



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:46 PM BST

PDB ID : 4DL1  
Title : Crystal Structure of human Myeloperoxidase with covalent thioxanthine analog  
Authors : Vajdos, F.; Varghese, A.  
Deposited on : 2012-02-05  
Resolution : 2.00 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

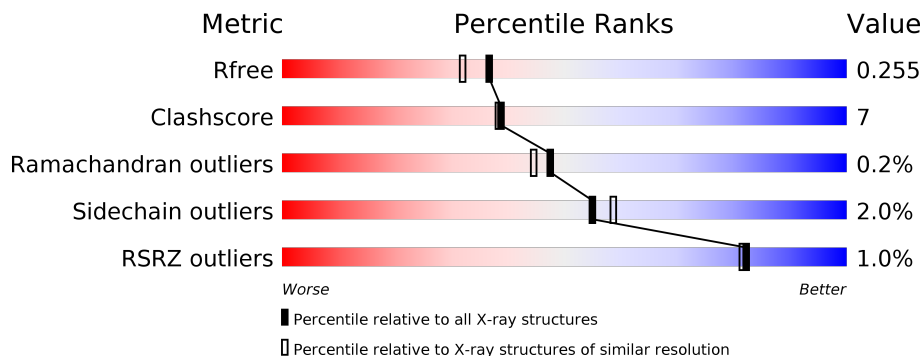
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 8085 (2.00-2.00)                                      |
| Clashscore            | 141614                      | 9178 (2.00-2.00)                                      |
| Ramachandran outliers | 138981                      | 9054 (2.00-2.00)                                      |
| Sidechain outliers    | 138945                      | 9053 (2.00-2.00)                                      |
| RSRZ outliers         | 127900                      | 7900 (2.00-2.00)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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     | 104    | <div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: red; margin-bottom: 2px;"></div> <div style="width: 100%; height: 10px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 10px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 10px; background-color: orange; margin-bottom: 2px;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>91%</span> <span>9%</span> </div> |
| 1   | B     | 104    | <div style="width: 100%; height: 10px; background-color: green; margin-bottom: 2px;"></div> <div style="width: 100%; height: 10px; background-color: yellow; margin-bottom: 2px;"></div> <div style="width: 100%; height: 10px; background-color: orange; margin-bottom: 2px;"></div>   |

83%
17%

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | M     | 104    | 2% 85% 14%       |
| 1   | N     | 104    | 85% 15%          |
| 2   | C     | 466    | 86% 13%          |
| 2   | D     | 466    | 2% 86% 13%       |
| 2   | G     | 466    | 2% 80% 18%       |
| 2   | H     | 466    | 2% 85% 15%       |
| 2   | K     | 466    | 2% 84% 15%       |
| 2   | L     | 466    | 2% 86% 13%       |
| 2   | O     | 466    | 2% 83% 16%       |
| 2   | P     | 466    | 2% 85% 14%       |
| 3   | Q     | 6      | 33% 50% 17%      |
| 3   | R     | 6      | 33% 67%          |
| 3   | S     | 6      | 17% 83%          |
| 3   | T     | 6      | 17% 67% 17%      |
| 3   | U     | 6      | 100%             |
| 3   | V     | 6      | 100%             |
| 3   | W     | 6      | 17% 83%          |
| 3   | X     | 6      | 83% 17%          |
| 4   | Y     | 5      | 20% 80%          |

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 40392 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Myeloperoxidase light chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 1   | A     | 104      | 838   | 529 | 148 | 156 | 5 | 0       | 0       | 0     |
| 1   | B     | 104      | 838   | 529 | 148 | 156 | 5 | 0       | 0       | 0     |
| 1   | E     | 104      | 838   | 529 | 148 | 156 | 5 | 0       | 0       | 0     |
| 1   | F     | 104      | 838   | 529 | 148 | 156 | 5 | 0       | 0       | 0     |
| 1   | I     | 104      | 838   | 529 | 148 | 156 | 5 | 0       | 0       | 0     |
| 1   | J     | 104      | 838   | 529 | 148 | 156 | 5 | 0       | 0       | 0     |
| 1   | M     | 104      | 838   | 529 | 148 | 156 | 5 | 0       | 0       | 0     |
| 1   | N     | 104      | 841   | 531 | 148 | 157 | 5 | 0       | 1       | 0     |

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

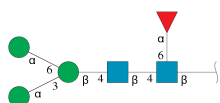
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 2   | C     | 465      | 3726  | 2348 | 686 | 665 | 27 | 0       | 1       | 0     |
| 2   | D     | 466      | 3729  | 2349 | 687 | 666 | 27 | 0       | 0       | 0     |
| 2   | G     | 465      | 3727  | 2348 | 686 | 666 | 27 | 0       | 0       | 0     |
| 2   | H     | 466      | 3729  | 2349 | 687 | 666 | 27 | 0       | 0       | 0     |
| 2   | K     | 465      | 3727  | 2348 | 686 | 666 | 27 | 0       | 0       | 0     |
| 2   | L     | 466      | 3730  | 2350 | 686 | 667 | 27 | 0       | 0       | 0     |

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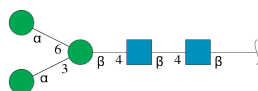
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 2   | O     | 466      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3729  | 2349 | 687 | 666 | 27 |         |         |       |
| 2   | P     | 466      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3733  | 2351 | 687 | 668 | 27 |         |         |       |

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
|     |       |          | Total | C  | N | O  |         |         |       |
| 3   | Q     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |
| 3   | R     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |
| 3   | S     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |
| 3   | T     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |
| 3   | U     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |
| 3   | V     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |
| 3   | W     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |
| 3   | X     | 6        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 71    | 40 | 2 | 29 |         |         |       |

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

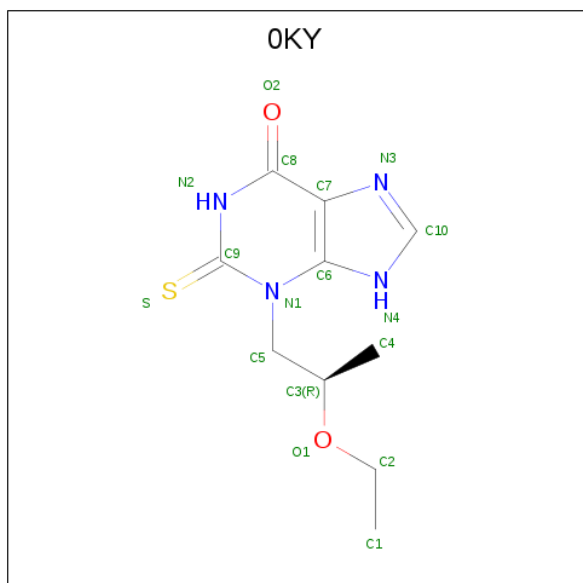


| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
|     |       |          | Total | C  | N | O  |         |         |       |
| 4   | Y     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | J     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | E     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | B     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | I     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | A     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | N     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | F     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 5   | M     | 1        | Total Cl<br>1 1 | 0       | 0       |

- Molecule 6 is 3-[(2R)-2-ethoxypropyl]-2-thioxo-1,2,3,9-tetrahydro-6H-purin-6-one (three-letter code: OKY) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub>S).



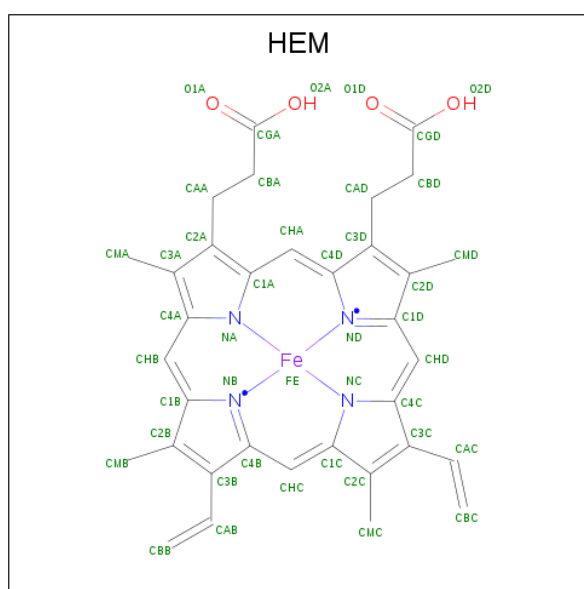
| Mol | Chain | Residues | Atoms                        | ZeroOcc | AltConf |
|-----|-------|----------|------------------------------|---------|---------|
| 6   | A     | 1        | Total C N O S<br>17 10 4 2 1 | 0       | 0       |
| 6   | B     | 1        | Total C N O S<br>17 10 4 2 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 6   | G     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 17    | 10 | 4 | 2 | 1 |         |         |
| 6   | H     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 17    | 10 | 4 | 2 | 1 |         |         |
| 6   | I     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 17    | 10 | 4 | 2 | 1 |         |         |
| 6   | J     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 17    | 10 | 4 | 2 | 1 |         |         |
| 6   | O     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 17    | 10 | 4 | 2 | 1 |         |         |
| 6   | P     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 17    | 10 | 4 | 2 | 1 |         |         |

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



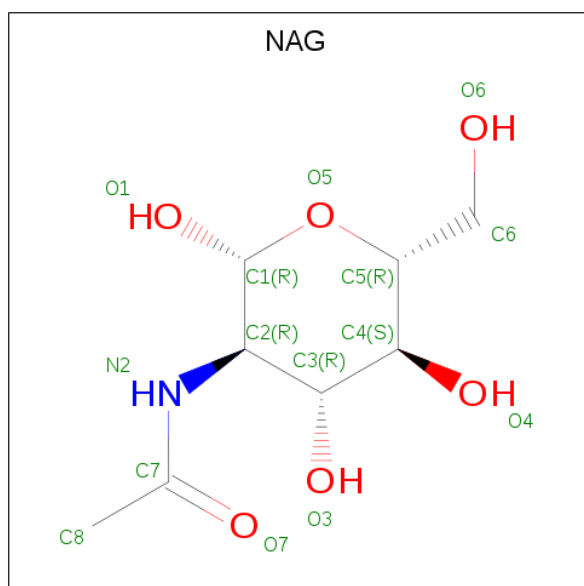
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 7   | C     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 7   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 7   | E     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 7   | F     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 7   | I     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|----|----|---|---------|---------|---|
| 7   | J     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 7   | M     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |
| 7   | N     | 1        | Total | C  | Fe | N | O       | 0       | 0 |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |   |

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



| 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   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | H     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 8   | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | K     | 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 |         |         |
| 8   | O     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | O     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 8   | P     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 9   | P     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | G     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | D     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | K     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | H     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | C     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | O     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 9   | L     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 10 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 10  | A     | 85       | Total | O   | 0       | 0       |
|     |       |          | 85    | 85  |         |         |
| 10  | C     | 337      | Total | O   | 0       | 0       |
|     |       |          | 337   | 337 |         |         |

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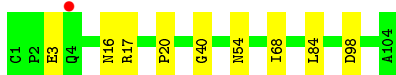
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| <b>Mol</b> | <b>Chain</b> | <b>Residues</b> | <b>Atoms</b> |          | <b>ZeroOcc</b> | <b>AltConf</b> |
|------------|--------------|-----------------|--------------|----------|----------------|----------------|
| 10         | B            | 76              | Total<br>76  | O<br>76  | 0              | 0              |
| 10         | D            | 268             | Total<br>268 | O<br>268 | 0              | 0              |
| 10         | E            | 63              | Total<br>63  | O<br>63  | 0              | 0              |
| 10         | G            | 245             | Total<br>245 | O<br>245 | 0              | 0              |
| 10         | F            | 73              | Total<br>73  | O<br>73  | 0              | 0              |
| 10         | H            | 196             | Total<br>196 | O<br>196 | 0              | 0              |
| 10         | I            | 75              | Total<br>75  | O<br>75  | 0              | 0              |
| 10         | K            | 212             | Total<br>212 | O<br>212 | 0              | 0              |
| 10         | J            | 69              | Total<br>69  | O<br>69  | 0              | 0              |
| 10         | L            | 250             | Total<br>250 | O<br>250 | 0              | 0              |
| 10         | M            | 68              | Total<br>68  | O<br>68  | 0              | 0              |
| 10         | O            | 225             | Total<br>225 | O<br>225 | 0              | 0              |
| 10         | N            | 61              | Total<br>61  | O<br>61  | 0              | 0              |
| 10         | P            | 217             | Total<br>217 | O<br>217 | 0              | 0              |

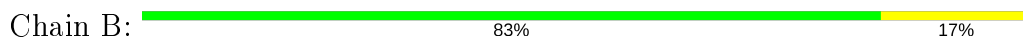
### 3 Residue-property plots [i](#)

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

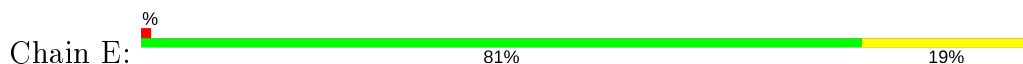
- Molecule 1: Myeloperoxidase light chain



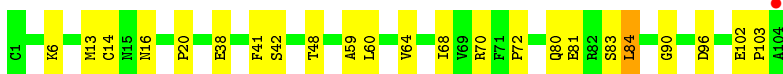
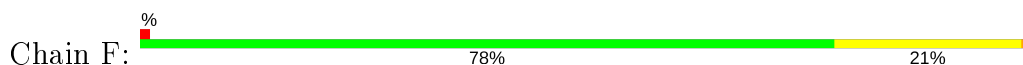
- Molecule 1: Myeloperoxidase light chain



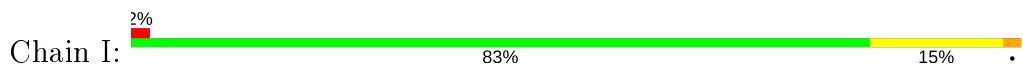
- Molecule 1: Myeloperoxidase light chain



- Molecule 1: Myeloperoxidase light chain



- Molecule 1: Myeloperoxidase light chain




- Molecule 1: Myeloperoxidase light chain

Chain J:  93% 6%




- Molecule 1: Myeloperoxidase light chain

Chain M:  2% 85% 14%




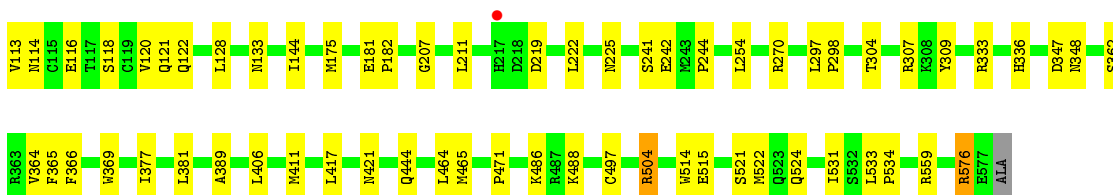
- Molecule 1: Myeloperoxidase light chain

Chain N:  85% 15%




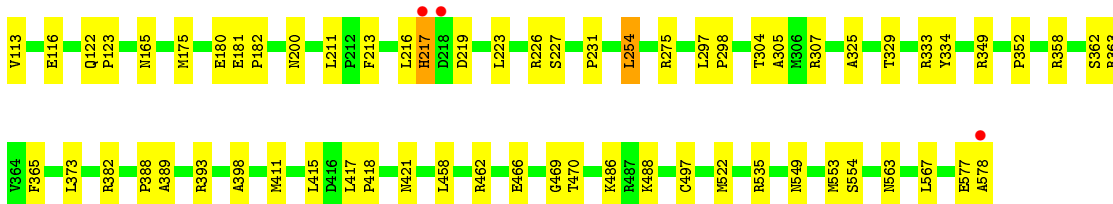
- Molecule 2: Myeloperoxidase heavy chain

Chain C:  86% 13%




- Molecule 2: Myeloperoxidase heavy chain

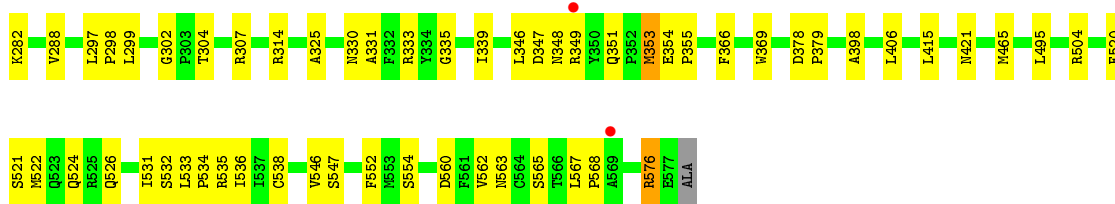
Chain D:  86% 13%



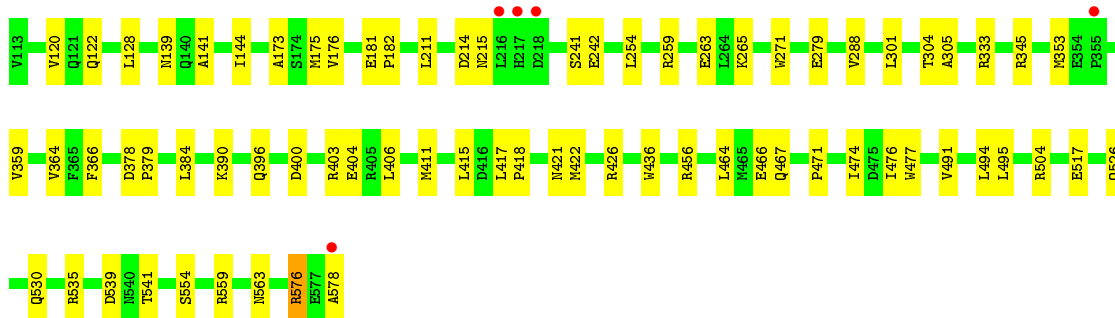
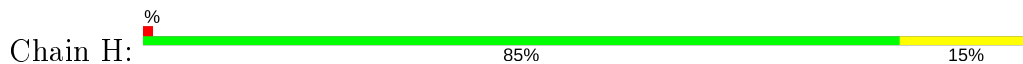
- Molecule 2: Myeloperoxidase heavy chain

Chain G:  80% 18%

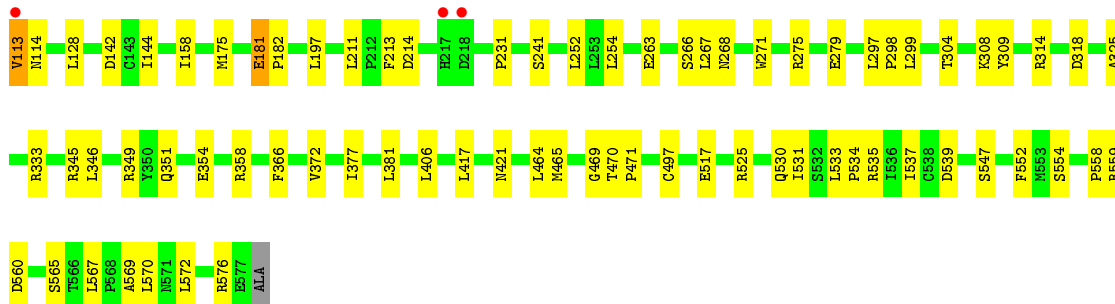
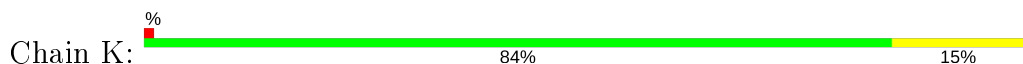




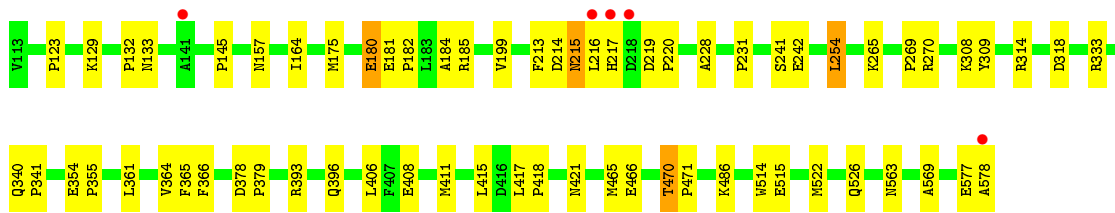
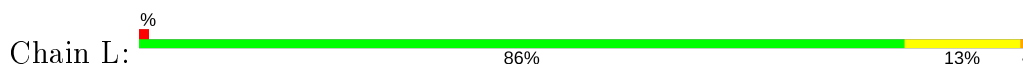
• Molecule 2: Myeloperoxidase heavy chain



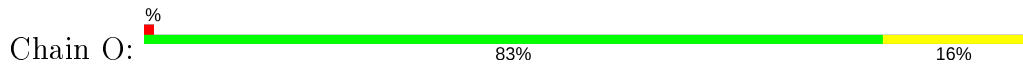
• Molecule 2: Myeloperoxidase heavy chain

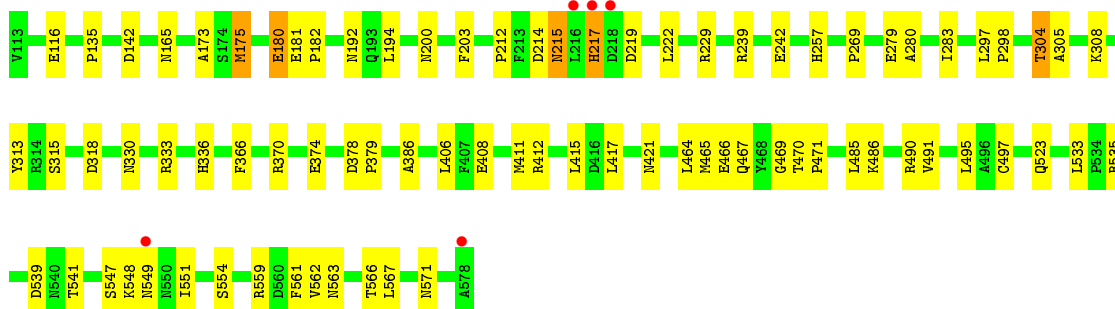


• Molecule 2: Myeloperoxidase heavy chain

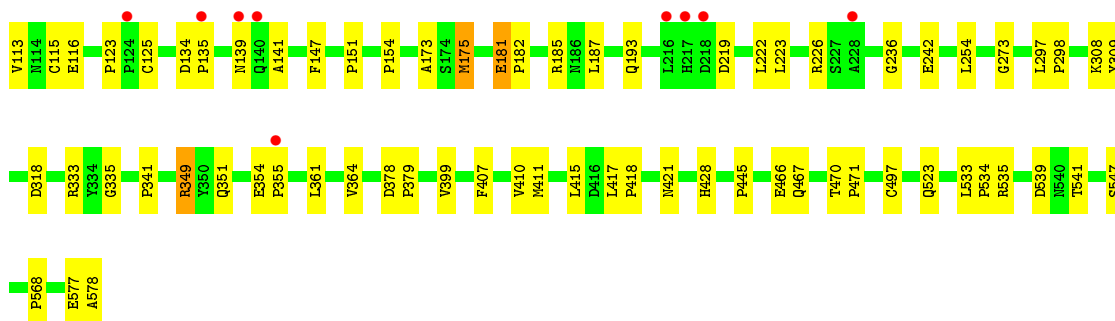
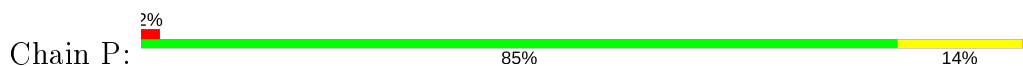


• Molecule 2: Myeloperoxidase heavy chain





- Molecule 2: Myeloperoxidase heavy chain



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



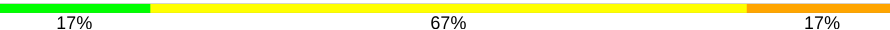
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

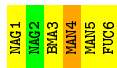


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  17% 67% 17%



- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%



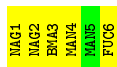
- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

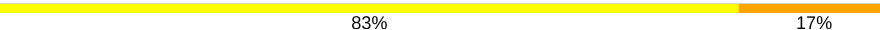


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  17% 83%

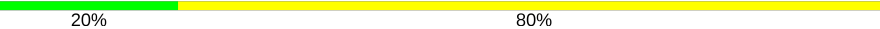


- Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  83% 17%



- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  20% 80%





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 63.83Å 242.64Å 151.50Å<br>90.00° 91.19° 90.00°              | Depositor        |
| Resolution (Å)  | 128.49 – 2.00<br>128.49 – 2.00                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.6 (128.49-2.00)<br>97.6 (128.49-2.00)                    | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.09  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.83 (at 2.00Å)   | Xtrriage         |
| Refinement program  | REFMAC  | Depositor        |
| R, $R_{free}$   | 0.190 , 0.246<br>0.205 , 0.255                              | Depositor<br>DCC |
| $R_{free}$ test set   | 15173 reflections (5.03%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 25.8  | Xtrriage         |
| Anisotropy  | 0.040   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 25.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$ | Xtrriage         |
| Estimated twinning fraction   | 0.086 for h,-k,-l   | Xtrriage         |
| $F_o, F_c$ correlation  | 0.94  | EDS              |
| Total number of atoms   | 40392   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 29.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5328e-03.*

<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: CSO, BMA, NAG, CL, CA, OKY, FUC, HEM, MAN

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     | 0.58         | 0/863   | 0.69        | 0/1174         |
| 1   | B     | 0.53         | 0/863   | 0.61        | 0/1174         |
| 1   | E     | 0.58         | 0/863   | 0.63        | 0/1174         |
| 1   | F     | 0.47         | 0/863   | 0.59        | 0/1174         |
| 1   | I     | 0.52         | 0/863   | 0.61        | 0/1174         |
| 1   | J     | 0.49         | 0/863   | 0.59        | 0/1174         |
| 1   | M     | 0.47         | 0/863   | 0.58        | 0/1174         |
| 1   | N     | 0.47         | 0/869   | 0.57        | 0/1183         |
| 2   | C     | 0.58         | 0/3807  | 0.61        | 0/5164         |
| 2   | D     | 0.51         | 0/3807  | 0.57        | 0/5163         |
| 2   | G     | 0.51         | 0/3805  | 0.58        | 0/5161         |
| 2   | H     | 0.44         | 0/3807  | 0.53        | 0/5163         |
| 2   | K     | 0.48         | 0/3805  | 0.55        | 0/5161         |
| 2   | L     | 0.48         | 0/3808  | 0.56        | 1/5164 (0.0%)  |
| 2   | O     | 0.45         | 0/3807  | 0.54        | 0/5163         |
| 2   | P     | 0.45         | 0/3811  | 0.52        | 0/5168         |
| All | All   | 0.50         | 0/37367 | 0.57        | 1/50708 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | I     | 0                   | 1                   |
| 2   | D     | 0                   | 1                   |
| 2   | G     | 0                   | 2                   |
| 2   | K     | 0                   | 1                   |
| 2   | L     | 0                   | 1                   |
| 2   | O     | 0                   | 3                   |
| All | All   | 0                   | 9                   |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|-----------|------|------------------------|---------------------|
| 2   | L     | 318 | ASP  | CB-CG-OD1 | 5.26 | 123.03                 | 118.30              |

There are no chirality outliers.

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | D     | 180 | GLU  | Peptide |
| 2   | G     | 180 | GLU  | Peptide |
| 2   | G     | 302 | GLY  | Peptide |
| 1   | I     | 2   | PRO  | Peptide |
| 2   | K     | 547 | SER  | Peptide |
| 2   | L     | 180 | GLU  | Peptide |
| 2   | O     | 180 | GLU  | Peptide |
| 2   | O     | 214 | ASP  | Peptide |
| 2   | O     | 215 | ASN  | Peptide |

## 5.2 Too-close contacts [i](#)

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     | 838   | 0        | 798      | 9       | 0            |
| 1   | B     | 838   | 0        | 798      | 18      | 0            |
| 1   | E     | 838   | 0        | 798      | 16      | 0            |
| 1   | F     | 838   | 0        | 798      | 27      | 0            |
| 1   | I     | 838   | 0        | 798      | 18      | 0            |
| 1   | J     | 838   | 0        | 798      | 5       | 0            |
| 1   | M     | 838   | 0        | 798      | 11      | 0            |
| 1   | N     | 841   | 0        | 803      | 11      | 0            |
| 2   | C     | 3726  | 0        | 3721     | 63      | 0            |
| 2   | D     | 3729  | 0        | 3721     | 45      | 0            |
| 2   | G     | 3727  | 0        | 3720     | 67      | 2            |
| 2   | H     | 3729  | 0        | 3721     | 70      | 0            |
| 2   | K     | 3727  | 0        | 3720     | 48      | 0            |
| 2   | L     | 3730  | 0        | 3721     | 47      | 0            |
| 2   | O     | 3729  | 0        | 3721     | 63      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | P     | 3733  | 0        | 3725     | 56      | 0            |
| 3   | Q     | 71    | 0        | 61       | 1       | 0            |
| 3   | R     | 71    | 0        | 61       | 0       | 0            |
| 3   | S     | 71    | 0        | 61       | 0       | 0            |
| 3   | T     | 71    | 0        | 61       | 1       | 0            |
| 3   | U     | 71    | 0        | 61       | 0       | 0            |
| 3   | V     | 71    | 0        | 61       | 0       | 0            |
| 3   | W     | 71    | 0        | 61       | 1       | 0            |
| 3   | X     | 71    | 0        | 61       | 2       | 0            |
| 4   | Y     | 61    | 0        | 52       | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | E     | 1     | 0        | 0        | 0       | 0            |
| 5   | F     | 1     | 0        | 0        | 0       | 0            |
| 5   | I     | 1     | 0        | 0        | 0       | 0            |
| 5   | J     | 1     | 0        | 0        | 0       | 0            |
| 5   | M     | 1     | 0        | 0        | 0       | 0            |
| 5   | N     | 1     | 0        | 0        | 0       | 0            |
| 6   | A     | 17    | 0        | 14       | 3       | 0            |
| 6   | B     | 17    | 0        | 14       | 4       | 0            |
| 6   | G     | 17    | 0        | 14       | 1       | 0            |
| 6   | H     | 17    | 0        | 14       | 5       | 0            |
| 6   | I     | 17    | 0        | 14       | 2       | 0            |
| 6   | J     | 17    | 0        | 14       | 1       | 0            |
| 6   | O     | 17    | 0        | 14       | 5       | 0            |
| 6   | P     | 17    | 0        | 14       | 4       | 0            |
| 7   | B     | 43    | 0        | 30       | 5       | 0            |
| 7   | C     | 43    | 0        | 30       | 6       | 0            |
| 7   | E     | 43    | 0        | 30       | 6       | 0            |
| 7   | F     | 43    | 0        | 30       | 5       | 0            |
| 7   | I     | 43    | 0        | 30       | 1       | 0            |
| 7   | J     | 43    | 0        | 30       | 5       | 0            |
| 7   | M     | 43    | 0        | 30       | 5       | 0            |
| 7   | N     | 43    | 0        | 30       | 7       | 0            |
| 8   | C     | 28    | 0        | 26       | 0       | 0            |
| 8   | D     | 28    | 0        | 26       | 1       | 0            |
| 8   | G     | 28    | 0        | 26       | 2       | 0            |
| 8   | H     | 28    | 0        | 26       | 0       | 0            |
| 8   | K     | 28    | 0        | 26       | 0       | 0            |
| 8   | L     | 28    | 0        | 26       | 0       | 0            |
| 8   | O     | 28    | 0        | 26       | 0       | 0            |
| 8   | P     | 14    | 0        | 13       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | C     | 1     | 0        | 0        | 0       | 0            |
| 9   | D     | 1     | 0        | 0        | 0       | 0            |
| 9   | G     | 1     | 0        | 0        | 0       | 0            |
| 9   | H     | 1     | 0        | 0        | 0       | 0            |
| 9   | K     | 1     | 0        | 0        | 0       | 0            |
| 9   | L     | 1     | 0        | 0        | 0       | 0            |
| 9   | O     | 1     | 0        | 0        | 0       | 0            |
| 9   | P     | 1     | 0        | 0        | 0       | 0            |
| 10  | A     | 85    | 0        | 0        | 1       | 0            |
| 10  | B     | 76    | 0        | 0        | 0       | 0            |
| 10  | C     | 337   | 0        | 0        | 17      | 0            |
| 10  | D     | 268   | 0        | 0        | 10      | 0            |
| 10  | E     | 63    | 0        | 0        | 4       | 0            |
| 10  | F     | 73    | 0        | 0        | 1       | 0            |
| 10  | G     | 245   | 0        | 0        | 13      | 0            |
| 10  | H     | 196   | 0        | 0        | 12      | 0            |
| 10  | I     | 75    | 0        | 0        | 1       | 0            |
| 10  | J     | 69    | 0        | 0        | 1       | 0            |
| 10  | K     | 212   | 0        | 0        | 9       | 1            |
| 10  | L     | 250   | 0        | 0        | 11      | 2            |
| 10  | M     | 68    | 0        | 0        | 2       | 0            |
| 10  | N     | 61    | 0        | 0        | 1       | 1            |
| 10  | O     | 225   | 0        | 0        | 16      | 0            |
| 10  | P     | 217   | 0        | 0        | 12      | 0            |
| All | All   | 40392 | 0        | 37246    | 563     | 3            |

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 7.

