



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:11 PM EDT

PDB ID : 2QJY / pdb\_00002qjy  
Title : Crystal structure of rhodobacter sphaeroides double mutant with stigmatellin and UQ2  
Authors : Esser, L.; Xia, D.  
Deposited on : 2007-07-09  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

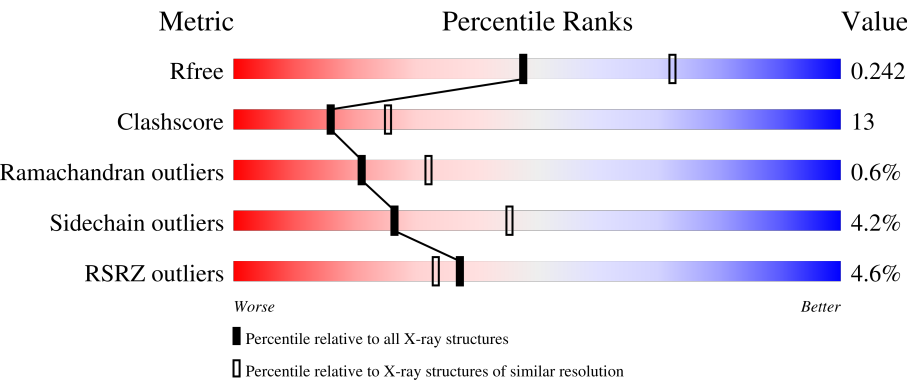
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 4912 (2.40-2.40)                                      |
| Clashscore            | 190562                      | 5391 (2.40-2.40)                                      |
| Ramachandran outliers | 187476                      | 5320 (2.40-2.40)                                      |
| Sidechain outliers    | 187428                      | 5321 (2.40-2.40)                                      |
| RSRZ outliers         | 180081                      | 4916 (2.40-2.40)                                      |

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

| Mol | Chain | Length | Quality of chain                                                     |
|-----|-------|--------|----------------------------------------------------------------------|
| 1   | A     | 445    | <div><div>2%</div><div>72%</div><div>21%</div><div>• •</div></div>   |
| 1   | D     | 445    | <div><div>2%</div><div>70%</div><div>24%</div><div>• •</div></div>   |
| 1   | G     | 445    | <div><div>2%</div><div>70%</div><div>23%</div><div>• •</div></div>   |
| 1   | J     | 445    | <div><div>3%</div><div>68%</div><div>25%</div><div>• • •</div></div> |
| 1   | M     | 445    | <div><div>2%</div><div>67%</div><div>26%</div><div>• •</div></div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | P     | 445    |                  |
| 2   | B     | 269    |                  |
| 2   | E     | 269    |                  |
| 2   | H     | 269    |                  |
| 2   | K     | 269    |                  |
| 2   | N     | 269    |                  |
| 2   | Q     | 269    |                  |
| 3   | C     | 187    |                  |
| 3   | F     | 187    |                  |
| 3   | I     | 187    |                  |
| 3   | L     | 187    |                  |
| 3   | O     | 187    |                  |
| 3   | R     | 187    |                  |

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 42656 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 Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3440  | 2322 | 548 | 555 | 15 |         |         |       |
| 1   | D     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3440  | 2322 | 548 | 555 | 15 |         |         |       |
| 1   | G     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3440  | 2322 | 548 | 555 | 15 |         |         |       |
| 1   | J     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3440  | 2322 | 548 | 555 | 15 |         |         |       |
| 1   | M     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3440  | 2322 | 548 | 555 | 15 |         |         |       |
| 1   | P     | 428      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3440  | 2322 | 548 | 555 | 15 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 287     | ARG      | SER    | engineered mutation | UNP Q02761 |
| D     | 287     | ARG      | SER    | engineered mutation | UNP Q02761 |
| G     | 287     | ARG      | SER    | engineered mutation | UNP Q02761 |
| J     | 287     | ARG      | SER    | engineered mutation | UNP Q02761 |
| M     | 287     | ARG      | SER    | engineered mutation | UNP Q02761 |
| P     | 287     | ARG      | SER    | engineered mutation | UNP Q02761 |

- Molecule 2 is a protein called Cytochrome c1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | B     | 256      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1953  | 1240 | 326 | 374 | 13 |         |         |       |
| 2   | E     | 256      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1953  | 1240 | 326 | 374 | 13 |         |         |       |
| 2   | H     | 256      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1953  | 1240 | 326 | 374 | 13 |         |         |       |

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| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 2   | K     | 256      | Total<br>1953 | C<br>1240 | N<br>326 | O<br>374 | S<br>13 | 0       | 0       | 0     |
| 2   | N     | 256      | Total<br>1953 | C<br>1240 | N<br>326 | O<br>374 | S<br>13 | 0       | 0       | 0     |
| 2   | Q     | 256      | Total<br>1953 | C<br>1240 | N<br>326 | O<br>374 | S<br>13 | 0       | 0       | 0     |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 264     | HIS      | -      | expression tag | UNP Q3IY11 |
| B     | 265     | HIS      | -      | expression tag | UNP Q3IY11 |
| B     | 266     | HIS      | -      | expression tag | UNP Q3IY11 |
| B     | 267     | HIS      | -      | expression tag | UNP Q3IY11 |
| B     | 268     | HIS      | -      | expression tag | UNP Q3IY11 |
| B     | 269     | HIS      | -      | expression tag | UNP Q3IY11 |
| E     | 264     | HIS      | -      | expression tag | UNP Q3IY11 |
| E     | 265     | HIS      | -      | expression tag | UNP Q3IY11 |
| E     | 266     | HIS      | -      | expression tag | UNP Q3IY11 |
| E     | 267     | HIS      | -      | expression tag | UNP Q3IY11 |
| E     | 268     | HIS      | -      | expression tag | UNP Q3IY11 |
| E     | 269     | HIS      | -      | expression tag | UNP Q3IY11 |
| H     | 264     | HIS      | -      | expression tag | UNP Q3IY11 |
| H     | 265     | HIS      | -      | expression tag | UNP Q3IY11 |
| H     | 266     | HIS      | -      | expression tag | UNP Q3IY11 |
| H     | 267     | HIS      | -      | expression tag | UNP Q3IY11 |
| H     | 268     | HIS      | -      | expression tag | UNP Q3IY11 |
| H     | 269     | HIS      | -      | expression tag | UNP Q3IY11 |
| K     | 264     | HIS      | -      | expression tag | UNP Q3IY11 |
| K     | 265     | HIS      | -      | expression tag | UNP Q3IY11 |
| K     | 266     | HIS      | -      | expression tag | UNP Q3IY11 |
| K     | 267     | HIS      | -      | expression tag | UNP Q3IY11 |
| K     | 268     | HIS      | -      | expression tag | UNP Q3IY11 |
| K     | 269     | HIS      | -      | expression tag | UNP Q3IY11 |
| N     | 264     | HIS      | -      | expression tag | UNP Q3IY11 |
| N     | 265     | HIS      | -      | expression tag | UNP Q3IY11 |
| N     | 266     | HIS      | -      | expression tag | UNP Q3IY11 |
| N     | 267     | HIS      | -      | expression tag | UNP Q3IY11 |
| N     | 268     | HIS      | -      | expression tag | UNP Q3IY11 |
| N     | 269     | HIS      | -      | expression tag | UNP Q3IY11 |
| Q     | 264     | HIS      | -      | expression tag | UNP Q3IY11 |
| Q     | 265     | HIS      | -      | expression tag | UNP Q3IY11 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| Q     | 266     | HIS      | -      | expression tag | UNP Q3IY11 |
| Q     | 267     | HIS      | -      | expression tag | UNP Q3IY11 |
| Q     | 268     | HIS      | -      | expression tag | UNP Q3IY11 |
| Q     | 269     | HIS      | -      | expression tag | UNP Q3IY11 |

- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 843 | 237 | 254 | 6 |         |         |       |
| 3   | F     | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 843 | 237 | 254 | 6 |         |         |       |
| 3   | I     | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 843 | 237 | 254 | 6 |         |         |       |
| 3   | L     | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 843 | 237 | 254 | 6 |         |         |       |
| 3   | O     | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 843 | 237 | 254 | 6 |         |         |       |
| 3   | R     | 179      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1340  | 843 | 237 | 254 | 6 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| C     | 135     | SER      | VAL    | engineered mutation | UNP Q02762 |
| F     | 135     | SER      | VAL    | engineered mutation | UNP Q02762 |
| I     | 135     | SER      | VAL    | engineered mutation | UNP Q02762 |
| L     | 135     | SER      | VAL    | engineered mutation | UNP Q02762 |
| O     | 135     | SER      | VAL    | engineered mutation | UNP Q02762 |
| R     | 135     | SER      | VAL    | engineered mutation | UNP Q02762 |

- Molecule 4 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

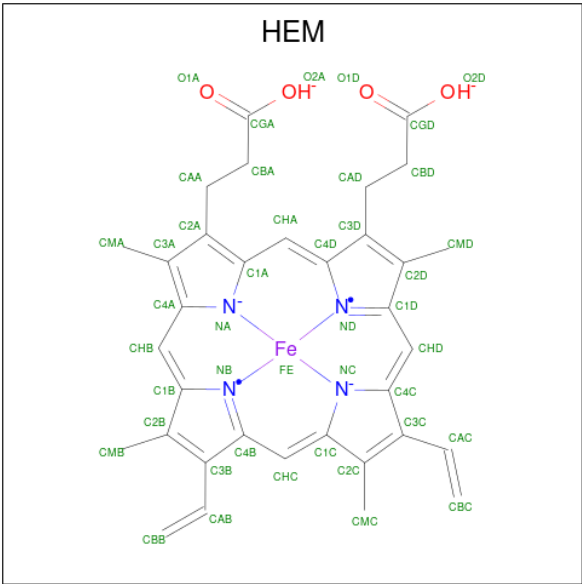
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | B     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | E     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | G     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | H     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | K     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | M     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | N     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 4   | Q     | 1        | Total | Sr | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



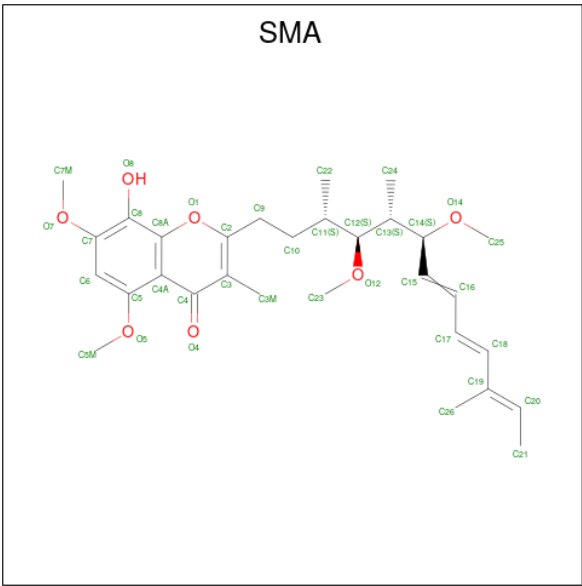
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 5   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

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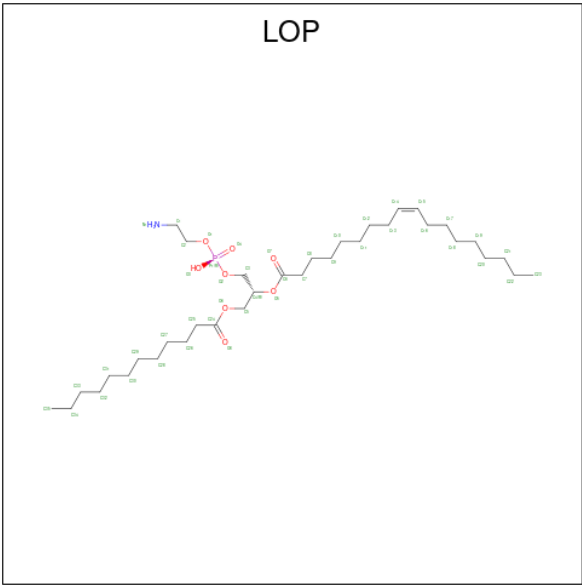
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 5   | G     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | G     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | H     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | J     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | J     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | K     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | M     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | M     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | N     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | P     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | P     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 5   | Q     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 6 is STIGMATELLIN A (CCD ID: SMA) (formula: C<sub>30</sub>H<sub>42</sub>O<sub>7</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |
| 6   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |
| 6   | G     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |
| 6   | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |
| 6   | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |
| 6   | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 37    | 30 | 7 |         |         |

- Molecule 7 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: C<sub>35</sub>H<sub>68</sub>NO<sub>8</sub>P).



