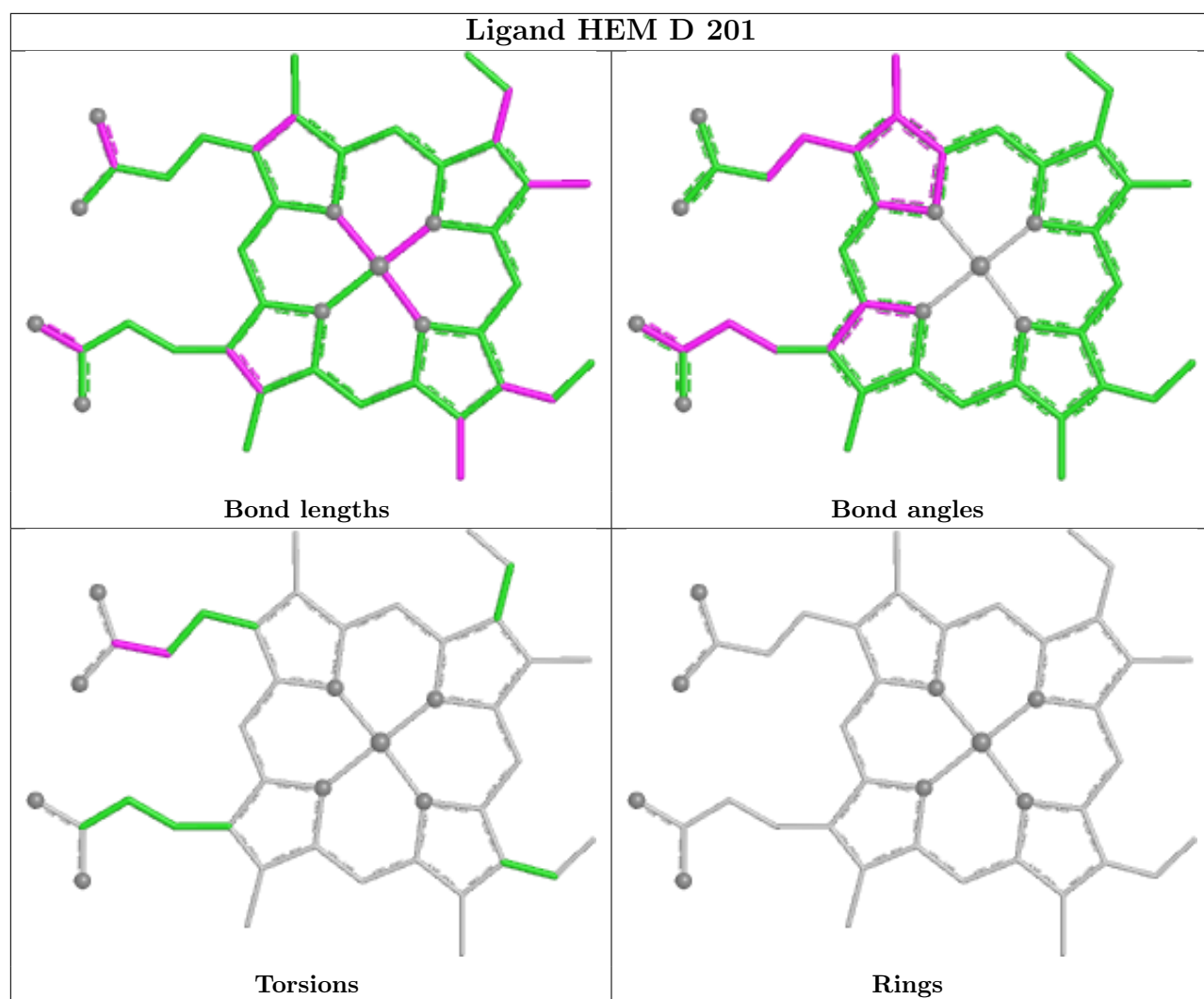
Rings





## Ligand HEM J 201





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9  |
|-----|-------|-----------------|--------|----------------|-----------------------|--------|
| 1   | A     | 141/141 (100%)  | -0.49  | 0 100 100      | 37, 56, 86, 124       | 0      |
| 1   | D     | 141/141 (100%)  | -0.40  | 4 (2%) 55 46   | 40, 57, 84, 103       | 0      |
| 1   | G     | 141/141 (100%)  | -0.39  | 1 (0%) 84 79   | 41, 60, 96, 132       | 0      |
| 1   | J     | 141/141 (100%)  | 1.51   | 42 (29%) 1 1   | 110, 156, 201, 300    | 0      |
| 2   | B     | 146/146 (100%)  | -0.17  | 5 (3%) 48 39   | 27, 84, 129, 196      | 1 (0%) |
| 2   | E     | 146/146 (100%)  | 0.06   | 7 (4%) 35 28   | 30, 93, 138, 233      | 1 (0%) |
| 2   | H     | 146/146 (100%)  | -0.15  | 5 (3%) 48 39   | 27, 85, 131, 204      | 1 (0%) |
| 2   | K     | 146/146 (100%)  | 1.60   | 39 (26%) 1 1   | 67, 182, 250, 268     | 1 (0%) |
| 3   | C     | 309/347 (89%)   | -0.20  | 1 (0%) 90 87   | 45, 81, 121, 186      | 0      |
| 3   | F     | 309/347 (89%)   | -0.26  | 1 (0%) 90 87   | 42, 72, 118, 165      | 1 (0%) |
| 3   | I     | 309/347 (89%)   | -0.24  | 7 (2%) 61 52   | 44, 67, 106, 133      | 0      |
| 3   | L     | 309/347 (89%)   | 0.14   | 9 (2%) 53 45   | 66, 103, 141, 187     | 1 (0%) |
| All | All   | 2384/2536 (94%) | 0.02   | 121 (5%) 33 26 | 27, 81, 176, 300      | 6 (0%) |