All (563) 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:C:465:MET:CE  | 2:C:471:PRO:HG3  | 1.79                     | 1.12              |
| 1:N:63:ALA:O    | 1:N:67:GLU:HG2   | 1.50                     | 1.09              |
| 1:F:84:LEU:HD22 | 2:H:384:LEU:HD23 | 1.35                     | 1.09              |
| 2:C:465:MET:HE3 | 2:C:471:PRO:HD3  | 1.34                     | 1.05              |
| 2:P:116:GLU:OE2 | 2:P:411:MET:HE3  | 1.57                     | 1.05              |
| 2:C:465:MET:HE1 | 2:C:471:PRO:CG   | 1.87                     | 1.04              |
| 2:C:465:MET:HE1 | 2:C:471:PRO:HG3  | 1.04                     | 1.04              |
| 1:F:84:LEU:CD2  | 2:H:384:LEU:HD23 | 1.94                     | 0.96              |
| 2:H:214:ASP:HB3 | 10:H:1865:HOH:O  | 1.66                     | 0.93              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:173:ALA:HA   | 2:H:175:MET:HE3  | 1.49                     | 0.92              |
| 2:O:465:MET:HE1  | 2:O:470:THR:HA   | 1.54                     | 0.89              |
| 2:G:211:LEU:HD23 | 2:G:254:LEU:HD13 | 1.55                     | 0.88              |
| 2:C:347:ASP:HB2  | 1:I:80:GLN:OE1   | 1.72                     | 0.88              |
| 2:C:465:MET:HE3  | 2:C:471:PRO:CD   | 2.05                     | 0.87              |
| 7:F:202:HEM:HMC2 | 7:F:202:HEM:HBC2 | 1.57                     | 0.86              |
| 2:C:465:MET:CE   | 2:C:471:PRO:CG   | 2.48                     | 0.86              |
| 2:P:411:MET:HE1  | 2:P:415:LEU:HD21 | 1.59                     | 0.83              |
| 2:C:531:ILE:C    | 2:C:531:ILE:HD12 | 1.98                     | 0.82              |
| 2:G:113:VAL:HG12 | 2:G:113:VAL:O    | 1.80                     | 0.81              |
| 2:O:200:ASN:HD22 | 2:O:203:PHE:H    | 1.27                     | 0.81              |
| 2:D:577:GLU:O    | 2:D:578:ALA:HB3  | 1.81                     | 0.81              |
| 2:C:465:MET:CE   | 2:C:471:PRO:HD3  | 2.12                     | 0.80              |
| 1:I:16:ASN:HD22  | 1:I:19:SER:H     | 1.29                     | 0.80              |
| 1:F:84:LEU:CD2   | 2:H:384:LEU:CD2  | 2.60                     | 0.79              |
| 2:L:181:GLU:O    | 2:L:181:GLU:OE2  | 2.01                     | 0.79              |
| 1:N:64:VAL:HG13  | 1:N:68:ILE:HD12  | 1.63                     | 0.79              |
| 2:H:175:MET:CE   | 2:H:288:VAL:HG11 | 2.13                     | 0.78              |
| 2:O:411:MET:HE2  | 2:O:415:LEU:HD21 | 1.64                     | 0.78              |
| 1:B:6:LYS:NZ     | 2:D:275:ARG:NH2  | 2.31                     | 0.78              |
| 6:O:610:OKY:H8   | 10:O:886:HOH:O   | 1.84                     | 0.78              |
| 2:P:116:GLU:OE2  | 2:P:411:MET:CE   | 2.31                     | 0.78              |
| 2:C:465:MET:CE   | 2:C:471:PRO:CD   | 2.61                     | 0.78              |
| 2:D:577:GLU:O    | 2:D:578:ALA:CB   | 2.32                     | 0.78              |
| 2:G:181:GLU:N    | 2:G:182:PRO:HD2  | 1.99                     | 0.77              |
| 2:C:348:ASN:ND2  | 1:I:77:THR:CG2   | 2.48                     | 0.77              |
| 2:K:535:ARG:NH1  | 2:K:567:LEU:O    | 2.19                     | 0.76              |
| 1:F:64:VAL:CG1   | 1:F:68:ILE:HD12  | 2.15                     | 0.76              |
| 1:M:83:SER:HB3   | 2:O:554:SER:O    | 1.85                     | 0.76              |
| 2:H:504:ARG:HB3  | 10:H:1750:HOH:O  | 1.84                     | 0.76              |
| 1:F:38:GLU:OE1   | 1:F:48:THR:OG1   | 2.04                     | 0.75              |
| 2:H:181:GLU:N    | 2:H:182:PRO:HD2  | 2.02                     | 0.75              |
| 2:C:486:LYS:HE3  | 10:C:992:HOH:O   | 1.86                     | 0.75              |
| 2:H:120:VAL:HG12 | 2:H:122:GLN:HG3  | 1.68                     | 0.75              |
| 2:H:175:MET:HE2  | 2:H:288:VAL:HG11 | 1.67                     | 0.75              |
| 1:F:84:LEU:HD23  | 2:H:384:LEU:CD2  | 2.17                     | 0.74              |
| 10:J:356:HOH:O   | 2:L:129:LYS:HE3  | 1.87                     | 0.73              |
| 2:C:304:THR:HG22 | 10:C:946:HOH:O   | 1.87                     | 0.73              |
| 2:P:113:VAL:O    | 2:P:113:VAL:HG13 | 1.86                     | 0.73              |
| 2:O:304:THR:HG22 | 10:O:860:HOH:O   | 1.87                     | 0.73              |
| 2:P:577:GLU:O    | 2:P:578:ALA:O    | 2.06                     | 0.73              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:466:GLU:OE1   | 10:P:910:HOH:O    | 2.05                     | 0.73              |
| 2:C:488:LYS:HD2   | 10:C:773:HOH:O    | 1.90                     | 0.72              |
| 7:C:601:HEM:HMC2  | 7:C:601:HEM:HBC2  | 1.72                     | 0.72              |
| 2:O:333:ARG:HH11  | 2:O:421:ASN:HD22  | 1.37                     | 0.72              |
| 7:N:202:HEM:HAA2  | 6:P:614:OKY:S     | 2.29                     | 0.72              |
| 7:B:202:HEM:HBA1  | 6:B:203:OKY:S     | 2.30                     | 0.71              |
| 2:K:465:MET:HE1   | 2:K:471:PRO:HD3   | 1.72                     | 0.71              |
| 1:B:6:LYS:NZ      | 2:D:275:ARG:HH21  | 1.88                     | 0.71              |
| 2:G:349:ARG:HG3   | 2:G:351:GLN:HG2   | 1.72                     | 0.70              |
| 1:M:16:ASN:HD22   | 1:M:19:SER:H      | 1.37                     | 0.70              |
| 2:G:333:ARG:HH11  | 2:G:421:ASN:HD22  | 1.39                     | 0.70              |
| 7:J:202:HEM:HMC2  | 7:J:202:HEM:HBC2  | 1.72                     | 0.69              |
| 2:C:348:ASN:ND2   | 1:I:77:THR:HG23   | 2.08                     | 0.69              |
| 7:J:202:HEM:HBB2  | 2:L:242:GLU:OE1   | 1.91                     | 0.69              |
| 1:M:68:ILE:HD13   | 2:O:464:LEU:HD23  | 1.74                     | 0.68              |
| 2:D:352:PRO:HD2   | 10:D:879:HOH:O    | 1.93                     | 0.68              |
| 2:P:182:PRO:HG2   | 10:P:830:HOH:O    | 1.94                     | 0.68              |
| 2:O:217:HIS:HE1   | 10:O:844:HOH:O    | 1.77                     | 0.68              |
| 7:E:1602:HEM:HMC2 | 7:E:1602:HEM:HBC2 | 1.75                     | 0.68              |
| 2:K:465:MET:HE1   | 2:K:470:THR:HA    | 1.75                     | 0.68              |
| 2:L:411:MET:CE    | 2:L:415:LEU:HD21  | 2.23                     | 0.68              |
| 1:E:67:GLU:OE1    | 1:E:67:GLU:HA     | 1.95                     | 0.67              |
| 7:F:202:HEM:HBC2  | 7:F:202:HEM:CMC   | 2.23                     | 0.67              |
| 2:D:181:GLU:N     | 2:D:182:PRO:HD2   | 2.10                     | 0.67              |
| 2:O:559:ARG:HD3   | 10:O:874:HOH:O    | 1.95                     | 0.67              |
| 6:H:610:OKY:C6    | 6:H:610:OKY:H11   | 2.24                     | 0.66              |
| 1:F:64:VAL:HG13   | 1:F:68:ILE:HD12   | 1.76                     | 0.66              |
| 2:G:531:ILE:HD12  | 2:G:531:ILE:C     | 2.15                     | 0.66              |
| 2:L:157:ASN:HB2   | 10:L:922:HOH:O    | 1.94                     | 0.66              |
| 2:H:406:LEU:HD22  | 2:H:417:LEU:HB2   | 1.77                     | 0.66              |
| 2:K:465:MET:HE3   | 10:K:857:HOH:O    | 1.94                     | 0.66              |
| 2:C:270:ARG:HG3   | 10:C:927:HOH:O    | 1.95                     | 0.66              |
| 2:H:436:TRP:CD1   | 2:H:476:ILE:HD13  | 2.30                     | 0.66              |
| 2:L:123:PRO:HA    | 10:L:869:HOH:O    | 1.95                     | 0.65              |
| 2:P:378:ASP:HB2   | 2:P:379:PRO:HD3   | 1.77                     | 0.65              |
| 1:I:68:ILE:HD13   | 2:K:464:LEU:HD23  | 1.78                     | 0.65              |
| 2:K:113:VAL:HA    | 10:K:765:HOH:O    | 1.95                     | 0.65              |
| 2:O:333:ARG:HH11  | 2:O:421:ASN:ND2   | 1.94                     | 0.65              |
| 2:G:333:ARG:HH11  | 2:G:421:ASN:ND2   | 1.93                     | 0.65              |
| 2:P:113:VAL:HG13  | 2:P:125:CYS:SG    | 2.36                     | 0.64              |
| 2:C:116:GLU:OE1   | 2:C:411:MET:CE    | 2.45                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:84:LEU:HD13  | 2:D:389:ALA:HA   | 1.80                     | 0.64              |
| 7:N:202:HEM:HBC2 | 7:N:202:HEM:HMC2 | 1.78                     | 0.64              |
| 2:P:181:GLU:HG2  | 10:P:893:HOH:O   | 1.97                     | 0.64              |
| 2:C:486:LYS:CE   | 10:C:992:HOH:O   | 2.45                     | 0.64              |
| 2:G:331:ALA:HB1  | 2:G:495:LEU:HD23 | 1.80                     | 0.64              |
| 2:O:563:ASN:HB3  | 10:O:785:HOH:O   | 1.98                     | 0.64              |
| 2:O:567:LEU:N    | 2:O:567:LEU:HD23 | 2.13                     | 0.64              |
| 2:P:123:PRO:HA   | 10:P:829:HOH:O   | 1.98                     | 0.63              |
| 2:G:353:MET:HG2  | 10:G:768:HOH:O   | 1.98                     | 0.63              |
| 1:N:16:ASN:O     | 1:N:20:PRO:HA    | 1.97                     | 0.63              |
| 2:H:301:LEU:HB3  | 2:H:305:ALA:HB3  | 1.81                     | 0.63              |
| 6:A:1602:0KY:C6  | 6:A:1602:0KY:H11 | 2.29                     | 0.63              |
| 2:P:242:GLU:HG3  | 6:P:614:0KY:O2   | 1.98                     | 0.63              |
| 10:H:1806:HOH:O  | 3:T:4:MAN:H61    | 1.98                     | 0.63              |
| 7:N:202:HEM:HBB2 | 7:N:202:HEM:HMB1 | 1.80                     | 0.62              |
| 2:P:113:VAL:O    | 2:P:113:VAL:CG1  | 2.47                     | 0.62              |
| 2:O:523:GLN:HG2  | 10:O:840:HOH:O   | 1.99                     | 0.62              |
| 6:H:610:0KY:H11  | 6:H:610:0KY:N4   | 2.15                     | 0.62              |
| 2:C:531:ILE:O    | 2:C:531:ILE:HD12 | 1.98                     | 0.62              |
| 7:B:202:HEM:HMC2 | 7:B:202:HEM:HBC2 | 1.80                     | 0.62              |
| 1:F:64:VAL:HG12  | 1:F:68:ILE:HD12  | 1.82                     | 0.62              |
| 1:M:70:ARG:CZ    | 10:M:1744:HOH:O  | 2.48                     | 0.62              |
| 2:H:211:LEU:HD23 | 2:H:254:LEU:HD22 | 1.82                     | 0.61              |
| 2:O:559:ARG:CD   | 10:O:874:HOH:O   | 2.49                     | 0.61              |
| 2:H:411:MET:HE2  | 2:H:415:LEU:HD21 | 1.82                     | 0.61              |
| 2:C:181:GLU:N    | 2:C:182:PRO:CD   | 2.63                     | 0.61              |
| 2:P:535:ARG:NH2  | 2:P:539:ASP:OD2  | 2.32                     | 0.61              |
| 2:K:211:LEU:HD23 | 2:K:254:LEU:HD22 | 1.82                     | 0.61              |
| 8:G:608:NAG:O3   | 8:G:608:NAG:O7   | 2.15                     | 0.60              |
| 2:P:354:GLU:OE1  | 2:P:355:PRO:O    | 2.18                     | 0.60              |
| 2:G:123:PRO:HA   | 10:G:867:HOH:O   | 2.02                     | 0.60              |
| 2:O:239:ARG:HG2  | 6:O:610:0KY:N3   | 2.17                     | 0.60              |
| 2:P:151:PRO:HG2  | 2:P:154:PRO:HG3  | 1.84                     | 0.60              |
| 1:I:16:ASN:ND2   | 1:I:19:SER:H     | 1.99                     | 0.59              |
| 2:K:181:GLU:N    | 2:K:182:PRO:CD   | 2.66                     | 0.59              |
| 2:H:411:MET:CE   | 2:H:415:LEU:HD21 | 2.32                     | 0.59              |
| 2:D:200:ASN:HB2  | 2:D:211:LEU:O    | 2.02                     | 0.59              |
| 2:H:259:ARG:O    | 2:H:263:GLU:HG3  | 2.03                     | 0.59              |
| 2:O:181:GLU:N    | 2:O:182:PRO:CD   | 2.66                     | 0.59              |
| 2:O:548:LYS:HZ3  | 2:O:562:VAL:CG1  | 2.15                     | 0.59              |
| 2:K:263:GLU:O    | 2:K:266:SER:HB2  | 2.02                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:P:411:MET:CE    | 2:P:415:LEU:HD21  | 2.30                     | 0.59              |
| 2:G:181:GLU:H     | 2:G:182:PRO:HD2   | 1.66                     | 0.58              |
| 2:L:569:ALA:HB3   | 10:L:896:HOH:O    | 2.03                     | 0.58              |
| 7:M:1602:HEM:HBC2 | 7:M:1602:HEM:HMC2 | 1.84                     | 0.58              |
| 2:P:193:GLN:NE2   | 2:P:273:GLY:H     | 2.01                     | 0.58              |
| 1:E:104:ALA:HA    | 10:E:1715:HOH:O   | 2.01                     | 0.58              |
| 1:B:6:LYS:HZ3     | 2:D:275:ARG:HH21  | 1.50                     | 0.58              |
| 1:F:96:ASP:OD2    | 2:H:175:MET:HE2   | 2.03                     | 0.58              |
| 2:G:113:VAL:CG1   | 2:G:113:VAL:O     | 2.50                     | 0.58              |
| 1:F:70:ARG:HH11   | 2:H:403:ARG:NH2   | 2.02                     | 0.58              |
| 2:H:422:MET:O     | 2:H:426:ARG:HG3   | 2.04                     | 0.58              |
| 7:E:1602:HEM:CMC  | 7:E:1602:HEM:HBC2 | 2.34                     | 0.58              |
| 2:P:308:LYS:HE3   | 3:W:4:MAN:O2      | 2.03                     | 0.58              |
| 2:C:211:LEU:HD23  | 2:C:254:LEU:HD13  | 1.85                     | 0.58              |
| 2:C:377:ILE:HD12  | 2:C:381:LEU:HD11  | 1.86                     | 0.57              |
| 2:D:116:GLU:OE2   | 2:D:411:MET:HE3   | 2.04                     | 0.57              |
| 2:H:175:MET:HE1   | 2:H:288:VAL:HG21  | 1.85                     | 0.57              |
| 2:P:115:CYS:HB2   | 2:P:147:PHE:CE1   | 2.39                     | 0.57              |
| 2:O:366:PHE:CZ    | 6:O:610:OKY:H9    | 2.40                     | 0.57              |
| 2:D:333:ARG:HH11  | 2:D:421:ASN:HD22  | 1.53                     | 0.57              |
| 2:L:157:ASN:CB    | 10:L:922:HOH:O    | 2.50                     | 0.57              |
| 2:C:522:MET:HE2   | 10:C:917:HOH:O    | 2.04                     | 0.57              |
| 2:O:465:MET:CE    | 2:O:469:GLY:O     | 2.53                     | 0.57              |
| 2:K:531:ILE:C     | 2:K:531:ILE:HD12  | 2.25                     | 0.57              |
| 2:C:116:GLU:OE1   | 2:C:411:MET:HE3   | 2.05                     | 0.57              |
| 2:C:576:ARG:HD2   | 10:C:970:HOH:O    | 2.04                     | 0.57              |
| 2:H:576:ARG:CG    | 2:H:578:ALA:HB2   | 2.35                     | 0.57              |
| 1:A:68:ILE:HD13   | 2:C:464:LEU:HD23  | 1.86                     | 0.57              |
| 2:G:211:LEU:CD2   | 2:G:254:LEU:HD13  | 2.30                     | 0.57              |
| 2:L:411:MET:HE2   | 2:L:415:LEU:HD21  | 1.86                     | 0.56              |
| 2:G:171:VAL:CG1   | 2:G:288:VAL:HG12  | 2.35                     | 0.56              |
| 2:C:219:ASP:HB3   | 2:C:222:LEU:HD12  | 1.87                     | 0.56              |
| 1:M:16:ASN:ND2    | 1:M:19:SER:H      | 2.03                     | 0.56              |
| 2:D:488:LYS:HD2   | 10:D:868:HOH:O    | 2.06                     | 0.56              |
| 2:H:120:VAL:CG1   | 2:H:122:GLN:HG3   | 2.34                     | 0.56              |
| 7:E:1602:HEM:CBC  | 2:G:335:GLY:HA3   | 2.35                     | 0.56              |
| 1:F:68:ILE:HD13   | 2:H:464:LEU:HD23  | 1.86                     | 0.56              |
| 2:K:271:TRP:CZ3   | 2:K:279:GLU:HG3   | 2.39                     | 0.56              |
| 1:I:13:MET:O      | 1:I:14:CYS:HB2    | 2.05                     | 0.56              |
| 10:M:1744:HOH:O   | 2:O:135:PRO:HG3   | 2.04                     | 0.56              |
| 2:O:200:ASN:ND2   | 2:O:203:PHE:H     | 2.02                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:465:MET:HE3  | 10:O:740:HOH:O   | 2.05                     | 0.56              |
| 2:L:314:ARG:HG2  | 10:L:853:HOH:O   | 2.06                     | 0.55              |
| 2:P:182:PRO:CG   | 10:P:822:HOH:O   | 2.54                     | 0.55              |
| 2:L:216:LEU:HD13 | 2:L:219:ASP:OD1  | 2.06                     | 0.55              |
| 2:D:181:GLU:N    | 2:D:182:PRO:CD   | 2.68                     | 0.55              |
| 2:O:386:ALA:HB2  | 2:O:561:PHE:CZ   | 2.40                     | 0.55              |
| 2:D:333:ARG:HH11 | 2:D:421:ASN:ND2  | 2.04                     | 0.55              |
| 2:G:226:ARG:HD3  | 10:G:810:HOH:O   | 2.06                     | 0.55              |
| 2:G:378:ASP:HB2  | 2:G:379:PRO:HD3  | 1.89                     | 0.55              |
| 1:A:54:ASN:HB2   | 10:A:1742:HOH:O  | 2.06                     | 0.55              |
| 1:I:5:ASP:N      | 1:I:5:ASP:OD1    | 2.40                     | 0.55              |
| 7:N:202:HEM:CAA  | 6:P:614:OKY:S    | 2.95                     | 0.55              |
| 2:D:382:ARG:NH2  | 10:D:949:HOH:O   | 2.25                     | 0.55              |
| 2:G:181:GLU:N    | 2:G:182:PRO:CD   | 2.68                     | 0.55              |
| 2:K:268:ASN:OD1  | 2:K:576:ARG:HA   | 2.07                     | 0.54              |
| 1:E:54:ASN:CB    | 10:E:1748:HOH:O  | 2.54                     | 0.54              |
| 2:C:531:ILE:C    | 2:C:531:ILE:CD1  | 2.70                     | 0.54              |
| 2:G:331:ALA:HB1  | 2:G:495:LEU:CD2  | 2.37                     | 0.54              |
| 2:C:121:GLN:NE2  | 10:C:1018:HOH:O  | 2.40                     | 0.54              |
| 2:K:142:ASP:HB3  | 10:K:825:HOH:O   | 2.07                     | 0.54              |
| 2:O:465:MET:HE3  | 2:O:469:GLY:O    | 2.07                     | 0.54              |
| 2:C:120:VAL:HG12 | 2:C:122:GLN:HG2  | 1.90                     | 0.54              |
| 1:J:56:PHE:CD2   | 2:L:470:THR:HG22 | 2.43                     | 0.54              |
| 2:P:407:PHE:O    | 2:P:410:VAL:HG22 | 2.08                     | 0.54              |
| 2:G:533:LEU:HB3  | 2:G:534:PRO:HD3  | 1.90                     | 0.54              |
| 2:L:361:LEU:HA   | 2:L:364:VAL:HG22 | 1.89                     | 0.54              |
| 2:C:133:ASN:HB3  | 2:H:517:GLU:OE2  | 2.08                     | 0.54              |
| 1:F:102:GLU:HB3  | 1:F:103:PRO:HD2  | 1.89                     | 0.53              |
| 2:G:521:SER:OG   | 2:G:524:GLN:HG3  | 2.08                     | 0.53              |
| 2:C:333:ARG:HH11 | 2:C:421:ASN:HD22 | 1.56                     | 0.53              |
| 10:P:702:HOH:O   | 3:X:4:MAN:H62    | 2.08                     | 0.53              |
| 1:A:68:ILE:CD1   | 2:C:464:LEU:HD23 | 2.38                     | 0.53              |
| 1:N:63:ALA:O     | 1:N:67:GLU:CG    | 2.41                     | 0.53              |
| 1:A:3:GLU:O      | 1:A:17:ARG:NH1   | 2.31                     | 0.53              |
| 2:D:182:PRO:HG2  | 10:D:800:HOH:O   | 2.07                     | 0.53              |
| 1:E:54:ASN:CG    | 10:E:1748:HOH:O  | 2.47                     | 0.53              |
| 2:L:217:HIS:CE1  | 10:L:868:HOH:O   | 2.61                     | 0.53              |
| 2:L:577:GLU:O    | 2:L:578:ALA:OXT  | 2.26                     | 0.53              |
| 2:D:535:ARG:NH1  | 2:D:567:LEU:O    | 2.42                     | 0.53              |
| 2:L:214:ASP:OD1  | 2:L:215:ASN:N    | 2.35                     | 0.53              |
| 1:E:69:VAL:CG1   | 2:G:398:ALA:HB3  | 2.39                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:G:307:ARG:HD3   | 10:G:835:HOH:O   | 2.08                     | 0.53              |
| 2:L:465:MET:SD    | 2:L:471:PRO:HD3  | 2.49                     | 0.53              |
| 2:H:175:MET:HE1   | 2:H:288:VAL:HG11 | 1.88                     | 0.52              |
| 1:I:54:ASN:HA     | 10:I:1731:HOH:O  | 2.10                     | 0.52              |
| 2:L:214:ASP:HB3   | 2:L:216:LEU:CD1  | 2.40                     | 0.52              |
| 1:N:80:GLN:HG3    | 1:N:80:GLN:O     | 2.08                     | 0.52              |
| 2:O:485:LEU:HD13  | 2:O:490:ARG:HA   | 1.92                     | 0.52              |
| 1:F:90:GLY:HA3    | 7:F:202:HEM:CBC  | 2.40                     | 0.52              |
| 2:C:348:ASN:HD21  | 1:I:77:THR:HG22  | 1.74                     | 0.52              |
| 2:G:406:LEU:HB3   | 2:G:415:LEU:HB2  | 1.92                     | 0.52              |
| 2:H:181:GLU:H     | 2:H:182:PRO:HD2  | 1.72                     | 0.52              |
| 2:C:348:ASN:HD21  | 1:I:77:THR:CG2   | 2.21                     | 0.52              |
| 7:N:202:HEM:HBB2  | 7:N:202:HEM:CMB  | 2.40                     | 0.52              |
| 2:H:333:ARG:HH11  | 2:H:421:ASN:HD22 | 1.57                     | 0.52              |
| 2:P:568:PRO:HA    | 10:P:804:HOH:O   | 2.09                     | 0.52              |
| 1:A:16:ASN:O      | 1:A:20:PRO:HA    | 2.10                     | 0.51              |
| 2:C:114:ASN:HA    | 10:C:715:HOH:O   | 2.10                     | 0.51              |
| 2:O:566:THR:C     | 2:O:567:LEU:HD23 | 2.30                     | 0.51              |
| 2:P:417:LEU:HB3   | 2:P:418:PRO:HD3  | 1.92                     | 0.51              |
| 2:G:267:LEU:HD13  | 2:G:576:ARG:HB2  | 1.93                     | 0.51              |
| 2:C:244:PRO:HD3   | 2:C:364:VAL:O    | 2.10                     | 0.51              |
| 2:G:354:GLU:OE1   | 2:G:354:GLU:HA   | 2.10                     | 0.51              |
| 2:H:535:ARG:NH2   | 2:H:539:ASP:OD2  | 2.42                     | 0.51              |
| 1:J:76:LEU:HD23   | 1:J:76:LEU:C     | 2.31                     | 0.51              |
| 2:K:213:PHE:CD1   | 2:K:231:PRO:HG2  | 2.45                     | 0.51              |
| 2:L:214:ASP:HB3   | 2:L:216:LEU:HD12 | 1.91                     | 0.51              |
| 1:I:52:LYS:HD3    | 2:O:412:ARG:O    | 2.11                     | 0.51              |
| 1:E:3:GLU:O       | 1:E:4:GLN:HB2    | 2.10                     | 0.51              |
| 2:K:535:ARG:NH2   | 2:K:539:ASP:OD2  | 2.40                     | 0.51              |
| 2:L:406:LEU:HD23  | 2:L:415:LEU:HB2  | 1.91                     | 0.51              |
| 7:M:1602:HEM:HBA1 | 6:O:610:OKY:S    | 2.51                     | 0.51              |
| 1:F:70:ARG:HH11   | 2:H:403:ARG:HH21 | 1.57                     | 0.51              |
| 2:O:378:ASP:HB2   | 2:O:379:PRO:HD3  | 1.92                     | 0.51              |
| 1:F:16:ASN:O      | 1:F:20:PRO:HA    | 2.11                     | 0.50              |
| 2:H:181:GLU:N     | 2:H:182:PRO:CD   | 2.71                     | 0.50              |
| 2:G:113:VAL:O     | 2:G:114:ASN:C    | 2.50                     | 0.50              |
| 2:H:333:ARG:HH11  | 2:H:421:ASN:ND2  | 2.08                     | 0.50              |
| 2:L:340:GLN:OE1   | 2:L:341:PRO:HD2  | 2.12                     | 0.50              |
| 2:D:307:ARG:NH1   | 10:D:940:HOH:O   | 2.44                     | 0.50              |
| 1:F:72:PRO:HA     | 10:F:373:HOH:O   | 2.11                     | 0.50              |
| 2:G:128:LEU:HB2   | 2:G:144:ILE:HB   | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:267:LEU:CD2   | 10:G:861:HOH:O    | 2.59                     | 0.50              |
| 2:O:336:HIS:CE1   | 2:O:417:LEU:HD21  | 2.47                     | 0.50              |
| 1:B:83:SER:HB3    | 2:D:554:SER:O     | 2.11                     | 0.50              |
| 2:H:378:ASP:OD1   | 2:H:541:THR:HB    | 2.12                     | 0.50              |
| 2:H:378:ASP:HB2   | 2:H:379:PRO:HD3   | 1.93                     | 0.50              |
| 2:P:181:GLU:N     | 2:P:182:PRO:HD2   | 2.26                     | 0.50              |
| 1:A:84:LEU:HD13   | 2:C:389:ALA:HA    | 1.94                     | 0.50              |
| 2:C:488:LYS:CE    | 10:C:773:HOH:O    | 2.60                     | 0.50              |
| 2:H:242:GLU:HG3   | 6:H:610:OKY:O2    | 2.12                     | 0.50              |
| 7:C:601:HEM:CMB   | 7:C:601:HEM:HBB2  | 2.41                     | 0.50              |
| 1:A:98:ASP:OD2    | 7:C:601:HEM:O1D   | 2.30                     | 0.50              |
| 2:G:355:PRO:HD2   | 10:G:761:HOH:O    | 2.12                     | 0.50              |
| 2:K:267:LEU:O     | 2:K:576:ARG:NH1   | 2.44                     | 0.50              |
| 2:K:308:LYS:NZ    | 10:K:909:HOH:O    | 2.40                     | 0.50              |
| 1:E:76:LEU:C      | 1:E:76:LEU:HD23   | 2.33                     | 0.49              |
| 1:F:59:ALA:HB2    | 2:H:467:GLN:O     | 2.12                     | 0.49              |
| 7:C:601:HEM:HBC2  | 7:C:601:HEM:CMC   | 2.40                     | 0.49              |
| 2:H:563:ASN:ND2   | 10:H:1826:HOH:O   | 2.45                     | 0.49              |
| 1:N:67:GLU:HG3    | 2:P:467:GLN:NE2   | 2.27                     | 0.49              |
| 2:O:192:ASN:CG    | 2:O:194:LEU:HD12  | 2.32                     | 0.49              |
| 2:O:486:LYS:CE    | 10:O:861:HOH:O    | 2.59                     | 0.49              |
| 7:N:202:HEM:HBC2  | 7:N:202:HEM:CMC   | 2.42                     | 0.49              |
| 2:L:181:GLU:N     | 2:L:182:PRO:CD    | 2.75                     | 0.49              |
| 1:B:16:ASN:O      | 1:B:20:PRO:HA     | 2.12                     | 0.49              |
| 2:H:576:ARG:HG3   | 2:H:578:ALA:HB2   | 1.94                     | 0.49              |
| 1:N:40:GLY:HA2    | 10:N:344:HOH:O    | 2.11                     | 0.49              |
| 6:A:1602:OKY:H2   | 10:C:702:HOH:O    | 2.11                     | 0.49              |
| 2:K:372:VAL:O     | 10:K:907:HOH:O    | 2.20                     | 0.49              |
| 2:K:525:ARG:HD3   | 10:K:811:HOH:O    | 2.12                     | 0.49              |
| 2:P:577:GLU:O     | 2:P:578:ALA:C     | 2.50                     | 0.49              |
| 2:C:559:ARG:HD2   | 10:C:784:HOH:O    | 2.13                     | 0.49              |
| 2:K:530:GLN:NE2   | 10:K:910:HOH:O    | 2.46                     | 0.49              |
| 1:E:81:GLU:HG2    | 10:E:1736:HOH:O   | 2.12                     | 0.49              |
| 2:H:417:LEU:HB3   | 2:H:418:PRO:HD3   | 1.95                     | 0.49              |
| 1:M:1:CYS:O       | 1:M:2:PRO:C       | 2.51                     | 0.49              |
| 2:P:219:ASP:HB3   | 2:P:222:LEU:HD12  | 1.95                     | 0.49              |
| 6:P:614:OKY:H14   | 10:P:897:HOH:O    | 2.13                     | 0.49              |
| 2:G:554:SER:HB3   | 2:G:560:ASP:HB3   | 1.94                     | 0.49              |
| 1:J:16:ASN:O      | 1:J:20:PRO:HA     | 2.12                     | 0.49              |
| 7:M:1602:HEM:HBB2 | 7:M:1602:HEM:HMB1 | 1.94                     | 0.49              |
| 2:H:128:LEU:HB2   | 2:H:144:ILE:HB    | 1.94                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:H:353:MET:CE    | 10:H:1849:HOH:O  | 2.60                     | 0.48              |
| 2:O:269:PRO:HD2   | 10:O:714:HOH:O   | 2.12                     | 0.48              |
| 2:C:116:GLU:OE1   | 2:C:411:MET:HE1  | 2.13                     | 0.48              |
| 1:E:92:LEU:HD22   | 2:G:249:MET:HB3  | 1.94                     | 0.48              |
| 1:N:41:PHE:CD1    | 1:N:42:SER:HB2   | 2.48                     | 0.48              |
| 2:P:115:CYS:HB2   | 2:P:147:PHE:CZ   | 2.48                     | 0.48              |
| 2:P:333:ARG:HH11  | 2:P:421:ASN:ND2  | 2.11                     | 0.48              |
| 6:H:610:0KY:C6    | 6:H:610:0KY:C4   | 2.90                     | 0.48              |
| 2:K:128:LEU:HB2   | 2:K:144:ILE:HB   | 1.94                     | 0.48              |
| 2:L:216:LEU:HD22  | 2:L:220:PRO:HD2  | 1.95                     | 0.48              |
| 2:L:569:ALA:CB    | 10:L:896:HOH:O   | 2.59                     | 0.48              |
| 2:C:488:LYS:CD    | 10:C:773:HOH:O   | 2.57                     | 0.48              |
| 7:C:601:HEM:HMB1  | 7:C:601:HEM:HBB2 | 1.95                     | 0.48              |
| 2:O:465:MET:HE1   | 2:O:471:PRO:HD3  | 1.96                     | 0.48              |
| 6:I:1603:0KY:C6   | 6:I:1603:0KY:H11 | 2.43                     | 0.48              |
| 2:L:563:ASN:HB3   | 10:L:749:HOH:O   | 2.14                     | 0.48              |
| 7:M:1602:HEM:HBC2 | 7:M:1602:HEM:CMC | 2.43                     | 0.48              |
| 2:C:333:ARG:HH11  | 2:C:421:ASN:ND2  | 2.11                     | 0.48              |
| 2:G:348:ASN:OD1   | 2:G:349:ARG:N    | 2.46                     | 0.48              |
| 2:H:182:PRO:HG2   | 10:H:1814:HOH:O  | 2.14                     | 0.48              |
| 7:M:1602:HEM:HBB2 | 7:M:1602:HEM:CMB | 2.43                     | 0.48              |
| 7:B:202:HEM:CMC   | 7:B:202:HEM:HBC2 | 2.43                     | 0.48              |
| 2:D:116:GLU:OE2   | 2:D:411:MET:CE   | 2.61                     | 0.48              |
| 2:H:345:ARG:NE    | 10:H:1849:HOH:O  | 2.47                     | 0.47              |
| 2:P:341:PRO:HD3   | 2:P:399:VAL:HG11 | 1.96                     | 0.47              |
| 1:E:83:SER:O      | 1:E:86:PHE:HB3   | 2.13                     | 0.47              |
| 2:G:532:SER:O     | 2:G:536:ILE:HG13 | 2.13                     | 0.47              |
| 2:H:436:TRP:HB3   | 2:H:494:LEU:HD11 | 1.96                     | 0.47              |
| 2:O:313:TYR:CZ    | 2:O:315:SER:HA   | 2.49                     | 0.47              |
| 2:C:297:LEU:N     | 2:C:298:PRO:CD   | 2.78                     | 0.47              |
| 2:P:139:ASN:OD1   | 2:P:141:ALA:HB3  | 2.14                     | 0.47              |
| 2:P:378:ASP:CB    | 2:P:379:PRO:HD3  | 2.45                     | 0.47              |
| 2:C:225:ASN:HB2   | 2:C:369:TRP:CE2  | 2.49                     | 0.47              |
| 2:G:241:SER:O     | 2:G:366:PHE:HA   | 2.14                     | 0.47              |
| 2:G:562:VAL:HG11  | 10:G:892:HOH:O   | 2.12                     | 0.47              |
| 2:P:333:ARG:HH11  | 2:P:421:ASN:HD22 | 1.62                     | 0.47              |
| 2:G:116:GLU:HG2   | 10:G:855:HOH:O   | 2.13                     | 0.47              |
| 1:I:16:ASN:O      | 1:I:20:PRO:HA    | 2.14                     | 0.47              |
| 2:O:549:ASN:ND2   | 10:O:899:HOH:O   | 2.40                     | 0.47              |
| 2:D:211:LEU:HD23  | 2:D:254:LEU:HD13 | 1.96                     | 0.47              |
| 1:F:68:ILE:HD13   | 2:H:464:LEU:CD2  | 2.44                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:576:ARG:HG2  | 2:H:578:ALA:HB2  | 1.96                     | 0.47              |
| 2:L:333:ARG:HH11 | 2:L:421:ASN:HD22 | 1.62                     | 0.47              |
| 2:O:242:GLU:HG3  | 6:O:610:OKY:O2   | 2.15                     | 0.47              |
| 2:G:259:ARG:O    | 2:G:263:GLU:HG3  | 2.15                     | 0.47              |
| 2:K:349:ARG:HB2  | 2:K:351:GLN:HG2  | 1.97                     | 0.47              |
| 2:O:215:ASN:HB3  | 10:O:822:HOH:O   | 2.13                     | 0.47              |
| 2:H:559:ARG:HB2  | 10:H:1785:HOH:O  | 2.15                     | 0.46              |
| 2:O:370:ARG:HG2  | 2:O:374:GLU:OE2  | 2.15                     | 0.46              |
| 1:B:64:VAL:HG13  | 1:B:68:ILE:HD12  | 1.97                     | 0.46              |
| 2:D:223:LEU:HA   | 2:D:226:ARG:NE   | 2.30                     | 0.46              |
| 1:E:5:ASP:OD1    | 1:E:5:ASP:N      | 2.47                     | 0.46              |
| 2:G:199:VAL:HG12 | 2:G:254:LEU:HD21 | 1.96                     | 0.46              |
| 2:H:241:SER:O    | 2:H:366:PHE:HA   | 2.15                     | 0.46              |
| 2:L:466:GLU:HB2  | 10:L:897:HOH:O   | 2.15                     | 0.46              |
| 2:D:305:ALA:HB2  | 2:D:486:LYS:HZ2  | 1.80                     | 0.46              |
| 7:J:202:HEM:HBC2 | 7:J:202:HEM:CMC  | 2.42                     | 0.46              |
| 2:L:265:LYS:HD2  | 2:L:269:PRO:HA   | 1.97                     | 0.46              |
| 2:P:297:LEU:N    | 2:P:298:PRO:CD   | 2.79                     | 0.46              |
| 2:P:361:LEU:O    | 2:P:364:VAL:HG22 | 2.16                     | 0.46              |
| 1:B:79:ASP:O     | 2:D:388:PRO:HB3  | 2.16                     | 0.46              |
| 2:G:297:LEU:N    | 2:G:298:PRO:CD   | 2.79                     | 0.46              |
| 1:I:83:SER:HB3   | 2:K:554:SER:O    | 2.16                     | 0.46              |
| 2:L:132:PRO:O    | 2:L:133:ASN:HB2  | 2.16                     | 0.46              |
| 2:C:504:ARG:HD3  | 3:Q:6:FUC:H62    | 1.98                     | 0.46              |
| 2:G:531:ILE:O    | 2:G:531:ILE:HD12 | 2.15                     | 0.46              |
| 2:L:213:PHE:CG   | 2:L:231:PRO:HG2  | 2.51                     | 0.46              |
| 7:N:202:HEM:CBC  | 2:P:335:GLY:HA3  | 2.46                     | 0.46              |
| 2:P:349:ARG:HG3  | 2:P:351:GLN:HG2  | 1.98                     | 0.46              |
| 2:C:128:LEU:N    | 2:C:128:LEU:HD12 | 2.31                     | 0.45              |
| 2:H:359:VAL:HG12 | 2:H:364:VAL:CG1  | 2.46                     | 0.45              |
| 1:M:13:MET:O     | 1:M:14:CYS:HB2   | 2.16                     | 0.45              |
| 7:B:202:HEM:CAA  | 6:B:203:OKY:S    | 3.05                     | 0.45              |
| 1:B:63:ALA:O     | 1:B:67:GLU:HG2   | 2.16                     | 0.45              |
| 2:C:307:ARG:HD3  | 10:C:857:HOH:O   | 2.15                     | 0.45              |
| 1:F:41:PHE:CD1   | 1:F:42:SER:HB2   | 2.52                     | 0.45              |
| 2:G:271:TRP:CZ3  | 2:G:279:GLU:HG3  | 2.51                     | 0.45              |
| 7:F:202:HEM:HAA2 | 6:H:610:OKY:S    | 2.56                     | 0.45              |
| 1:J:98:ASP:OD2   | 7:J:202:HEM:O1D  | 2.34                     | 0.45              |
| 2:K:213:PHE:CG   | 2:K:231:PRO:HG2  | 2.52                     | 0.45              |
| 1:M:11:THR:O     | 1:M:24:ALA:HA    | 2.17                     | 0.45              |
| 1:A:40:GLY:HA2   | 1:B:20:PRO:HD2   | 1.99                     | 0.45              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:E:1602:HEM:HBA1 | 6:G:610:0KY:S    | 2.55                     | 0.45              |
| 2:G:267:LEU:HD22  | 2:G:576:ARG:NH2  | 2.31                     | 0.45              |
| 2:O:533:LEU:HD23  | 2:O:551:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:32:TRP:CE2    | 2:D:325:ALA:HB2  | 2.52                     | 0.45              |
| 2:G:171:VAL:HG12  | 2:G:288:VAL:HG12 | 1.99                     | 0.45              |
| 1:J:41:PHE:CD1    | 1:J:42:SER:HB2   | 2.51                     | 0.45              |
| 2:K:377:ILE:HD12  | 2:K:381:LEU:HD11 | 1.98                     | 0.45              |
| 1:F:70:ARG:NH1    | 2:H:403:ARG:HH21 | 2.15                     | 0.45              |
| 2:L:333:ARG:HH11  | 2:L:421:ASN:ND2  | 2.15                     | 0.45              |
| 2:C:533:LEU:N     | 2:C:534:PRO:HD2  | 2.32                     | 0.45              |
| 2:O:336:HIS:CE1   | 2:O:417:LEU:HD11 | 2.51                     | 0.45              |
| 2:D:417:LEU:HB3   | 2:D:418:PRO:HD3  | 1.99                     | 0.45              |
| 2:P:411:MET:SD    | 2:P:415:LEU:HD11 | 2.57                     | 0.45              |
| 2:C:406:LEU:HD22  | 2:C:417:LEU:HB2  | 1.98                     | 0.44              |
| 2:K:333:ARG:HH11  | 2:K:421:ASN:ND2  | 2.14                     | 0.44              |
| 2:K:241:SER:O     | 2:K:366:PHE:HA   | 2.17                     | 0.44              |
| 2:L:241:SER:O     | 2:L:366:PHE:HA   | 2.18                     | 0.44              |
| 2:D:213:PHE:CG    | 2:D:231:PRO:HG2  | 2.52                     | 0.44              |
| 1:E:88:GLN:OE1    | 2:G:245:GLU:HB2  | 2.17                     | 0.44              |
| 2:G:157:ASN:OD1   | 2:G:158:ILE:HG13 | 2.18                     | 0.44              |
| 1:I:32:TRP:CE2    | 2:K:325:ALA:HB2  | 2.52                     | 0.44              |
| 2:K:275:ARG:CD    | 10:K:847:HOH:O   | 2.64                     | 0.44              |
| 7:I:1602:HEM:HAA2 | 6:I:1603:0KY:S   | 2.58                     | 0.44              |
| 2:K:406:LEU:HD22  | 2:K:417:LEU:HB2  | 1.98                     | 0.44              |
| 2:K:354:GLU:OE1   | 2:K:354:GLU:HA   | 2.17                     | 0.44              |
| 2:P:181:GLU:N     | 2:P:182:PRO:CD   | 2.81                     | 0.44              |
| 2:C:336:HIS:CE1   | 2:C:417:LEU:HD21 | 2.53                     | 0.44              |
| 2:H:301:LEU:HB3   | 2:H:305:ALA:CB   | 2.46                     | 0.44              |
| 2:K:308:LYS:HD3   | 2:K:309:TYR:CZ   | 2.52                     | 0.44              |
| 2:O:200:ASN:HD22  | 2:O:203:PHE:N    | 2.06                     | 0.44              |
| 2:O:406:LEU:HD23  | 2:O:415:LEU:HB2  | 1.99                     | 0.44              |
| 2:C:241:SER:O     | 2:C:366:PHE:HA   | 2.17                     | 0.44              |
| 2:H:175:MET:HG3   | 2:H:176:VAL:HG23 | 1.99                     | 0.44              |
| 2:C:333:ARG:HD3   | 2:C:421:ASN:ND2  | 2.32                     | 0.44              |
| 1:F:13:MET:O      | 1:F:14:CYS:HB2   | 2.18                     | 0.44              |
| 2:G:172:ASP:O     | 2:G:173:ALA:HB3  | 2.18                     | 0.44              |
| 2:K:197:LEU:HB2   | 2:K:254:LEU:HD12 | 2.00                     | 0.44              |
| 1:N:64:VAL:CG1    | 1:N:68:ILE:HD12  | 2.41                     | 0.44              |
| 2:P:173:ALA:HA    | 2:P:175:MET:SD   | 2.57                     | 0.44              |
| 2:C:362:SER:HA    | 2:C:365:PHE:CE1  | 2.52                     | 0.44              |
| 2:O:465:MET:CE    | 2:O:471:PRO:HD3  | 2.47                     | 0.44              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:P:523:GLN:HG2   | 10:P:817:HOH:O   | 2.18                     | 0.44              |
| 6:A:1602:OKY:S    | 7:C:601:HEM:HAA2 | 2.58                     | 0.43              |
| 1:E:31:ARG:CZ     | 1:E:35:ALA:HB2   | 2.48                     | 0.43              |
| 2:K:570:LEU:HD23  | 2:K:572:LEU:HD21 | 1.99                     | 0.43              |
| 2:L:199:VAL:HG12  | 2:L:254:LEU:HD21 | 2.00                     | 0.43              |
| 2:L:270:ARG:HD3   | 10:L:872:HOH:O   | 2.17                     | 0.43              |
| 1:B:56:PHE:CD1    | 2:D:469:GLY:HA3  | 2.52                     | 0.43              |
| 2:G:299:LEU:CD1   | 2:G:299:LEU:N    | 2.81                     | 0.43              |
| 1:F:68:ILE:CD1    | 2:H:464:LEU:HD23 | 2.47                     | 0.43              |
| 2:O:571:ASN:HA    | 10:O:828:HOH:O   | 2.17                     | 0.43              |
| 2:H:456:ARG:NH2   | 10:H:1827:HOH:O  | 2.52                     | 0.43              |
| 2:C:128:LEU:HB2   | 2:C:144:ILE:HB   | 2.01                     | 0.43              |
| 2:C:304:THR:HG21  | 10:C:977:HOH:O   | 2.18                     | 0.43              |
| 2:G:181:GLU:HB2   | 10:G:752:HOH:O   | 2.17                     | 0.43              |
| 2:C:242:GLU:O     | 2:C:365:PHE:HA   | 2.18                     | 0.43              |
| 2:K:554:SER:HB3   | 2:K:560:ASP:HB3  | 2.00                     | 0.43              |
| 2:P:354:GLU:HB3   | 2:P:355:PRO:HA   | 2.00                     | 0.43              |
| 1:F:96:ASP:OD2    | 2:H:175:MET:CE   | 2.65                     | 0.43              |
| 2:H:390:LYS:NZ    | 2:H:396:GLN:O    | 2.37                     | 0.43              |
| 7:J:202:HEM:HAA2  | 6:J:203:OKY:S    | 2.59                     | 0.43              |
| 2:K:569:ALA:O     | 2:K:570:LEU:C    | 2.56                     | 0.43              |
| 2:O:465:MET:HE1   | 2:O:469:GLY:O    | 2.19                     | 0.43              |
| 7:B:202:HEM:CBA   | 6:B:203:OKY:S    | 3.03                     | 0.43              |
| 2:K:377:ILE:O     | 2:K:381:LEU:HG   | 2.19                     | 0.43              |
| 2:L:181:GLU:OE2   | 2:L:184:ALA:HB3  | 2.18                     | 0.43              |
| 2:L:378:ASP:HB2   | 2:L:379:PRO:HD3  | 2.00                     | 0.43              |
| 2:G:533:LEU:N     | 2:G:534:PRO:CD   | 2.82                     | 0.43              |
| 2:P:309:TYR:CZ    | 2:P:497:CYS:HA   | 2.54                     | 0.43              |
| 2:G:504:ARG:HB3   | 10:G:736:HOH:O   | 2.19                     | 0.43              |
| 2:G:567:LEU:HA    | 2:G:568:PRO:HD3  | 1.91                     | 0.43              |
| 2:K:299:LEU:CD2   | 2:K:552:PHE:HB2  | 2.49                     | 0.43              |
| 2:K:158:ILE:HD13  | 2:L:164:ILE:HD13 | 2.01                     | 0.43              |
| 2:O:535:ARG:NH2   | 2:O:539:ASP:OD2  | 2.50                     | 0.43              |
| 2:O:559:ARG:HD2   | 10:O:874:HOH:O   | 2.18                     | 0.43              |
| 6:B:203:OKY:H11   | 6:B:203:OKY:C6   | 2.49                     | 0.42              |
| 1:B:29:PHE:CZ     | 2:D:329:THR:HG21 | 2.53                     | 0.42              |
| 2:L:514:TRP:CE2   | 2:L:515:GLU:HG3  | 2.54                     | 0.42              |
| 1:M:59:ALA:HB2    | 2:O:467:GLN:O    | 2.18                     | 0.42              |
| 1:E:13:MET:O      | 1:E:14:CYS:HB2   | 2.19                     | 0.42              |
| 7:E:1602:HEM:HBB2 | 2:G:242:GLU:OE1  | 2.18                     | 0.42              |
| 2:H:353:MET:HE2   | 10:H:1849:HOH:O  | 2.18                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:347:ASP:CB   | 1:I:80:GLN:OE1   | 2.54                     | 0.42              |
| 2:G:225:ASN:C    | 2:G:225:ASN:OD1  | 2.58                     | 0.42              |
| 2:G:369:TRP:CZ3  | 8:G:608:NAG:H2   | 2.54                     | 0.42              |
| 2:H:271:TRP:CZ3  | 2:H:279:GLU:HG3  | 2.55                     | 0.42              |
| 2:H:491:VAL:HB   | 2:H:495:LEU:HB2  | 2.01                     | 0.42              |
| 2:H:530:GLN:HG3  | 10:H:1829:HOH:O  | 2.19                     | 0.42              |
| 2:D:122:GLN:O    | 2:D:123:PRO:C    | 2.56                     | 0.42              |
| 1:F:83:SER:HB3   | 2:H:554:SER:O    | 2.20                     | 0.42              |
| 2:G:304:THR:HG23 | 10:G:814:HOH:O   | 2.19                     | 0.42              |
| 2:H:139:ASN:OD1  | 2:H:141:ALA:HB3  | 2.19                     | 0.42              |
| 2:L:228:ALA:HB3  | 10:L:739:HOH:O   | 2.19                     | 0.42              |
| 2:O:212:PRO:HB3  | 10:O:848:HOH:O   | 2.19                     | 0.42              |
| 2:O:318:ASP:OD1  | 2:O:318:ASP:C    | 2.57                     | 0.42              |
| 1:B:29:PHE:CE1   | 2:D:165:ASN:HB2  | 2.55                     | 0.42              |
| 1:B:6:LYS:HZ2    | 2:D:275:ARG:NH2  | 2.13                     | 0.42              |
| 2:G:314:ARG:HD3  | 2:G:314:ARG:HA   | 1.86                     | 0.42              |
| 2:H:411:MET:HE2  | 2:H:415:LEU:CD2  | 2.48                     | 0.42              |
| 2:K:297:LEU:N    | 2:K:298:PRO:CD   | 2.83                     | 0.42              |
| 2:K:465:MET:HE3  | 2:K:469:GLY:O    | 2.19                     | 0.42              |
| 2:O:304:THR:CG2  | 10:O:860:HOH:O   | 2.59                     | 0.42              |
| 2:D:486:LYS:NZ   | 10:D:881:HOH:O   | 2.53                     | 0.42              |
| 2:K:558:PRO:O    | 2:K:559:ARG:C    | 2.58                     | 0.42              |
| 2:D:549:ASN:HB3  | 10:D:930:HOH:O   | 2.20                     | 0.42              |
| 2:G:565:SER:C    | 2:G:567:LEU:H    | 2.23                     | 0.42              |
| 2:K:181:GLU:HB2  | 10:K:801:HOH:O   | 2.20                     | 0.42              |
| 2:K:309:TYR:CZ   | 2:K:497:CYS:HA   | 2.55                     | 0.42              |
| 2:O:535:ARG:HD2  | 2:O:535:ARG:HA   | 1.93                     | 0.42              |
| 2:O:378:ASP:OD1  | 2:O:541:THR:HB   | 2.20                     | 0.42              |
| 2:O:308:LYS:NZ   | 3:X:4:MAN:O6     | 2.49                     | 0.42              |
| 2:C:309:TYR:OH   | 2:C:497:CYS:HB2  | 2.19                     | 0.41              |
| 2:D:304:THR:HG22 | 10:D:881:HOH:O   | 2.20                     | 0.41              |
| 1:B:69:VAL:CG1   | 2:D:398:ALA:HB3  | 2.50                     | 0.41              |
| 2:D:393:ARG:CD   | 10:D:756:HOH:O   | 2.68                     | 0.41              |
| 2:G:465:MET:HE3  | 10:G:873:HOH:O   | 2.20                     | 0.41              |
| 2:H:471:PRO:HA   | 2:H:474:ILE:HG13 | 2.02                     | 0.41              |
| 2:L:522:MET:O    | 2:L:526:GLN:HG3  | 2.20                     | 0.41              |
| 2:O:279:GLU:O    | 2:O:283:ILE:HG13 | 2.19                     | 0.41              |
| 2:L:308:LYS:HD3  | 2:L:309:TYR:CE2  | 2.56                     | 0.41              |
| 1:M:29:PHE:CE1   | 2:O:165:ASN:HB2  | 2.55                     | 0.41              |
| 1:E:82:ARG:HA    | 2:G:552:PHE:O    | 2.20                     | 0.41              |
| 2:C:521:SER:OG   | 2:C:524:GLN:HG3  | 2.19                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:D:113:VAL:HG21  | 2:D:122:GLN:HB2  | 2.01                     | 0.41              |
| 1:I:4:GLN:HA      | 1:I:17:ARG:HH12  | 1.85                     | 0.41              |
| 1:N:53:ARG:O      | 1:N:54:ASN:C     | 2.59                     | 0.41              |
| 2:P:187:LEU:HD11  | 2:P:236:GLY:HA2  | 2.02                     | 0.41              |
| 1:A:20:PRO:HD2    | 1:B:40:GLY:HA2   | 2.03                     | 0.41              |
| 7:E:1602:HEM:HBC2 | 2:G:335:GLY:HA3  | 2.03                     | 0.41              |
| 2:L:354:GLU:HB3   | 2:L:355:PRO:HA   | 2.01                     | 0.41              |
| 2:L:417:LEU:HB3   | 2:L:418:PRO:HD3  | 2.03                     | 0.41              |
| 2:P:181:GLU:OE1   | 2:P:185:ARG:NH1  | 2.54                     | 0.41              |
| 2:P:223:LEU:HD22  | 2:P:226:ARG:HH12 | 1.85                     | 0.41              |
| 2:C:113:VAL:O     | 10:C:996:HOH:O   | 2.22                     | 0.41              |
| 2:L:242:GLU:O     | 2:L:365:PHE:HA   | 2.20                     | 0.41              |
| 1:M:10:ILE:HD13   | 1:M:10:ILE:HA    | 1.86                     | 0.41              |
| 2:O:491:VAL:HB    | 2:O:495:LEU:HB2  | 2.03                     | 0.41              |
| 2:P:113:VAL:CG1   | 2:P:125:CYS:SG   | 3.08                     | 0.41              |
| 2:P:378:ASP:OD1   | 2:P:541:THR:HB   | 2.21                     | 0.41              |
| 1:B:13:MET:O      | 1:B:14:CYS:HB2   | 2.21                     | 0.41              |
| 2:C:514:TRP:CE2   | 2:C:515:GLU:HG3  | 2.56                     | 0.41              |
| 1:F:38:GLU:CD     | 1:F:48:THR:HG1   | 2.14                     | 0.41              |
| 2:K:345:ARG:O     | 2:K:346:LEU:HD23 | 2.21                     | 0.41              |
| 2:O:548:LYS:HZ3   | 2:O:562:VAL:HG12 | 1.84                     | 0.41              |
| 2:P:182:PRO:HG3   | 10:P:822:HOH:O   | 2.19                     | 0.41              |
| 2:G:282:LYS:HG2   | 2:G:520:PHE:CZ   | 2.56                     | 0.41              |
| 2:H:175:MET:HE1   | 2:H:288:VAL:CG2  | 2.49                     | 0.41              |
| 2:H:214:ASP:OD1   | 2:H:215:ASN:N    | 2.53                     | 0.41              |
| 2:L:393:ARG:HB2   | 2:L:396:GLN:HB2  | 2.02                     | 0.41              |
| 2:O:257:HIS:CE1   | 2:O:280:ALA:HB3  | 2.56                     | 0.41              |
| 2:P:181:GLU:CG    | 10:P:893:HOH:O   | 2.62                     | 0.41              |
| 2:P:182:PRO:HG2   | 10:P:822:HOH:O   | 2.19                     | 0.41              |
| 2:P:445:PRO:O     | 2:P:471:PRO:HG2  | 2.21                     | 0.41              |
| 2:D:362:SER:HA    | 2:D:365:PHE:CE1  | 2.56                     | 0.41              |
| 2:D:411:MET:HE1   | 2:D:415:LEU:HD21 | 2.03                     | 0.41              |
| 2:G:346:LEU:HA    | 2:G:346:LEU:HD23 | 1.92                     | 0.41              |
| 1:I:84:LEU:HD12   | 1:I:84:LEU:HA    | 1.94                     | 0.41              |
| 2:O:305:ALA:HB2   | 2:O:486:LYS:HE3  | 2.02                     | 0.41              |
| 1:E:32:TRP:CE2    | 2:G:325:ALA:HB2  | 2.56                     | 0.40              |
| 2:G:339:ILE:HG23  | 10:G:754:HOH:O   | 2.20                     | 0.40              |
| 2:L:181:GLU:HG3   | 2:L:185:ARG:NH2  | 2.36                     | 0.40              |
| 2:O:173:ALA:HA    | 2:O:175:MET:SD   | 2.62                     | 0.40              |
| 7:F:202:HEM:HMC2  | 7:F:202:HEM:CBC  | 2.41                     | 0.40              |
| 2:G:535:ARG:O     | 2:G:538:CYS:HB2  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:476:ILE:HG23 | 2:H:477:TRP:N    | 2.35                     | 0.40              |
| 2:K:252:LEU:HD11 | 2:K:537:ILE:HA   | 2.02                     | 0.40              |
| 1:N:100:THR:HG21 | 2:P:428:HIS:CE1  | 2.55                     | 0.40              |
| 2:D:458:LEU:O    | 2:D:462:ARG:HG3  | 2.21                     | 0.40              |
| 2:D:563:ASN:HB3  | 10:D:948:HOH:O   | 2.20                     | 0.40              |
| 2:K:533:LEU:HB3  | 2:K:534:PRO:HD3  | 2.03                     | 0.40              |
| 2:L:145:PRO:HG2  | 2:L:411:MET:HE1  | 2.02                     | 0.40              |
| 2:C:207:GLY:N    | 10:C:1013:HOH:O  | 2.46                     | 0.40              |
| 2:D:297:LEU:N    | 2:D:298:PRO:CD   | 2.85                     | 0.40              |
| 2:D:373:LEU:HD13 | 8:D:608:NAG:H61  | 2.04                     | 0.40              |
| 1:F:64:VAL:HG13  | 1:F:68:ILE:CD1   | 2.45                     | 0.40              |
| 2:G:347:ASP:OD1  | 2:G:347:ASP:C    | 2.58                     | 0.40              |
| 2:P:134:ASP:CG   | 2:P:135:PRO:HD2  | 2.42                     | 0.40              |
| 2:D:216:LEU:HA   | 2:D:216:LEU:HD23 | 1.95                     | 0.40              |
| 1:F:80:GLN:HB2   | 1:F:81:GLU:OE2   | 2.21                     | 0.40              |
| 2:H:304:THR:HG22 | 10:H:1789:HOH:O  | 2.22                     | 0.40              |
| 2:H:400:ASP:O    | 2:H:404:GLU:HB2  | 2.22                     | 0.40              |
| 2:K:517:GLU:HA   | 2:K:517:GLU:OE1  | 2.22                     | 0.40              |
| 2:O:219:ASP:HB3  | 2:O:222:LEU:HD12 | 2.03                     | 0.40              |
| 2:O:297:LEU:N    | 2:O:298:PRO:HD2  | 2.36                     | 0.40              |
| 2:P:533:LEU:N    | 2:P:534:PRO:CD   | 2.85                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------------|--------------------------|-------------------|
| 10:K:879:HOH:O  | 10:N:346:HOH:O[1_455] | 2.12                     | 0.08              |
| 2:G:208:ARG:NH2 | 10:L:946:HOH:O[1_456] | 2.13                     | 0.07              |
| 2:G:522:MET:SD  | 10:L:904:HOH:O[1_556] | 2.14                     | 0.06              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 102/104 (98%)   | 101 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 1   | B     | 102/104 (98%)   | 100 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 1   | E     | 102/104 (98%)   | 95 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 1   | F     | 102/104 (98%)   | 98 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 1   | I     | 102/104 (98%)   | 97 (95%)   | 4 (4%)   | 1 (1%)   | 15          | 9   |
| 1   | J     | 102/104 (98%)   | 100 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 1   | M     | 102/104 (98%)   | 98 (96%)   | 2 (2%)   | 2 (2%)   | 7           | 3   |
| 1   | N     | 103/104 (99%)   | 100 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 2   | C     | 463/466 (99%)   | 449 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 2   | D     | 463/466 (99%)   | 443 (96%)  | 19 (4%)  | 1 (0%)   | 47          | 44  |
| 2   | G     | 462/466 (99%)   | 440 (95%)  | 19 (4%)  | 3 (1%)   | 25          | 19  |
| 2   | H     | 463/466 (99%)   | 442 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 2   | K     | 462/466 (99%)   | 438 (95%)  | 23 (5%)  | 1 (0%)   | 47          | 44  |
| 2   | L     | 463/466 (99%)   | 447 (96%)  | 16 (4%)  | 0        | 100         | 100 |
| 2   | O     | 463/466 (99%)   | 442 (96%)  | 19 (4%)  | 2 (0%)   | 34          | 30  |
| 2   | P     | 463/466 (99%)   | 447 (96%)  | 16 (4%)  | 0        | 100         | 100 |
| All | All   | 4519/4560 (99%) | 4337 (96%) | 172 (4%) | 10 (0%)  | 47          | 44  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 114 | ASN  |
| 2   | G     | 142 | ASP  |
| 1   | I     | 3   | GLU  |
| 2   | K     | 114 | ASN  |
| 1   | M     | 3   | GLU  |
| 2   | D     | 217 | HIS  |
| 2   | G     | 217 | HIS  |
| 2   | O     | 142 | ASP  |
| 1   | M     | 2   | PRO  |
| 2   | O     | 217 | HIS  |