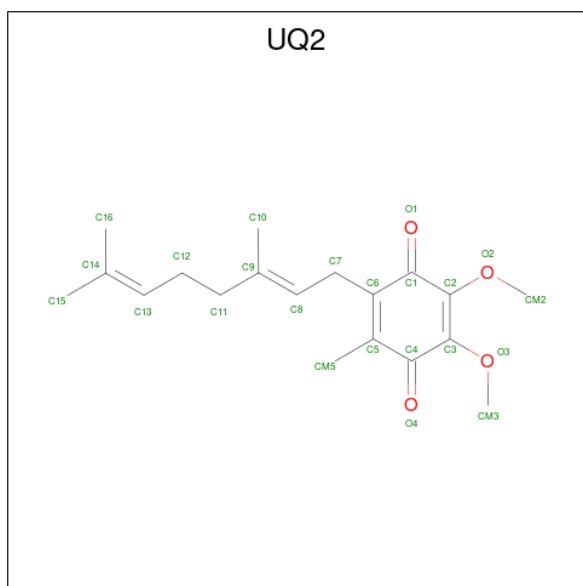
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 7   | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |         |
| 7   | D     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |         |
| 7   | G     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |         |
| 7   | J     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |         |
| 7   | M     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |         |

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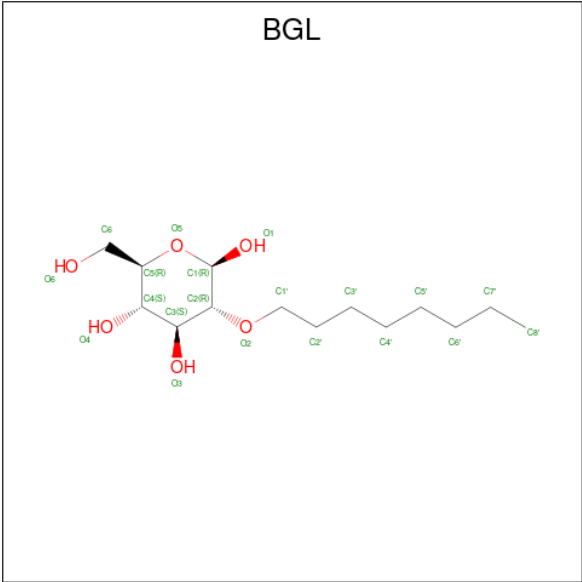
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 7   | P     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |         |

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



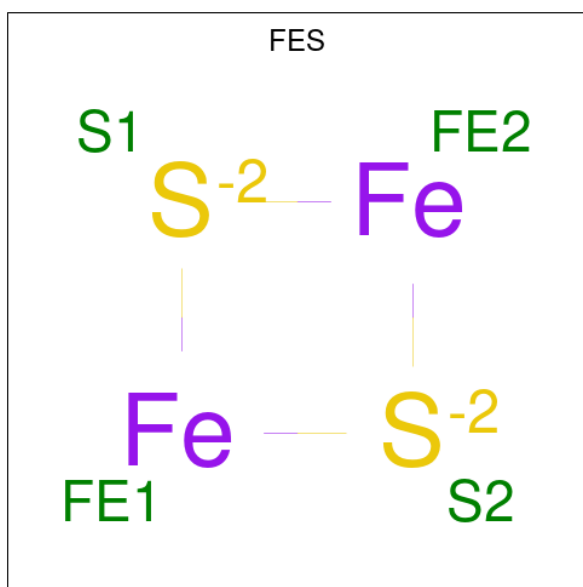
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 8   | A     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |
| 8   | D     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |
| 8   | G     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |
| 8   | J     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |
| 8   | M     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |
| 8   | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 23    | 19 | 4 |         |         |

- Molecule 9 is 2-O-octyl-beta-D-glucopyranose (CCD ID: BGL) (formula:  $C_{14}H_{28}O_6$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9   | B     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 9   | E     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 9   | G     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 9   | K     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 9   | N     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |
| 9   | P     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 20    | 14 | 6 |         |         |

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 10  | C     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 10  | F     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 10  | I     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 10  | L     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 10  | O     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |
| 10  | R     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 11  | I     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 11  | R     | 1        | Total | Cl | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 12 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 12  | R     | 1        | Total | Na | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

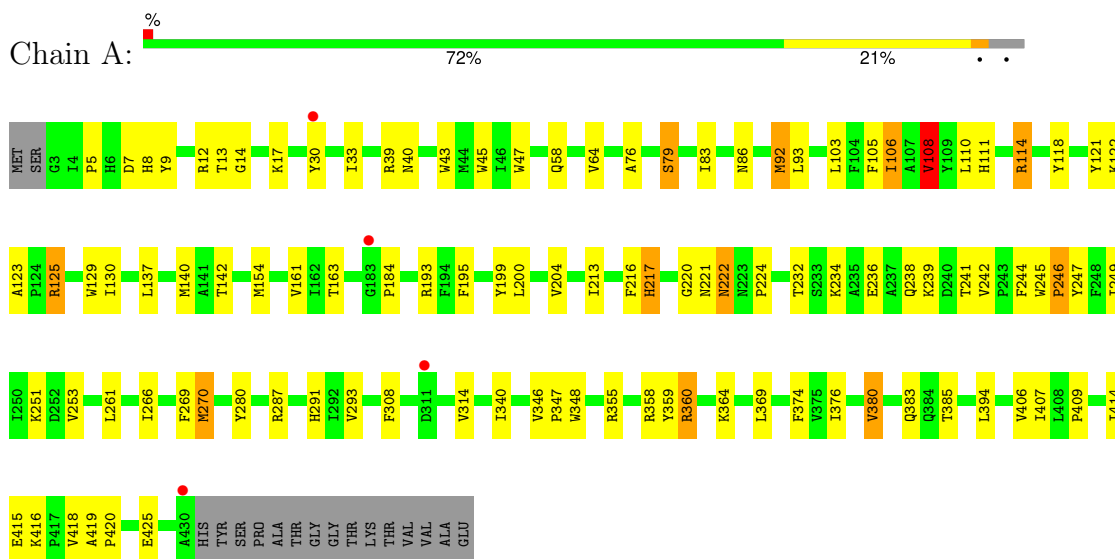
- Molecule 13 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 13  | A     | 73       | Total O<br>73 73 | 0       | 0       |
| 13  | B     | 19       | Total O<br>19 19 | 0       | 0       |
| 13  | C     | 47       | Total O<br>47 47 | 0       | 0       |
| 13  | D     | 64       | Total O<br>64 64 | 0       | 0       |
| 13  | E     | 14       | Total O<br>14 14 | 0       | 0       |
| 13  | F     | 36       | Total O<br>36 36 | 0       | 0       |
| 13  | G     | 68       | Total O<br>68 68 | 0       | 0       |
| 13  | H     | 35       | Total O<br>35 35 | 0       | 0       |
| 13  | I     | 42       | Total O<br>42 42 | 0       | 0       |
| 13  | J     | 55       | Total O<br>55 55 | 0       | 0       |
| 13  | K     | 17       | Total O<br>17 17 | 0       | 0       |
| 13  | L     | 42       | Total O<br>42 42 | 0       | 0       |
| 13  | M     | 34       | Total O<br>34 34 | 0       | 0       |
| 13  | N     | 11       | Total O<br>11 11 | 0       | 0       |
| 13  | O     | 41       | Total O<br>41 41 | 0       | 0       |
| 13  | P     | 60       | Total O<br>60 60 | 0       | 0       |
| 13  | Q     | 16       | Total O<br>16 16 | 0       | 0       |
| 13  | R     | 24       | Total O<br>24 24 | 0       | 0       |