All (121) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 109 | LEU  | 6.9  |
| 1   | J     | 121 | VAL  | 5.8  |
| 2   | K     | 11  | VAL  | 5.3  |
| 1   | J     | 117 | PHE  | 4.7  |
| 3   | L     | 229 | ALA  | 4.6  |
| 1   | J     | 108 | THR  | 4.5  |
| 1   | J     | 10  | VAL  | 4.4  |
| 2   | K     | 65  | LYS  | 4.2  |
| 2   | K     | 20  | VAL  | 4.1  |
| 2   | K     | 7   | GLU  | 4.0  |
| 2   | H     | 125 | ASN  | 3.9  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 3   | L     | 149    | HIS  | 3.8  |
| 1   | J     | 69     | ALA  | 3.8  |
| 2   | E     | 101[A] | GLU  | 3.6  |
| 1   | J     | 30     | GLU  | 3.5  |
| 3   | L     | 151    | ASN  | 3.5  |
| 1   | J     | 48     | LEU  | 3.5  |
| 2   | E     | 2      | HIS  | 3.4  |
| 2   | H     | 1      | VAL  | 3.3  |
| 2   | K     | 2      | HIS  | 3.2  |
| 1   | J     | 14     | TRP  | 3.2  |
| 2   | K     | 10     | ALA  | 3.2  |
| 1   | J     | 21     | ALA  | 3.1  |
| 1   | J     | 28     | ALA  | 3.1  |
| 1   | J     | 19     | GLY  | 3.1  |
| 2   | K     | 8      | LYS  | 3.1  |
| 1   | J     | 1      | VAL  | 3.1  |
| 2   | B     | 125    | ASN  | 3.1  |
| 1   | J     | 110    | ALA  | 3.0  |
| 2   | K     | 71     | PHE  | 3.0  |
| 2   | E     | 125    | ASN  | 3.0  |
| 1   | J     | 111    | ALA  | 3.0  |
| 2   | K     | 68     | LEU  | 3.0  |
| 1   | J     | 43     | PHE  | 3.0  |
| 2   | K     | 145    | TYR  | 2.9  |
| 3   | L     | 97     | VAL  | 2.9  |
| 2   | K     | 143    | HIS  | 2.9  |
| 1   | D     | 53     | ASP  | 2.9  |
| 2   | K     | 5      | ALA  | 2.9  |
| 2   | K     | 15     | TRP  | 2.8  |
| 2   | K     | 109    | VAL  | 2.8  |
| 2   | K     | 112    | VAL  | 2.8  |
| 2   | K     | 125    | ASN  | 2.8  |
| 2   | K     | 91     | LEU  | 2.8  |
| 2   | K     | 1      | VAL  | 2.8  |
| 1   | J     | 51     | GLY  | 2.8  |
| 2   | B     | 144    | LYS  | 2.8  |
| 1   | J     | 46     | PHE  | 2.7  |
| 3   | L     | 106    | GLY  | 2.7  |
| 2   | K     | 101[A] | GLU  | 2.7  |
| 1   | J     | 112    | HIS  | 2.7  |
| 2   | K     | 146    | HIS  | 2.7  |
| 2   | K     | 127    | GLN  | 2.7  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | J     | 16     | LYS  | 2.7  |
| 2   | K     | 120    | HIS  | 2.6  |
| 2   | K     | 144    | LYS  | 2.6  |
| 1   | J     | 32     | MET  | 2.6  |
| 1   | J     | 57     | ALA  | 2.6  |
| 1   | D     | 1      | VAL  | 2.6  |
| 1   | J     | 136    | LEU  | 2.6  |
| 1   | J     | 102    | SER  | 2.5  |
| 1   | J     | 37     | PRO  | 2.5  |
| 1   | J     | 132    | VAL  | 2.5  |
| 2   | K     | 69     | GLN  | 2.5  |
| 3   | I     | 53     | GLN  | 2.5  |
| 2   | E     | 144    | LYS  | 2.5  |
| 3   | I     | 346    | ASP  | 2.5  |
| 2   | K     | 23     | VAL  | 2.5  |
| 1   | J     | 80     | LEU  | 2.4  |
| 1   | J     | 128    | PHE  | 2.4  |
| 2   | K     | 82     | LYS  | 2.4  |
| 1   | J     | 105    | LEU  | 2.4  |
| 2   | K     | 74     | GLY  | 2.4  |
| 3   | I     | 256    | GLY  | 2.4  |
| 3   | L     | 53     | GLN  | 2.4  |
| 2   | B     | 146    | HIS  | 2.4  |
| 3   | L     | 230    | ASN  | 2.4  |
| 2   | K     | 75     | LEU  | 2.4  |
| 2   | B     | 101[A] | GLU  | 2.3  |
| 2   | H     | 2      | HIS  | 2.3  |
| 2   | K     | 34     | VAL  | 2.3  |
| 1   | J     | 26     | ALA  | 2.3  |
| 1   | J     | 49     | SER  | 2.3  |
| 2   | B     | 2      | HIS  | 2.3  |
| 2   | K     | 63     | HIS  | 2.3  |
| 2   | K     | 18     | VAL  | 2.3  |
| 2   | H     | 101[A] | GLU  | 2.3  |
| 2   | E     | 82     | LYS  | 2.3  |
| 2   | K     | 14     | LEU  | 2.2  |
| 1   | D     | 16     | LYS  | 2.2  |
| 3   | I     | 150    | LYS  | 2.2  |
| 2   | K     | 122    | PHE  | 2.2  |
| 3   | I     | 247    | GLN  | 2.2  |
| 1   | G     | 50     | HIS  | 2.2  |
| 1   | J     | 93     | VAL  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | E     | 1   | VAL  | 2.2  |
| 2   | K     | 130 | PHE  | 2.2  |
| 2   | K     | 87  | LYS  | 2.2  |
| 1   | J     | 106 | LEU  | 2.2  |
| 1   | J     | 113 | HIS  | 2.2  |
| 1   | J     | 17  | VAL  | 2.2  |
| 2   | H     | 17  | LYS  | 2.2  |
| 1   | J     | 24  | HIS  | 2.1  |
| 3   | L     | 104 | MET  | 2.1  |
| 2   | K     | 102 | ASN  | 2.1  |
| 1   | J     | 35  | GLY  | 2.1  |
| 3   | C     | 258 | THR  | 2.1  |
| 2   | K     | 41  | PHE  | 2.1  |
| 1   | J     | 104 | CYS  | 2.1  |
| 2   | K     | 126 | VAL  | 2.1  |
| 1   | D     | 50  | HIS  | 2.1  |
| 2   | K     | 133 | VAL  | 2.1  |
| 3   | I     | 97  | VAL  | 2.1  |
| 1   | J     | 83  | LEU  | 2.1  |
| 1   | J     | 116 | ASP  | 2.1  |
| 2   | E     | 8   | LYS  | 2.0  |
| 1   | J     | 55  | VAL  | 2.0  |
| 3   | L     | 152 | ASP  | 2.0  |
| 3   | F     | 201 | GLU  | 2.0  |
| 1   | J     | 34  | LEU  | 2.0  |
| 3   | I     | 151 | ASN  | 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](#)