### 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     | 90/90 (100%)     | 90 (100%)  | 0        | 100         | 100 |
| 1   | B     | 90/90 (100%)     | 89 (99%)   | 1 (1%)   | 73          | 78  |
| 1   | E     | 90/90 (100%)     | 89 (99%)   | 1 (1%)   | 73          | 78  |
| 1   | F     | 90/90 (100%)     | 87 (97%)   | 3 (3%)   | 38          | 37  |
| 1   | I     | 90/90 (100%)     | 88 (98%)   | 2 (2%)   | 52          | 55  |
| 1   | J     | 90/90 (100%)     | 89 (99%)   | 1 (1%)   | 73          | 78  |
| 1   | M     | 90/90 (100%)     | 89 (99%)   | 1 (1%)   | 73          | 78  |
| 1   | N     | 91/90 (101%)     | 88 (97%)   | 3 (3%)   | 38          | 37  |
| 2   | C     | 410/410 (100%)   | 405 (99%)  | 5 (1%)   | 71          | 76  |
| 2   | D     | 409/410 (100%)   | 395 (97%)  | 14 (3%)  | 37          | 36  |
| 2   | G     | 410/410 (100%)   | 398 (97%)  | 12 (3%)  | 42          | 43  |
| 2   | H     | 409/410 (100%)   | 405 (99%)  | 4 (1%)   | 76          | 81  |
| 2   | K     | 410/410 (100%)   | 401 (98%)  | 9 (2%)   | 52          | 55  |
| 2   | L     | 409/410 (100%)   | 402 (98%)  | 7 (2%)   | 60          | 65  |
| 2   | O     | 409/410 (100%)   | 399 (98%)  | 10 (2%)  | 49          | 51  |
| 2   | P     | 410/410 (100%)   | 403 (98%)  | 7 (2%)   | 60          | 65  |
| All | All   | 3997/4000 (100%) | 3917 (98%) | 80 (2%)  | 55          | 58  |

All (80) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 118 | SER  |
| 2   | C     | 175 | MET  |
| 2   | C     | 444 | GLN  |
| 2   | C     | 504 | ARG  |
| 2   | C     | 576 | ARG  |
| 1   | B     | 75  | GLN  |
| 2   | D     | 175 | MET  |
| 2   | D     | 217 | HIS  |
| 2   | D     | 219 | ASP  |
| 2   | D     | 227 | SER  |
| 2   | D     | 254 | LEU  |
| 2   | D     | 334 | TYR  |
| 2   | D     | 349 | ARG  |
| 2   | D     | 358 | ARG  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | D            | 363        | ARG         |
| 2          | D            | 466        | GLU         |
| 2          | D            | 470        | THR         |
| 2          | D            | 497        | CYS         |
| 2          | D            | 522        | MET         |
| 2          | D            | 553        | MET         |
| 1          | E            | 42         | SER         |
| 2          | G            | 142        | ASP         |
| 2          | G            | 175        | MET         |
| 2          | G            | 227        | SER         |
| 2          | G            | 243        | MET         |
| 2          | G            | 267        | LEU         |
| 2          | G            | 330        | ASN         |
| 2          | G            | 353        | MET         |
| 2          | G            | 526        | GLN         |
| 2          | G            | 546        | VAL         |
| 2          | G            | 547        | SER         |
| 2          | G            | 563        | ASN         |
| 2          | G            | 576        | ARG         |
| 1          | F            | 6          | LYS         |
| 1          | F            | 60         | LEU         |
| 1          | F            | 84         | LEU         |
| 2          | H            | 265        | LYS         |
| 2          | H            | 466        | GLU         |
| 2          | H            | 526        | GLN         |
| 2          | H            | 576        | ARG         |
| 1          | I            | 5          | ASP         |
| 1          | I            | 52         | LYS         |
| 2          | K            | 113        | VAL         |
| 2          | K            | 175        | MET         |
| 2          | K            | 181        | GLU         |
| 2          | K            | 214        | ASP         |
| 2          | K            | 304        | THR         |
| 2          | K            | 314        | ARG         |
| 2          | K            | 318        | ASP         |
| 2          | K            | 358        | ARG         |
| 2          | K            | 565        | SER         |
| 1          | J            | 42         | SER         |
| 2          | L            | 175        | MET         |
| 2          | L            | 180        | GLU         |
| 2          | L            | 215        | ASN         |
| 2          | L            | 254        | LEU         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 408 | GLU  |
| 2   | L     | 470 | THR  |
| 2   | L     | 486 | LYS  |
| 1   | M     | 80  | GLN  |
| 2   | O     | 116 | GLU  |
| 2   | O     | 175 | MET  |
| 2   | O     | 180 | GLU  |
| 2   | O     | 229 | ARG  |
| 2   | O     | 304 | THR  |
| 2   | O     | 330 | ASN  |
| 2   | O     | 408 | GLU  |
| 2   | O     | 466 | GLU  |
| 2   | O     | 497 | CYS  |
| 2   | O     | 547 | SER  |
| 1   | N     | 60  | LEU  |
| 1   | N     | 75  | GLN  |
| 1   | N     | 81  | GLU  |
| 2   | P     | 175 | MET  |
| 2   | P     | 181 | GLU  |
| 2   | P     | 254 | LEU  |
| 2   | P     | 318 | ASP  |
| 2   | P     | 349 | ARG  |
| 2   | P     | 470 | THR  |
| 2   | P     | 547 | SER  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 121 | GLN  |
| 2   | C     | 133 | ASN  |
| 2   | C     | 348 | ASN  |
| 2   | C     | 421 | ASN  |
| 2   | D     | 140 | GLN  |
| 2   | D     | 201 | GLN  |
| 2   | D     | 421 | ASN  |
| 2   | D     | 467 | GLN  |
| 2   | D     | 549 | ASN  |
| 1   | E     | 26  | ASN  |
| 2   | G     | 121 | GLN  |
| 2   | G     | 206 | ASN  |
| 2   | G     | 351 | GLN  |
| 2   | G     | 421 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 549 | ASN  |
| 1   | F     | 26  | ASN  |
| 2   | H     | 140 | GLN  |
| 2   | H     | 157 | ASN  |
| 2   | H     | 201 | GLN  |
| 2   | H     | 563 | ASN  |
| 1   | I     | 16  | ASN  |
| 2   | K     | 133 | ASN  |
| 2   | K     | 201 | GLN  |
| 2   | K     | 421 | ASN  |
| 2   | K     | 530 | GLN  |
| 2   | K     | 549 | ASN  |
| 2   | L     | 121 | GLN  |
| 2   | L     | 193 | GLN  |
| 2   | L     | 201 | GLN  |
| 2   | L     | 215 | ASN  |
| 2   | L     | 217 | HIS  |
| 2   | L     | 421 | ASN  |
| 1   | M     | 16  | ASN  |
| 2   | O     | 140 | GLN  |
| 2   | O     | 200 | ASN  |
| 2   | O     | 217 | HIS  |
| 2   | O     | 356 | ASN  |
| 2   | O     | 421 | ASN  |
| 2   | O     | 549 | ASN  |
| 1   | N     | 26  | ASN  |
| 2   | P     | 193 | GLN  |
| 2   | P     | 217 | HIS  |
| 2   | P     | 421 | ASN  |
| 2   | P     | 467 | GLN  |
| 2   | P     | 549 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | CSO  | D     | 150 | 2    | 3,6,7        | 0.60 | 0           | 0,6,8       | 0.00 | -           |
| 2   | CSO  | G     | 150 | 2    | 3,6,7        | 0.77 | 0           | 0,6,8       | 0.00 | -           |
| 2   | CSO  | C     | 150 | 2    | 3,6,7        | 0.76 | 0           | 0,6,8       | 0.00 | -           |
| 2   | CSO  | L     | 150 | 2    | 3,6,7        | 0.56 | 0           | 0,6,8       | 0.00 | -           |
| 2   | CSO  | O     | 150 | 2    | 3,6,7        | 0.45 | 0           | 0,6,8       | 0.00 | -           |
| 2   | CSO  | H     | 150 | 2    | 3,6,7        | 0.58 | 0           | 0,6,8       | 0.00 | -           |
| 2   | CSO  | K     | 150 | 2    | 3,6,7        | 0.59 | 0           | 0,6,8       | 0.00 | -           |
| 2   | CSO  | P     | 150 | 2    | 3,6,7        | 0.70 | 0           | 0,6,8       | 0.00 | -           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 2   | CSO  | D     | 150 | 2    | -       | 0/1/5/7  | -     |
| 2   | CSO  | G     | 150 | 2    | -       | 0/1/5/7  | -     |
| 2   | CSO  | C     | 150 | 2    | -       | 0/1/5/7  | -     |
| 2   | CSO  | L     | 150 | 2    | -       | 0/1/5/7  | -     |
| 2   | CSO  | O     | 150 | 2    | -       | 0/1/5/7  | -     |
| 2   | CSO  | H     | 150 | 2    | -       | 0/1/5/7  | -     |
| 2   | CSO  | K     | 150 | 2    | -       | 0/1/5/7  | -     |
| 2   | CSO  | P     | 150 | 2    | -       | 0/1/5/7  | -     |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

53 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 |
| 3   | NAG  | Q     | 1   | 3,2  | 14,14,15     | 0.48 | 0        | 17,19,21    | 1.70 | 2 (11%)  |
| 3   | NAG  | Q     | 2   | 3    | 14,14,15     | 0.70 | 0        | 17,19,21    | 1.04 | 0        |
| 3   | BMA  | Q     | 3   | 3    | 11,11,12     | 0.47 | 0        | 15,15,17    | 1.04 | 1 (6%)   |
| 3   | MAN  | Q     | 4   | 3    | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.01 | 0        |
| 3   | MAN  | Q     | 5   | 3    | 11,11,12     | 0.76 | 0        | 15,15,17    | 1.06 | 1 (6%)   |
| 3   | FUC  | Q     | 6   | 3    | 10,10,11     | 0.89 | 0        | 14,14,16    | 1.47 | 1 (7%)   |
| 3   | NAG  | R     | 1   | 3,2  | 14,14,15     | 0.66 | 0        | 17,19,21    | 1.45 | 2 (11%)  |
| 3   | NAG  | R     | 2   | 3    | 14,14,15     | 0.75 | 0        | 17,19,21    | 0.81 | 0        |
| 3   | BMA  | R     | 3   | 3    | 11,11,12     | 0.54 | 0        | 15,15,17    | 1.50 | 3 (20%)  |
| 3   | MAN  | R     | 4   | 3    | 11,11,12     | 0.62 | 0        | 15,15,17    | 0.89 | 0        |
| 3   | MAN  | R     | 5   | 3    | 11,11,12     | 0.56 | 0        | 15,15,17    | 1.29 | 2 (13%)  |
| 3   | FUC  | R     | 6   | 3    | 10,10,11     | 0.76 | 0        | 14,14,16    | 1.41 | 1 (7%)   |
| 3   | NAG  | S     | 1   | 3,2  | 14,14,15     | 0.57 | 0        | 17,19,21    | 1.82 | 4 (23%)  |
| 3   | NAG  | S     | 2   | 3    | 14,14,15     | 0.56 | 0        | 17,19,21    | 1.07 | 1 (5%)   |
| 3   | BMA  | S     | 3   | 3    | 11,11,12     | 0.40 | 0        | 15,15,17    | 1.28 | 2 (13%)  |
| 3   | MAN  | S     | 4   | 3    | 11,11,12     | 0.63 | 0        | 15,15,17    | 0.92 | 0        |
| 3   | MAN  | S     | 5   | 3    | 11,11,12     | 0.45 | 0        | 15,15,17    | 1.04 | 1 (6%)   |
| 3   | FUC  | S     | 6   | 3    | 10,10,11     | 0.85 | 1 (10%)  | 14,14,16    | 1.40 | 2 (14%)  |
| 3   | NAG  | T     | 1   | 3,2  | 14,14,15     | 0.50 | 0        | 17,19,21    | 1.33 | 1 (5%)   |
| 3   | NAG  | T     | 2   | 3    | 14,14,15     | 0.61 | 0        | 17,19,21    | 0.90 | 0        |
| 3   | BMA  | T     | 3   | 3    | 11,11,12     | 0.40 | 0        | 15,15,17    | 0.81 | 1 (6%)   |
| 3   | MAN  | T     | 4   | 3    | 11,11,12     | 0.66 | 0        | 15,15,17    | 0.95 | 1 (6%)   |
| 3   | MAN  | T     | 5   | 3    | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.05 | 1 (6%)   |
| 3   | FUC  | T     | 6   | 3    | 10,10,11     | 1.06 | 1 (10%)  | 14,14,16    | 1.38 | 3 (21%)  |
| 3   | NAG  | U     | 1   | 3,2  | 14,14,15     | 0.57 | 0        | 17,19,21    | 1.50 | 1 (5%)   |
| 3   | NAG  | U     | 2   | 3    | 14,14,15     | 0.88 | 1 (7%)   | 17,19,21    | 1.16 | 0        |
| 3   | BMA  | U     | 3   | 3    | 11,11,12     | 0.56 | 0        | 15,15,17    | 1.27 | 1 (6%)   |
| 3   | MAN  | U     | 4   | 3    | 11,11,12     | 0.52 | 0        | 15,15,17    | 0.82 | 1 (6%)   |
| 3   | MAN  | U     | 5   | 3    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.12 | 1 (6%)   |
| 3   | FUC  | U     | 6   | 3    | 10,10,11     | 0.70 | 0        | 14,14,16    | 1.38 | 2 (14%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NAG  | V     | 1   | 3,2  | 14,14,15     | 0.49 | 0        | 17,19,21    | 1.57 | 4 (23%)  |
| 3   | NAG  | V     | 2   | 3    | 14,14,15     | 0.76 | 0        | 17,19,21    | 1.23 | 1 (5%)   |
| 3   | BMA  | V     | 3   | 3    | 11,11,12     | 0.47 | 0        | 15,15,17    | 1.26 | 1 (6%)   |
| 3   | MAN  | V     | 4   | 3    | 11,11,12     | 0.64 | 0        | 15,15,17    | 1.23 | 2 (13%)  |
| 3   | MAN  | V     | 5   | 3    | 11,11,12     | 0.46 | 0        | 15,15,17    | 1.33 | 1 (6%)   |
| 3   | FUC  | V     | 6   | 3    | 10,10,11     | 0.81 | 0        | 14,14,16    | 1.06 | 1 (7%)   |
| 3   | NAG  | W     | 1   | 3,2  | 14,14,15     | 0.63 | 0        | 17,19,21    | 1.71 | 2 (11%)  |
| 3   | NAG  | W     | 2   | 3    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 1.26 | 2 (11%)  |
| 3   | BMA  | W     | 3   | 3    | 11,11,12     | 0.49 | 0        | 15,15,17    | 1.19 | 2 (13%)  |
| 3   | MAN  | W     | 4   | 3    | 11,11,12     | 0.72 | 0        | 15,15,17    | 0.69 | 0        |
| 3   | MAN  | W     | 5   | 3    | 11,11,12     | 0.64 | 0        | 15,15,17    | 0.78 | 0        |
| 3   | FUC  | W     | 6   | 3    | 10,10,11     | 0.77 | 0        | 14,14,16    | 1.47 | 2 (14%)  |
| 3   | NAG  | X     | 1   | 3,2  | 14,14,15     | 0.53 | 0        | 17,19,21    | 1.58 | 4 (23%)  |
| 3   | NAG  | X     | 2   | 3    | 14,14,15     | 0.60 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 3   | BMA  | X     | 3   | 3    | 11,11,12     | 0.38 | 0        | 15,15,17    | 1.29 | 1 (6%)   |
| 3   | MAN  | X     | 4   | 3    | 11,11,12     | 0.57 | 0        | 15,15,17    | 1.29 | 3 (20%)  |
| 3   | MAN  | X     | 5   | 3    | 11,11,12     | 0.62 | 0        | 15,15,17    | 0.99 | 1 (6%)   |
| 3   | FUC  | X     | 6   | 3    | 10,10,11     | 1.09 | 1 (10%)  | 14,14,16    | 0.94 | 0        |
| 4   | NAG  | Y     | 1   | 2,4  | 14,14,15     | 0.69 | 0        | 17,19,21    | 0.95 | 1 (5%)   |
| 4   | NAG  | Y     | 2   | 4    | 14,14,15     | 0.74 | 0        | 17,19,21    | 0.91 | 0        |
| 4   | BMA  | Y     | 3   | 4    | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.92 | 1 (6%)   |
| 4   | MAN  | Y     | 4   | 4    | 11,11,12     | 0.49 | 0        | 15,15,17    | 1.00 | 1 (6%)   |
| 4   | MAN  | Y     | 5   | 4    | 11,11,12     | 0.64 | 0        | 15,15,17    | 0.95 | 1 (6%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | Q     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Q     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | Q     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | Q     | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | Q     | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | FUC  | Q     | 6   | 3    | -       | -         | 0/1/1/1 |
| 3   | NAG  | R     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | R     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | BMA  | R     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | R     | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | R     | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | FUC  | R     | 6   | 3    | -       | -         | 0/1/1/1 |
| 3   | NAG  | S     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | S     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | S     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | S     | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | S     | 5   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | FUC  | S     | 6   | 3    | -       | -         | 0/1/1/1 |
| 3   | NAG  | T     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | T     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | BMA  | T     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | T     | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | T     | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | FUC  | T     | 6   | 3    | -       | -         | 0/1/1/1 |
| 3   | NAG  | U     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | U     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | U     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | U     | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | U     | 5   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | FUC  | U     | 6   | 3    | -       | -         | 0/1/1/1 |
| 3   | NAG  | V     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | V     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | V     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | V     | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | V     | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | FUC  | V     | 6   | 3    | -       | -         | 0/1/1/1 |
| 3   | NAG  | W     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | W     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | W     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | W     | 4   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | MAN  | W     | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | FUC  | W     | 6   | 3    | -       | -         | 0/1/1/1 |
| 3   | NAG  | X     | 1   | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | X     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | X     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | X     | 4   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | MAN  | X     | 5   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | FUC  | X     | 6   | 3    | -       | -         | 0/1/1/1 |
| 4   | NAG  | Y     | 1   | 2,4  | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | Y     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | BMA  | Y     | 3   | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | Y     | 4   | 4    | -       | 2/2/19/22 | 0/1/1/1 |
| 4   | MAN  | Y     | 5   | 4    | -       | 2/2/19/22 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | X     | 6   | FUC  | O5-C1 | -2.68 | 1.39        | 1.43     |
| 3   | T     | 6   | FUC  | O5-C1 | -2.66 | 1.39        | 1.43     |
| 3   | U     | 2   | NAG  | O5-C1 | -2.26 | 1.40        | 1.43     |
| 3   | S     | 6   | FUC  | O5-C1 | -2.17 | 1.40        | 1.43     |
| 3   | W     | 2   | NAG  | C1-C2 | 2.13  | 1.55        | 1.52     |