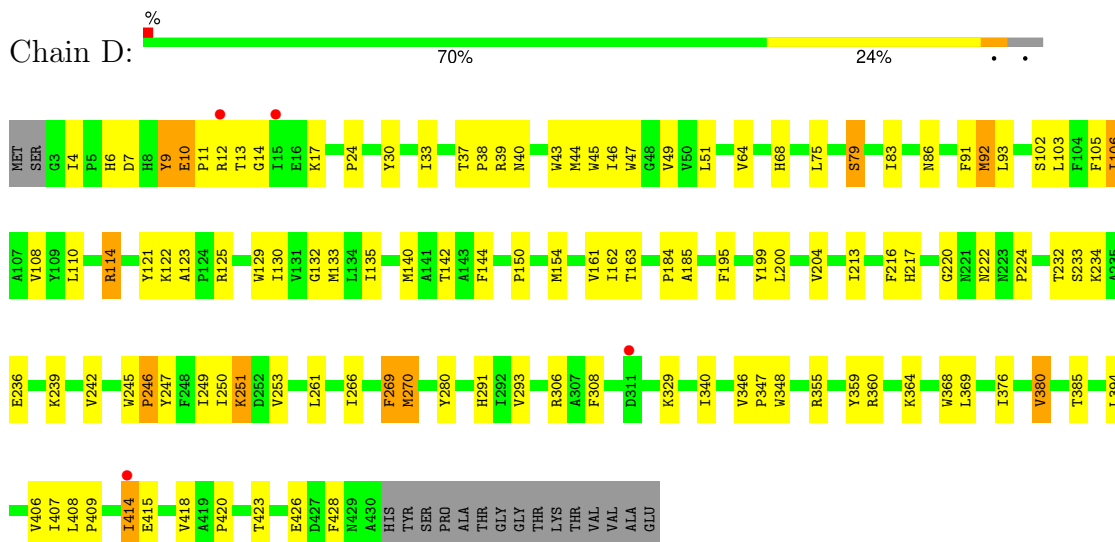
### 3 Residue-property plots

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

#### • Molecule 1: Cytochrome b



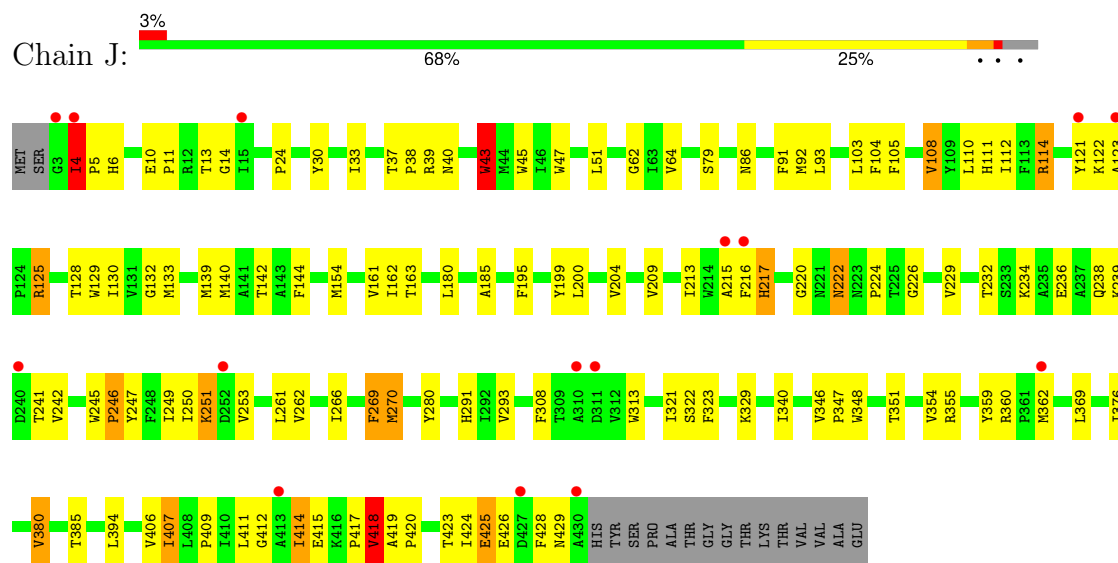
#### • Molecule 1: Cytochrome b



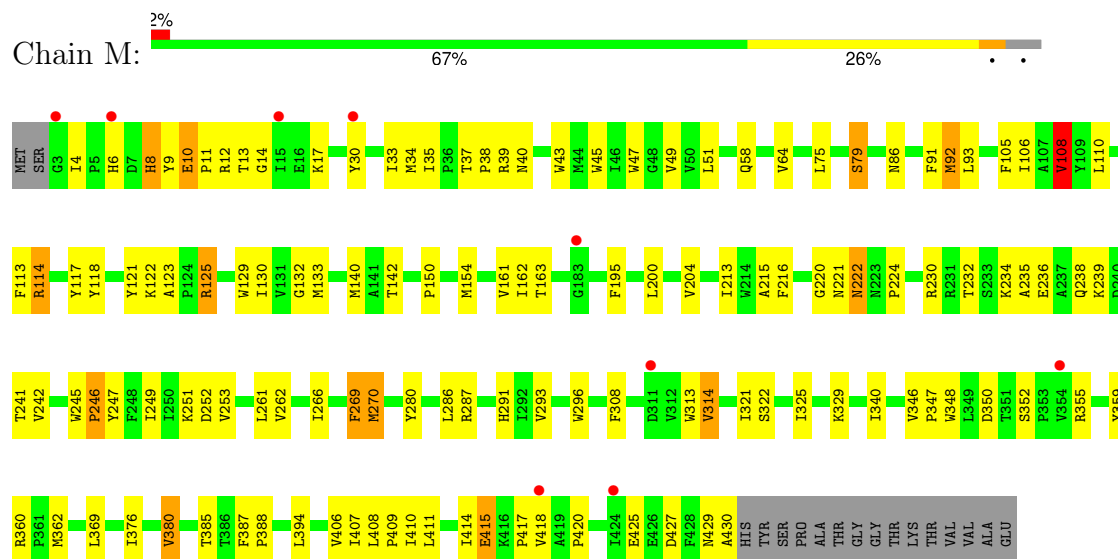
#### • Molecule 1: Cytochrome b



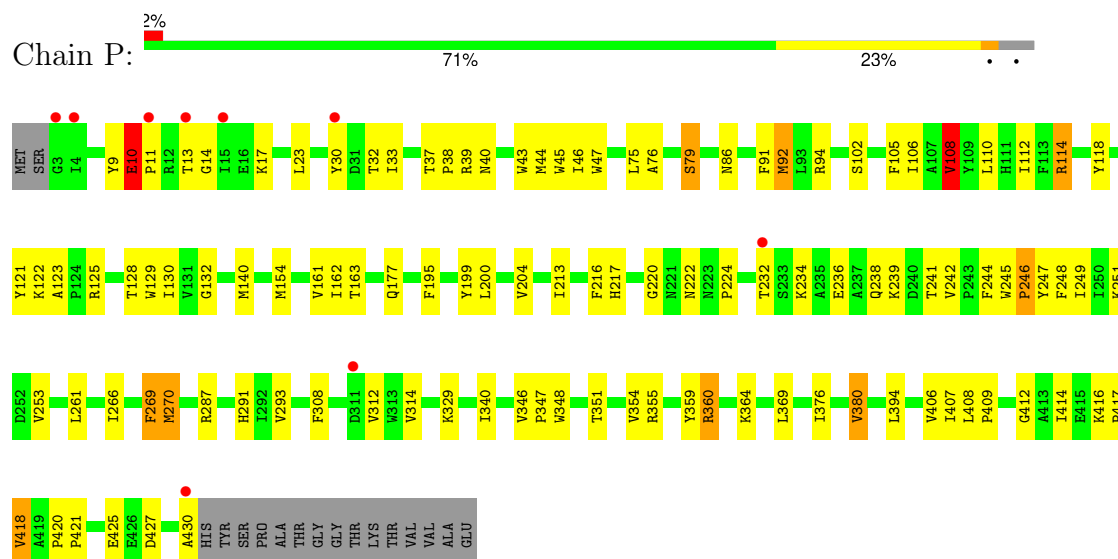
- Molecule 1: Cytochrome b



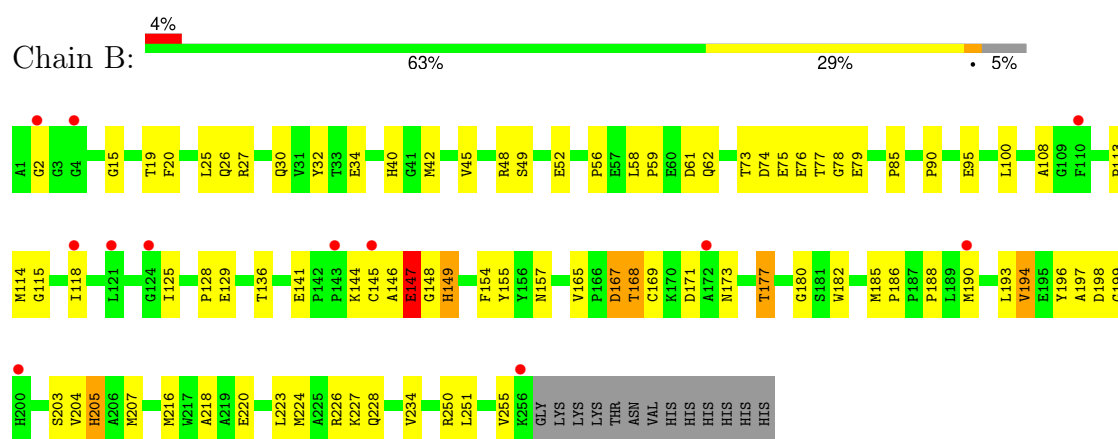
- Molecule 1: Cytochrome b