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  | O     | 2   | 14/15 | 0.45 | 0.19 | 161,161,161,161            | 0     |
| 4   | NAG  | Q     | 2   | 14/15 | 0.45 | 0.15 | 168,168,168,168            | 0     |

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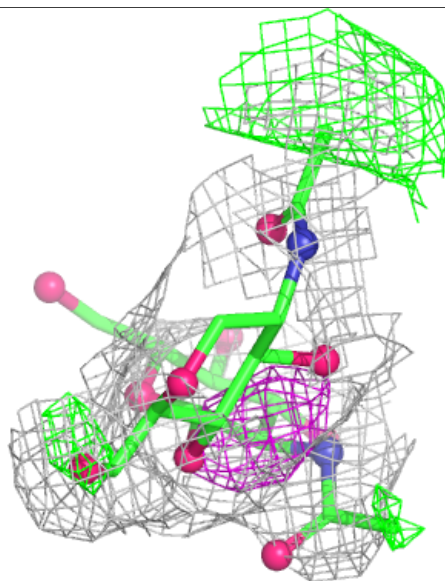
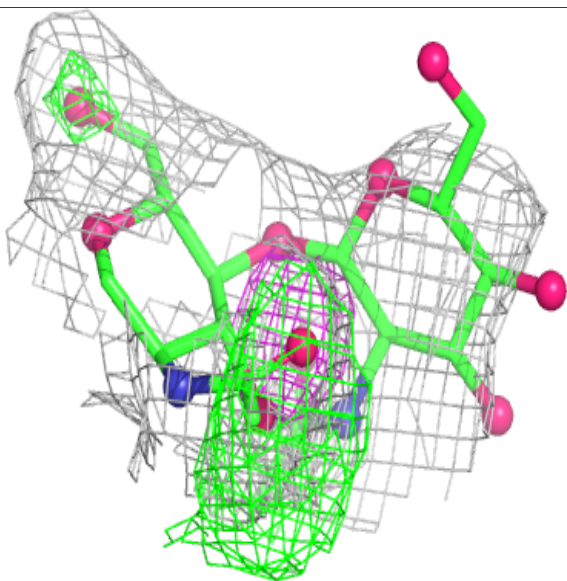
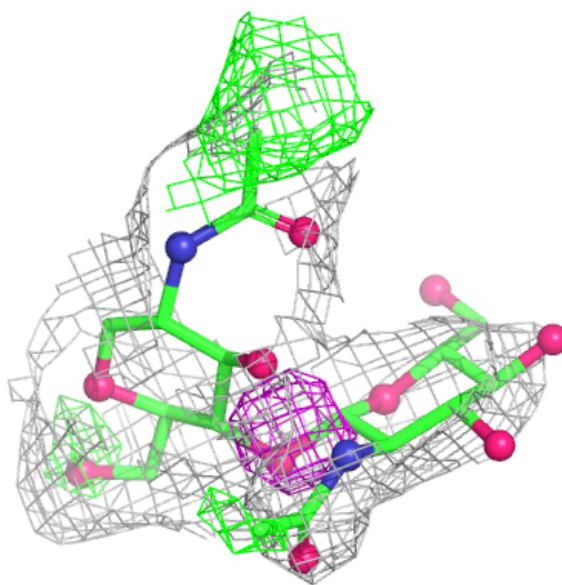
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | NAG  | M     | 1   | 14/15 | 0.48 | 0.15 | 122,122,122,122             | 0     |
| 4   | NAG  | M     | 2   | 14/15 | 0.49 | 0.17 | 180,180,180,180             | 0     |
| 4   | NAG  | O     | 1   | 14/15 | 0.51 | 0.19 | 118,118,118,118             | 0     |
| 4   | NAG  | Q     | 1   | 14/15 | 0.55 | 0.17 | 126,126,126,126             | 0     |
| 5   | FUC  | S     | 2   | 10/11 | 0.63 | 0.22 | 188,188,188,188             | 0     |
| 5   | NAG  | S     | 1   | 14/15 | 0.64 | 0.19 | 212,212,212,212             | 0     |
| 5   | NAG  | P     | 1   | 14/15 | 0.67 | 0.18 | 135,135,135,135             | 0     |
| 5   | FUC  | P     | 2   | 10/11 | 0.71 | 0.23 | 149,149,149,149             | 0     |
| 5   | NAG  | N     | 1   | 14/15 | 0.74 | 0.18 | 138,138,138,138             | 0     |
| 5   | FUC  | N     | 2   | 10/11 | 0.76 | 0.17 | 138,138,138,138             | 0     |
| 5   | FUC  | R     | 2   | 10/11 | 0.81 | 0.17 | 148,148,148,148             | 0     |
| 5   | NAG  | R     | 1   | 14/15 | 0.83 | 0.17 | 141,141,141,141             | 0     |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