All (68) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | W     | 1   | NAG  | C1-O5-C5 | 5.95  | 120.25      | 112.19   |
| 3   | U     | 1   | NAG  | O5-C1-C2 | -5.29 | 102.94      | 111.29   |
| 3   | Q     | 1   | NAG  | O5-C1-C2 | -4.67 | 103.91      | 111.29   |
| 3   | V     | 5   | MAN  | O5-C5-C6 | 4.17  | 113.74      | 107.20   |
| 3   | Q     | 6   | FUC  | C1-C2-C3 | -4.07 | 104.66      | 109.67   |
| 3   | Q     | 1   | NAG  | C1-O5-C5 | 3.95  | 117.54      | 112.19   |
| 3   | S     | 1   | NAG  | C1-O5-C5 | 3.89  | 117.47      | 112.19   |
| 3   | S     | 6   | FUC  | C1-C2-C3 | -3.87 | 104.91      | 109.67   |
| 3   | S     | 1   | NAG  | O5-C1-C2 | -3.84 | 105.22      | 111.29   |
| 3   | V     | 1   | NAG  | O5-C1-C2 | -3.80 | 105.29      | 111.29   |
| 3   | W     | 6   | FUC  | C1-C2-C3 | -3.76 | 105.05      | 109.67   |
| 3   | T     | 1   | NAG  | O5-C1-C2 | -3.60 | 105.60      | 111.29   |
| 3   | X     | 3   | BMA  | C1-C2-C3 | 3.52  | 113.99      | 109.67   |
| 3   | S     | 3   | BMA  | C1-C2-C3 | 3.49  | 113.96      | 109.67   |
| 3   | R     | 5   | MAN  | O5-C5-C6 | 3.49  | 112.67      | 107.20   |
| 3   | R     | 1   | NAG  | C1-O5-C5 | 3.37  | 116.75      | 112.19   |
| 3   | R     | 6   | FUC  | C6-C5-C4 | -3.30 | 106.98      | 113.07   |
| 3   | V     | 3   | BMA  | O5-C5-C6 | 3.20  | 112.22      | 107.20   |
| 3   | X     | 1   | NAG  | O5-C1-C2 | -3.19 | 106.25      | 111.29   |
| 3   | W     | 3   | BMA  | C1-C2-C3 | 3.18  | 113.57      | 109.67   |
| 4   | Y     | 4   | MAN  | C1-O5-C5 | 3.11  | 116.40      | 112.19   |
| 3   | R     | 1   | NAG  | O5-C1-C2 | -3.10 | 106.39      | 111.29   |
| 3   | S     | 2   | NAG  | C4-C3-C2 | -3.03 | 106.57      | 111.02   |
| 3   | X     | 1   | NAG  | C1-O5-C5 | 2.99  | 116.24      | 112.19   |
| 3   | R     | 3   | BMA  | O3-C3-C2 | -2.94 | 104.36      | 109.99   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | X     | 5   | MAN  | C1-O5-C5 | 2.94  | 116.17      | 112.19   |
| 3   | R     | 3   | BMA  | C1-C2-C3 | 2.86  | 113.18      | 109.67   |
| 3   | U     | 3   | BMA  | O5-C1-C2 | -2.84 | 106.38      | 110.77   |
| 3   | R     | 3   | BMA  | O2-C2-C3 | -2.82 | 104.48      | 110.14   |
| 3   | T     | 6   | FUC  | C1-C2-C3 | -2.76 | 106.28      | 109.67   |
| 3   | W     | 2   | NAG  | O3-C3-C2 | 2.67  | 115.00      | 109.47   |
| 3   | T     | 6   | FUC  | C6-C5-C4 | -2.62 | 108.23      | 113.07   |
| 3   | T     | 4   | MAN  | C1-O5-C5 | 2.59  | 115.70      | 112.19   |
| 3   | U     | 6   | FUC  | C1-C2-C3 | -2.59 | 106.48      | 109.67   |
| 3   | X     | 1   | NAG  | C1-C2-N2 | 2.57  | 114.88      | 110.49   |
| 3   | V     | 4   | MAN  | C2-C3-C4 | -2.54 | 106.50      | 110.89   |
| 3   | Q     | 5   | MAN  | O5-C5-C6 | 2.49  | 111.10      | 107.20   |
| 3   | V     | 2   | NAG  | O5-C1-C2 | -2.44 | 107.44      | 111.29   |
| 3   | Q     | 3   | BMA  | C1-C2-C3 | 2.42  | 112.64      | 109.67   |
| 3   | V     | 6   | FUC  | O5-C5-C4 | 2.41  | 113.84      | 109.52   |
| 3   | S     | 3   | BMA  | O5-C5-C6 | 2.39  | 110.95      | 107.20   |
| 3   | T     | 5   | MAN  | C1-O5-C5 | 2.38  | 115.42      | 112.19   |
| 3   | X     | 4   | MAN  | C6-C5-C4 | -2.38 | 107.44      | 113.00   |
| 3   | W     | 2   | NAG  | C4-C3-C2 | -2.35 | 107.57      | 111.02   |
| 3   | W     | 1   | NAG  | O4-C4-C3 | -2.35 | 104.91      | 110.35   |
| 3   | U     | 4   | MAN  | O5-C5-C6 | 2.35  | 110.89      | 107.20   |
| 4   | Y     | 5   | MAN  | C1-C2-C3 | 2.30  | 112.49      | 109.67   |
| 3   | V     | 1   | NAG  | C6-C5-C4 | -2.30 | 107.63      | 113.00   |
| 3   | X     | 4   | MAN  | C3-C4-C5 | 2.30  | 114.33      | 110.24   |
| 4   | Y     | 3   | BMA  | C1-C2-C3 | 2.29  | 112.48      | 109.67   |
| 3   | X     | 4   | MAN  | C1-O5-C5 | 2.27  | 115.26      | 112.19   |
| 3   | V     | 1   | NAG  | O5-C5-C6 | 2.26  | 110.75      | 107.20   |
| 3   | W     | 3   | BMA  | O5-C5-C6 | 2.25  | 110.72      | 107.20   |
| 3   | S     | 6   | FUC  | O5-C5-C6 | 2.24  | 112.14      | 107.33   |
| 3   | S     | 1   | NAG  | O4-C4-C3 | -2.24 | 105.18      | 110.35   |
| 3   | V     | 4   | MAN  | C1-O5-C5 | 2.22  | 115.20      | 112.19   |
| 3   | S     | 5   | MAN  | O5-C5-C6 | 2.21  | 110.66      | 107.20   |
| 3   | V     | 1   | NAG  | O4-C4-C3 | -2.15 | 105.39      | 110.35   |
| 3   | T     | 3   | BMA  | O5-C1-C2 | -2.15 | 107.46      | 110.77   |
| 3   | U     | 5   | MAN  | O5-C5-C6 | 2.12  | 110.53      | 107.20   |
| 3   | U     | 6   | FUC  | C3-C4-C5 | 2.11  | 113.06      | 109.77   |
| 3   | R     | 5   | MAN  | C1-O5-C5 | 2.09  | 115.03      | 112.19   |
| 3   | W     | 6   | FUC  | C6-C5-C4 | -2.09 | 109.22      | 113.07   |
| 3   | S     | 1   | NAG  | O3-C3-C2 | 2.09  | 113.78      | 109.47   |
| 4   | Y     | 1   | NAG  | C1-C2-N2 | 2.08  | 114.04      | 110.49   |
| 3   | T     | 6   | FUC  | C3-C4-C5 | 2.06  | 112.98      | 109.77   |
| 3   | X     | 1   | NAG  | O4-C4-C3 | -2.05 | 105.60      | 110.35   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | X     | 2   | NAG  | O7-C7-C8 | -2.05 | 118.25      | 122.06   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

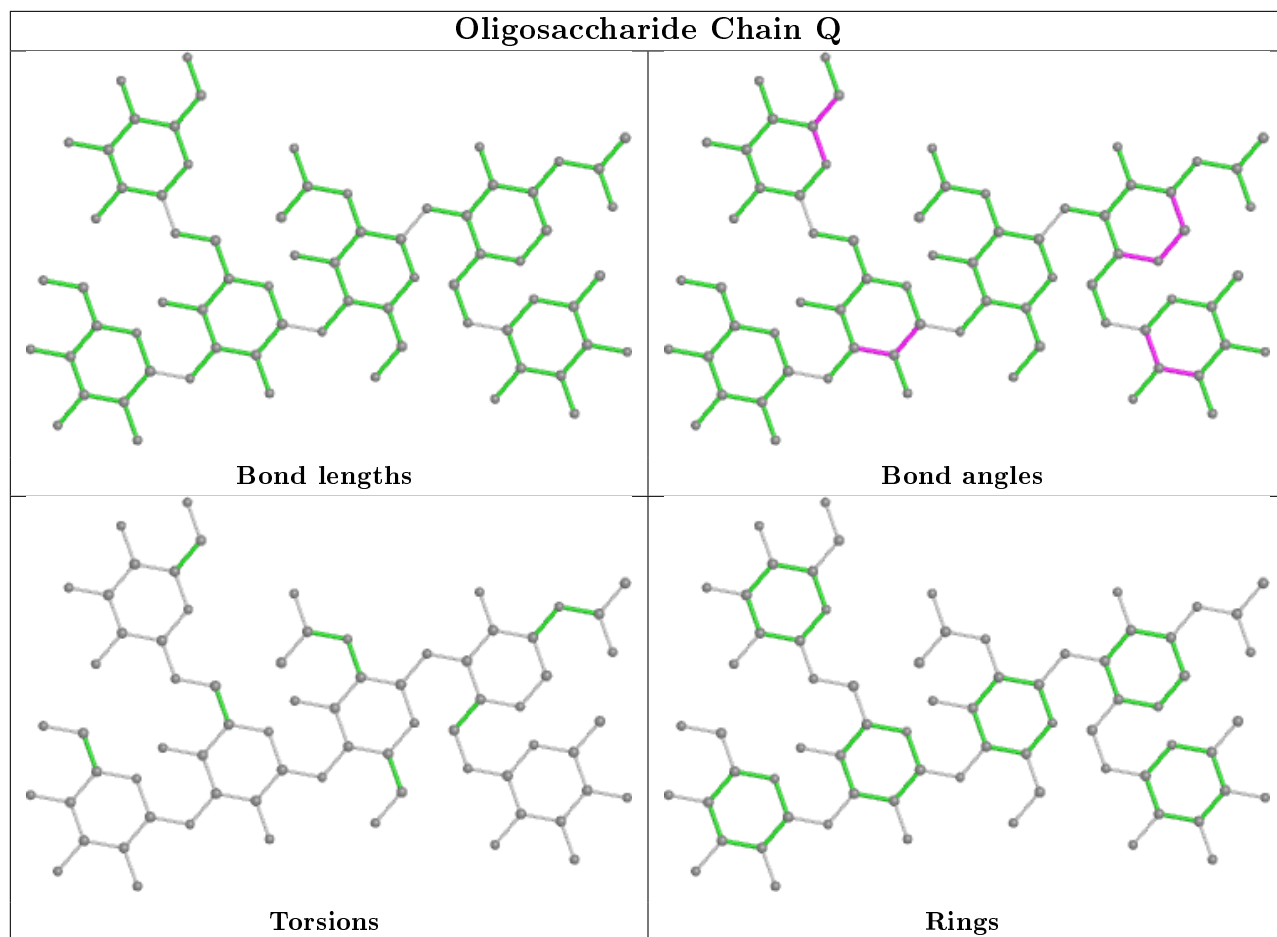
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | Y     | 5   | MAN  | C4-C5-C6-O6 |
| 3   | S     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | W     | 4   | MAN  | O5-C5-C6-O6 |
| 4   | Y     | 5   | MAN  | O5-C5-C6-O6 |
| 4   | Y     | 4   | MAN  | C4-C5-C6-O6 |
| 3   | S     | 4   | MAN  | C4-C5-C6-O6 |
| 3   | W     | 4   | MAN  | C4-C5-C6-O6 |
| 3   | V     | 4   | MAN  | C4-C5-C6-O6 |
| 4   | Y     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | U     | 5   | MAN  | C4-C5-C6-O6 |
| 3   | U     | 5   | MAN  | O5-C5-C6-O6 |
| 3   | U     | 4   | MAN  | C4-C5-C6-O6 |
| 3   | V     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | R     | 4   | MAN  | C4-C5-C6-O6 |
| 3   | T     | 4   | MAN  | C4-C5-C6-O6 |
| 3   | T     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | R     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | U     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | T     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | S     | 5   | MAN  | C4-C5-C6-O6 |

There are no ring outliers.

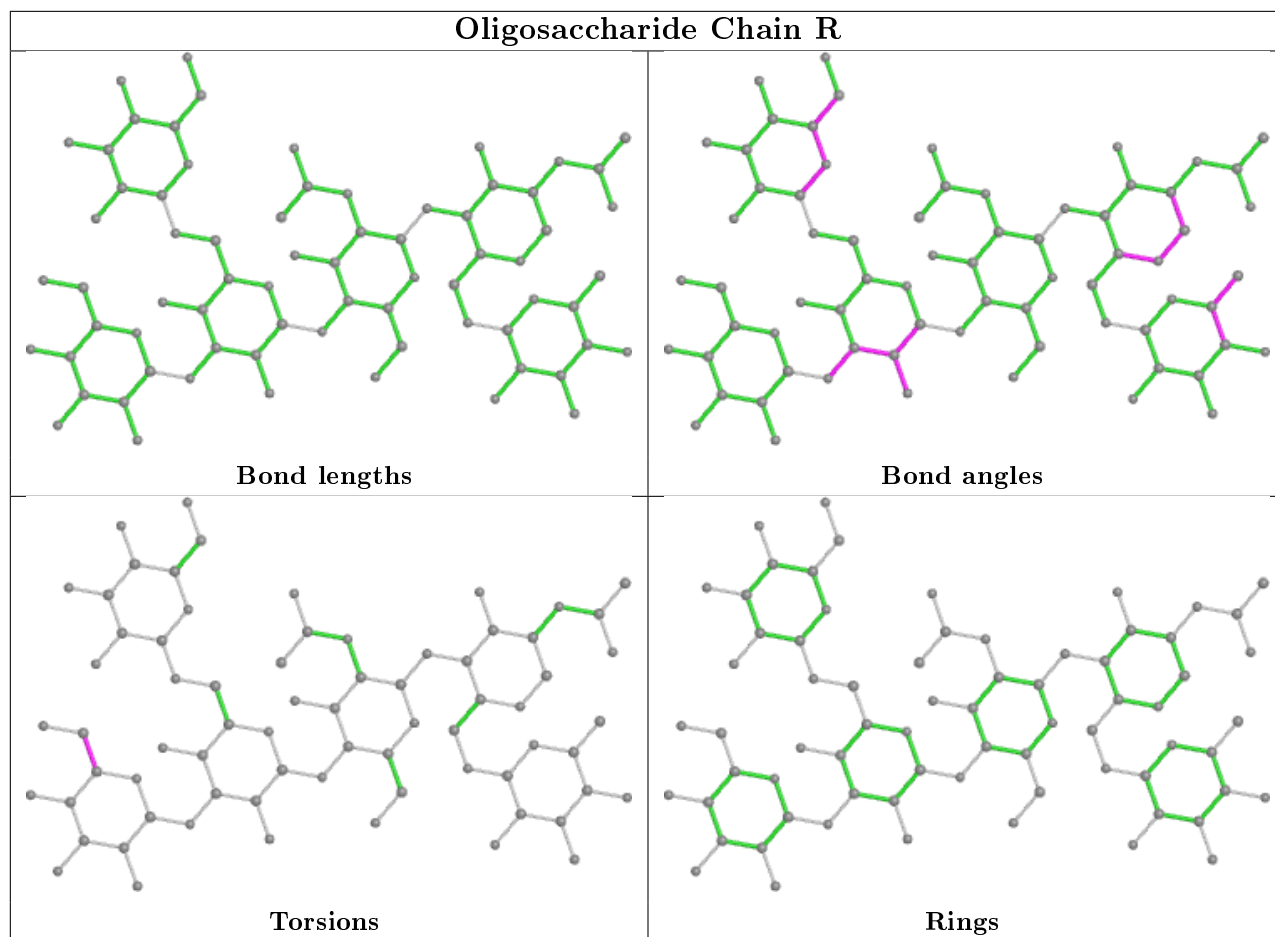
4 monomers are involved in 5 short contacts:

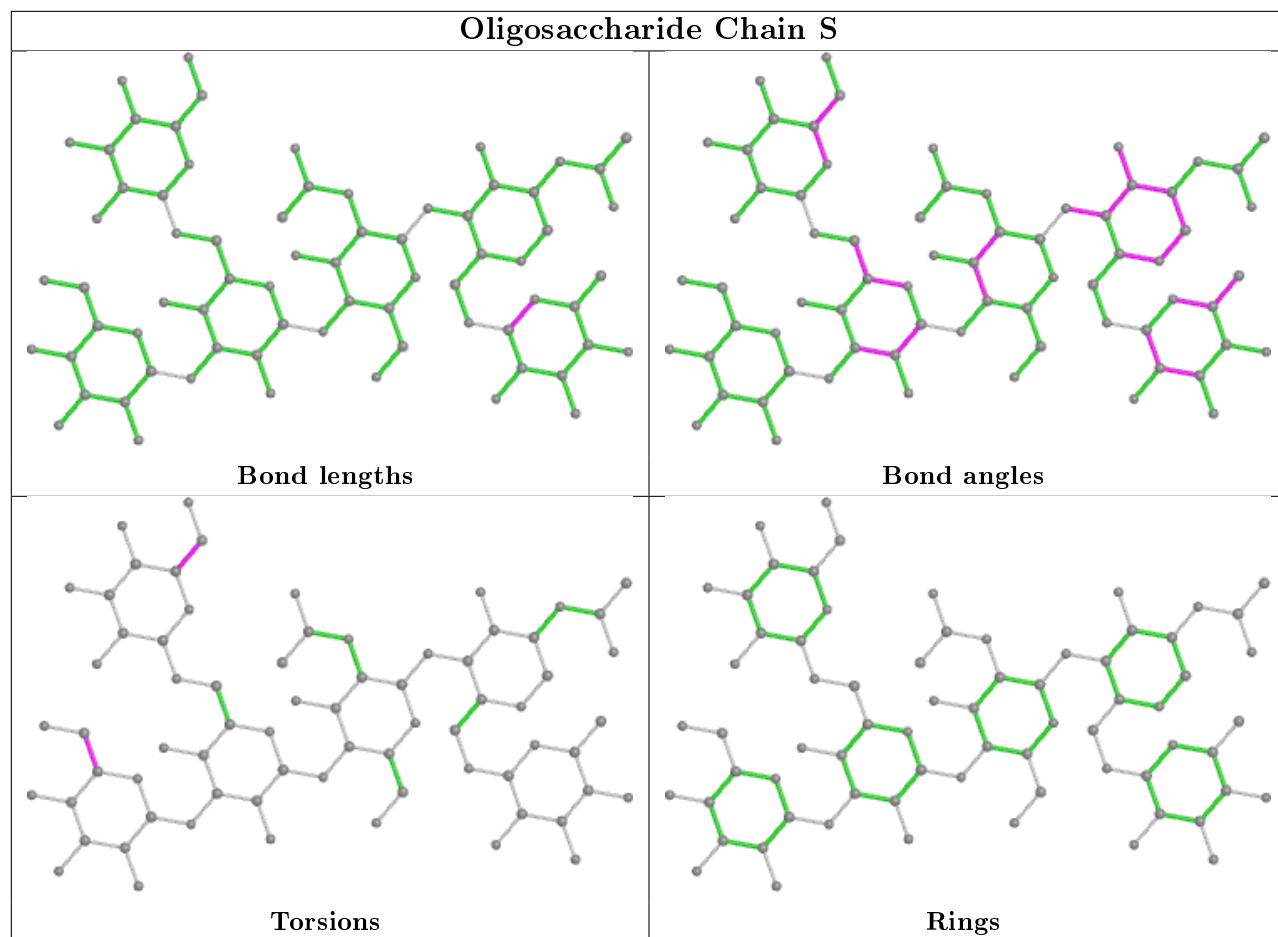
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | X     | 4   | MAN  | 2       | 0            |
| 3   | W     | 4   | MAN  | 1       | 0            |
| 3   | Q     | 6   | FUC  | 1       | 0            |
| 3   | T     | 4   | MAN  | 1       | 0            |

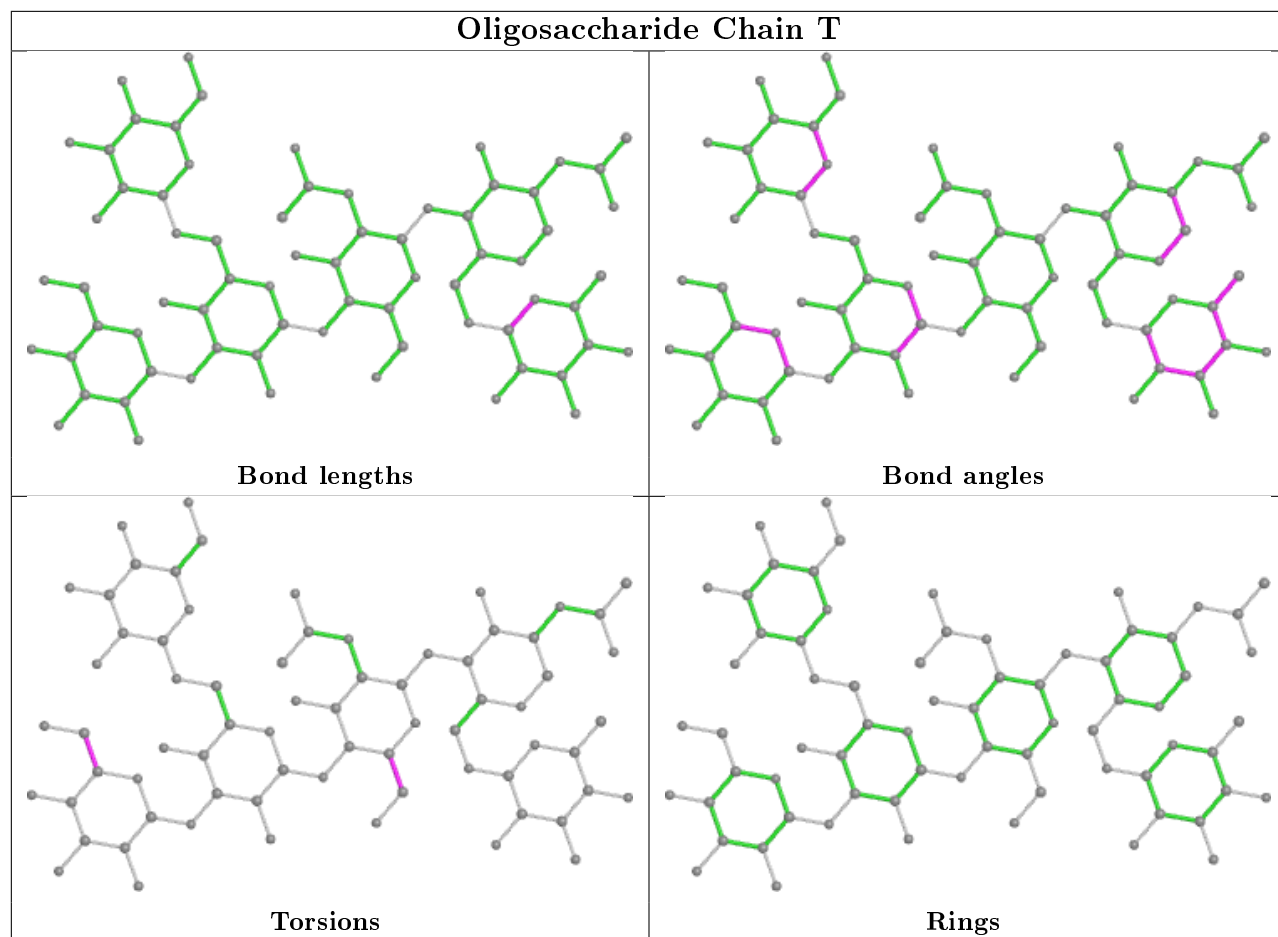
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

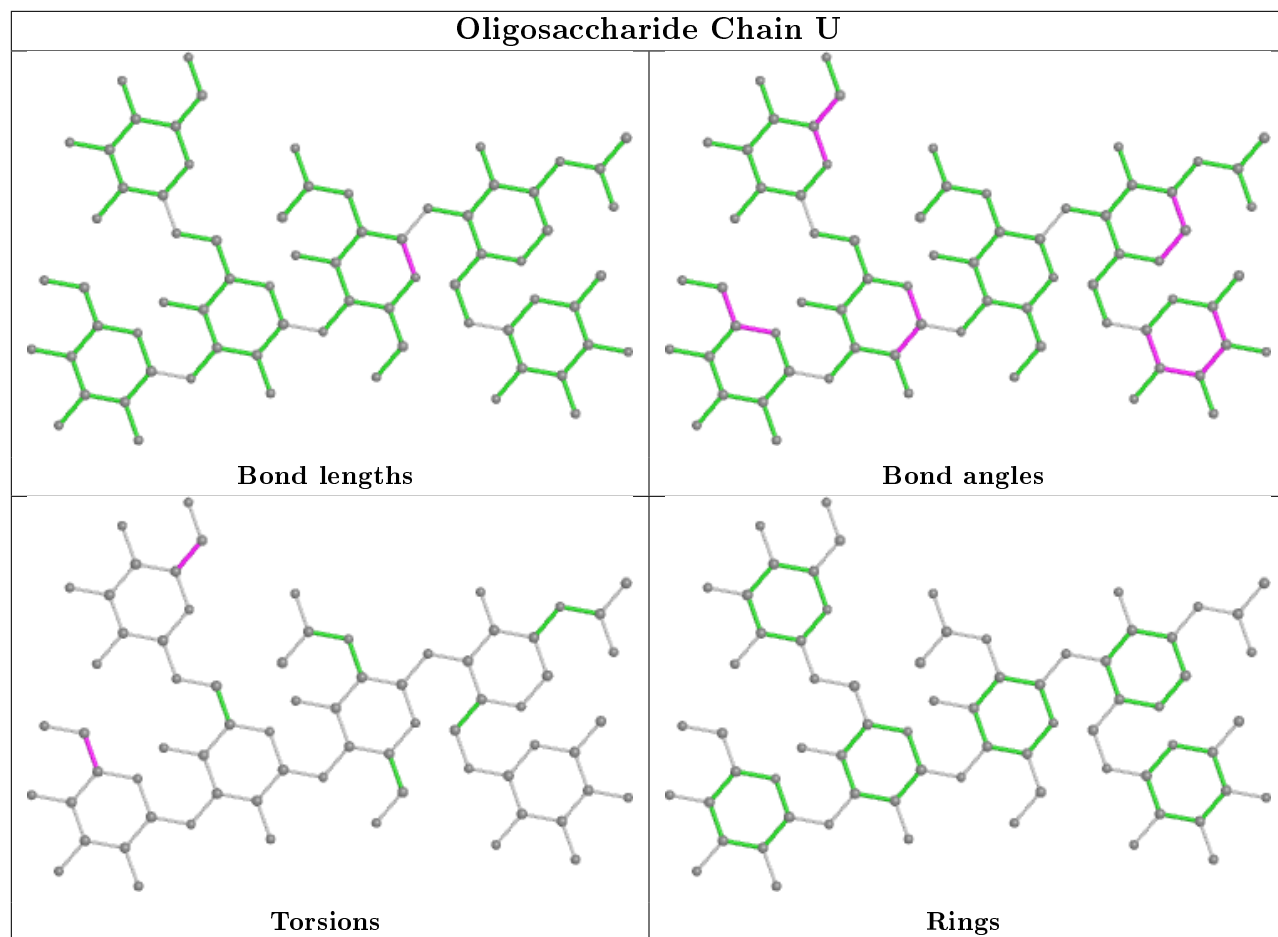


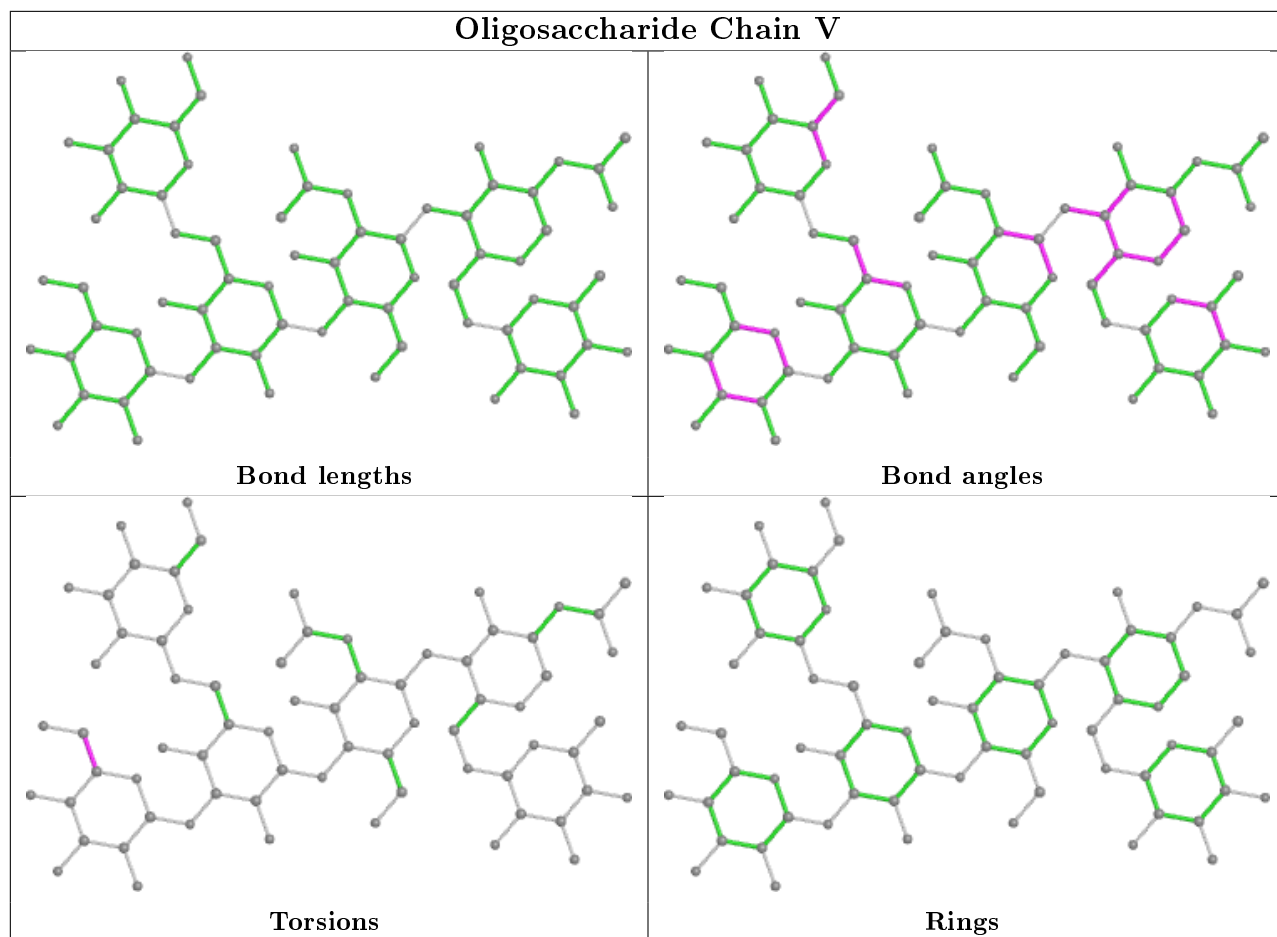


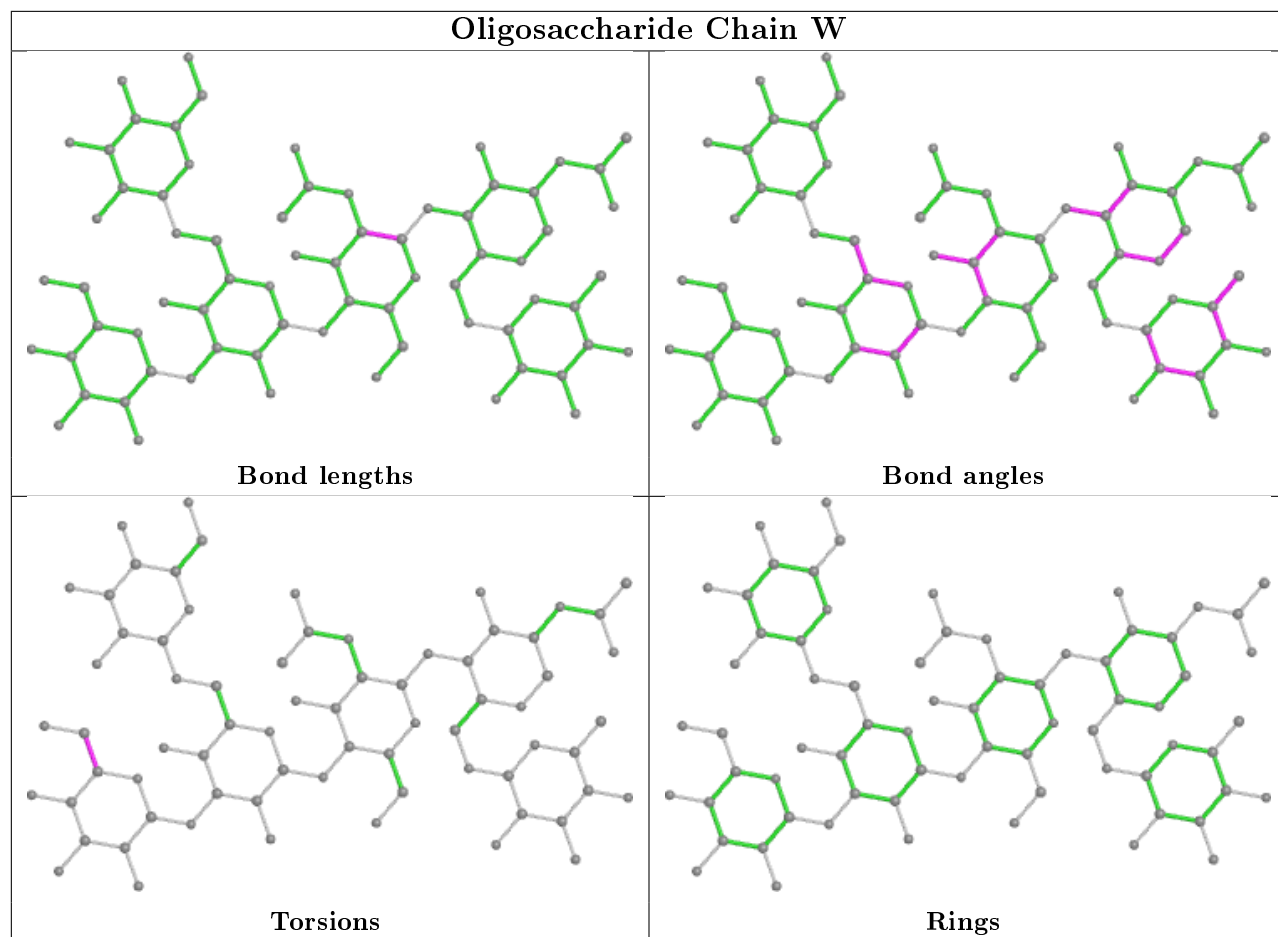


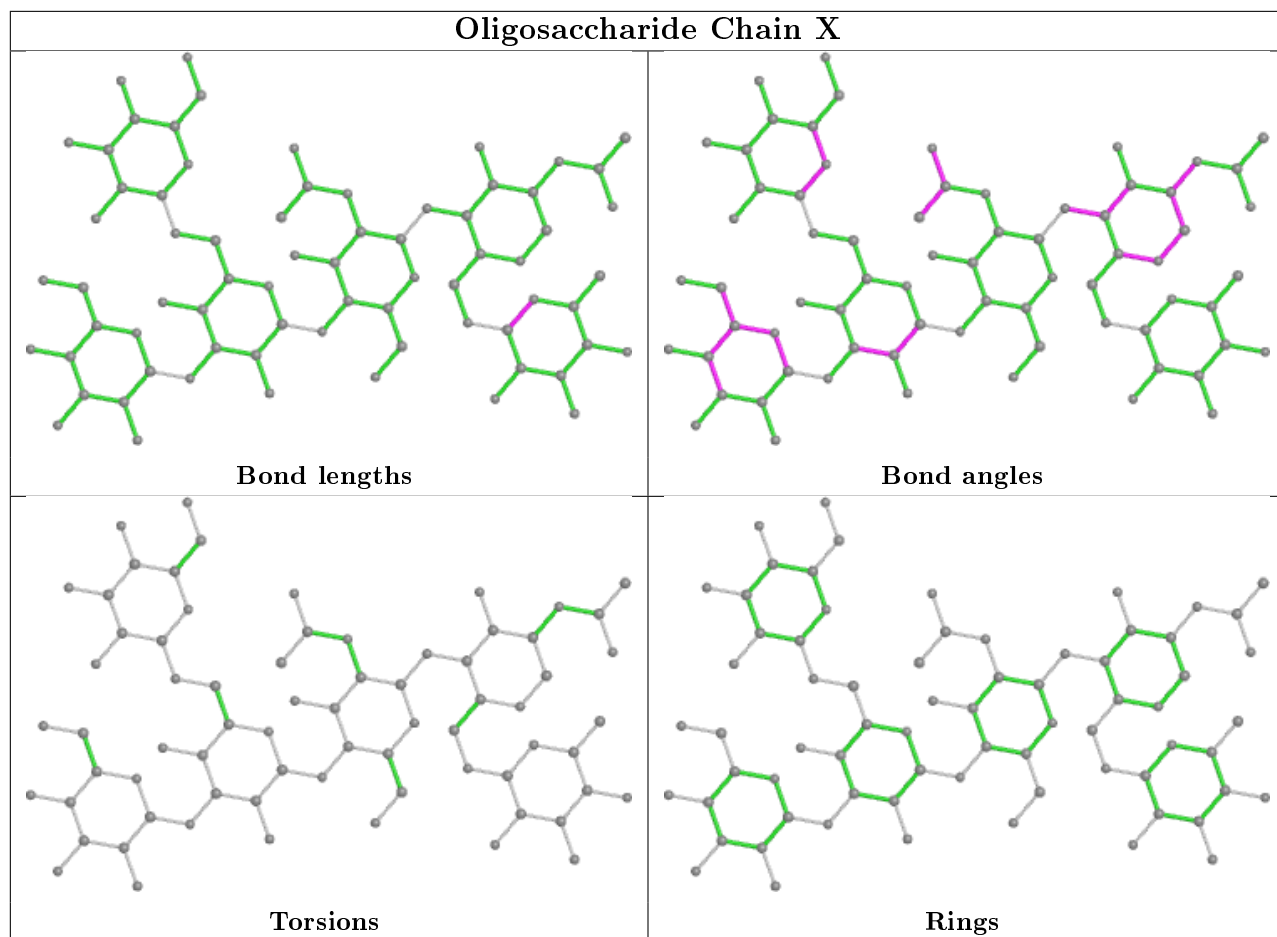


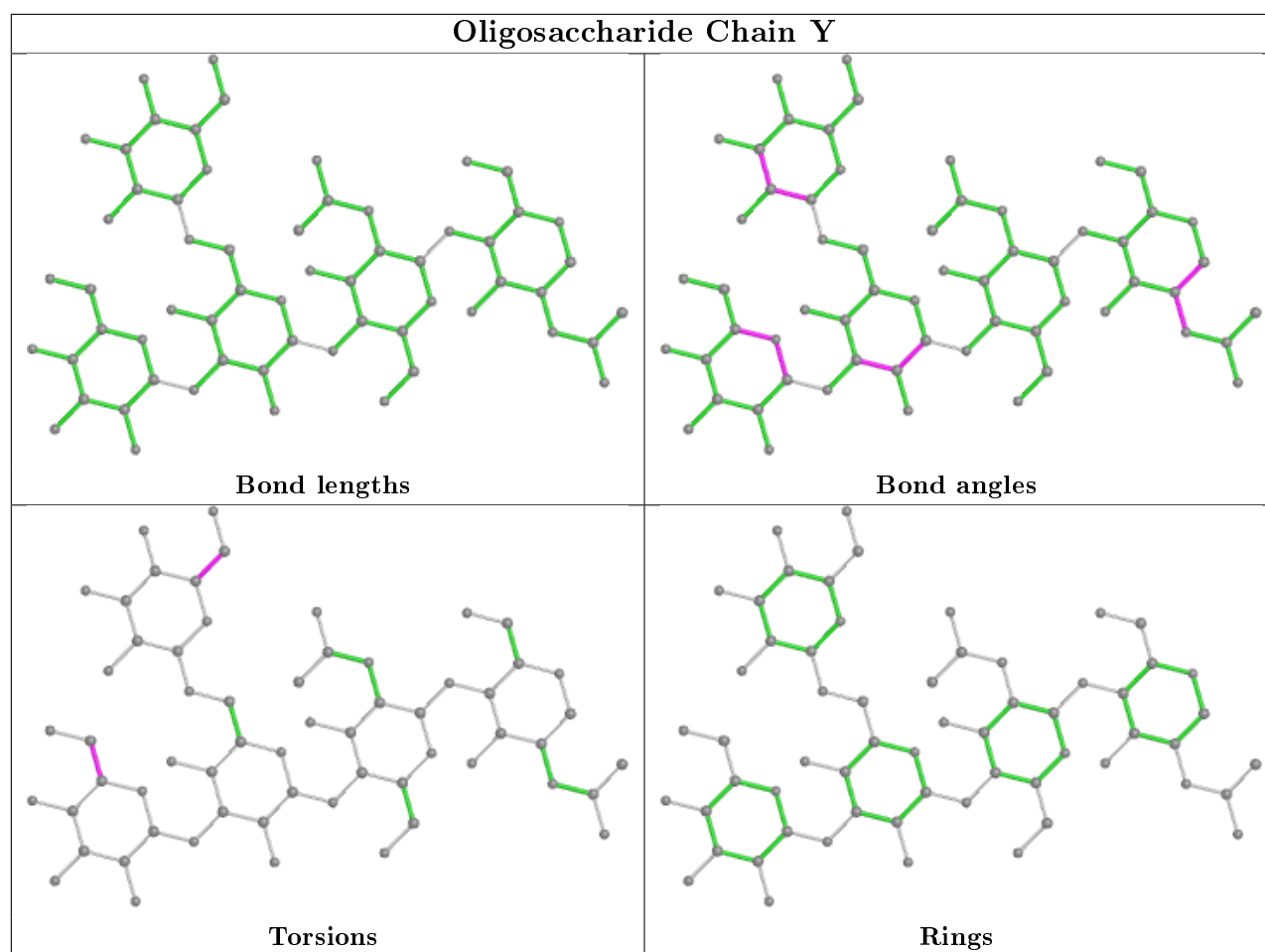












## 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 16 are monoatomic - leaving 31 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |       | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 7   | HEM  | J     | 202  | 1,2,6 | 27,50,50     | 2.08 | 5 (18%)     | 17,82,82    | 1.69 | 6 (35%)     |
| 7   | HEM  | C     | 601  | 1,2,6 | 27,50,50     | 2.15 | 6 (22%)     | 17,82,82    | 1.49 | 4 (23%)     |
| 7   | HEM  | E     | 1602 | 1,2,6 | 27,50,50     | 2.19 | 6 (22%)     | 17,82,82    | 1.45 | 2 (11%)     |
| 8   | NAG  | O     | 608  | 2     | 14,14,15     | 0.50 | 0           | 17,19,21    | 0.87 | 1 (5%)      |
| 8   | NAG  | P     | 608  | 2     | 14,14,15     | 0.49 | 0           | 17,19,21    | 1.05 | 1 (5%)      |



| Mol | Type | Chain | Res  | Link     | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|----------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |          | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | OKY  | P     | 614  | 7        | 10,18,18     | 2.46 | 4 (40%)  | 8,25,25     | 3.65 | 4 (50%)  |
| 7   | HEM  | N     | 202  | 1,2,6    | 27,50,50     | 2.17 | 6 (22%)  | 17,82,82    | 1.56 | 5 (29%)  |
| 8   | NAG  | L     | 607  | 2        | 14,14,15     | 0.45 | 0        | 17,19,21    | 1.46 | 2 (11%)  |
| 8   | NAG  | G     | 608  | 2        | 14,14,15     | 0.63 | 0        | 17,19,21    | 0.75 | 0        |
| 6   | OKY  | H     | 610  | 7        | 10,18,18     | 2.50 | 4 (40%)  | 8,25,25     | 3.62 | 5 (62%)  |
| 6   | OKY  | J     | 203  | 7        | 10,18,18     | 2.50 | 4 (40%)  | 8,25,25     | 3.48 | 4 (50%)  |
| 6   | OKY  | B     | 203  | 7        | 10,18,18     | 2.43 | 4 (40%)  | 8,25,25     | 3.50 | 4 (50%)  |
| 8   | NAG  | D     | 607  | 2        | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.98 | 1 (5%)   |
| 8   | NAG  | C     | 609  | 2        | 14,14,15     | 0.62 | 0        | 17,19,21    | 1.18 | 1 (5%)   |
| 7   | HEM  | F     | 202  | 1,2,6    | 27,50,50     | 2.17 | 7 (25%)  | 17,82,82    | 1.47 | 4 (23%)  |
| 8   | NAG  | C     | 608  | 2        | 14,14,15     | 0.56 | 0        | 17,19,21    | 1.15 | 1 (5%)   |
| 6   | OKY  | G     | 610  | 7        | 10,18,18     | 2.39 | 4 (40%)  | 8,25,25     | 3.32 | 4 (50%)  |
| 6   | OKY  | A     | 1602 | 7        | 10,18,18     | 2.50 | 4 (40%)  | 8,25,25     | 3.59 | 5 (62%)  |
| 7   | HEM  | I     | 1602 | 1,10,2,6 | 27,50,50     | 2.08 | 6 (22%)  | 17,82,82    | 1.50 | 4 (23%)  |
| 6   | OKY  | O     | 610  | 7        | 10,18,18     | 2.52 | 4 (40%)  | 8,25,25     | 3.71 | 5 (62%)  |
| 8   | NAG  | D     | 608  | 2        | 14,14,15     | 0.56 | 0        | 17,19,21    | 0.97 | 0        |
| 7   | HEM  | M     | 1602 | 1,2,6    | 27,50,50     | 2.13 | 7 (25%)  | 17,82,82    | 1.31 | 3 (17%)  |
| 8   | NAG  | K     | 607  | 2        | 14,14,15     | 0.63 | 0        | 17,19,21    | 1.19 | 1 (5%)   |
| 8   | NAG  | K     | 608  | 2        | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.98 | 1 (5%)   |
| 8   | NAG  | H     | 608  | 2        | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.67 | 0        |
| 8   | NAG  | L     | 608  | 2        | 14,14,15     | 0.71 | 0        | 17,19,21    | 1.08 | 1 (5%)   |
| 7   | HEM  | B     | 202  | 1,10,2,6 | 27,50,50     | 2.19 | 8 (29%)  | 17,82,82    | 1.29 | 1 (5%)   |
| 6   | OKY  | I     | 1603 | 7        | 10,18,18     | 2.41 | 4 (40%)  | 8,25,25     | 3.56 | 5 (62%)  |
| 8   | NAG  | H     | 607  | 2        | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.99 | 0        |
| 8   | NAG  | G     | 607  | 2        | 14,14,15     | 0.61 | 0        | 17,19,21    | 0.85 | 0        |
| 8   | NAG  | O     | 607  | 2        | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.79 | 0        |