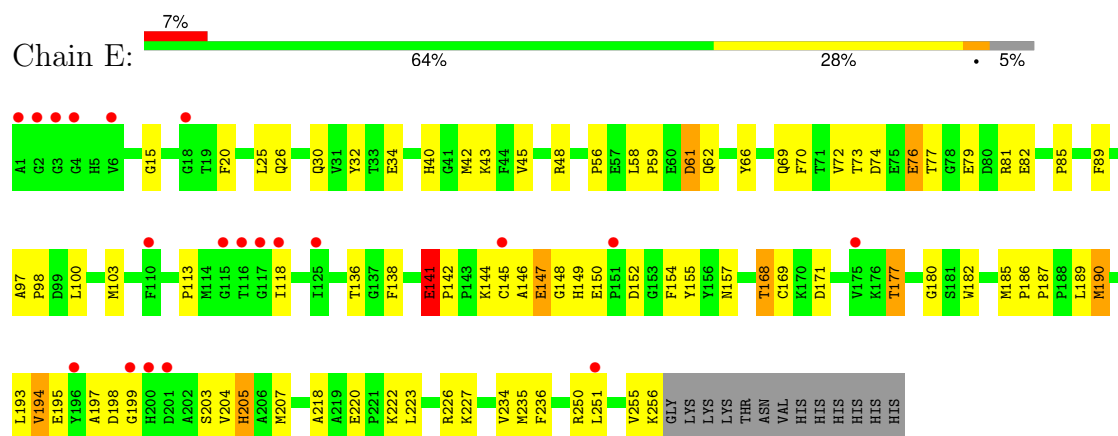
- Molecule 1: Cytochrome b



- Molecule 2: Cytochrome c1

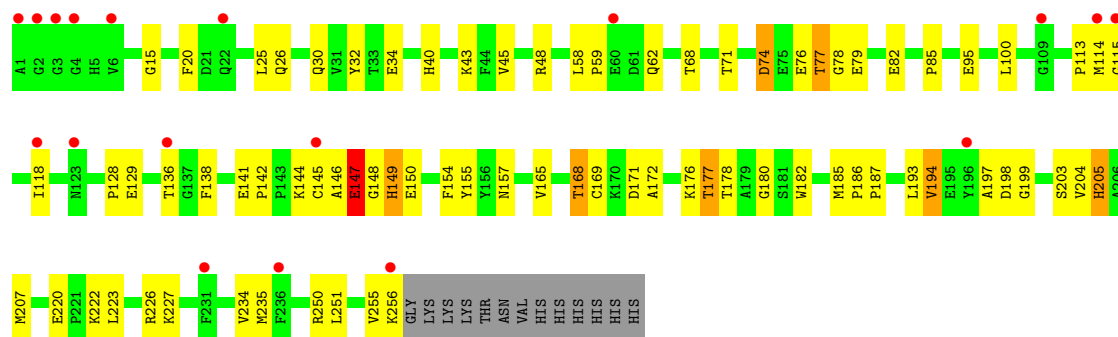


- Molecule 2: Cytochrome c1

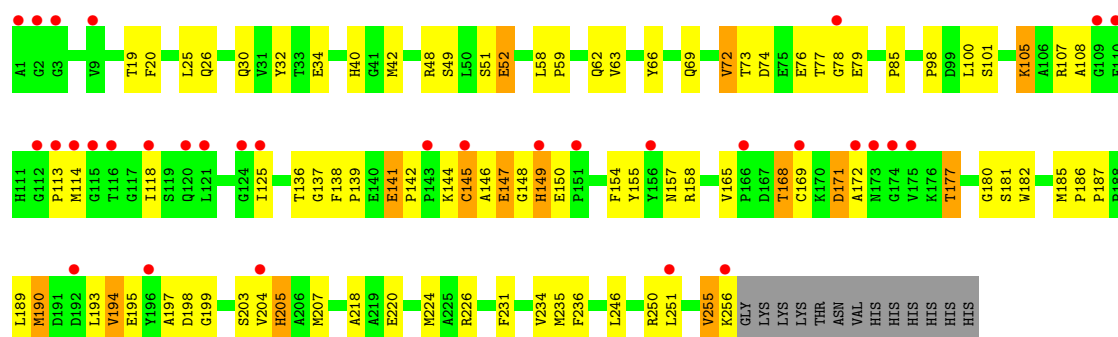


- Molecule 2: Cytochrome c1

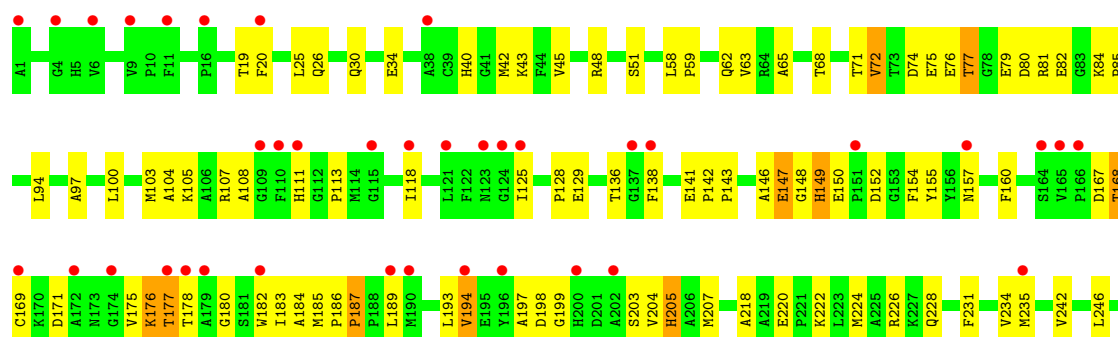




• Molecule 2: Cytochrome c1

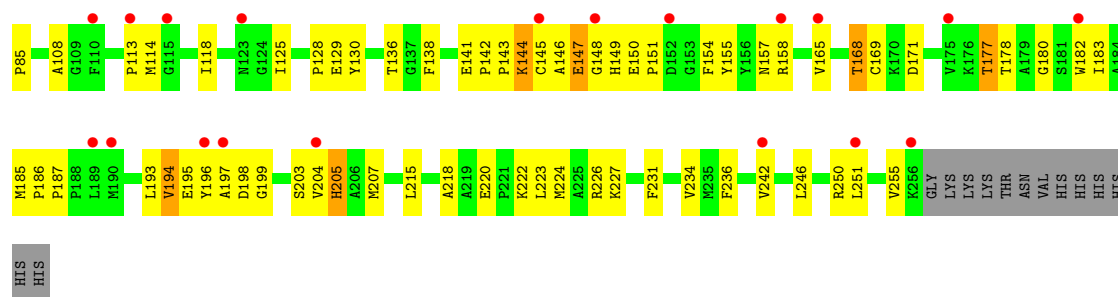


• Molecule 2: Cytochrome c1

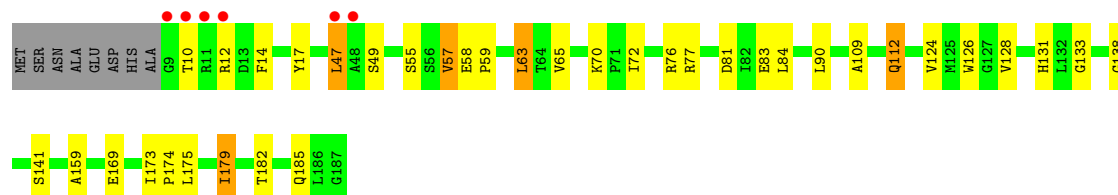
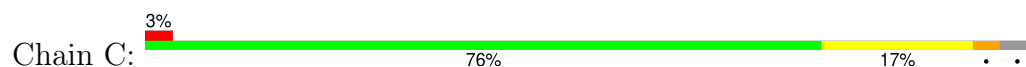


• Molecule 2: Cytochrome c1