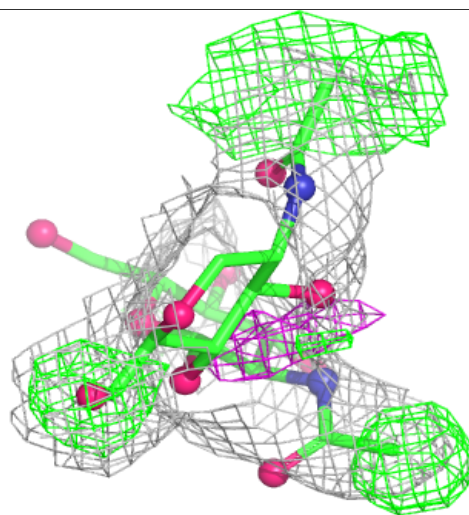
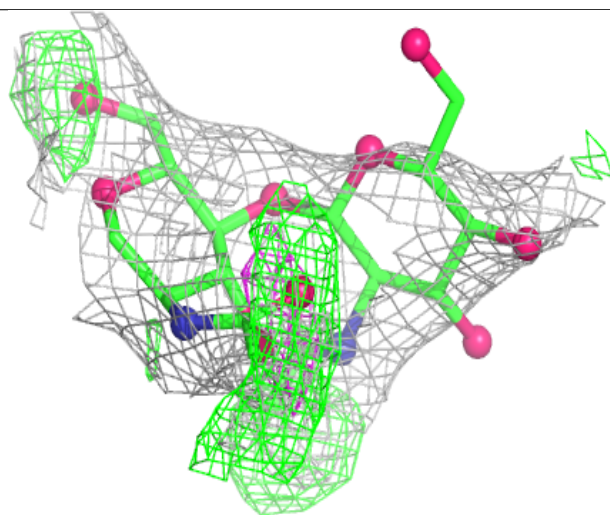
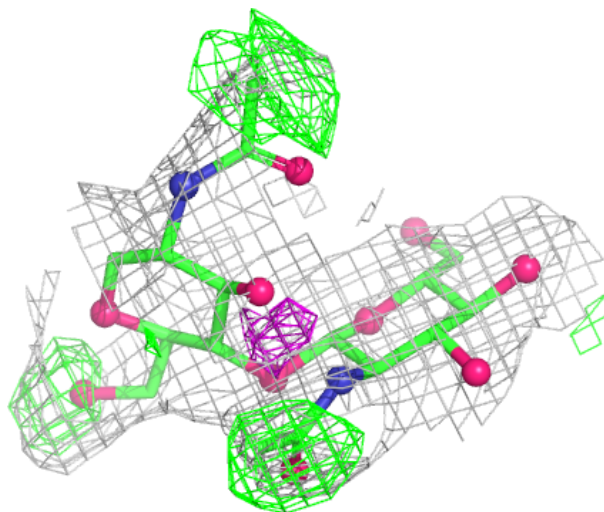
**Electron density around Chain M:**

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



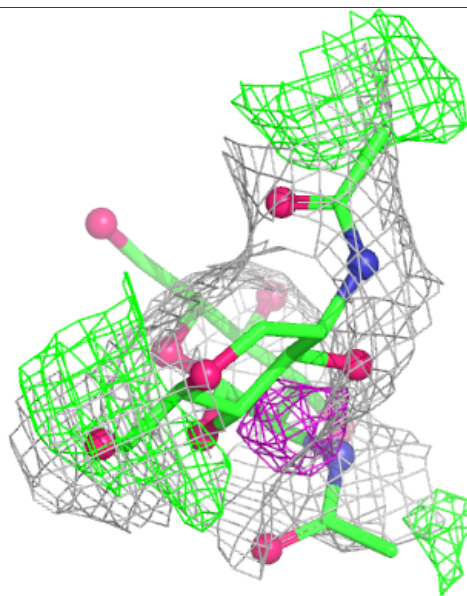
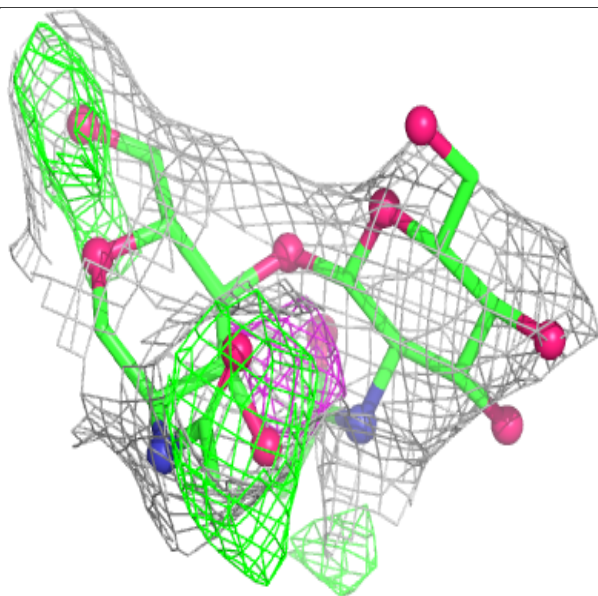
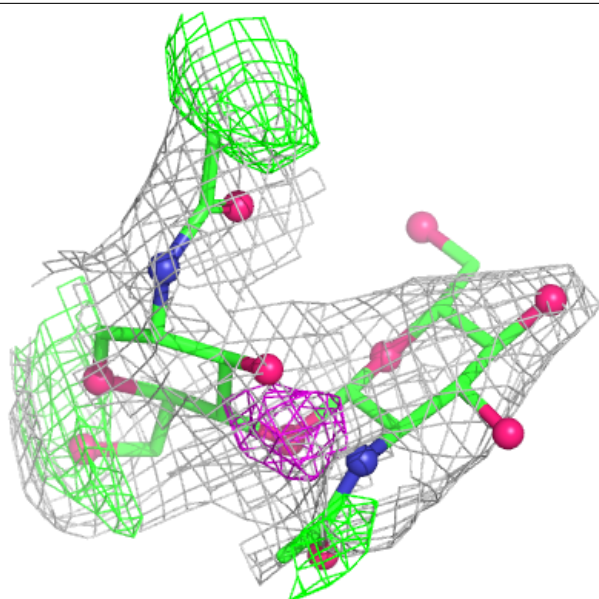
**Electron density around Chain O:**