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   |
|-----|------|-------|------|-------|---------|-----------|---------|
| 7   | HEM  | J     | 202  | 1,2,6 | -       | 0/6/54/54 | -       |
| 7   | HEM  | C     | 601  | 1,2,6 | -       | 0/6/54/54 | -       |
| 7   | HEM  | E     | 1602 | 1,2,6 | -       | 0/6/54/54 | -       |
| 8   | NAG  | O     | 608  | 2     | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | P     | 608  | 2     | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link     | Chirals | Torsions  | Rings   |
|-----|------|-------|------|----------|---------|-----------|---------|
| 6   | OKY  | P     | 614  | 7        | -       | 2/7/7/7   | 0/2/2/2 |
| 7   | HEM  | N     | 202  | 1,2,6    | -       | 0/6/54/54 | -       |
| 8   | NAG  | L     | 607  | 2        | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | G     | 608  | 2        | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | OKY  | H     | 610  | 7        | -       | 5/7/7/7   | 0/2/2/2 |
| 6   | OKY  | J     | 203  | 7        | -       | 2/7/7/7   | 0/2/2/2 |
| 6   | OKY  | B     | 203  | 7        | -       | 2/7/7/7   | 0/2/2/2 |
| 8   | NAG  | D     | 607  | 2        | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 609  | 2        | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | HEM  | F     | 202  | 1,2,6    | -       | 0/6/54/54 | -       |
| 8   | NAG  | C     | 608  | 2        | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | OKY  | G     | 610  | 7        | -       | 0/7/7/7   | 0/2/2/2 |
| 6   | OKY  | A     | 1602 | 7        | -       | 4/7/7/7   | 0/2/2/2 |
| 7   | HEM  | I     | 1602 | 1,10,2,6 | -       | 0/6/54/54 | -       |
| 6   | OKY  | O     | 610  | 7        | -       | 2/7/7/7   | 0/2/2/2 |
| 8   | NAG  | D     | 608  | 2        | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | HEM  | M     | 1602 | 1,2,6    | -       | 2/6/54/54 | -       |
| 8   | NAG  | K     | 607  | 2        | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | K     | 608  | 2        | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | H     | 608  | 2        | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | L     | 608  | 2        | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | HEM  | B     | 202  | 1,10,2,6 | -       | 0/6/54/54 | -       |
| 6   | OKY  | I     | 1603 | 7        | -       | 3/7/7/7   | 0/2/2/2 |
| 8   | NAG  | H     | 607  | 2        | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | G     | 607  | 2        | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | O     | 607  | 2        | -       | 0/6/23/26 | 0/1/1/1 |

All (83) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | N     | 202  | HEM  | C3D-C2D | 5.33  | 1.53        | 1.37     |
| 7   | E     | 1602 | HEM  | C3B-C2B | -5.30 | 1.33        | 1.40     |
| 7   | F     | 202  | HEM  | C3D-C2D | 5.18  | 1.53        | 1.37     |
| 7   | J     | 202  | HEM  | C3D-C2D | 5.15  | 1.52        | 1.37     |
| 7   | C     | 601  | HEM  | C3D-C2D | 5.14  | 1.52        | 1.37     |
| 7   | I     | 1602 | HEM  | C3B-C2B | -4.96 | 1.33        | 1.40     |
| 7   | F     | 202  | HEM  | C3B-C2B | -4.88 | 1.33        | 1.40     |
| 6   | O     | 610  | OKY  | O2-C8   | 4.87  | 1.36        | 1.24     |
| 6   | P     | 614  | OKY  | O2-C8   | 4.86  | 1.36        | 1.24     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 7   | C     | 601  | HEM  | C3B-C2B | -4.85 | 1.33        | 1.40     |
| 6   | A     | 1602 | 0KY  | O2-C8   | 4.83  | 1.36        | 1.24     |
| 7   | M     | 1602 | HEM  | C3D-C2D | 4.83  | 1.52        | 1.37     |
| 6   | H     | 610  | 0KY  | O2-C8   | 4.81  | 1.36        | 1.24     |
| 7   | I     | 1602 | HEM  | C3D-C2D | 4.77  | 1.51        | 1.37     |
| 7   | E     | 1602 | HEM  | C3C-C2C | -4.75 | 1.33        | 1.40     |
| 6   | J     | 203  | 0KY  | O2-C8   | 4.75  | 1.36        | 1.24     |
| 6   | J     | 203  | 0KY  | C8-C7   | 4.70  | 1.49        | 1.41     |
| 6   | I     | 1603 | 0KY  | O2-C8   | 4.69  | 1.36        | 1.24     |
| 6   | B     | 203  | 0KY  | O2-C8   | 4.68  | 1.36        | 1.24     |
| 7   | B     | 202  | HEM  | C3D-C2D | 4.68  | 1.51        | 1.37     |
| 6   | G     | 610  | 0KY  | O2-C8   | 4.59  | 1.36        | 1.24     |
| 6   | A     | 1602 | 0KY  | C8-C7   | 4.55  | 1.49        | 1.41     |
| 6   | H     | 610  | 0KY  | C8-C7   | 4.48  | 1.49        | 1.41     |
| 6   | O     | 610  | 0KY  | C8-C7   | 4.46  | 1.49        | 1.41     |
| 6   | I     | 1603 | 0KY  | C8-C7   | 4.46  | 1.49        | 1.41     |
| 7   | E     | 1602 | HEM  | C3D-C2D | 4.43  | 1.50        | 1.37     |
| 6   | B     | 203  | 0KY  | C8-C7   | 4.42  | 1.49        | 1.41     |
| 7   | N     | 202  | HEM  | C3C-C2C | -4.39 | 1.34        | 1.40     |
| 7   | J     | 202  | HEM  | C3B-C2B | -4.36 | 1.34        | 1.40     |
| 7   | B     | 202  | HEM  | C3C-C2C | -4.33 | 1.34        | 1.40     |
| 6   | P     | 614  | 0KY  | C8-C7   | 4.31  | 1.48        | 1.41     |
| 7   | B     | 202  | HEM  | C3B-C2B | -4.20 | 1.34        | 1.40     |
| 7   | I     | 1602 | HEM  | C3C-C2C | -4.15 | 1.34        | 1.40     |
| 6   | G     | 610  | 0KY  | C8-C7   | 4.14  | 1.48        | 1.41     |
| 7   | C     | 601  | HEM  | C3C-C2C | -4.14 | 1.34        | 1.40     |
| 7   | M     | 1602 | HEM  | C3B-C2B | -4.00 | 1.34        | 1.40     |
| 7   | N     | 202  | HEM  | C3B-C2B | -3.97 | 1.34        | 1.40     |
| 7   | F     | 202  | HEM  | C3C-C2C | -3.97 | 1.34        | 1.40     |
| 7   | E     | 1602 | HEM  | C3B-CAB | 3.95  | 1.56        | 1.47     |
| 7   | B     | 202  | HEM  | C3B-CAB | 3.94  | 1.56        | 1.47     |
| 7   | M     | 1602 | HEM  | C3B-CAB | 3.93  | 1.55        | 1.47     |
| 7   | M     | 1602 | HEM  | C3C-C2C | -3.85 | 1.35        | 1.40     |
| 7   | C     | 601  | HEM  | C3B-CAB | 3.82  | 1.55        | 1.47     |
| 7   | B     | 202  | HEM  | C3C-CAC | 3.82  | 1.55        | 1.47     |
| 7   | N     | 202  | HEM  | C3C-CAC | 3.81  | 1.55        | 1.47     |
| 7   | N     | 202  | HEM  | C3B-CAB | 3.76  | 1.55        | 1.47     |
| 7   | F     | 202  | HEM  | C3B-CAB | 3.70  | 1.55        | 1.47     |
| 7   | J     | 202  | HEM  | C3C-C2C | -3.69 | 1.35        | 1.40     |
| 7   | J     | 202  | HEM  | C3C-CAC | 3.60  | 1.55        | 1.47     |
| 7   | J     | 202  | HEM  | C3B-CAB | 3.59  | 1.55        | 1.47     |
| 7   | I     | 1602 | HEM  | C3B-CAB | 3.59  | 1.55        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 7   | M     | 1602 | HEM  | C3C-CAC | 3.27 | 1.54        | 1.47     |
| 7   | F     | 202  | HEM  | CAA-C2A | 3.17 | 1.56        | 1.52     |
| 6   | O     | 610  | OKY  | C9-S    | 3.15 | 1.73        | 1.66     |
| 6   | J     | 203  | OKY  | C9-S    | 3.11 | 1.73        | 1.66     |
| 6   | P     | 614  | OKY  | C9-S    | 3.10 | 1.73        | 1.66     |
| 7   | I     | 1602 | HEM  | C3C-CAC | 3.08 | 1.54        | 1.47     |
| 7   | C     | 601  | HEM  | C3C-CAC | 3.06 | 1.54        | 1.47     |
| 6   | B     | 203  | OKY  | C9-S    | 3.04 | 1.73        | 1.66     |
| 7   | F     | 202  | HEM  | C3C-CAC | 2.92 | 1.53        | 1.47     |
| 6   | G     | 610  | OKY  | C9-S    | 2.92 | 1.72        | 1.66     |
| 6   | H     | 610  | OKY  | C9-S    | 2.89 | 1.72        | 1.66     |
| 7   | E     | 1602 | HEM  | C3C-CAC | 2.80 | 1.53        | 1.47     |
| 6   | A     | 1602 | OKY  | C9-S    | 2.72 | 1.72        | 1.66     |
| 7   | C     | 601  | HEM  | CAA-C2A | 2.71 | 1.56        | 1.52     |
| 7   | B     | 202  | HEM  | CAA-C2A | 2.71 | 1.56        | 1.52     |
| 6   | I     | 1603 | OKY  | C9-S    | 2.58 | 1.72        | 1.66     |
| 6   | A     | 1602 | OKY  | C7-C6   | 2.58 | 1.47        | 1.40     |
| 6   | O     | 610  | OKY  | C7-C6   | 2.54 | 1.47        | 1.40     |
| 7   | M     | 1602 | HEM  | CAA-C2A | 2.53 | 1.55        | 1.52     |
| 6   | I     | 1603 | OKY  | C7-C6   | 2.52 | 1.47        | 1.40     |
| 7   | N     | 202  | HEM  | CAA-C2A | 2.49 | 1.55        | 1.52     |
| 6   | G     | 610  | OKY  | C7-C6   | 2.46 | 1.47        | 1.40     |
| 6   | H     | 610  | OKY  | C7-C6   | 2.46 | 1.47        | 1.40     |
| 7   | I     | 1602 | HEM  | CAA-C2A | 2.40 | 1.55        | 1.52     |
| 7   | M     | 1602 | HEM  | C1D-ND  | 2.37 | 1.41        | 1.36     |
| 6   | P     | 614  | OKY  | C7-C6   | 2.35 | 1.47        | 1.40     |
| 6   | J     | 203  | OKY  | C7-C6   | 2.28 | 1.46        | 1.40     |
| 7   | E     | 1602 | HEM  | CAA-C2A | 2.25 | 1.55        | 1.52     |
| 6   | B     | 203  | OKY  | C7-C6   | 2.23 | 1.46        | 1.40     |
| 7   | F     | 202  | HEM  | C1D-ND  | 2.06 | 1.40        | 1.36     |
| 7   | B     | 202  | HEM  | CMC-C2C | 2.05 | 1.56        | 1.51     |
| 7   | B     | 202  | HEM  | CAD-C3D | 2.04 | 1.55        | 1.52     |

All (75) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 6   | O     | 610  | OKY  | C9-N2-C8 | 7.33 | 123.43      | 115.93   |
| 6   | P     | 614  | OKY  | C9-N2-C8 | 7.22 | 123.31      | 115.93   |
| 6   | B     | 203  | OKY  | C9-N2-C8 | 6.86 | 122.94      | 115.93   |
| 6   | A     | 1602 | OKY  | C9-N2-C8 | 6.77 | 122.86      | 115.93   |
| 6   | I     | 1603 | OKY  | C9-N2-C8 | 6.74 | 122.83      | 115.93   |
| 6   | H     | 610  | OKY  | C9-N2-C8 | 6.64 | 122.72      | 115.93   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | J     | 203  | OKY  | C9-N2-C8    | 6.59  | 122.67      | 115.93   |
| 6   | G     | 610  | OKY  | C9-N2-C8    | 6.32  | 122.39      | 115.93   |
| 6   | O     | 610  | OKY  | C7-C8-N2    | -4.53 | 117.23      | 123.43   |
| 6   | A     | 1602 | OKY  | C7-C8-N2    | -4.45 | 117.34      | 123.43   |
| 6   | P     | 614  | OKY  | C7-C8-N2    | -4.43 | 117.38      | 123.43   |
| 6   | I     | 1603 | OKY  | C7-C8-N2    | -4.39 | 117.42      | 123.43   |
| 6   | J     | 203  | OKY  | C6-C7-N3    | -4.13 | 105.10      | 109.40   |
| 6   | G     | 610  | OKY  | C7-C8-N2    | -4.13 | 117.79      | 123.43   |
| 6   | H     | 610  | OKY  | C8-C7-C6    | -4.12 | 116.87      | 120.80   |
| 6   | B     | 203  | OKY  | C8-C7-C6    | -4.06 | 116.92      | 120.80   |
| 6   | B     | 203  | OKY  | C7-C8-N2    | -4.05 | 117.89      | 123.43   |
| 6   | J     | 203  | OKY  | C7-C8-N2    | -4.01 | 117.95      | 123.43   |
| 6   | H     | 610  | OKY  | C7-C8-N2    | -3.98 | 117.98      | 123.43   |
| 6   | P     | 614  | OKY  | C8-C7-C6    | -3.97 | 117.00      | 120.80   |
| 6   | P     | 614  | OKY  | C6-C7-N3    | -3.93 | 105.31      | 109.40   |
| 6   | B     | 203  | OKY  | C6-C7-N3    | -3.92 | 105.31      | 109.40   |
| 6   | J     | 203  | OKY  | C8-C7-C6    | -3.91 | 117.07      | 120.80   |
| 6   | A     | 1602 | OKY  | C6-C7-N3    | -3.89 | 105.34      | 109.40   |
| 6   | O     | 610  | OKY  | C6-C7-N3    | -3.87 | 105.37      | 109.40   |
| 6   | O     | 610  | OKY  | C8-C7-C6    | -3.81 | 117.16      | 120.80   |
| 6   | G     | 610  | OKY  | C8-C7-C6    | -3.78 | 117.19      | 120.80   |
| 8   | L     | 607  | NAG  | C1-O5-C5    | 3.74  | 117.26      | 112.19   |
| 6   | I     | 1603 | OKY  | C8-C7-C6    | -3.73 | 117.23      | 120.80   |
| 6   | H     | 610  | OKY  | C5-N1-C6    | 3.72  | 121.74      | 118.41   |
| 6   | I     | 1603 | OKY  | C6-C7-N3    | -3.71 | 105.53      | 109.40   |
| 6   | G     | 610  | OKY  | C6-C7-N3    | -3.65 | 105.60      | 109.40   |
| 6   | A     | 1602 | OKY  | C8-C7-C6    | -3.60 | 117.36      | 120.80   |
| 6   | H     | 610  | OKY  | C6-C7-N3    | -3.32 | 105.94      | 109.40   |
| 7   | E     | 1602 | HEM  | CMA-C3A-C4A | -3.13 | 123.65      | 128.46   |
| 7   | I     | 1602 | HEM  | CMC-C2C-C3C | 3.05  | 130.39      | 124.68   |
| 7   | C     | 601  | HEM  | CMA-C3A-C4A | -3.02 | 123.82      | 128.46   |
| 7   | J     | 202  | HEM  | CBA-CAA-C2A | -2.87 | 107.19      | 112.49   |
| 7   | F     | 202  | HEM  | CMC-C2C-C3C | 2.79  | 129.90      | 124.68   |
| 7   | E     | 1602 | HEM  | CBA-CAA-C2A | -2.78 | 107.36      | 112.49   |
| 7   | F     | 202  | HEM  | CMA-C3A-C4A | -2.71 | 124.30      | 128.46   |
| 6   | I     | 1603 | OKY  | C5-N1-C6    | 2.56  | 120.70      | 118.41   |
| 7   | N     | 202  | HEM  | CBD-CAD-C3D | -2.54 | 107.80      | 112.48   |
| 7   | M     | 1602 | HEM  | CMB-C2B-C3B | 2.49  | 129.34      | 124.68   |
| 7   | I     | 1602 | HEM  | C3C-C4C-NC  | -2.45 | 106.31      | 110.94   |
| 7   | N     | 202  | HEM  | CBA-CAA-C2A | -2.42 | 108.02      | 112.49   |
| 8   | C     | 608  | NAG  | C1-O5-C5    | 2.42  | 115.47      | 112.19   |
| 7   | C     | 601  | HEM  | C4A-C3A-C2A | 2.41  | 108.67      | 107.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | F     | 202  | HEM  | C4A-C3A-C2A | 2.40  | 108.67      | 107.00   |
| 7   | J     | 202  | HEM  | CMA-C3A-C4A | -2.40 | 124.78      | 128.46   |
| 6   | A     | 1602 | 0KY  | C5-N1-C6    | 2.35  | 120.51      | 118.41   |
| 7   | N     | 202  | HEM  | C4A-C3A-C2A | 2.32  | 108.61      | 107.00   |
| 7   | N     | 202  | HEM  | CAD-CBD-CGD | -2.32 | 108.78      | 112.67   |
| 7   | B     | 202  | HEM  | CMA-C3A-C4A | -2.31 | 124.92      | 128.46   |
| 7   | J     | 202  | HEM  | C3C-C4C-NC  | -2.28 | 106.63      | 110.94   |
| 8   | C     | 609  | NAG  | O7-C7-C8    | -2.27 | 117.85      | 122.06   |
| 7   | J     | 202  | HEM  | CMC-C2C-C3C | 2.26  | 128.91      | 124.68   |
| 7   | J     | 202  | HEM  | C4C-C3C-C2C | 2.26  | 108.48      | 106.90   |
| 8   | D     | 607  | NAG  | O4-C4-C5    | 2.21  | 114.80      | 109.30   |
| 7   | I     | 1602 | HEM  | CAD-CBD-CGD | -2.21 | 108.95      | 112.67   |
| 7   | I     | 1602 | HEM  | CMA-C3A-C4A | -2.20 | 125.09      | 128.46   |
| 8   | P     | 608  | NAG  | C3-C4-C5    | -2.18 | 106.35      | 110.24   |
| 7   | F     | 202  | HEM  | C3C-C4C-NC  | -2.18 | 106.83      | 110.94   |
| 7   | M     | 1602 | HEM  | C4C-C3C-C2C | 2.17  | 108.41      | 106.90   |
| 8   | L     | 608  | NAG  | O5-C5-C4    | -2.14 | 105.61      | 110.83   |
| 7   | N     | 202  | HEM  | C1D-C2D-C3D | -2.14 | 105.51      | 107.00   |
| 7   | J     | 202  | HEM  | CBD-CAD-C3D | -2.10 | 108.60      | 112.48   |
| 6   | O     | 610  | 0KY  | C5-N1-C6    | 2.05  | 120.25      | 118.41   |
| 8   | K     | 607  | NAG  | O7-C7-C8    | -2.05 | 118.25      | 122.06   |
| 8   | K     | 608  | NAG  | O7-C7-C8    | -2.04 | 118.28      | 122.06   |
| 8   | L     | 607  | NAG  | O5-C1-C2    | -2.03 | 108.08      | 111.29   |
| 7   | C     | 601  | HEM  | CAD-CBD-CGD | -2.01 | 109.29      | 112.67   |
| 8   | O     | 608  | NAG  | O5-C5-C6    | 2.01  | 110.36      | 107.20   |
| 7   | M     | 1602 | HEM  | CAD-CBD-CGD | -2.01 | 109.30      | 112.67   |
| 7   | C     | 601  | HEM  | CMB-C2B-C3B | 2.00  | 128.42      | 124.68   |

There are no chirality outliers.

All (37) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 6   | H     | 610  | 0KY  | C3-C5-N1-C9 |
| 6   | H     | 610  | 0KY  | C3-C5-N1-C6 |
| 6   | H     | 610  | 0KY  | O1-C3-C5-N1 |
| 6   | H     | 610  | 0KY  | C1-C2-O1-C3 |
| 6   | J     | 203  | 0KY  | C4-C3-C5-N1 |
| 6   | B     | 203  | 0KY  | O1-C3-C5-N1 |
| 6   | A     | 1602 | 0KY  | C3-C5-N1-C9 |
| 6   | A     | 1602 | 0KY  | C3-C5-N1-C6 |
| 6   | O     | 610  | 0KY  | O1-C3-C5-N1 |
| 6   | O     | 610  | 0KY  | C4-C3-C5-N1 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | I     | 1603 | 0KY  | C3-C5-N1-C9     |
| 6   | I     | 1603 | 0KY  | O1-C3-C5-N1     |
| 8   | G     | 608  | NAG  | C1-C2-N2-C7     |
| 8   | C     | 609  | NAG  | O5-C5-C6-O6     |
| 8   | O     | 608  | NAG  | O5-C5-C6-O6     |
| 8   | C     | 609  | NAG  | C4-C5-C6-O6     |
| 8   | L     | 608  | NAG  | C4-C5-C6-O6     |
| 6   | P     | 614  | 0KY  | C1-C2-O1-C3     |
| 8   | O     | 608  | NAG  | C4-C5-C6-O6     |
| 8   | P     | 608  | NAG  | C4-C5-C6-O6     |
| 8   | L     | 608  | NAG  | O5-C5-C6-O6     |
| 8   | L     | 607  | NAG  | C4-C5-C6-O6     |
| 8   | L     | 607  | NAG  | O5-C5-C6-O6     |
| 8   | P     | 608  | NAG  | O5-C5-C6-O6     |
| 8   | K     | 608  | NAG  | C4-C5-C6-O6     |
| 6   | H     | 610  | 0KY  | C4-C3-C5-N1     |
| 6   | B     | 203  | 0KY  | C4-C3-C5-N1     |
| 6   | A     | 1602 | 0KY  | C4-C3-C5-N1     |
| 6   | I     | 1603 | 0KY  | C4-C3-C5-N1     |
| 8   | G     | 608  | NAG  | C3-C2-N2-C7     |
| 6   | J     | 203  | 0KY  | O1-C3-C5-N1     |
| 8   | K     | 608  | NAG  | O5-C5-C6-O6     |
| 7   | M     | 1602 | HEM  | C1A-C2A-CAA-CBA |
| 7   | M     | 1602 | HEM  | C3A-C2A-CAA-CBA |
| 6   | P     | 614  | 0KY  | C4-C3-C5-N1     |
| 6   | A     | 1602 | 0KY  | O1-C3-C5-N1     |
| 8   | D     | 607  | NAG  | C4-C5-C6-O6     |

There are no ring outliers.

18 monomers are involved in 57 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 7   | J     | 202  | HEM  | 5       | 0            |
| 7   | C     | 601  | HEM  | 6       | 0            |
| 7   | E     | 1602 | HEM  | 6       | 0            |
| 6   | P     | 614  | 0KY  | 4       | 0            |
| 7   | N     | 202  | HEM  | 7       | 0            |
| 8   | G     | 608  | NAG  | 2       | 0            |
| 6   | H     | 610  | 0KY  | 5       | 0            |
| 6   | J     | 203  | 0KY  | 1       | 0            |
| 6   | B     | 203  | 0KY  | 4       | 0            |
| 7   | F     | 202  | HEM  | 5       | 0            |

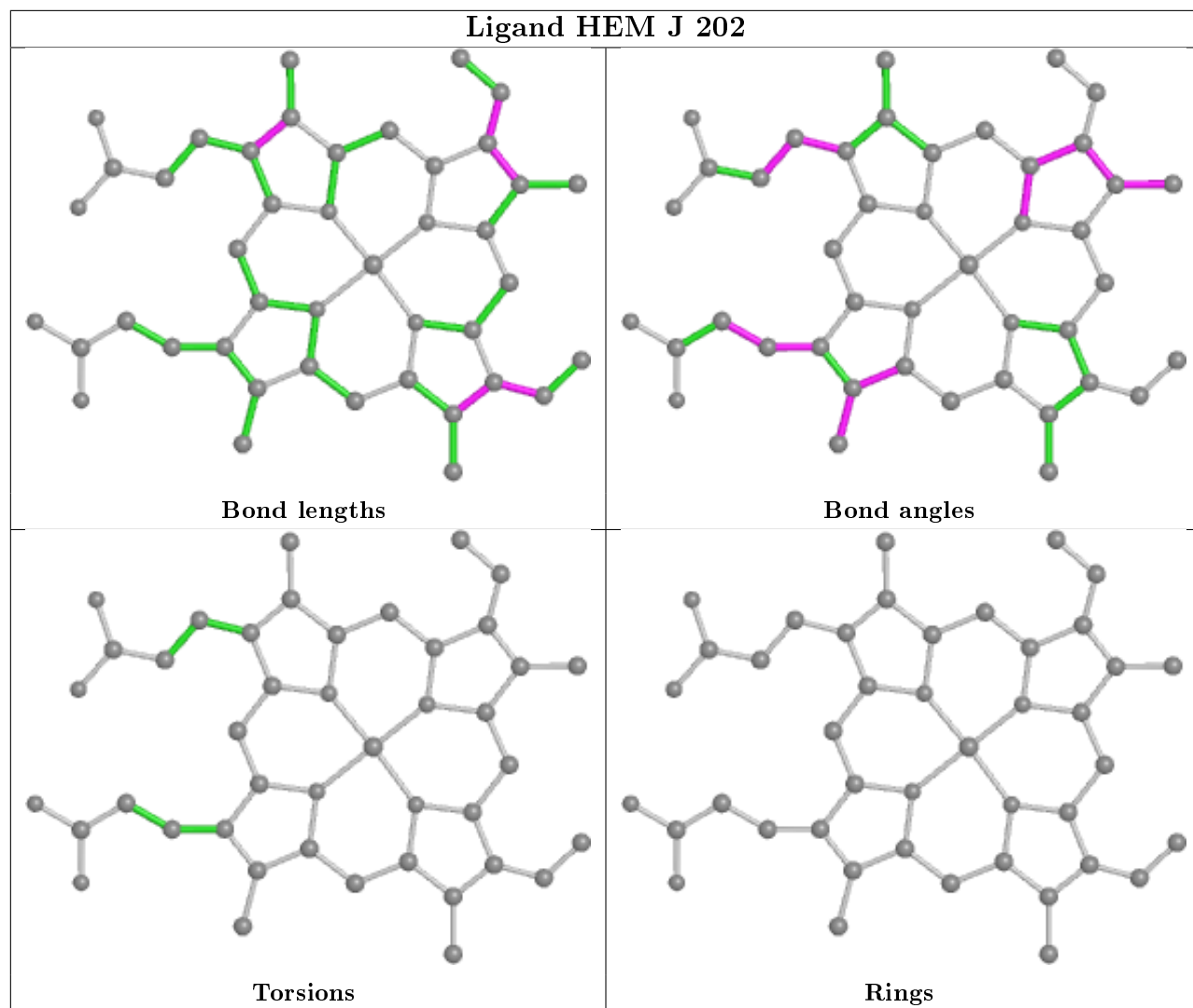
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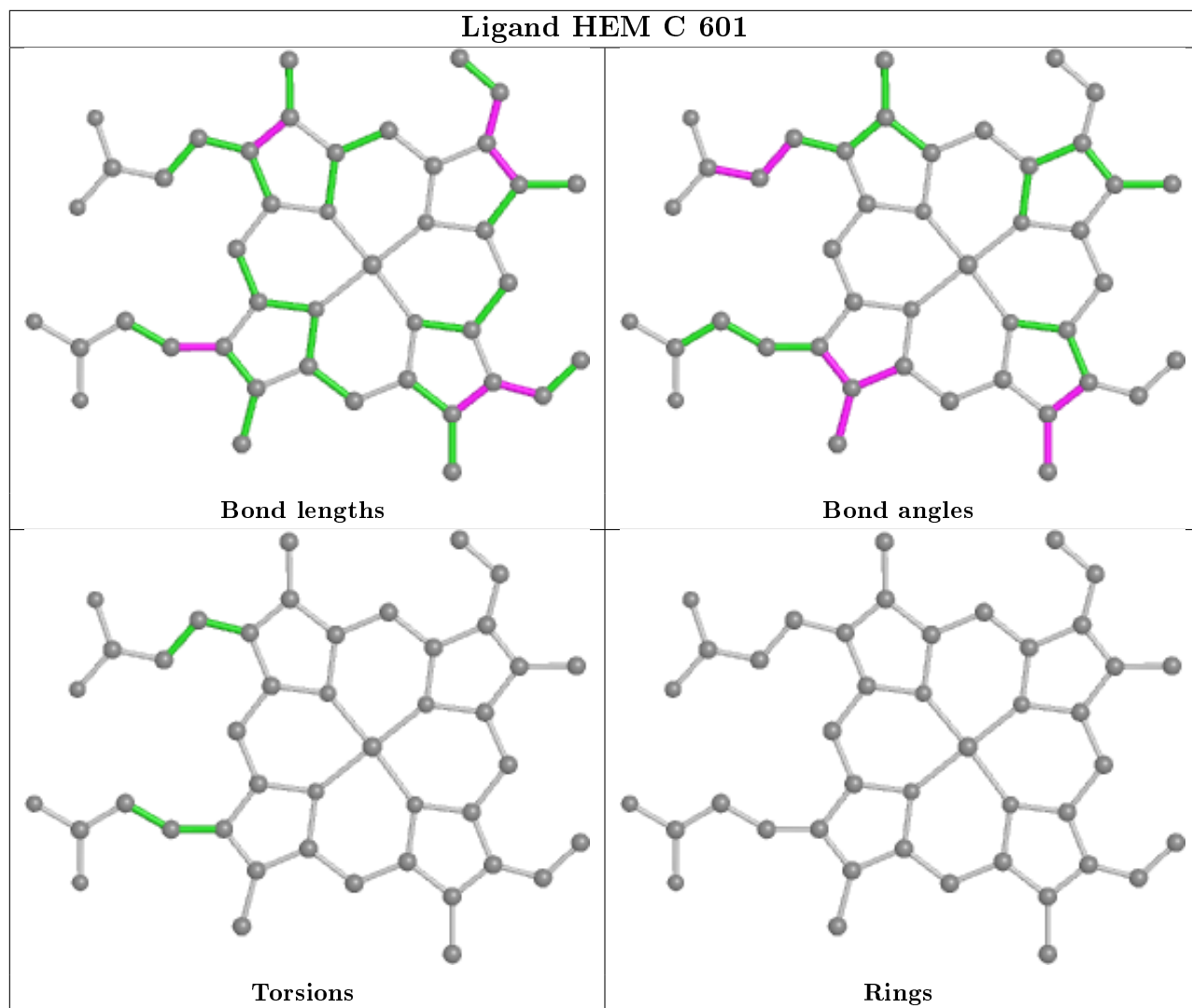
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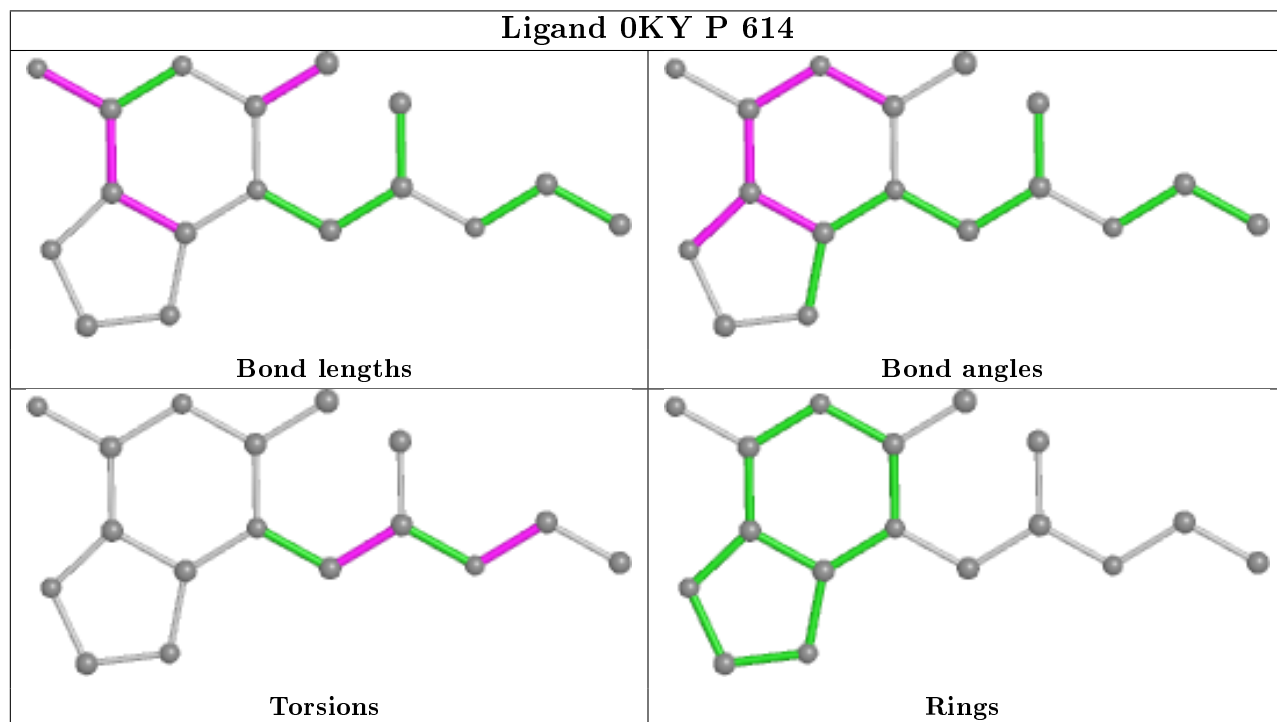
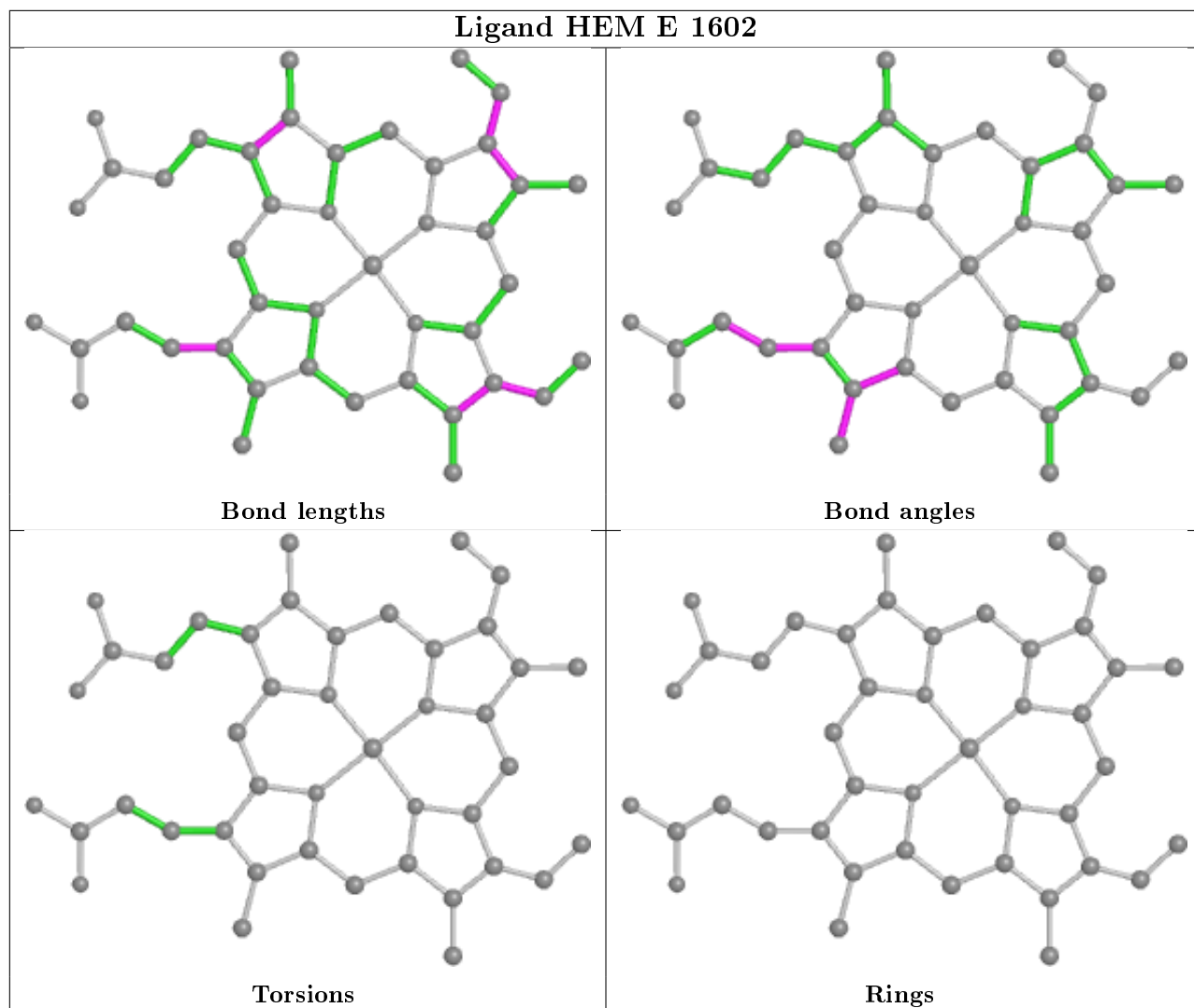
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | G     | 610  | 0KY  | 1       | 0            |
| 6   | A     | 1602 | 0KY  | 3       | 0            |
| 7   | I     | 1602 | HEM  | 1       | 0            |
| 6   | O     | 610  | 0KY  | 5       | 0            |
| 8   | D     | 608  | NAG  | 1       | 0            |
| 7   | M     | 1602 | HEM  | 5       | 0            |
| 7   | B     | 202  | HEM  | 5       | 0            |
| 6   | I     | 1603 | 0KY  | 2       | 0            |