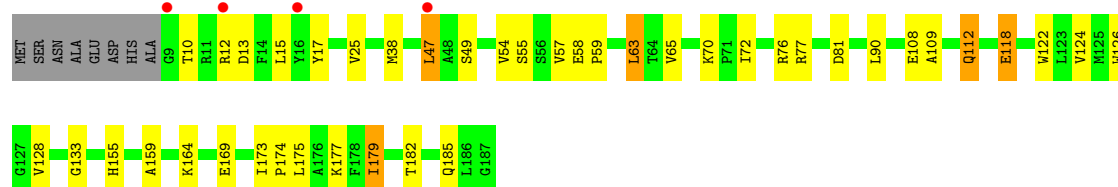




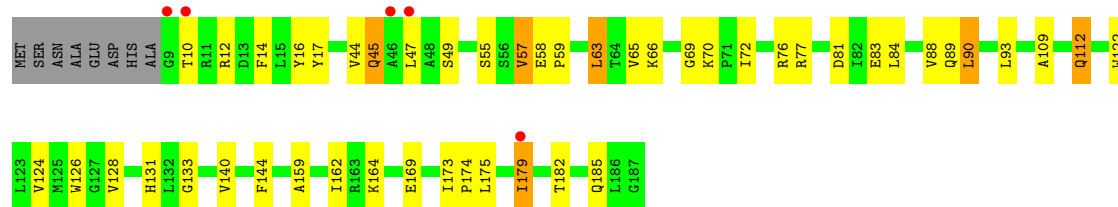
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



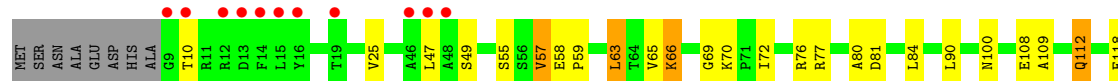
- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

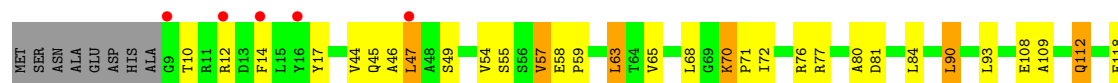


- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

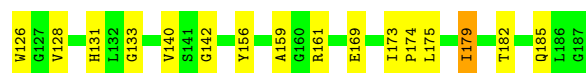
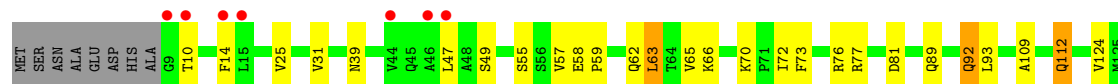
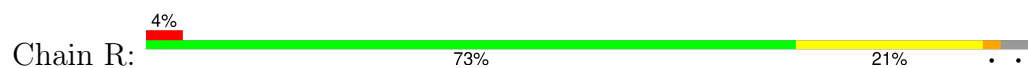




- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



- Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 351.89Å 147.04Å 161.31Å<br>90.00° 104.25° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 18.00 – 2.40<br>18.00 – 2.40                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.7 (18.00-2.40)<br>93.1 (18.00-2.40)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | 0.11                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.48 (at 2.34Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.226 , 0.251<br>0.225 , 0.242                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 9798 reflections (1.70%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.289                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 52.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 42656                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 70.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UQ2, BGL, HEM, FES, SMA, SR, NA, CL, LOP

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     | 0.47         | 0/3570         | 1.03        | 28/4897 (0.6%)   |
| 1   | D     | 0.48         | 0/3570         | 1.03        | 26/4897 (0.5%)   |
| 1   | G     | 0.47         | 0/3570         | 1.04        | 31/4897 (0.6%)   |
| 1   | J     | 0.48         | 0/3570         | 1.04        | 29/4897 (0.6%)   |
| 1   | M     | 0.45         | 0/3570         | 1.03        | 29/4897 (0.6%)   |
| 1   | P     | 0.47         | 0/3570         | 1.03        | 31/4897 (0.6%)   |
| 2   | B     | 0.44         | 0/2010         | 1.03        | 6/2733 (0.2%)    |
| 2   | E     | 0.43         | 0/2010         | 1.02        | 7/2733 (0.3%)    |
| 2   | H     | 0.45         | 0/2010         | 1.02        | 7/2733 (0.3%)    |
| 2   | K     | 0.42         | 0/2010         | 1.01        | 6/2733 (0.2%)    |
| 2   | N     | 0.41         | 0/2010         | 1.02        | 7/2733 (0.3%)    |
| 2   | Q     | 0.43         | 0/2010         | 0.99        | 3/2733 (0.1%)    |
| 3   | C     | 0.46         | 0/1370         | 1.05        | 6/1866 (0.3%)    |
| 3   | F     | 0.48         | 0/1370         | 1.05        | 6/1866 (0.3%)    |
| 3   | I     | 0.51         | 1/1370 (0.1%)  | 1.14        | 13/1866 (0.7%)   |
| 3   | L     | 0.47         | 0/1370         | 1.03        | 6/1866 (0.3%)    |
| 3   | O     | 0.46         | 0/1370         | 1.04        | 5/1866 (0.3%)    |
| 3   | R     | 0.45         | 0/1370         | 1.05        | 7/1866 (0.4%)    |
| All | All   | 0.46         | 1/41700 (0.0%) | 1.03        | 253/56976 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 1                   |
| 2   | E     | 0                   | 1                   |
| 2   | H     | 0                   | 1                   |
| 2   | K     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | I     | 44  | VAL  | CA-C  | 5.01 | 1.59        | 1.52     |