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



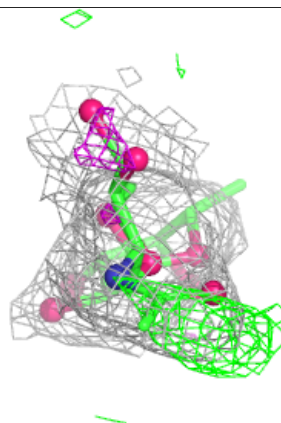
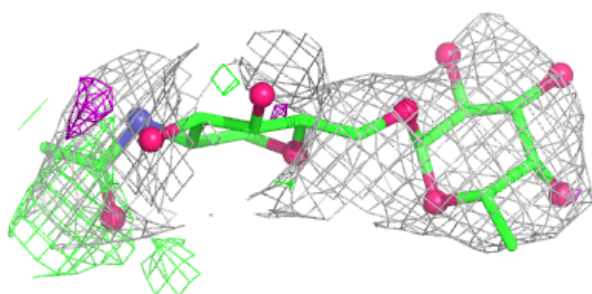
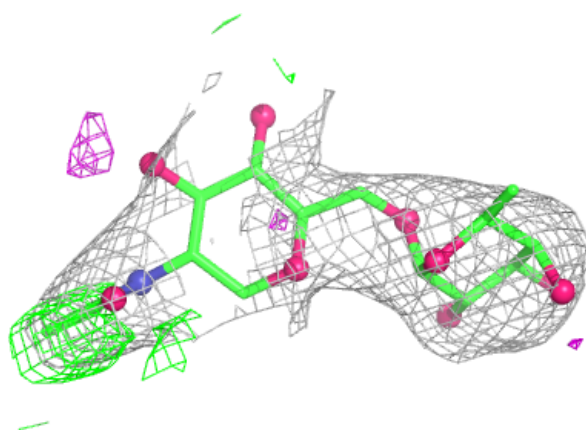
**Electron density around Chain Q:**

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

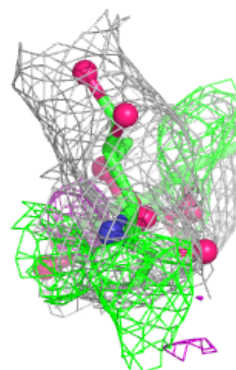
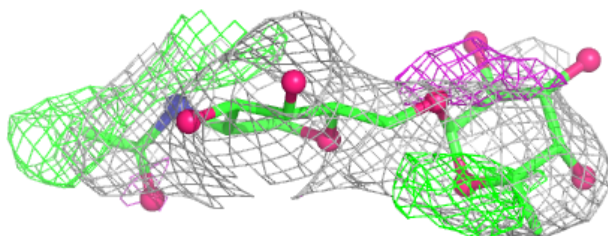
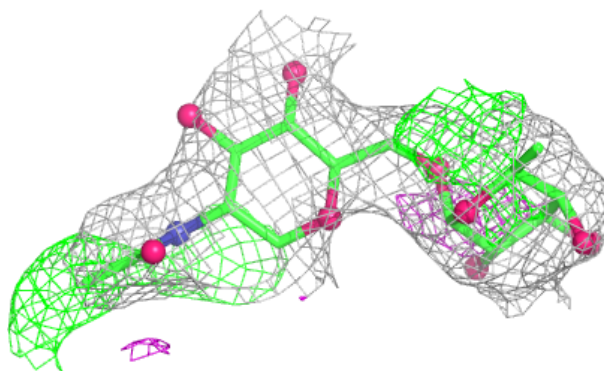


**Electron density around Chain N:**

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

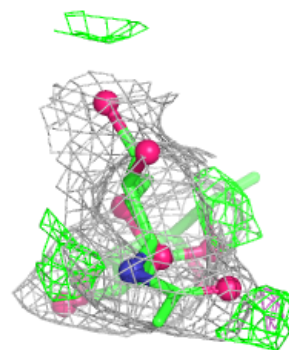
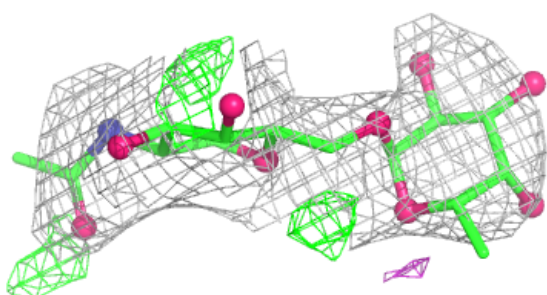
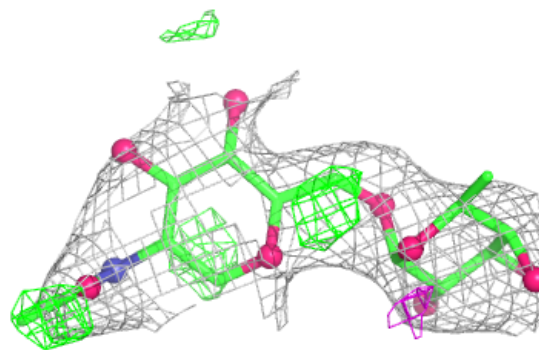
**Electron density around Chain P:**

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

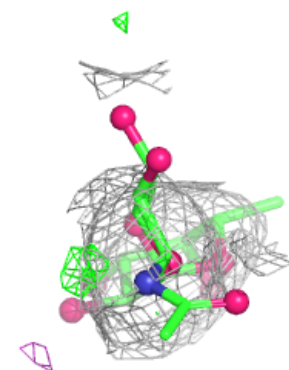
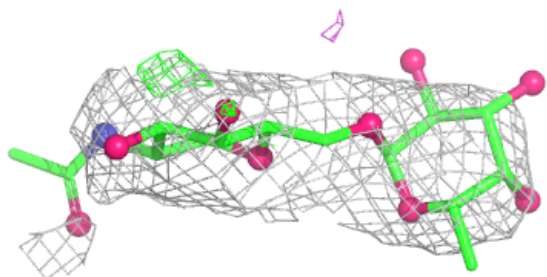
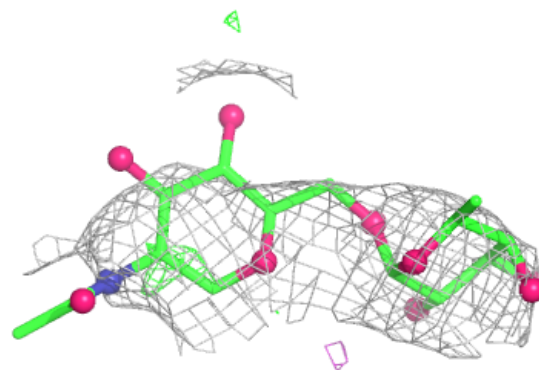