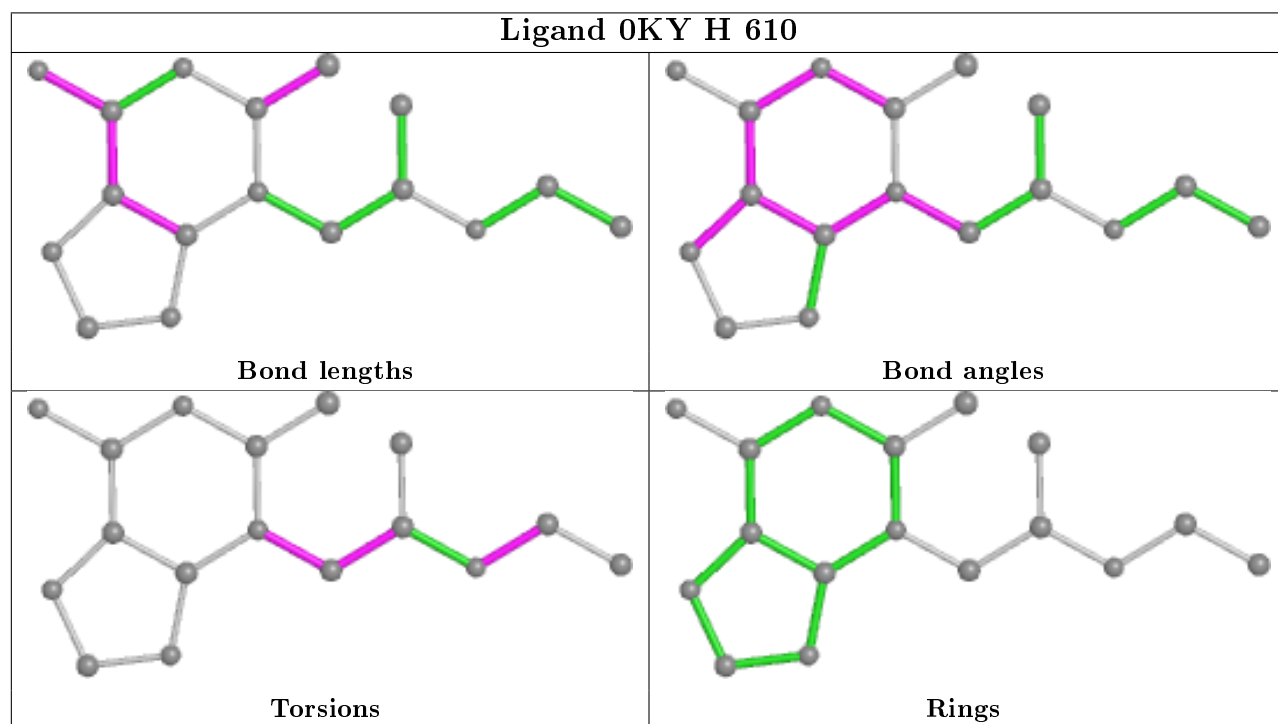
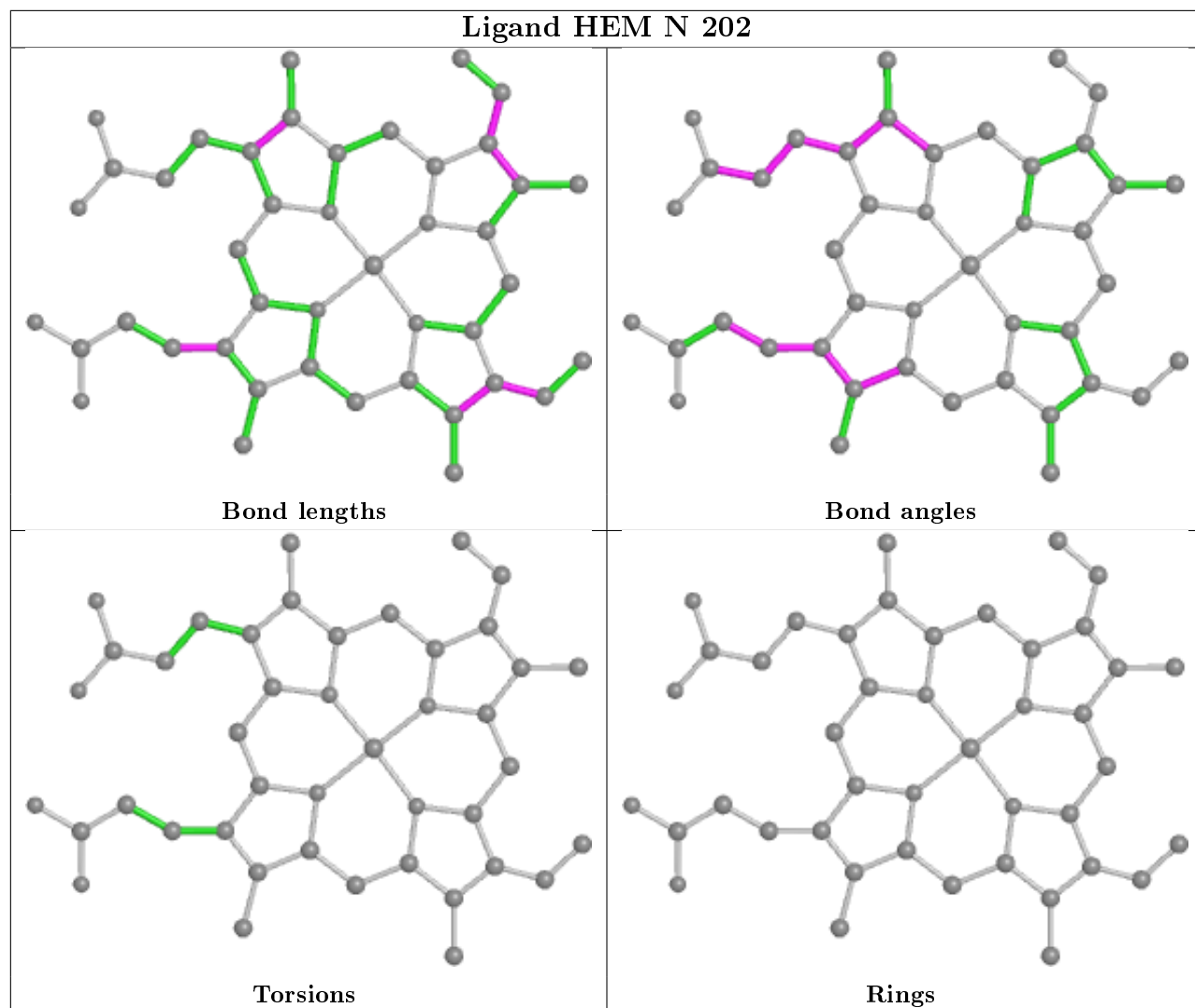
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

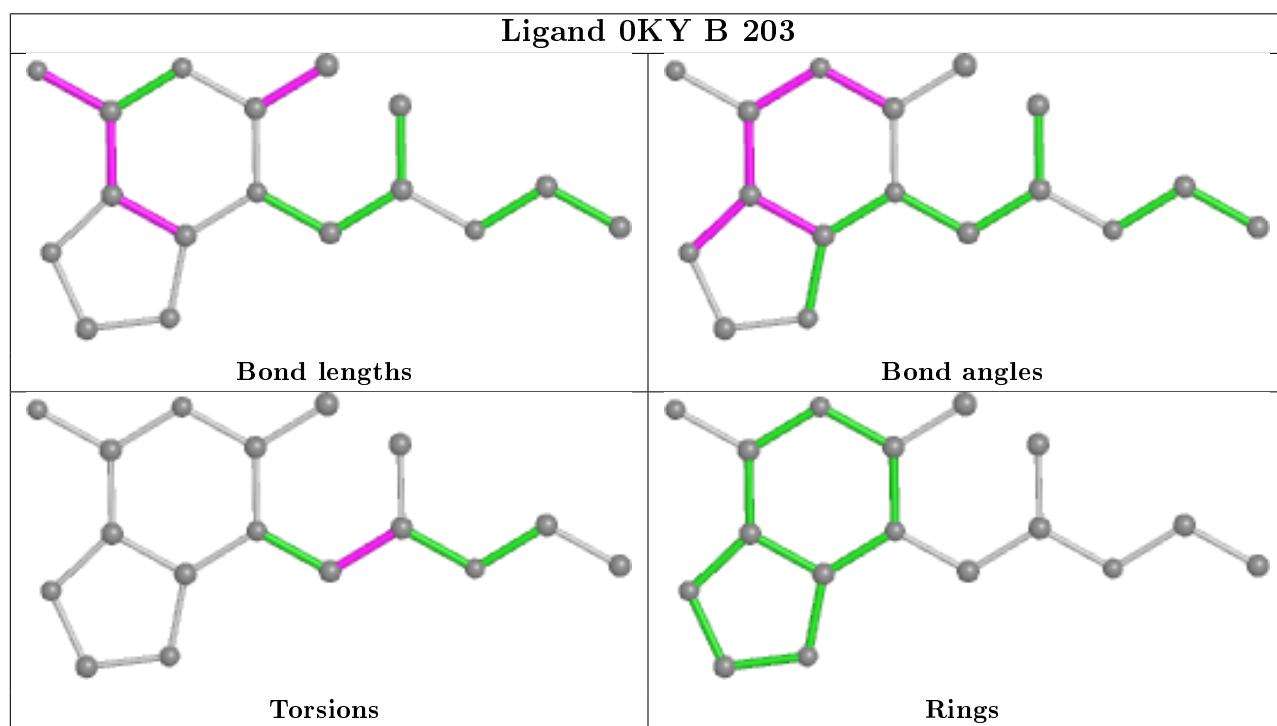
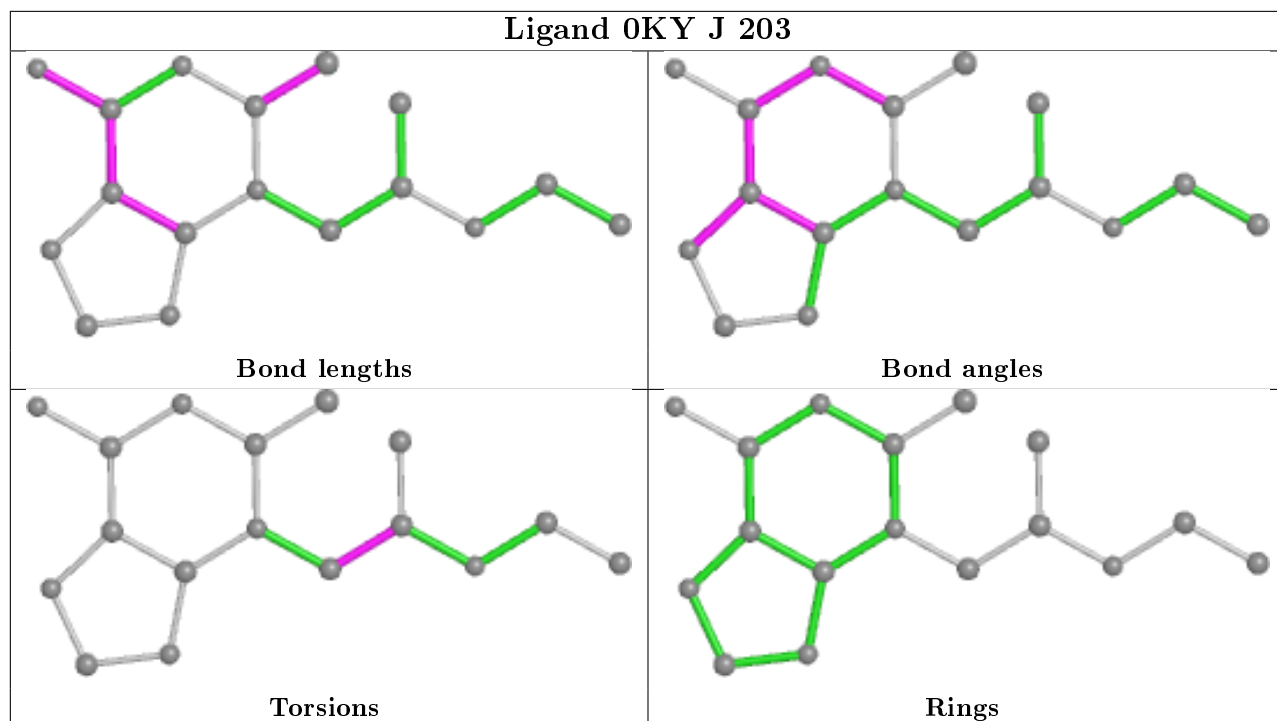


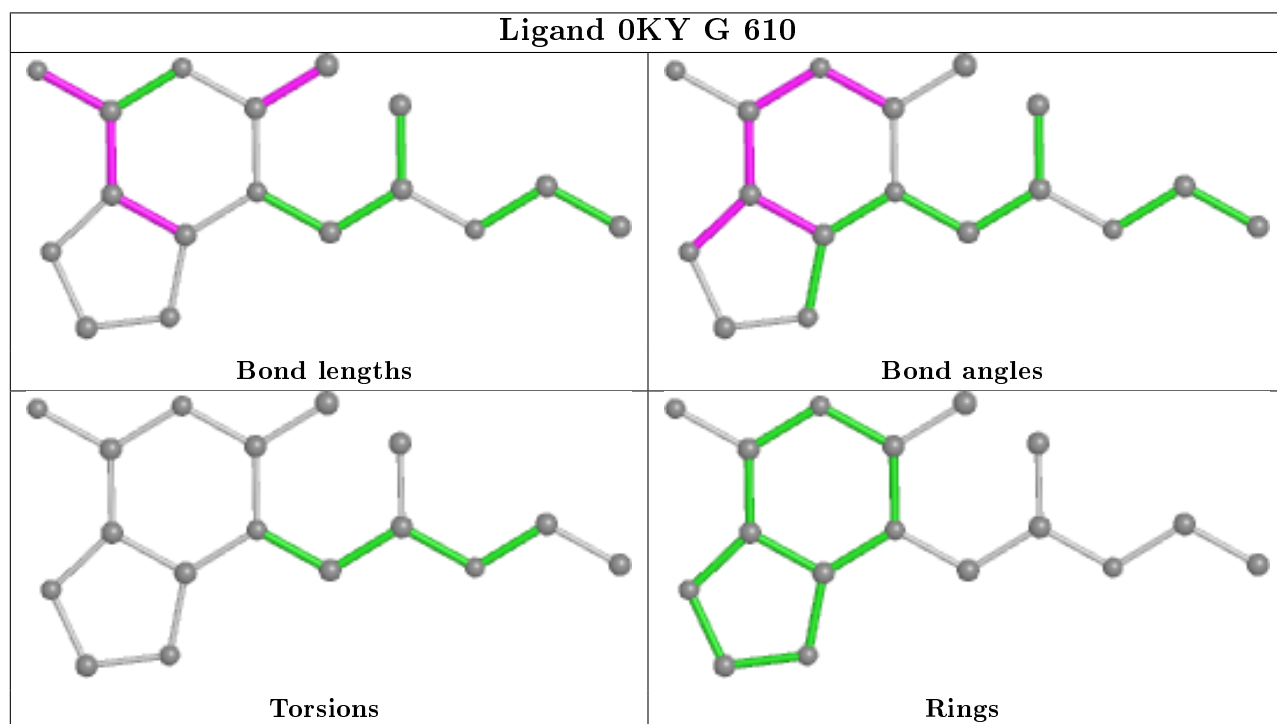
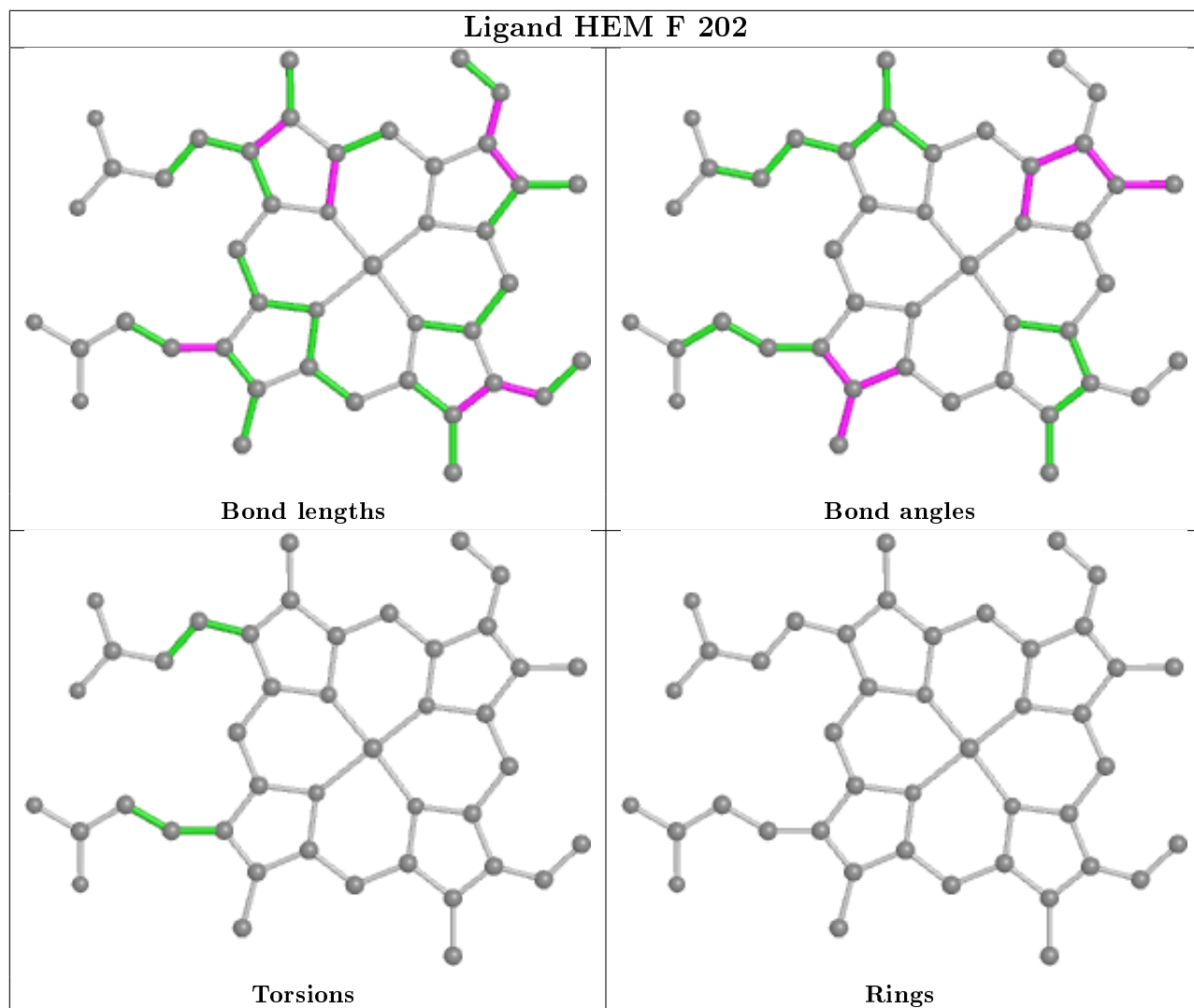


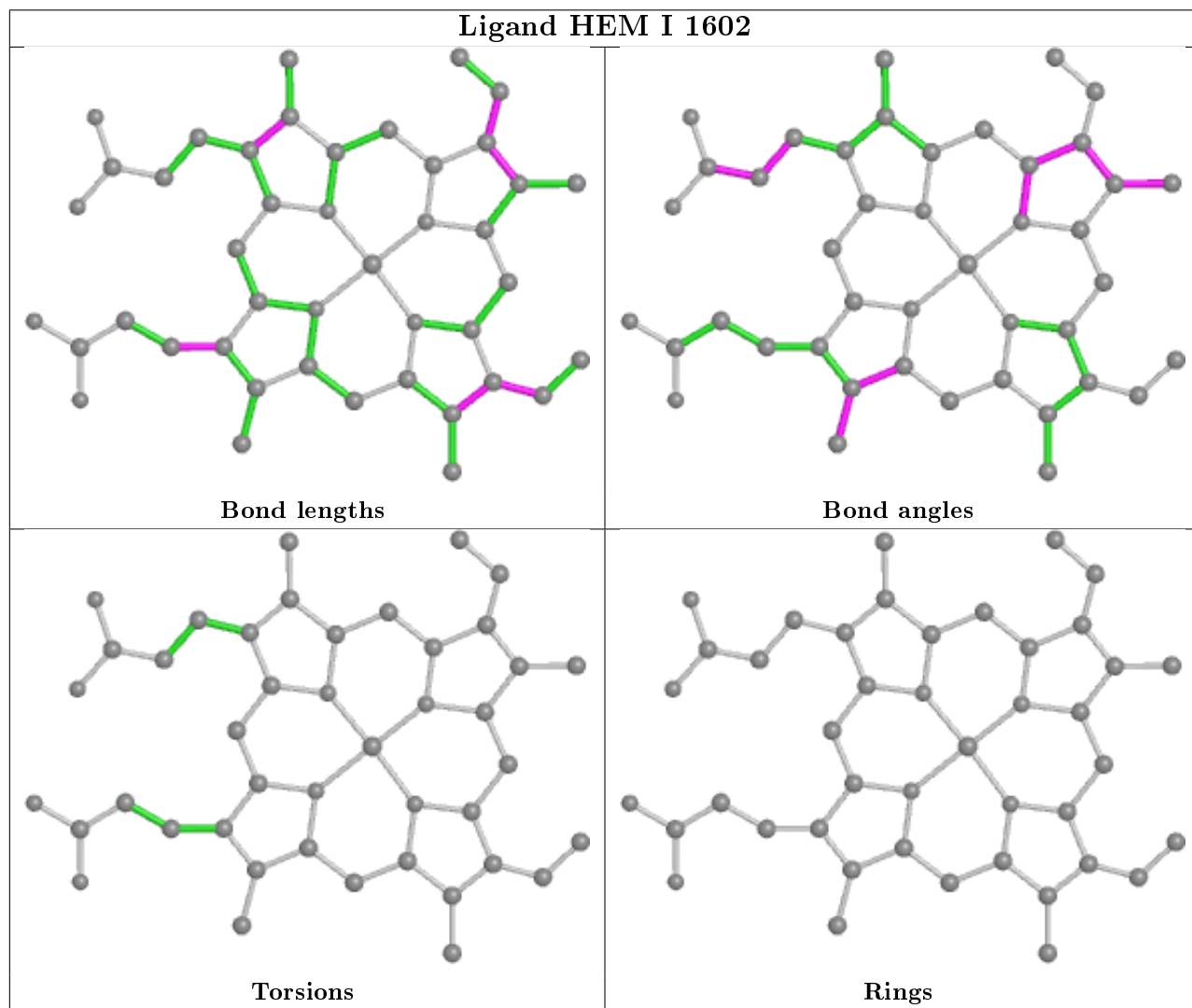
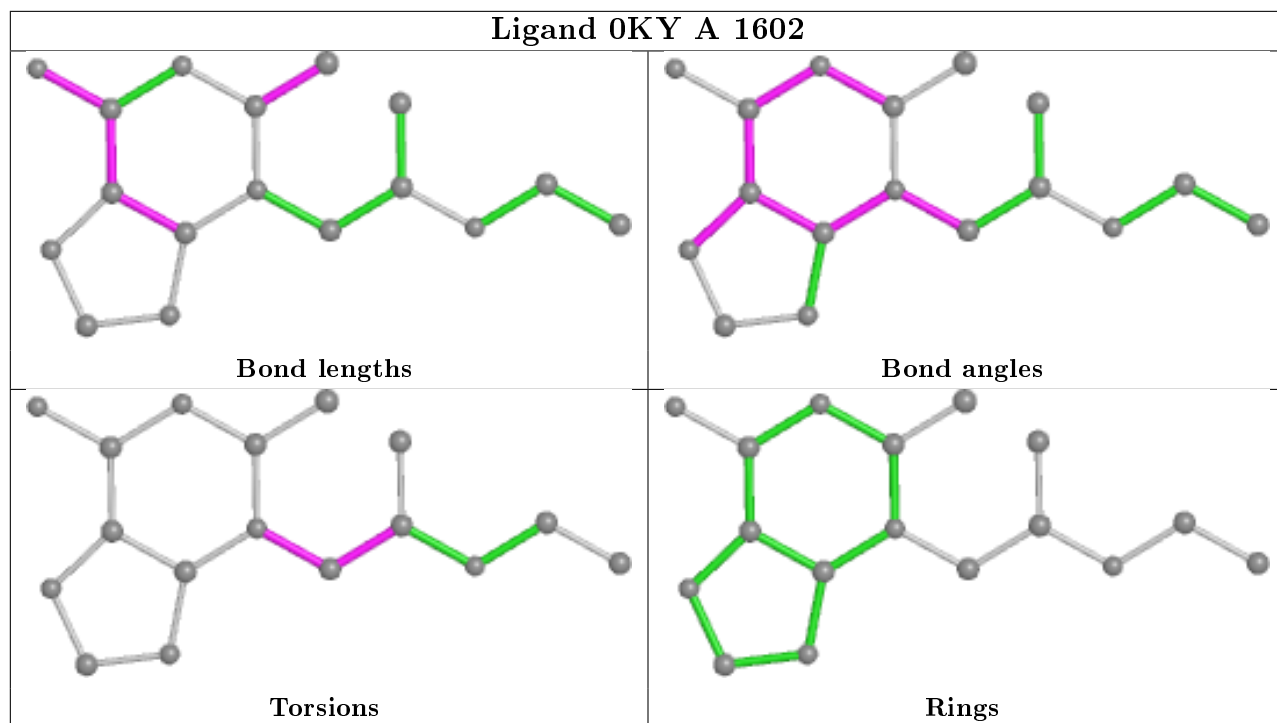


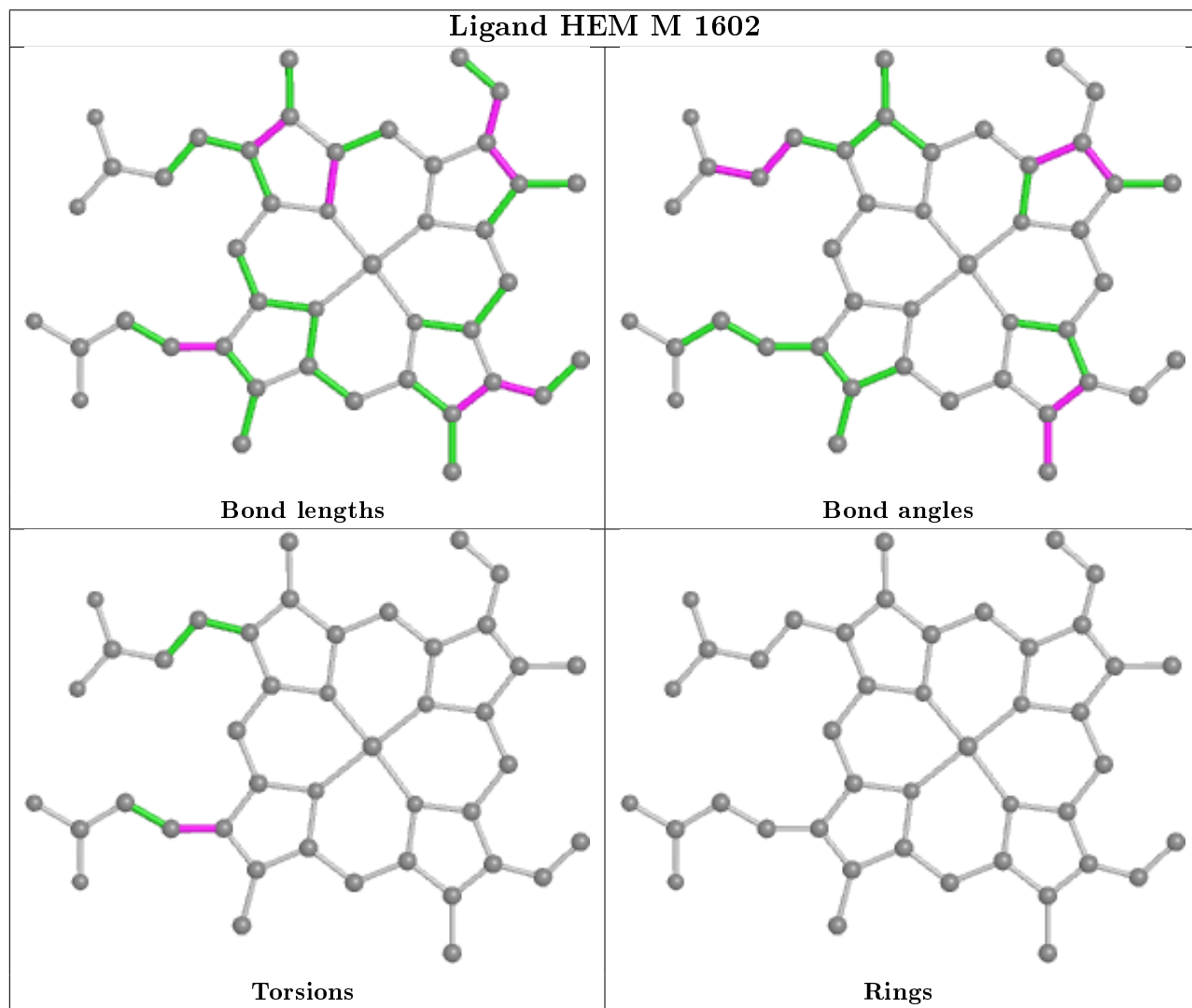
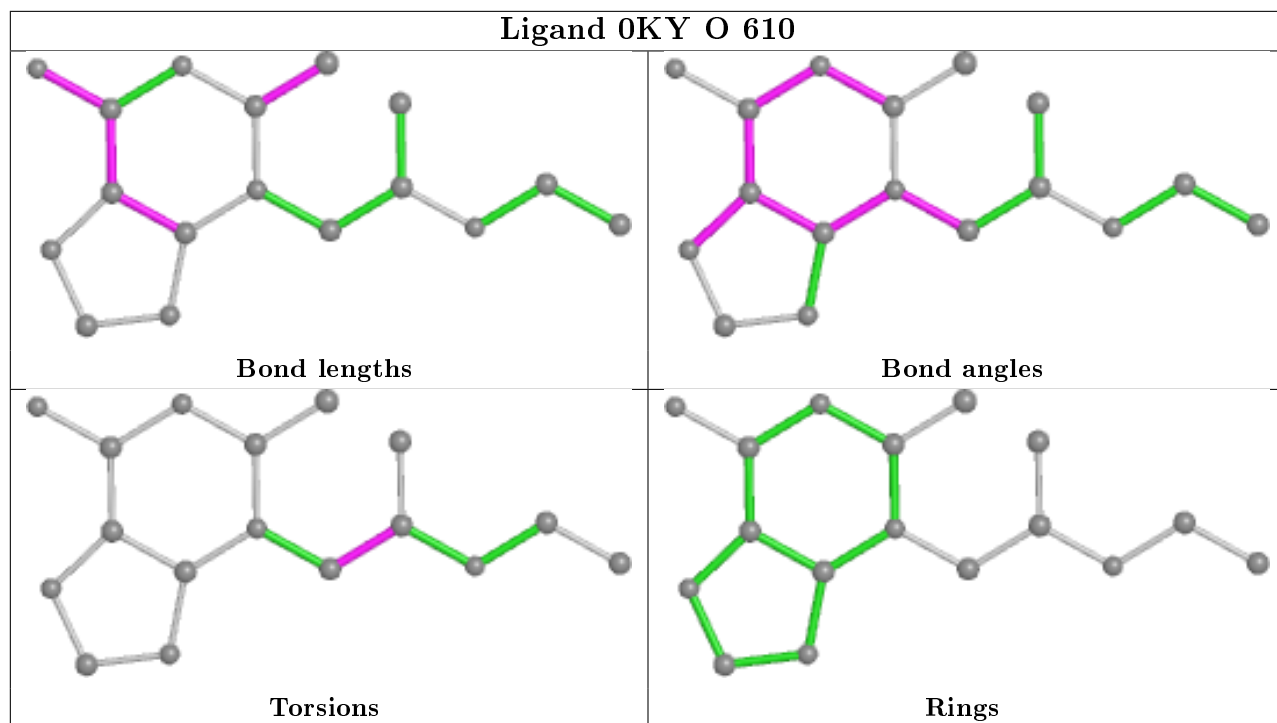




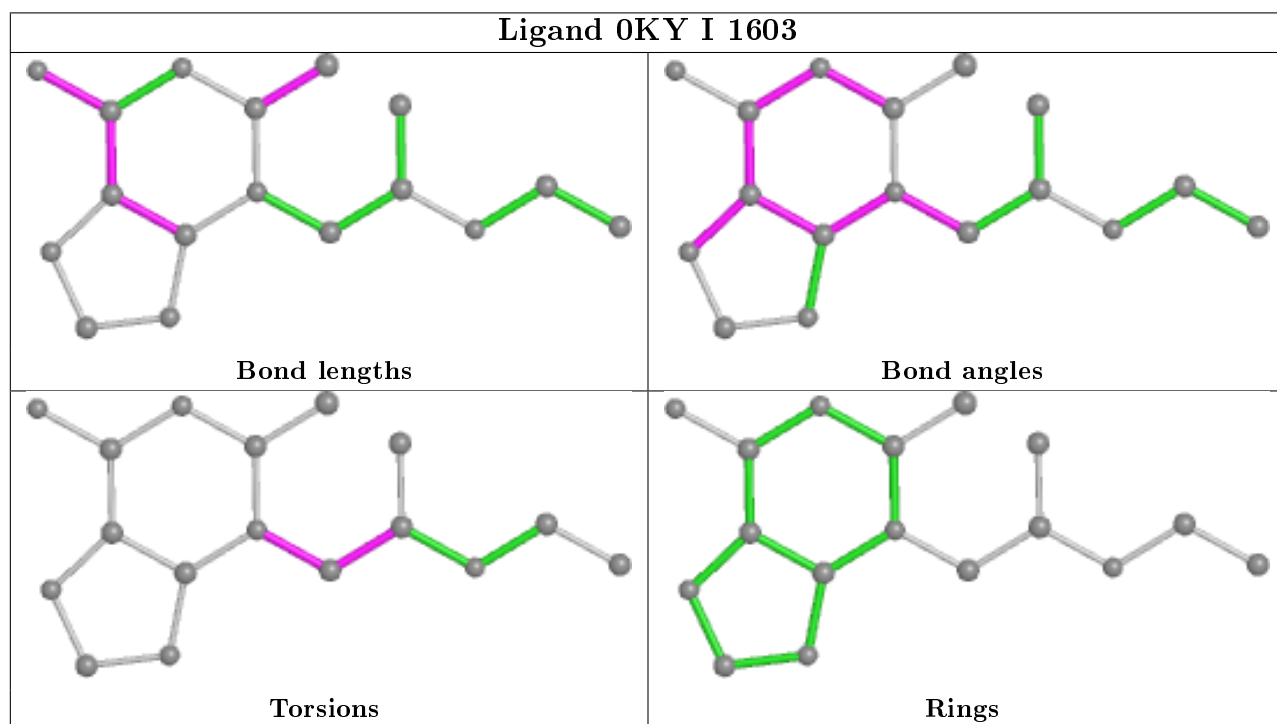
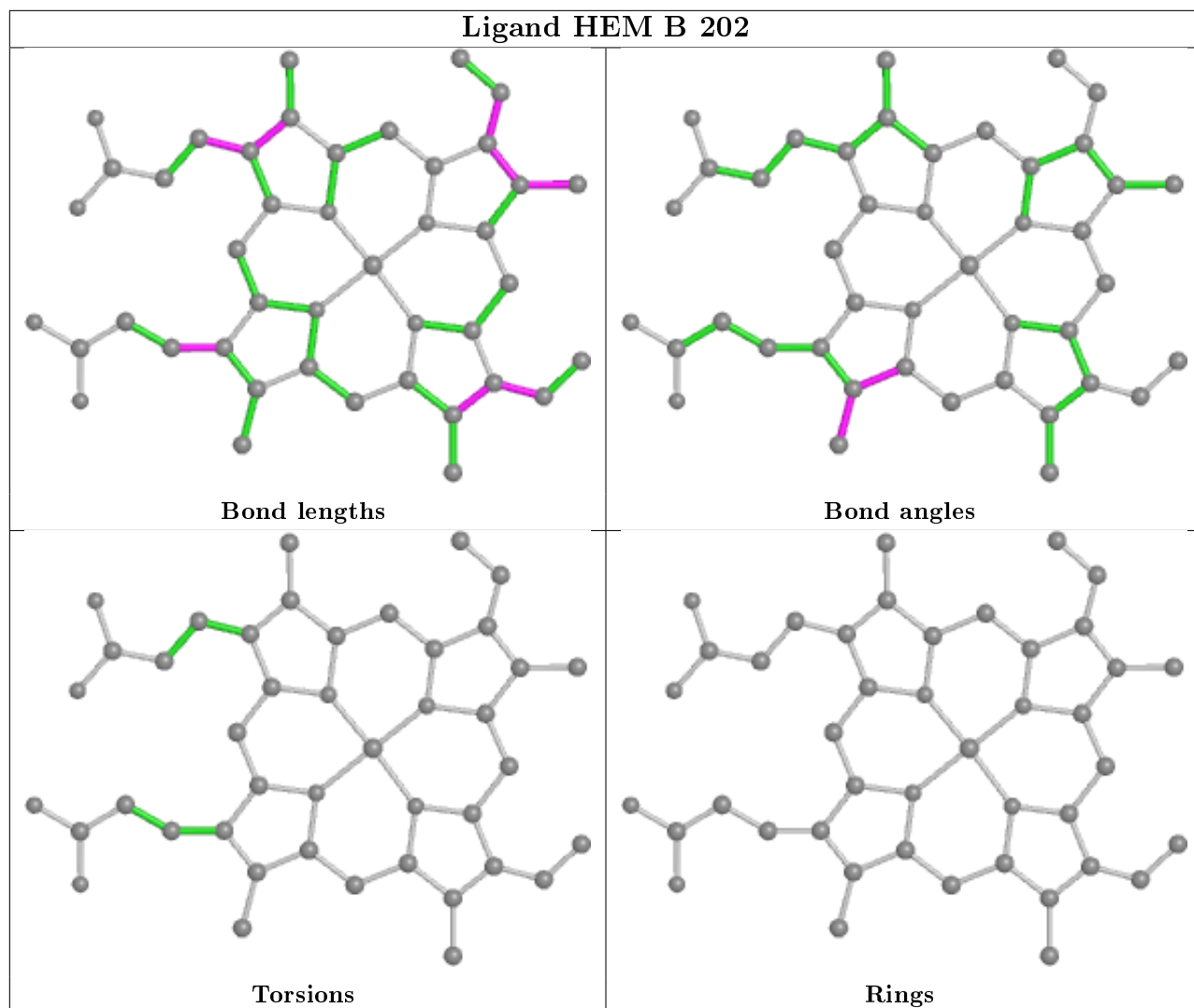