**Electron density around Chain R:**

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

**Electron density around Chain S:**

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



## 6.4 Ligands ⓘ

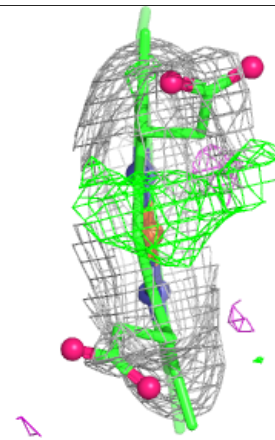
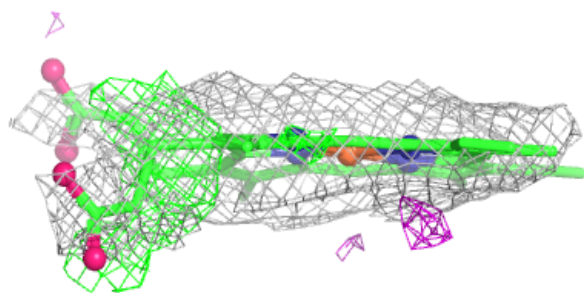
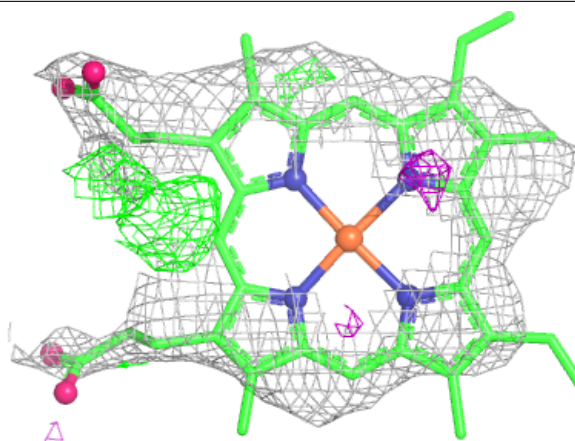
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 8   | NAG  | L     | 1001 | 14/15 | 0.19 | 0.18 | 138,138,138,138            | 0     |
| 8   | NAG  | C     | 1003 | 14/15 | 0.44 | 0.19 | 172,172,172,172            | 0     |
| 8   | NAG  | F     | 1003 | 14/15 | 0.58 | 0.16 | 174,174,174,174            | 0     |
| 8   | NAG  | I     | 1003 | 14/15 | 0.68 | 0.15 | 164,164,164,164            | 0     |
| 8   | NAG  | I     | 1004 | 14/15 | 0.70 | 0.17 | 150,150,150,150            | 0     |
| 8   | NAG  | F     | 1004 | 14/15 | 0.70 | 0.16 | 144,144,144,144            | 0     |
| 8   | NAG  | L     | 1002 | 14/15 | 0.74 | 0.15 | 171,171,171,171            | 0     |
| 7   | OXY  | J     | 202  | 2/2   | 0.80 | 0.21 | 225,225,225,229            | 0     |
| 8   | NAG  | C     | 1004 | 14/15 | 0.82 | 0.14 | 159,159,159,159            | 0     |
| 6   | HEM  | K     | 201  | 43/43 | 0.89 | 0.17 | 167,186,195,199            | 0     |
| 6   | HEM  | J     | 201  | 43/43 | 0.93 | 0.17 | 183,186,190,191            | 0     |
| 6   | HEM  | E     | 201  | 43/43 | 0.97 | 0.10 | 95,101,114,121             | 0     |
| 7   | OXY  | E     | 202  | 2/2   | 0.97 | 0.12 | 146,146,146,148            | 0     |
| 6   | HEM  | B     | 201  | 43/43 | 0.97 | 0.09 | 76,80,95,103               | 0     |
| 7   | OXY  | K     | 202  | 2/2   | 0.97 | 0.31 | 292,292,292,295            | 0     |
| 7   | OXY  | G     | 202  | 2/2   | 0.98 | 0.20 | 101,101,101,105            | 0     |
| 7   | OXY  | H     | 202  | 2/2   | 0.98 | 0.12 | 174,174,174,176            | 0     |
| 7   | OXY  | B     | 202  | 2/2   | 0.98 | 0.17 | 121,121,121,123            | 0     |
| 6   | HEM  | H     | 201  | 43/43 | 0.98 | 0.09 | 83,87,101,109              | 0     |
| 6   | HEM  | D     | 201  | 43/43 | 0.99 | 0.07 | 45,51,57,59                | 0     |
| 7   | OXY  | D     | 202  | 2/2   | 0.99 | 0.08 | 84,84,84,88                | 0     |
| 6   | HEM  | A     | 201  | 43/43 | 0.99 | 0.05 | 45,54,62,63                | 0     |
| 6   | HEM  | G     | 201  | 43/43 | 0.99 | 0.06 | 41,58,62,64                | 0     |
| 7   | OXY  | A     | 202  | 2/2   | 0.99 | 0.13 | 92,92,92,96                | 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.