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 104/104 (100%)  | -0.39  | 1 (0%) 82 81  | 12, 18, 40, 58        | 0       |
| 1   | B     | 104/104 (100%)  | -0.39  | 0 100 100     | 14, 24, 40, 53        | 0       |
| 1   | E     | 104/104 (100%)  | -0.30  | 1 (0%) 82 81  | 15, 23, 47, 67        | 0       |
| 1   | F     | 104/104 (100%)  | -0.20  | 1 (0%) 82 81  | 16, 30, 51, 56        | 0       |
| 1   | I     | 104/104 (100%)  | -0.40  | 2 (1%) 66 65  | 16, 24, 44, 65        | 0       |
| 1   | J     | 104/104 (100%)  | -0.27  | 0 100 100     | 16, 26, 45, 52        | 0       |
| 1   | M     | 104/104 (100%)  | -0.25  | 2 (1%) 66 65  | 16, 26, 49, 67        | 0       |
| 1   | N     | 104/104 (100%)  | -0.17  | 0 100 100     | 16, 32, 56, 63        | 0       |
| 2   | C     | 464/466 (99%)   | -0.47  | 1 (0%) 95 94  | 11, 20, 36, 58        | 0       |
| 2   | D     | 465/466 (99%)   | -0.32  | 3 (0%) 89 88  | 13, 26, 45, 63        | 0       |
| 2   | G     | 464/466 (99%)   | -0.27  | 6 (1%) 77 76  | 12, 29, 52, 67        | 0       |
| 2   | H     | 465/466 (99%)   | -0.14  | 5 (1%) 80 79  | 17, 33, 54, 72        | 0       |
| 2   | K     | 464/466 (99%)   | -0.27  | 3 (0%) 89 88  | 12, 29, 54, 73        | 0       |
| 2   | L     | 465/466 (99%)   | -0.29  | 5 (1%) 80 79  | 15, 27, 44, 65        | 0       |
| 2   | O     | 465/466 (99%)   | -0.30  | 5 (1%) 80 79  | 17, 30, 52, 67        | 0       |
| 2   | P     | 465/466 (99%)   | -0.21  | 9 (1%) 66 65  | 17, 31, 59, 77        | 0       |
| All | All   | 4549/4560 (99%) | -0.29  | 44 (0%) 82 81 | 11, 28, 51, 77        | 0       |

All (44) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | O     | 578 | ALA  | 7.4  |
| 2   | D     | 217 | HIS  | 5.4  |
| 2   | H     | 217 | HIS  | 5.4  |
| 2   | G     | 218 | ASP  | 4.8  |
| 1   | M     | 4   | GLN  | 4.7  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 2          | G            | 217        | HIS         | 4.5         |
| 2          | L            | 578        | ALA         | 4.2         |
| 2          | O            | 218        | ASP         | 4.1         |
| 2          | P            | 218        | ASP         | 4.0         |
| 2          | L            | 217        | HIS         | 4.0         |
| 2          | P            | 140        | GLN         | 3.2         |
| 2          | K            | 218        | ASP         | 2.9         |
| 2          | L            | 218        | ASP         | 2.9         |
| 1          | E            | 3          | GLU         | 2.7         |
| 1          | I            | 3          | GLU         | 2.7         |
| 2          | K            | 113        | VAL         | 2.7         |
| 1          | A            | 4          | GLN         | 2.7         |
| 2          | P            | 217        | HIS         | 2.7         |
| 2          | H            | 578        | ALA         | 2.6         |
| 2          | L            | 141        | ALA         | 2.5         |
| 2          | P            | 216        | LEU         | 2.5         |
| 2          | G            | 113        | VAL         | 2.5         |
| 2          | O            | 217        | HIS         | 2.5         |
| 2          | L            | 216        | LEU         | 2.4         |
| 2          | P            | 228        | ALA         | 2.4         |
| 2          | G            | 216        | LEU         | 2.4         |
| 2          | G            | 349        | ARG         | 2.3         |
| 2          | C            | 217        | HIS         | 2.3         |
| 1          | I            | 4          | GLN         | 2.3         |
| 2          | K            | 217        | HIS         | 2.2         |
| 2          | D            | 578        | ALA         | 2.2         |
| 1          | F            | 104        | ALA         | 2.2         |
| 2          | O            | 549        | ASN         | 2.2         |
| 2          | G            | 569        | ALA         | 2.2         |
| 2          | H            | 355        | PRO         | 2.2         |
| 2          | P            | 124        | PRO         | 2.1         |
| 2          | P            | 135        | PRO         | 2.1         |
| 2          | P            | 355        | PRO         | 2.1         |
| 1          | M            | 3          | GLU         | 2.1         |
| 2          | H            | 216        | LEU         | 2.1         |
| 2          | H            | 218        | ASP         | 2.0         |
| 2          | O            | 216        | LEU         | 2.0         |
| 2          | P            | 139        | ASN         | 2.0         |
| 2          | D            | 218        | ASP         | 2.0         |

## 6.2 Non-standard residues in protein, DNA, RNA chains [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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | CSO  | L     | 150 | 7/8   | 0.95 | 0.09 | 22,24,25,30                | 0     |
| 2   | CSO  | K     | 150 | 7/8   | 0.95 | 0.09 | 22,24,26,30                | 0     |
| 2   | CSO  | H     | 150 | 7/8   | 0.96 | 0.09 | 21,24,29,34                | 0     |
| 2   | CSO  | O     | 150 | 7/8   | 0.96 | 0.10 | 19,20,28,28                | 0     |
| 2   | CSO  | G     | 150 | 7/8   | 0.97 | 0.06 | 15,16,25,26                | 0     |
| 2   | CSO  | C     | 150 | 7/8   | 0.97 | 0.08 | 14,15,22,24                | 0     |
| 2   | CSO  | D     | 150 | 7/8   | 0.97 | 0.08 | 17,19,23,24                | 0     |
| 2   | CSO  | P     | 150 | 7/8   | 0.97 | 0.06 | 26,29,33,36                | 0     |

## 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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | MAN  | X     | 4   | 11/12 | 0.80 | 0.15 | 44,54,61,62                | 0     |
| 3   | MAN  | U     | 4   | 11/12 | 0.83 | 0.18 | 45,53,54,57                | 0     |
| 4   | MAN  | Y     | 5   | 11/12 | 0.87 | 0.11 | 46,52,57,57                | 0     |
| 4   | MAN  | Y     | 4   | 11/12 | 0.88 | 0.11 | 43,45,47,51                | 0     |
| 3   | MAN  | T     | 4   | 11/12 | 0.88 | 0.23 | 46,51,53,54                | 0     |
| 3   | MAN  | Q     | 4   | 11/12 | 0.88 | 0.13 | 47,52,54,56                | 0     |
| 3   | BMA  | S     | 3   | 11/12 | 0.89 | 0.12 | 36,42,46,49                | 0     |
| 3   | FUC  | W     | 6   | 10/11 | 0.90 | 0.13 | 36,37,39,40                | 0     |
| 3   | MAN  | V     | 4   | 11/12 | 0.91 | 0.15 | 39,46,48,49                | 0     |
| 3   | MAN  | W     | 4   | 11/12 | 0.91 | 0.12 | 51,55,64,70                | 0     |
| 3   | MAN  | V     | 5   | 11/12 | 0.91 | 0.12 | 26,30,33,33                | 0     |
| 3   | MAN  | S     | 5   | 11/12 | 0.92 | 0.10 | 34,38,39,39                | 0     |
| 3   | NAG  | W     | 1   | 14/15 | 0.92 | 0.10 | 28,33,41,45                | 0     |
| 3   | MAN  | R     | 4   | 11/12 | 0.92 | 0.11 | 44,49,54,54                | 0     |
| 3   | BMA  | V     | 3   | 11/12 | 0.93 | 0.10 | 21,26,31,36                | 0     |
| 3   | MAN  | W     | 5   | 11/12 | 0.93 | 0.11 | 29,35,37,38                | 0     |
| 4   | BMA  | Y     | 3   | 11/12 | 0.93 | 0.09 | 28,33,39,46                | 0     |
| 3   | MAN  | U     | 5   | 11/12 | 0.93 | 0.11 | 24,30,34,34                | 0     |
| 3   | MAN  | T     | 5   | 11/12 | 0.93 | 0.10 | 28,33,37,40                | 0     |

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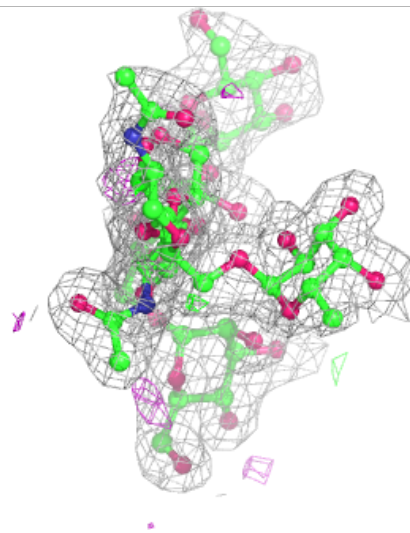
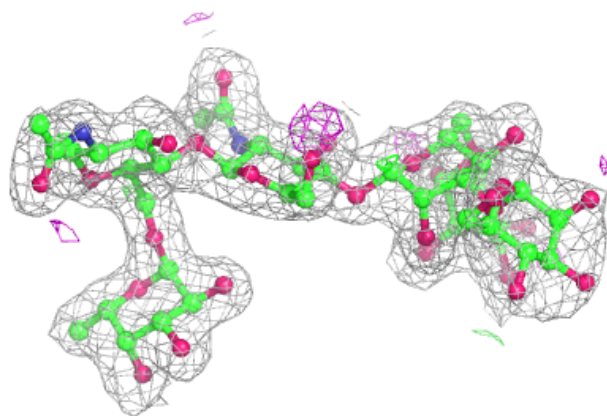
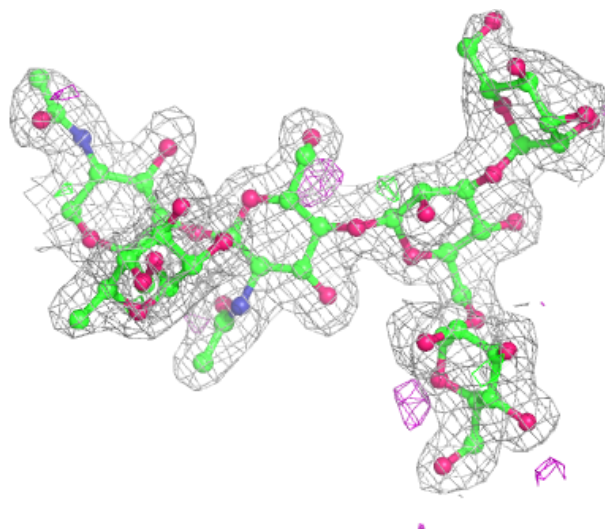
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | BMA  | W     | 3   | 11/12 | 0.94 | 0.08 | 35,37,40,44                 | 0     |
| 3   | MAN  | X     | 5   | 11/12 | 0.94 | 0.11 | 28,34,36,37                 | 0     |
| 3   | BMA  | Q     | 3   | 11/12 | 0.94 | 0.07 | 24,28,32,36                 | 0     |
| 3   | MAN  | S     | 4   | 11/12 | 0.94 | 0.09 | 58,63,67,67                 | 0     |
| 3   | FUC  | S     | 6   | 10/11 | 0.94 | 0.11 | 29,36,39,42                 | 0     |
| 3   | BMA  | U     | 3   | 11/12 | 0.94 | 0.11 | 22,25,31,37                 | 0     |
| 3   | NAG  | S     | 1   | 14/15 | 0.94 | 0.11 | 29,34,41,42                 | 0     |
| 3   | FUC  | V     | 6   | 10/11 | 0.94 | 0.11 | 26,29,30,31                 | 0     |
| 3   | FUC  | T     | 6   | 10/11 | 0.94 | 0.10 | 24,27,31,38                 | 0     |
| 3   | NAG  | T     | 1   | 14/15 | 0.95 | 0.10 | 19,24,31,34                 | 0     |
| 3   | FUC  | Q     | 6   | 10/11 | 0.95 | 0.08 | 23,27,29,32                 | 0     |
| 3   | MAN  | R     | 5   | 11/12 | 0.95 | 0.10 | 23,28,32,33                 | 0     |
| 3   | NAG  | R     | 1   | 14/15 | 0.95 | 0.10 | 15,21,28,32                 | 0     |
| 3   | NAG  | U     | 2   | 14/15 | 0.95 | 0.11 | 18,23,27,27                 | 0     |
| 3   | BMA  | T     | 3   | 11/12 | 0.95 | 0.12 | 25,27,33,38                 | 0     |
| 3   | NAG  | X     | 1   | 14/15 | 0.95 | 0.09 | 25,28,39,40                 | 0     |
| 3   | FUC  | R     | 6   | 10/11 | 0.95 | 0.10 | 18,22,26,27                 | 0     |
| 3   | FUC  | U     | 6   | 10/11 | 0.95 | 0.08 | 28,31,34,35                 | 0     |
| 3   | BMA  | X     | 3   | 11/12 | 0.95 | 0.09 | 24,31,36,41                 | 0     |
| 3   | NAG  | W     | 2   | 14/15 | 0.95 | 0.10 | 22,30,38,42                 | 0     |
| 3   | FUC  | X     | 6   | 10/11 | 0.96 | 0.09 | 28,30,31,33                 | 0     |
| 3   | NAG  | T     | 2   | 14/15 | 0.96 | 0.09 | 21,25,27,27                 | 0     |
| 3   | NAG  | Q     | 1   | 14/15 | 0.96 | 0.10 | 17,21,28,30                 | 0     |
| 4   | NAG  | Y     | 1   | 14/15 | 0.96 | 0.07 | 23,27,30,30                 | 0     |
| 3   | NAG  | X     | 2   | 14/15 | 0.96 | 0.08 | 19,25,28,30                 | 0     |
| 3   | NAG  | V     | 1   | 14/15 | 0.96 | 0.10 | 16,21,28,30                 | 0     |
| 3   | NAG  | V     | 2   | 14/15 | 0.96 | 0.08 | 15,17,20,22                 | 0     |
| 3   | NAG  | U     | 1   | 14/15 | 0.96 | 0.09 | 19,25,32,33                 | 0     |
| 3   | NAG  | S     | 2   | 14/15 | 0.97 | 0.08 | 29,31,35,37                 | 0     |
| 4   | NAG  | Y     | 2   | 14/15 | 0.97 | 0.11 | 28,30,36,37                 | 0     |
| 3   | NAG  | Q     | 2   | 14/15 | 0.97 | 0.10 | 14,22,27,28                 | 0     |
| 3   | BMA  | R     | 3   | 11/12 | 0.97 | 0.09 | 18,22,26,31                 | 0     |
| 3   | MAN  | Q     | 5   | 11/12 | 0.97 | 0.07 | 24,29,31,31                 | 0     |
| 3   | NAG  | R     | 2   | 14/15 | 0.98 | 0.09 | 15,18,22,22                 | 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.

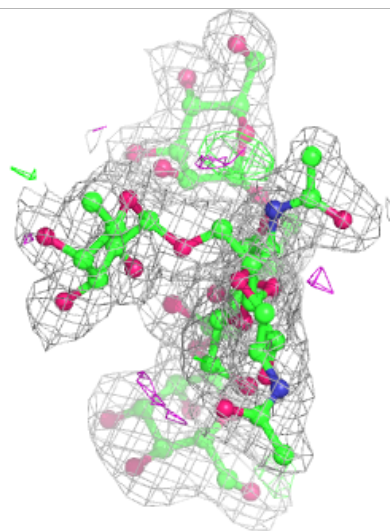
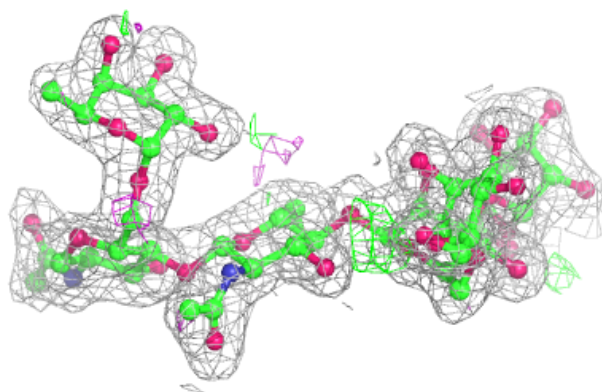
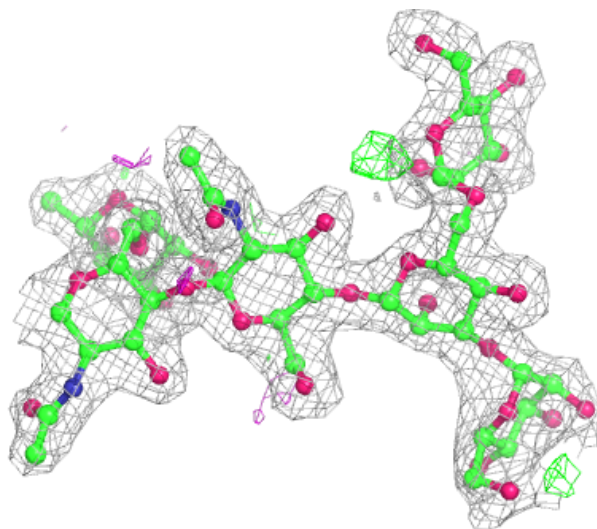
**Electron density around Chain Q:**

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



**Electron density around Chain R:**

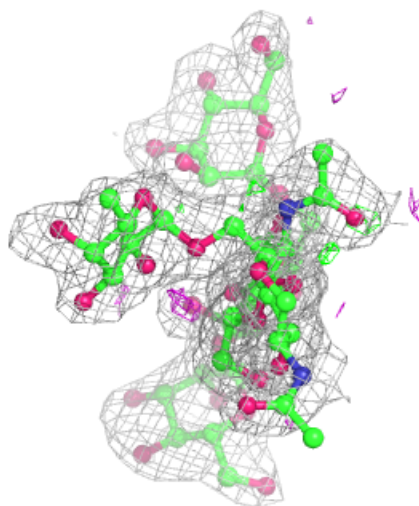
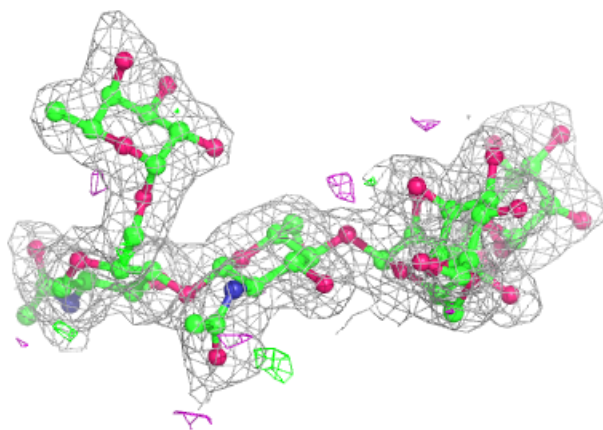
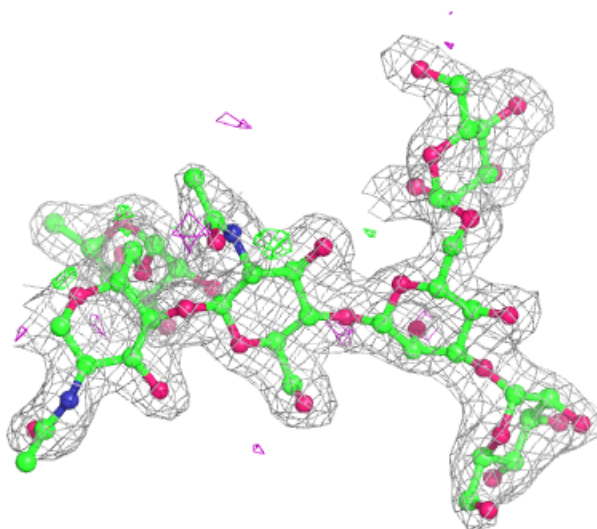
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





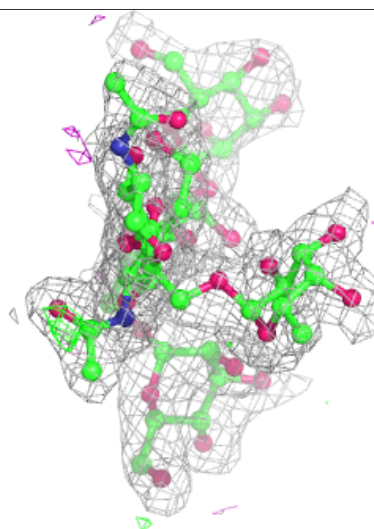
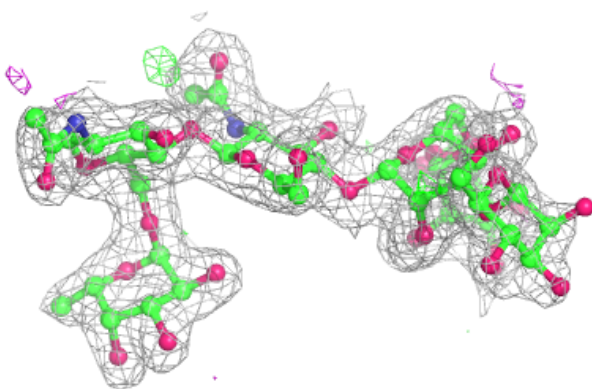
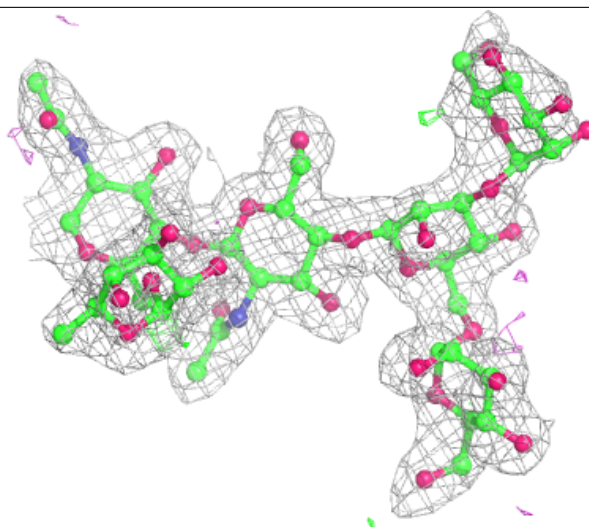
**Electron density around Chain S:**

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



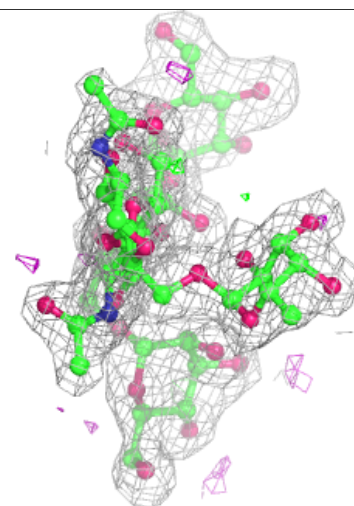
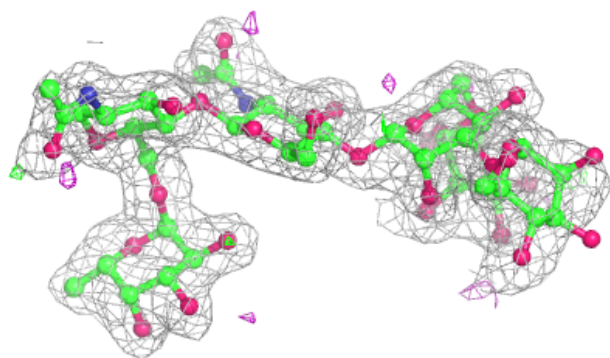
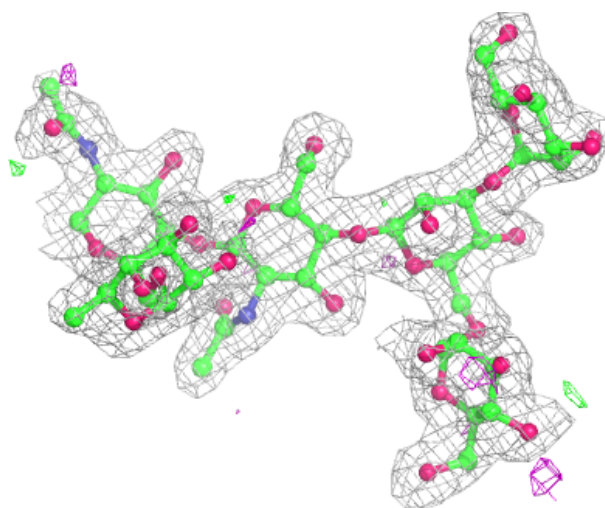
**Electron density around Chain T:**

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



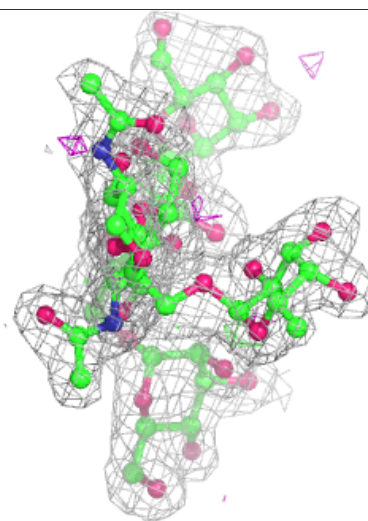
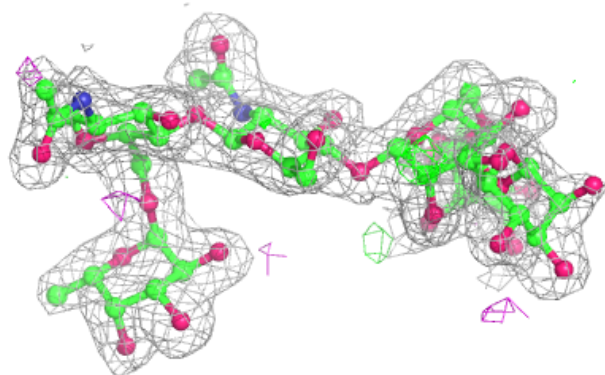
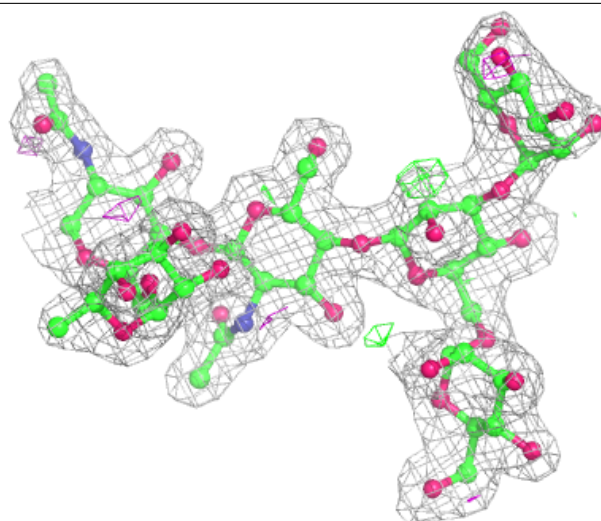
**Electron density around Chain U:**

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



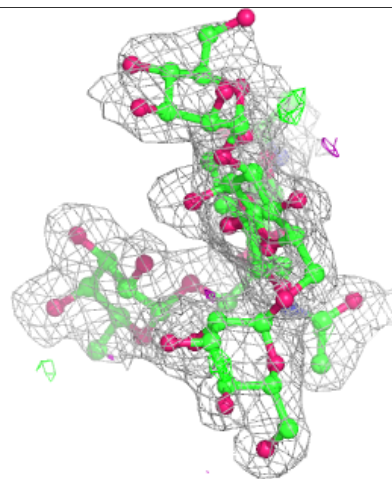
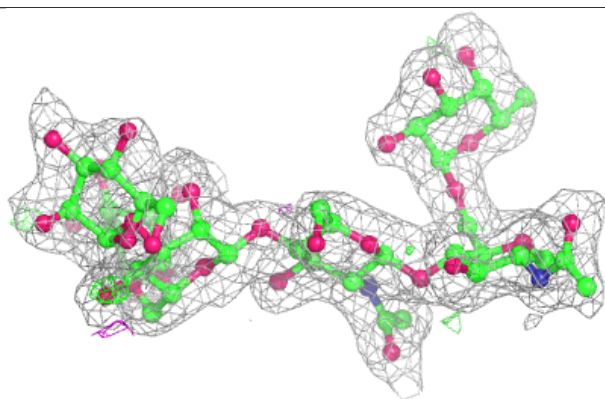
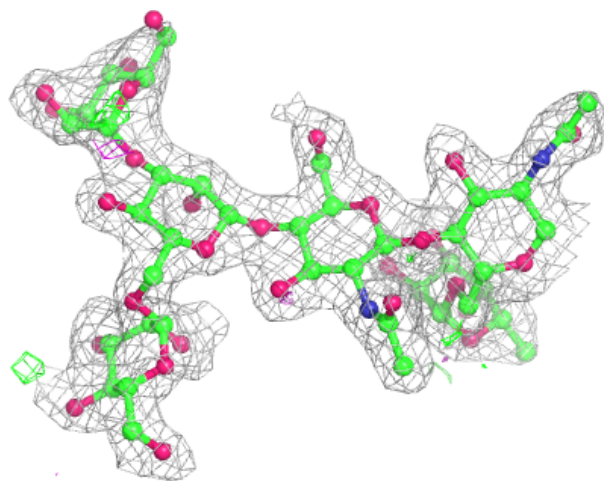
**Electron density around Chain V:**

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



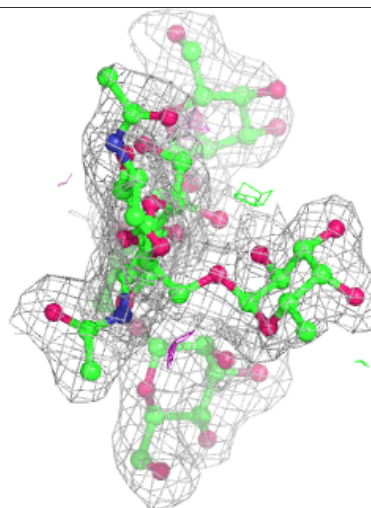
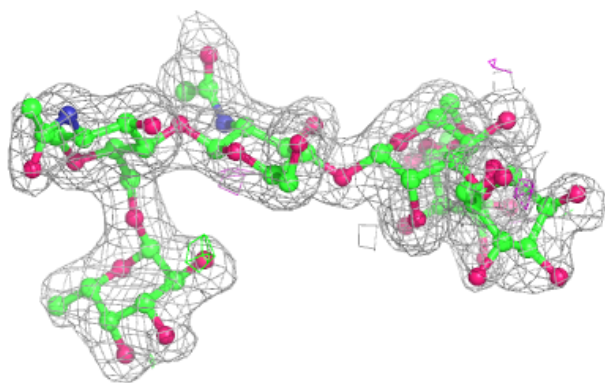
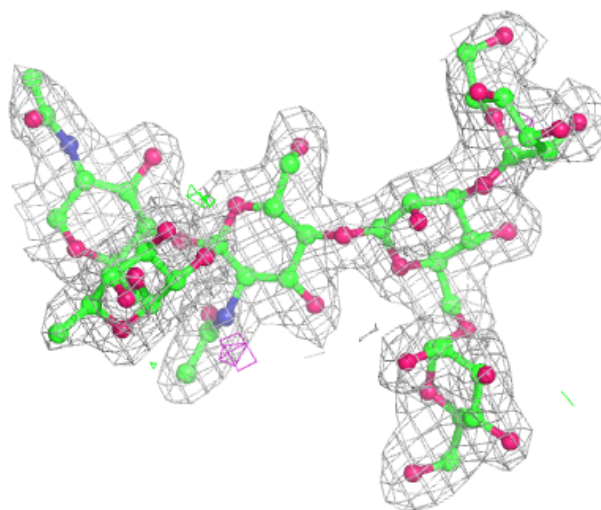
**Electron density around Chain W:**

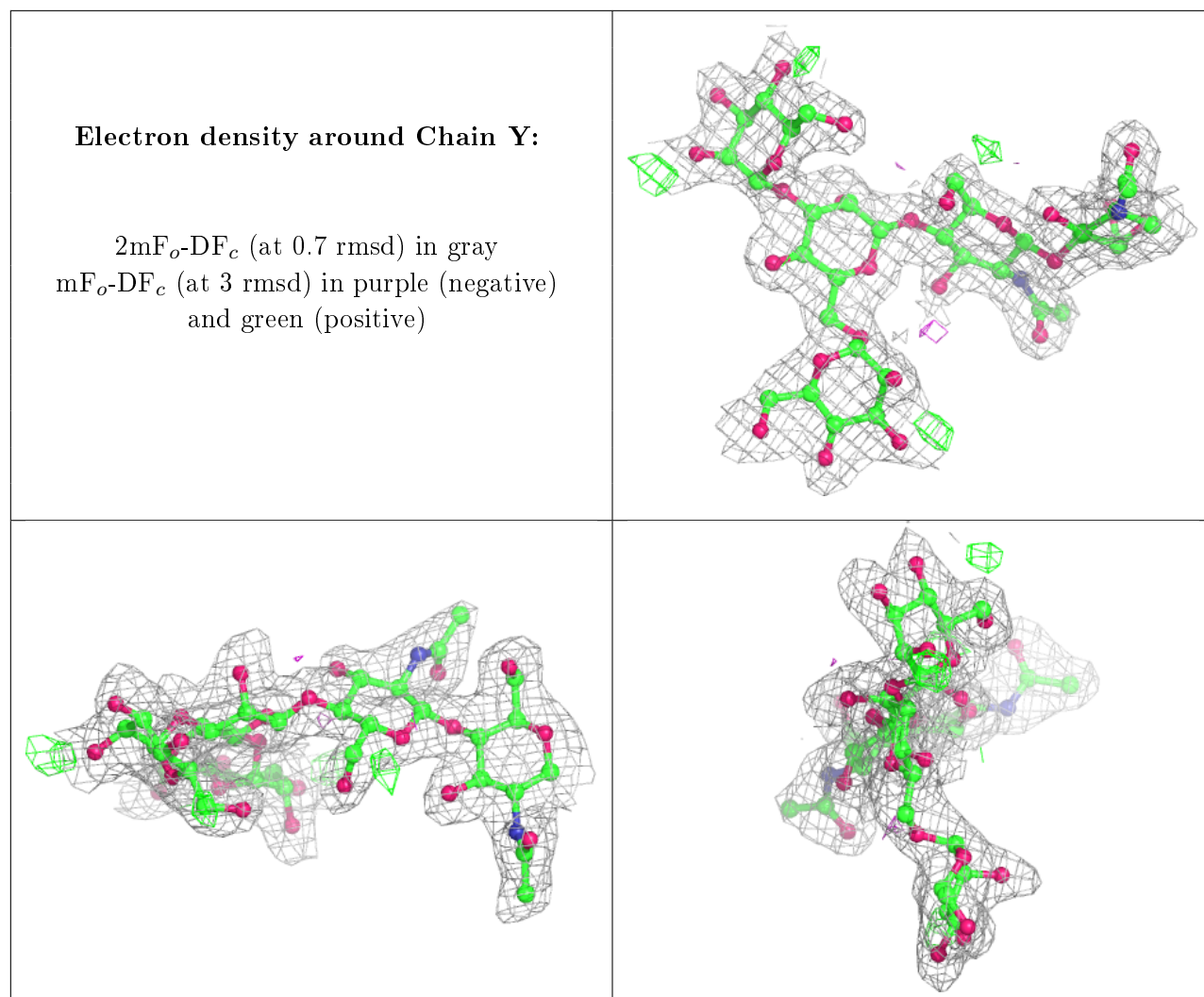
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain X:**

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





## 6.4 Ligands [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 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 8   | NAG  | O     | 608  | 14/15 | 0.71 | 0.26 | 71,75,81,84                | 0     |
| 6   | 0KY  | H     | 610  | 17/17 | 0.79 | 0.28 | 52,67,75,75                | 0     |
| 6   | 0KY  | O     | 610  | 17/17 | 0.79 | 0.26 | 53,61,70,70                | 0     |
| 8   | NAG  | C     | 609  | 14/15 | 0.80 | 0.17 | 54,62,66,66                | 0     |
| 6   | 0KY  | P     | 614  | 17/17 | 0.81 | 0.36 | 68,78,87,88                | 0     |
| 6   | 0KY  | J     | 203  | 17/17 | 0.83 | 0.27 | 50,61,68,68                | 0     |
| 8   | NAG  | H     | 608  | 14/15 | 0.83 | 0.17 | 62,66,70,72                | 0     |
| 6   | 0KY  | I     | 1603 | 17/17 | 0.84 | 0.19 | 43,59,63,64                | 0     |
| 6   | 0KY  | A     | 1602 | 17/17 | 0.85 | 0.20 | 36,43,48,49                | 0     |