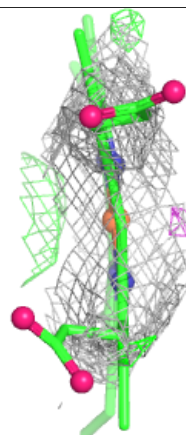
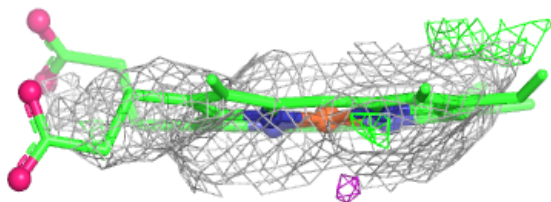
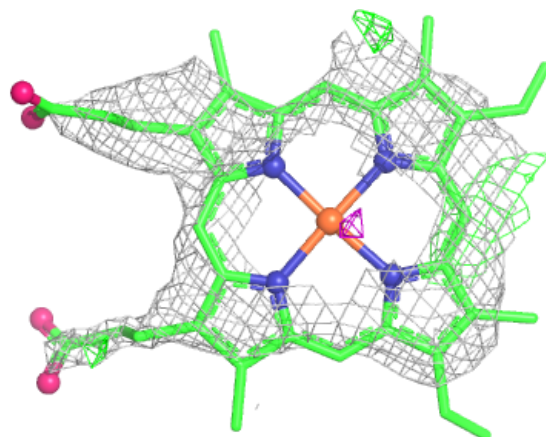
**Electron density around HEM K 201:**

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



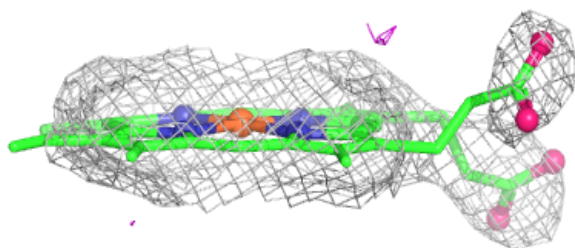
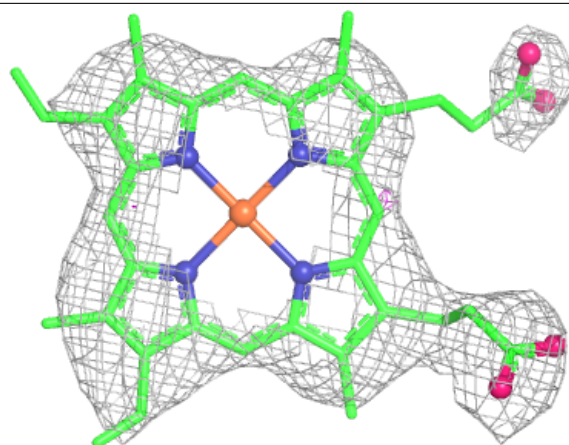
**Electron density around HEM J 201:**

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



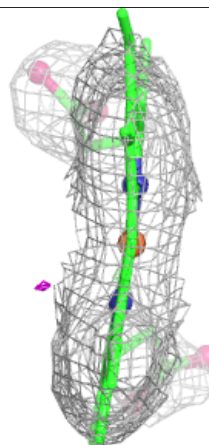
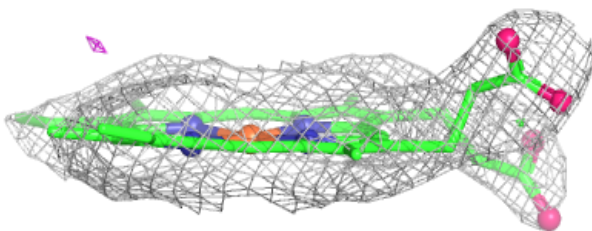
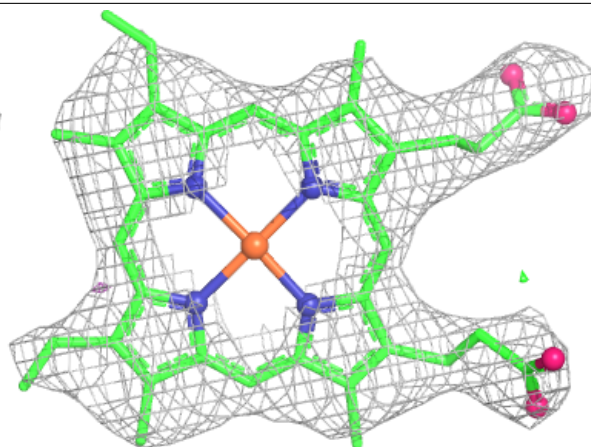
**Electron density around HEM E 201:**

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



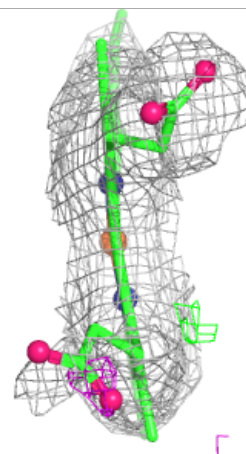
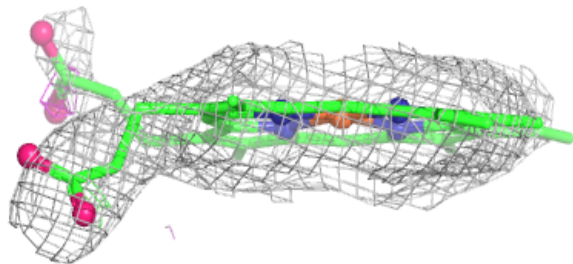
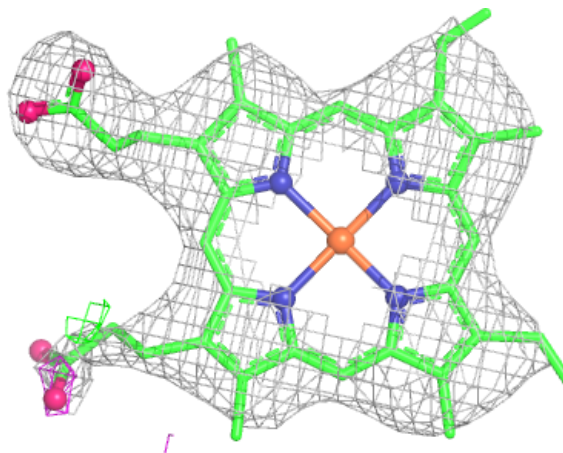
**Electron density around HEM B 201:**