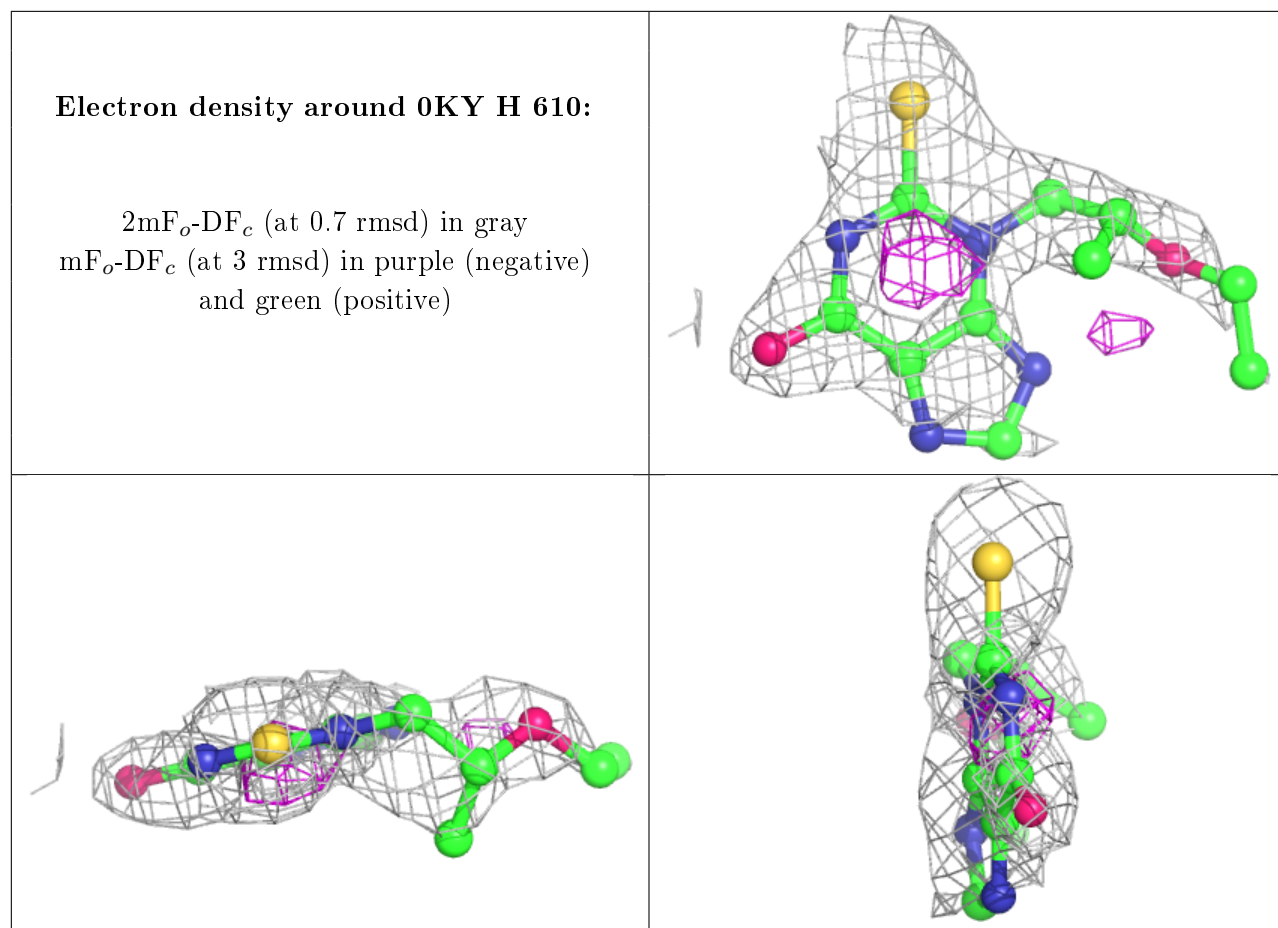
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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 6   | OKY  | B     | 203  | 17/17 | 0.85 | 0.29 | 50,64,66,67                 | 0     |
| 8   | NAG  | P     | 608  | 14/15 | 0.86 | 0.18 | 56,61,65,66                 | 0     |
| 8   | NAG  | D     | 608  | 14/15 | 0.86 | 0.16 | 46,53,55,57                 | 0     |
| 6   | OKY  | G     | 610  | 17/17 | 0.88 | 0.19 | 38,53,62,62                 | 0     |
| 8   | NAG  | K     | 607  | 14/15 | 0.88 | 0.12 | 40,49,53,54                 | 0     |
| 8   | NAG  | K     | 608  | 14/15 | 0.89 | 0.15 | 49,56,60,61                 | 0     |
| 8   | NAG  | G     | 608  | 14/15 | 0.90 | 0.11 | 60,67,69,69                 | 0     |
| 8   | NAG  | D     | 607  | 14/15 | 0.92 | 0.09 | 24,26,30,36                 | 0     |
| 8   | NAG  | G     | 607  | 14/15 | 0.92 | 0.11 | 32,36,41,43                 | 0     |
| 8   | NAG  | L     | 607  | 14/15 | 0.92 | 0.10 | 27,35,38,39                 | 0     |
| 8   | NAG  | L     | 608  | 14/15 | 0.93 | 0.12 | 50,56,59,60                 | 0     |
| 8   | NAG  | H     | 607  | 14/15 | 0.93 | 0.10 | 31,37,42,45                 | 0     |
| 8   | NAG  | C     | 608  | 14/15 | 0.95 | 0.09 | 19,25,29,30                 | 0     |
| 8   | NAG  | O     | 607  | 14/15 | 0.95 | 0.09 | 26,28,31,34                 | 0     |
| 7   | HEM  | F     | 202  | 43/43 | 0.95 | 0.11 | 22,29,33,38                 | 0     |
| 7   | HEM  | J     | 202  | 43/43 | 0.96 | 0.10 | 18,24,29,33                 | 0     |
| 7   | HEM  | N     | 202  | 43/43 | 0.96 | 0.10 | 21,30,36,43                 | 0     |
| 7   | HEM  | I     | 1602 | 43/43 | 0.97 | 0.11 | 11,20,24,28                 | 0     |
| 7   | HEM  | C     | 601  | 43/43 | 0.98 | 0.10 | 11,15,20,27                 | 0     |
| 7   | HEM  | M     | 1602 | 43/43 | 0.98 | 0.10 | 17,25,28,29                 | 0     |
| 5   | CL   | F     | 201  | 1/1   | 0.98 | 0.12 | 25,25,25,25                 | 0     |
| 7   | HEM  | E     | 1602 | 43/43 | 0.98 | 0.11 | 13,19,27,28                 | 0     |
| 7   | HEM  | B     | 202  | 43/43 | 0.98 | 0.10 | 15,21,27,35                 | 0     |
| 5   | CL   | M     | 1601 | 1/1   | 0.99 | 0.07 | 18,18,18,18                 | 0     |
| 9   | CA   | C     | 610  | 1/1   | 0.99 | 0.07 | 14,14,14,14                 | 0     |
| 9   | CA   | L     | 609  | 1/1   | 0.99 | 0.08 | 20,20,20,20                 | 0     |
| 9   | CA   | K     | 609  | 1/1   | 0.99 | 0.08 | 24,24,24,24                 | 0     |
| 9   | CA   | O     | 609  | 1/1   | 0.99 | 0.05 | 21,21,21,21                 | 0     |
| 5   | CL   | E     | 1601 | 1/1   | 0.99 | 0.09 | 18,18,18,18                 | 0     |
| 9   | CA   | G     | 609  | 1/1   | 0.99 | 0.08 | 22,22,22,22                 | 0     |
| 5   | CL   | J     | 201  | 1/1   | 0.99 | 0.06 | 20,20,20,20                 | 0     |
| 9   | CA   | P     | 601  | 1/1   | 1.00 | 0.05 | 19,19,19,19                 | 0     |
| 9   | CA   | D     | 609  | 1/1   | 1.00 | 0.09 | 16,16,16,16                 | 0     |
| 5   | CL   | A     | 1601 | 1/1   | 1.00 | 0.07 | 16,16,16,16                 | 0     |
| 9   | CA   | H     | 609  | 1/1   | 1.00 | 0.11 | 19,19,19,19                 | 0     |
| 5   | CL   | N     | 201  | 1/1   | 1.00 | 0.04 | 21,21,21,21                 | 0     |
| 5   | CL   | B     | 201  | 1/1   | 1.00 | 0.08 | 14,14,14,14                 | 0     |
| 5   | CL   | I     | 1601 | 1/1   | 1.00 | 0.09 | 14,14,14,14                 | 0     |

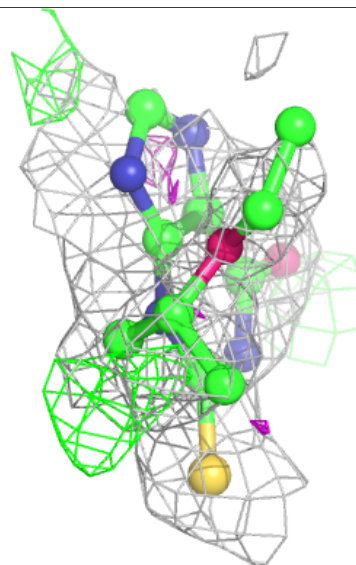
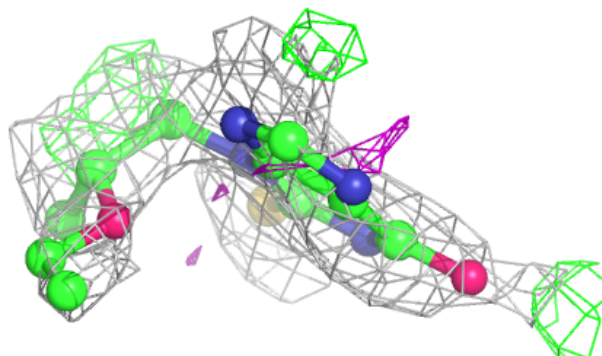
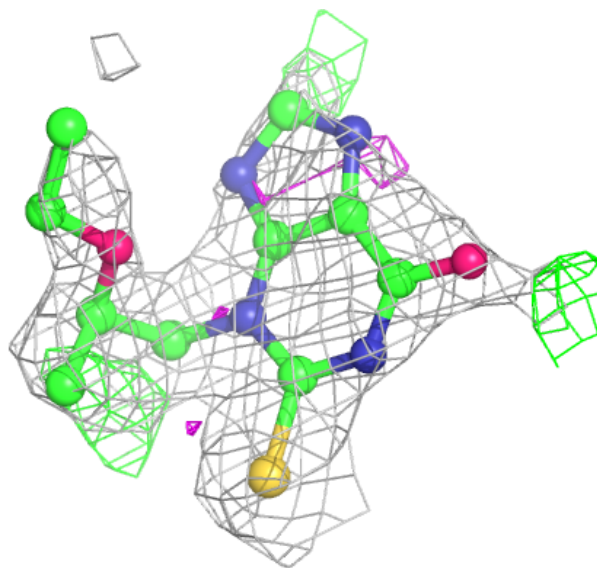
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





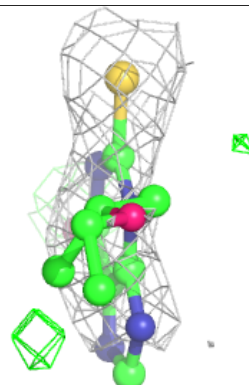
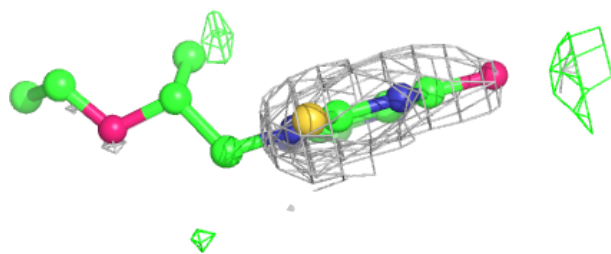
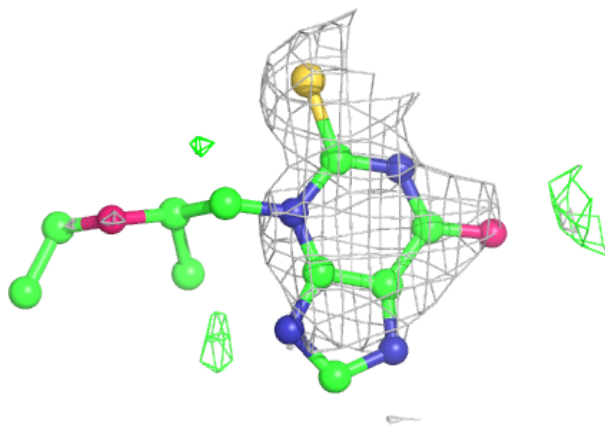
**Electron density around 0KY O 610:**

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



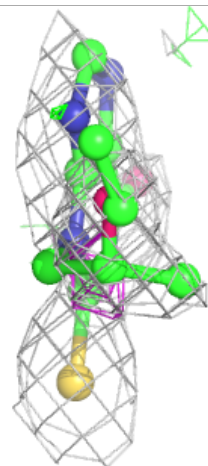
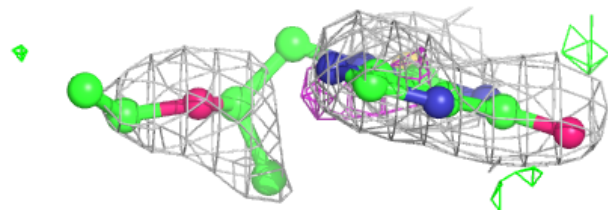
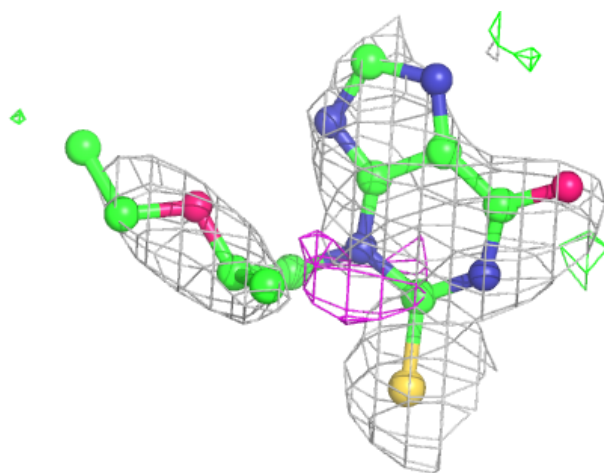
**Electron density around 0KY P 614:**

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



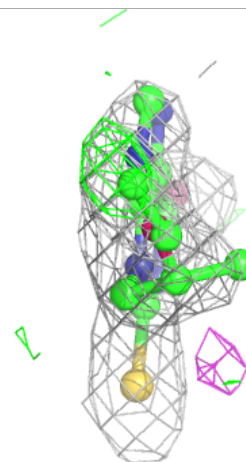
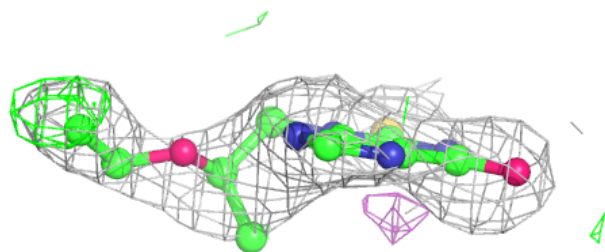
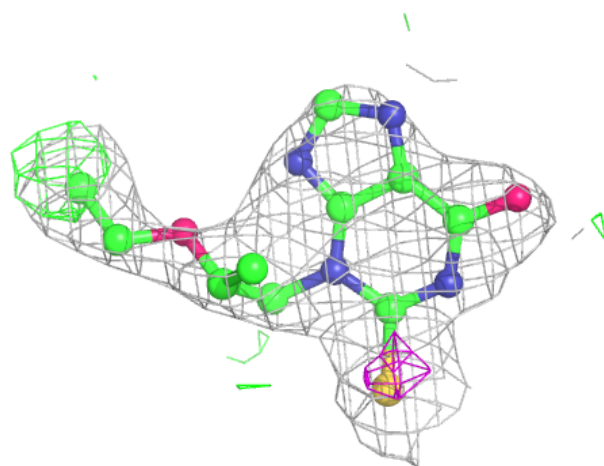
**Electron density around 0KY J 203:**

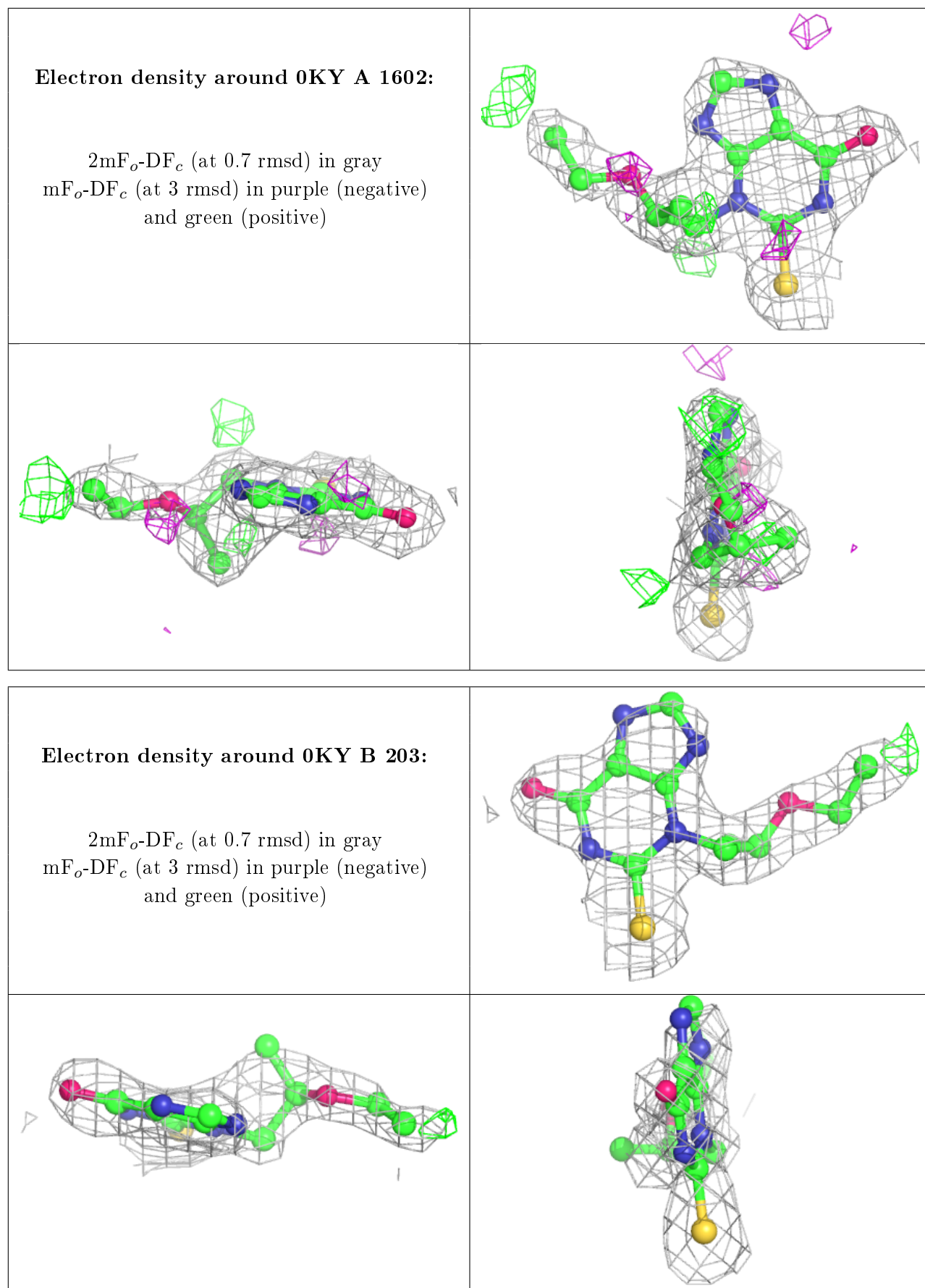
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 0KY I 1603:**

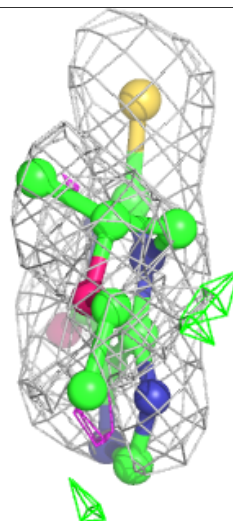
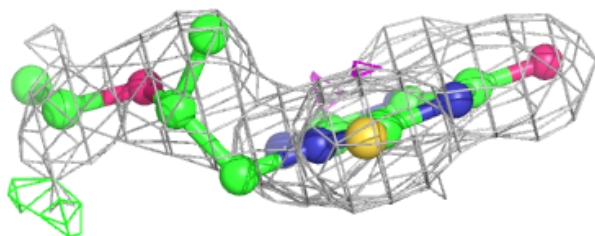
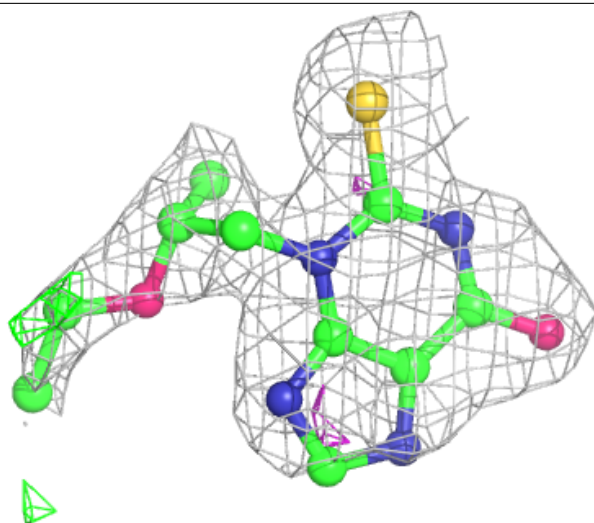
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





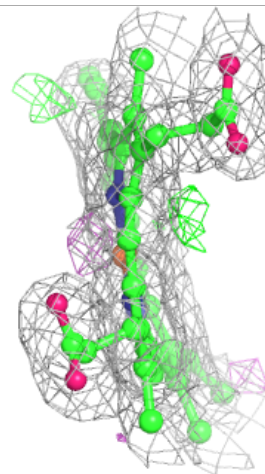
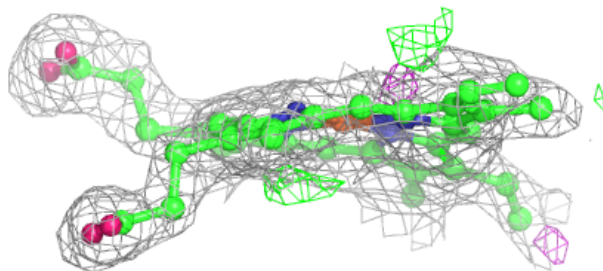
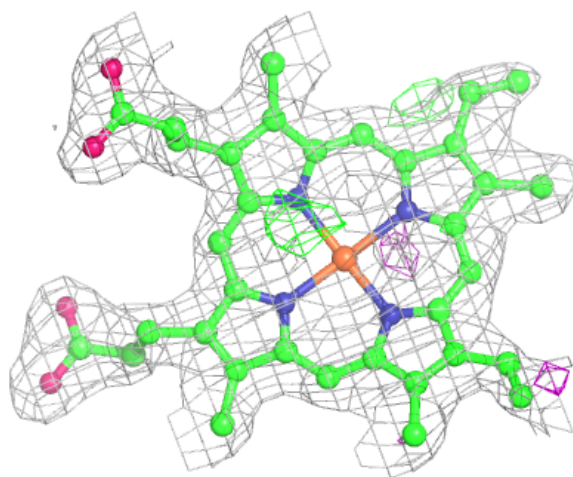
**Electron density around 0KY G 610:**

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and green (positive)



**Electron density around HEM F 202:**

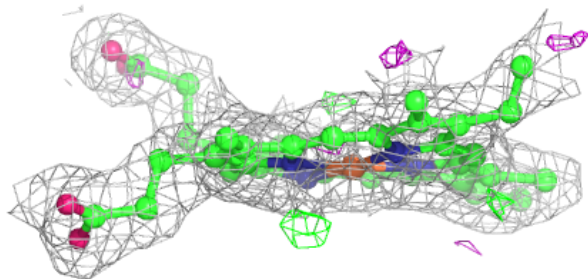
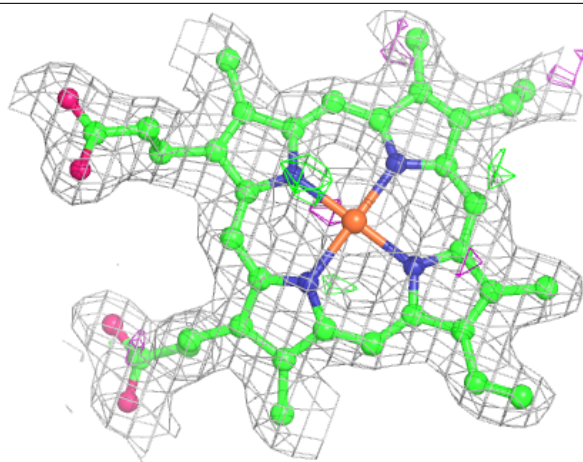
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





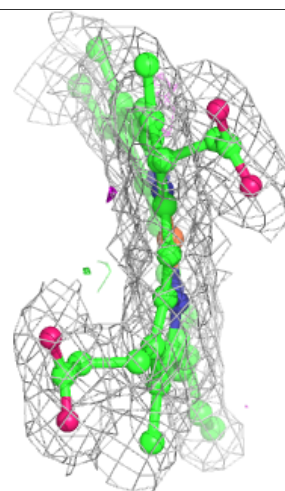
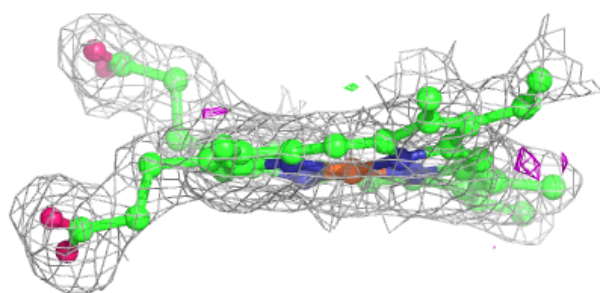
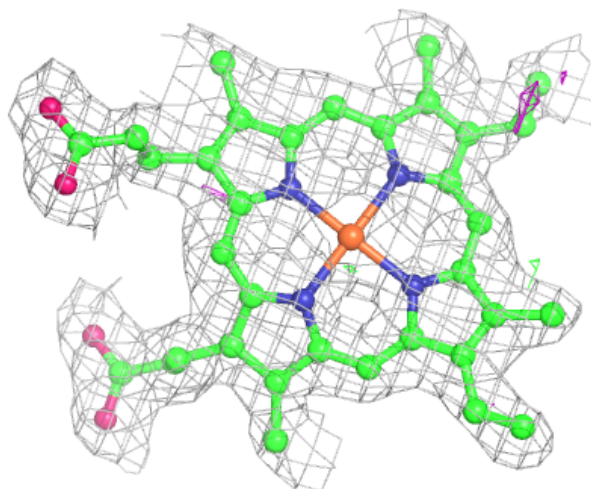
**Electron density around HEM J 202:**

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



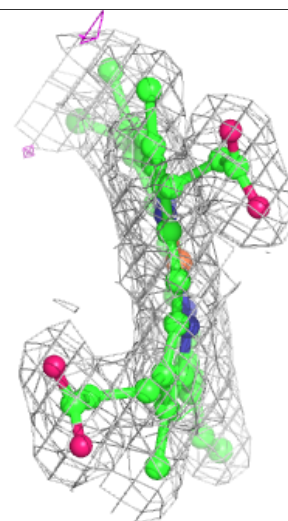
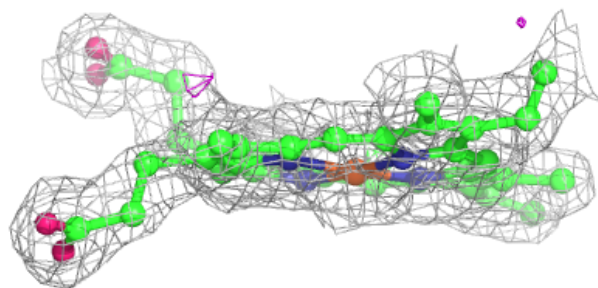
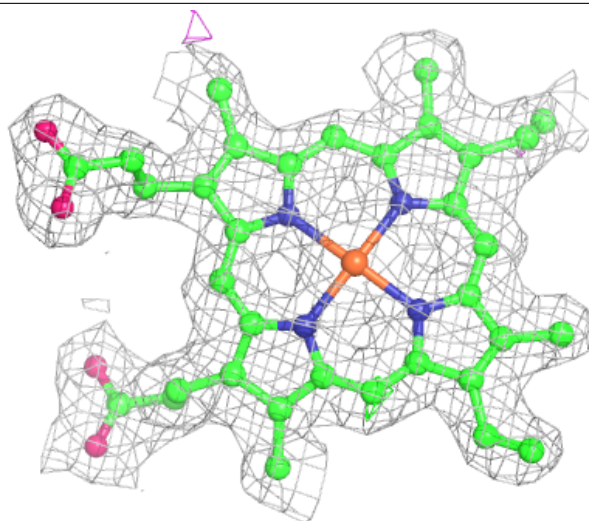
**Electron density around HEM N 202:**

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



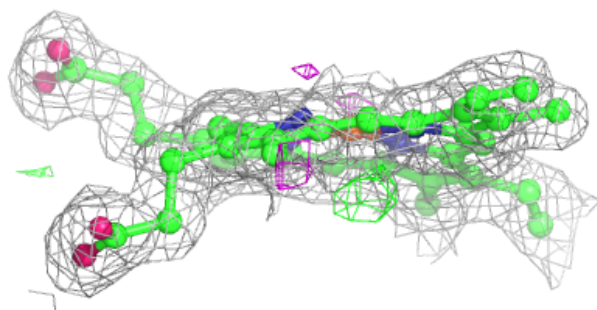
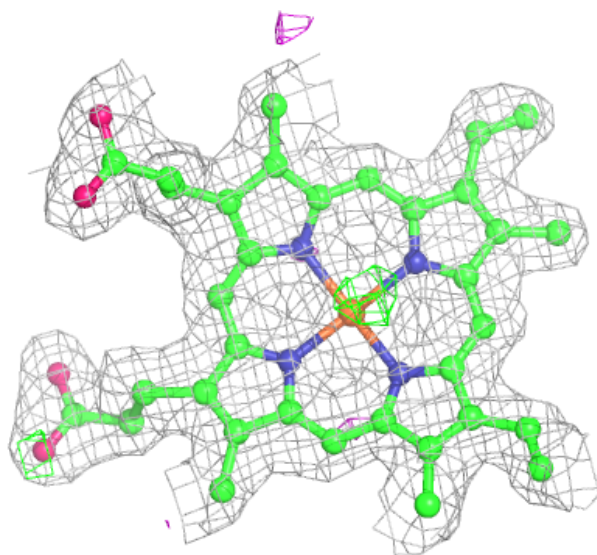
**Electron density around HEM I 1602:**

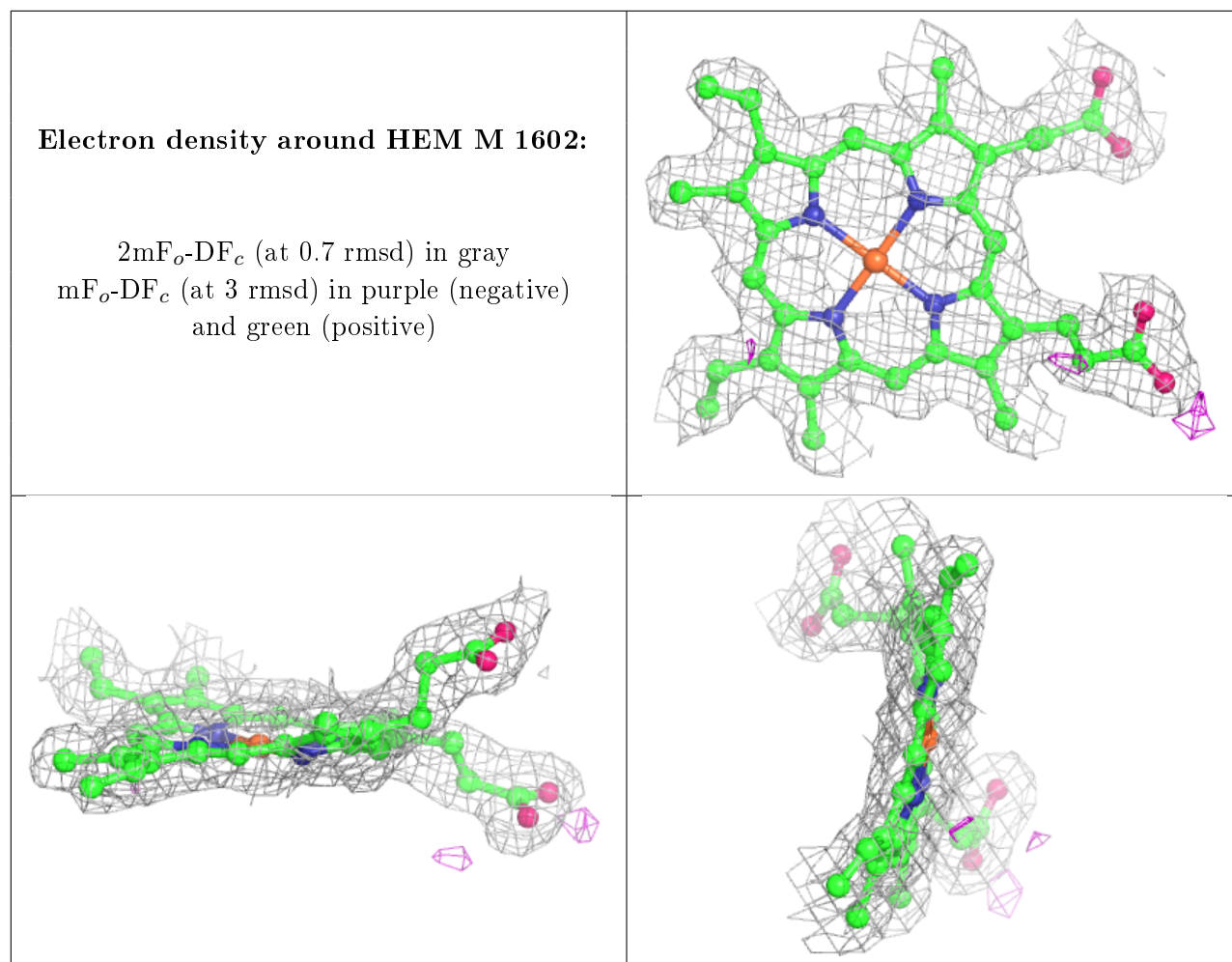
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 601:**

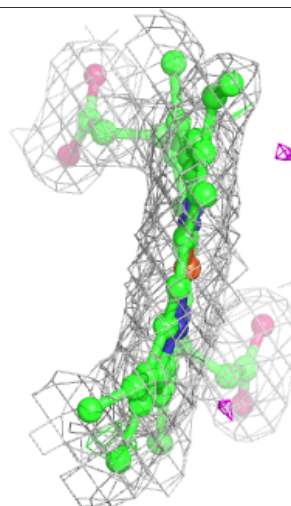
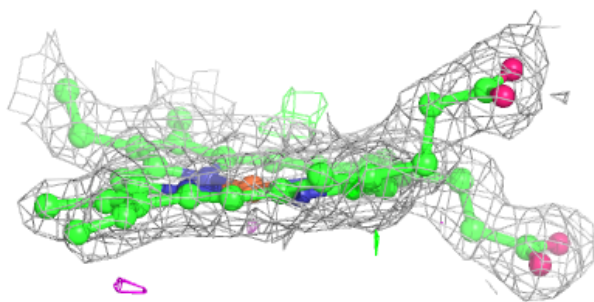
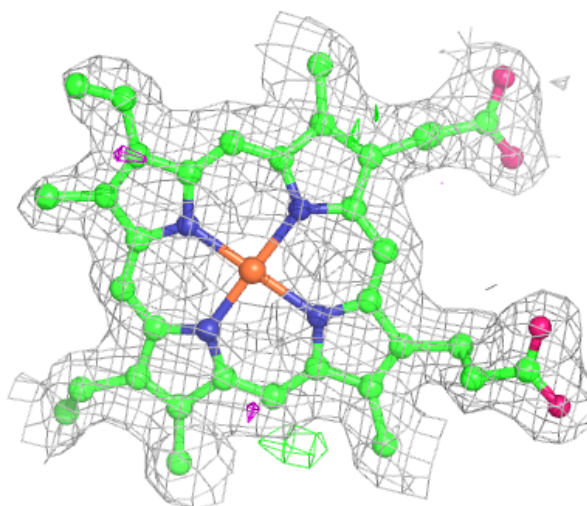
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

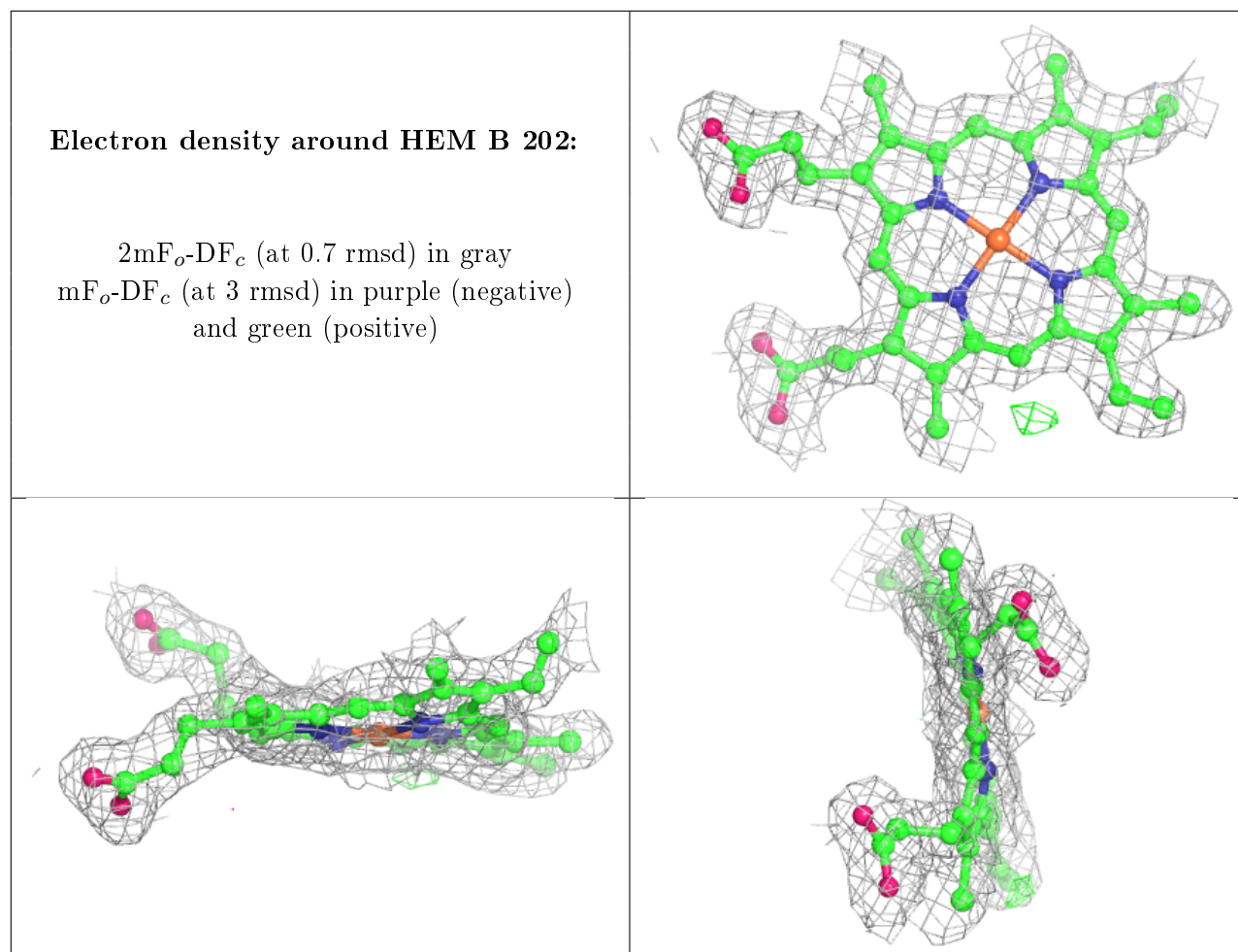




**Electron density around HEM E 1602:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.