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



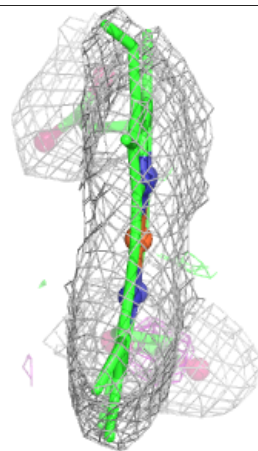
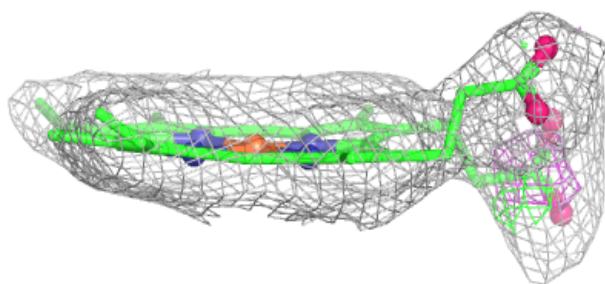
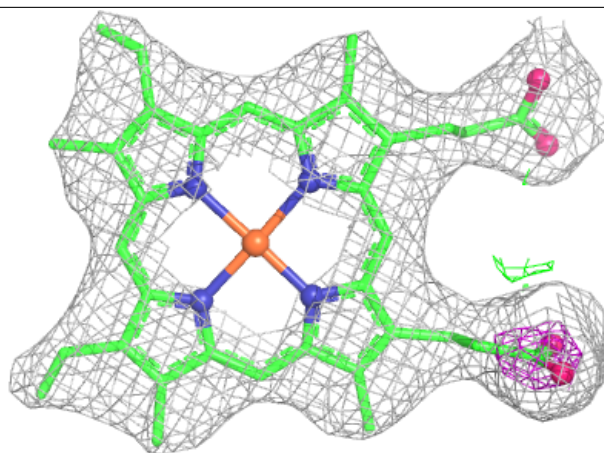
**Electron density around HEM H 201:**

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



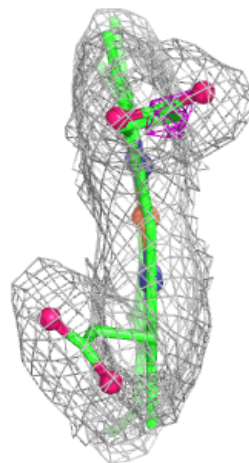
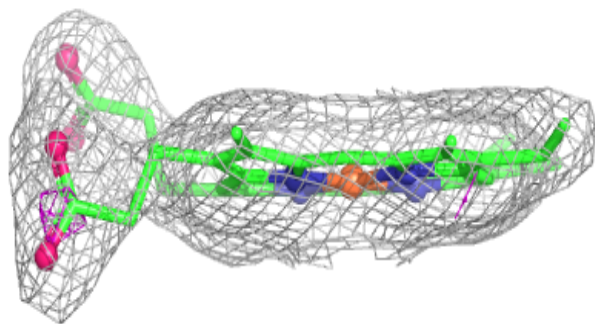
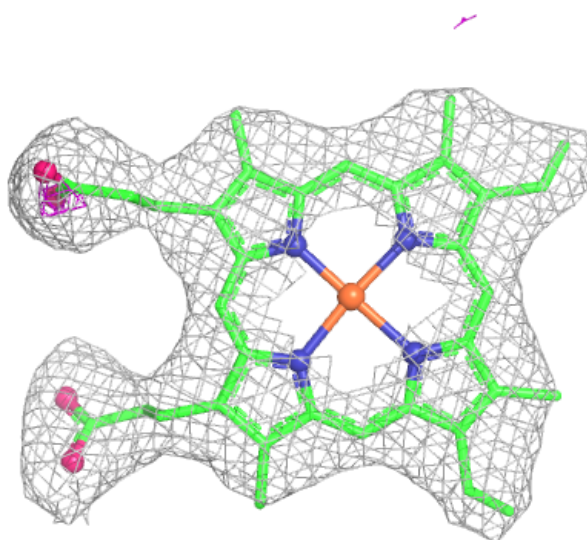
**Electron density around HEM D 201:**

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



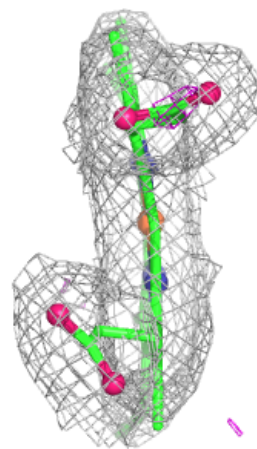
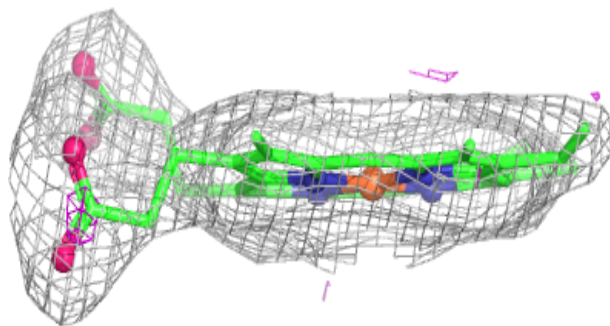
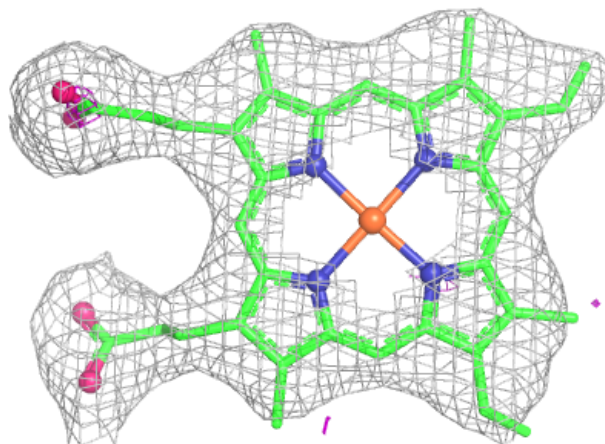
**Electron density around HEM A 201:**

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



**Electron density around HEM G 201:**

$2mF_o-DF_c$  (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.