All (253) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | I     | 44  | VAL  | N-CA-C  | 14.17 | 123.85      | 110.53   |
| 3   | O     | 133 | GLY  | N-CA-C  | 9.60  | 126.12      | 114.69   |
| 3   | R     | 133 | GLY  | N-CA-C  | 9.45  | 125.94      | 114.69   |
| 3   | I     | 133 | GLY  | N-CA-C  | 9.41  | 125.89      | 114.69   |
| 3   | F     | 133 | GLY  | N-CA-C  | 9.17  | 125.60      | 114.69   |
| 1   | J     | 313 | TRP  | N-CA-C  | 8.97  | 121.13      | 111.36   |
| 3   | C     | 133 | GLY  | N-CA-C  | 8.96  | 125.35      | 114.69   |
| 3   | L     | 133 | GLY  | N-CA-C  | 8.93  | 125.31      | 114.69   |
| 1   | G     | 9   | TYR  | N-CA-C  | 8.66  | 122.45      | 110.24   |
| 1   | P     | 108 | VAL  | CB-CA-C | -8.29 | 100.78      | 112.22   |
| 1   | J     | 4   | ILE  | N-CA-C  | 8.15  | 116.60      | 109.02   |
| 1   | G     | 108 | VAL  | CB-CA-C | -7.88 | 101.34      | 112.22   |
| 3   | F     | 169 | GLU  | N-CA-C  | 7.74  | 119.77      | 108.86   |
| 3   | I     | 169 | GLU  | N-CA-C  | 7.63  | 119.62      | 108.86   |
| 3   | I     | 93  | LEU  | N-CA-C  | 7.61  | 122.41      | 110.32   |
| 3   | O     | 169 | GLU  | N-CA-C  | 7.59  | 119.56      | 108.86   |
| 1   | P     | 10  | GLU  | CA-C-N  | 7.54  | 128.72      | 119.98   |
| 1   | P     | 10  | GLU  | C-N-CA  | 7.54  | 128.72      | 119.98   |
| 3   | L     | 169 | GLU  | N-CA-C  | 7.50  | 119.44      | 108.86   |
| 3   | C     | 169 | GLU  | N-CA-C  | 7.50  | 119.44      | 108.86   |
| 2   | K     | 78  | GLY  | N-CA-C  | -7.41 | 105.62      | 115.40   |
| 3   | R     | 169 | GLU  | N-CA-C  | 7.38  | 119.26      | 108.86   |
| 2   | H     | 144 | LYS  | N-CA-C  | 7.36  | 119.30      | 111.28   |
| 1   | G     | 407 | ILE  | N-CA-C  | 7.29  | 118.02      | 110.36   |
| 2   | B     | 78  | GLY  | N-CA-C  | -7.29 | 106.16      | 115.42   |
| 1   | M     | 407 | ILE  | N-CA-C  | 7.25  | 117.97      | 110.36   |
| 1   | D     | 407 | ILE  | N-CA-C  | 7.14  | 117.86      | 110.36   |
| 1   | J     | 125 | ARG  | N-CA-C  | 7.14  | 120.54      | 112.97   |
| 1   | M     | 125 | ARG  | N-CA-C  | 7.08  | 120.86      | 112.93   |
| 2   | K     | 105 | LYS  | N-CA-C  | -7.00 | 105.67      | 114.56   |
| 1   | G     | 200 | LEU  | N-CA-C  | 6.99  | 118.69      | 111.14   |
| 1   | M     | 108 | VAL  | CB-CA-C | -6.90 | 102.70      | 112.22   |
| 2   | N     | 43  | LYS  | N-CA-C  | 6.90  | 121.31      | 112.34   |
| 1   | A     | 125 | ARG  | N-CA-C  | 6.87  | 120.62      | 112.93   |
| 2   | K     | 76  | GLU  | N-CA-C  | -6.86 | 103.94      | 112.72   |
| 1   | P     | 125 | ARG  | N-CA-C  | 6.79  | 120.53      | 112.93   |
| 2   | K     | 193 | LEU  | N-CA-C  | -6.76 | 105.03      | 113.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | M     | 200 | LEU  | N-CA-C  | 6.75  | 118.42      | 111.14   |
| 2   | Q     | 193 | LEU  | N-CA-C  | -6.74 | 105.06      | 113.28   |
| 1   | M     | 313 | TRP  | N-CA-C  | 6.74  | 118.63      | 111.28   |
| 1   | D     | 125 | ARG  | N-CA-C  | 6.73  | 120.47      | 112.93   |
| 2   | E     | 193 | LEU  | N-CA-C  | -6.73 | 105.07      | 113.28   |
| 2   | N     | 193 | LEU  | N-CA-C  | -6.70 | 105.07      | 113.18   |
| 1   | M     | 321 | ILE  | CB-CA-C | -6.70 | 103.26      | 112.04   |
| 3   | R     | 93  | LEU  | N-CA-C  | 6.67  | 120.93      | 110.32   |
| 2   | B     | 193 | LEU  | N-CA-C  | -6.66 | 105.16      | 113.28   |
| 1   | G     | 125 | ARG  | N-CA-C  | 6.61  | 120.33      | 112.93   |
| 2   | H     | 193 | LEU  | N-CA-C  | -6.61 | 105.18      | 113.18   |
| 2   | H     | 43  | LYS  | N-CA-C  | 6.61  | 120.93      | 112.34   |
| 1   | J     | 200 | LEU  | N-CA-C  | 6.57  | 118.23      | 111.14   |
| 1   | J     | 407 | ILE  | N-CA-C  | 6.55  | 117.23      | 110.36   |
| 1   | P     | 200 | LEU  | N-CA-C  | 6.51  | 118.17      | 111.14   |
| 1   | J     | 415 | GLU  | N-CA-C  | 6.50  | 120.09      | 110.48   |
| 1   | P     | 232 | THR  | N-CA-C  | 6.46  | 119.14      | 111.71   |
| 1   | D     | 200 | LEU  | N-CA-C  | 6.45  | 118.11      | 111.14   |
| 2   | B     | 75  | GLU  | N-CA-C  | 6.44  | 120.40      | 112.54   |
| 1   | P     | 407 | ILE  | N-CA-C  | 6.42  | 117.10      | 110.36   |
| 1   | A     | 232 | THR  | N-CA-C  | 6.40  | 119.07      | 111.71   |
| 1   | G     | 232 | THR  | N-CA-C  | 6.36  | 119.02      | 111.71   |
| 1   | M     | 232 | THR  | N-CA-C  | 6.36  | 119.02      | 111.71   |
| 1   | J     | 232 | THR  | N-CA-C  | 6.35  | 119.01      | 111.71   |
| 1   | D     | 232 | THR  | N-CA-C  | 6.34  | 119.01      | 111.71   |
| 2   | Q     | 43  | LYS  | N-CA-C  | 6.30  | 120.53      | 112.34   |
| 1   | A     | 200 | LEU  | N-CA-C  | 6.30  | 117.94      | 111.14   |
| 1   | G     | 220 | GLY  | N-CA-C  | -6.29 | 104.86      | 112.48   |
| 1   | D     | 308 | PHE  | N-CA-C  | 6.26  | 119.45      | 108.56   |
| 1   | A     | 269 | PHE  | N-CA-C  | 6.22  | 121.15      | 113.50   |
| 1   | A     | 163 | THR  | N-CA-C  | -6.22 | 105.18      | 112.89   |
| 1   | A     | 308 | PHE  | N-CA-C  | 6.21  | 119.37      | 108.56   |
| 1   | P     | 163 | THR  | N-CA-C  | -6.21 | 105.20      | 112.89   |
| 1   | M     | 270 | MET  | CA-C-N  | 6.20  | 125.88      | 119.56   |
| 1   | M     | 270 | MET  | C-N-CA  | 6.20  | 125.88      | 119.56   |
| 1   | P     | 308 | PHE  | N-CA-C  | 6.13  | 119.23      | 108.56   |
| 1   | A     | 270 | MET  | CA-C-N  | 6.11  | 125.79      | 119.56   |
| 1   | A     | 270 | MET  | C-N-CA  | 6.11  | 125.79      | 119.56   |
| 1   | G     | 270 | MET  | CA-C-N  | 6.10  | 125.78      | 119.56   |
| 1   | G     | 270 | MET  | C-N-CA  | 6.10  | 125.78      | 119.56   |
| 1   | M     | 220 | GLY  | N-CA-C  | -6.06 | 105.15      | 112.48   |
| 1   | M     | 10  | GLU  | CA-C-N  | 6.06  | 127.01      | 119.98   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | M     | 10  | GLU  | C-N-CA | 6.06  | 127.01      | 119.98   |
| 1   | P     | 270 | MET  | CA-C-N | 6.06  | 125.74      | 119.56   |
| 1   | P     | 270 | MET  | C-N-CA | 6.06  | 125.74      | 119.56   |
| 1   | J     | 308 | PHE  | N-CA-C | 6.04  | 119.06      | 108.56   |
| 1   | M     | 308 | PHE  | N-CA-C | 6.03  | 119.05      | 108.56   |
| 1   | A     | 407 | ILE  | N-CA-C | 6.02  | 117.48      | 110.62   |
| 1   | P     | 220 | GLY  | N-CA-C | -6.02 | 105.20      | 112.48   |
| 1   | D     | 220 | GLY  | N-CA-C | -6.01 | 105.21      | 112.48   |
| 1   | D     | 415 | GLU  | N-CA-C | 5.99  | 119.35      | 110.48   |
| 1   | A     | 220 | GLY  | N-CA-C | -5.99 | 105.23      | 112.48   |
| 1   | P     | 360 | ARG  | CA-C-N | 5.99  | 125.70      | 119.05   |
| 1   | P     | 360 | ARG  | C-N-CA | 5.99  | 125.70      | 119.05   |
| 1   | A     | 40  | ASN  | N-CA-C | 5.99  | 120.20      | 113.02   |
| 1   | J     | 270 | MET  | CA-C-N | 5.97  | 125.65      | 119.56   |
| 1   | J     | 270 | MET  | C-N-CA | 5.97  | 125.65      | 119.56   |
| 1   | P     | 414 | ILE  | N-CA-C | 5.97  | 120.56      | 113.22   |
| 1   | G     | 269 | PHE  | N-CA-C | 5.96  | 120.83      | 113.50   |
| 1   | D     | 270 | MET  | CA-C-N | 5.96  | 125.64      | 119.56   |
| 1   | D     | 270 | MET  | C-N-CA | 5.96  | 125.64      | 119.56   |
| 1   | J     | 220 | GLY  | N-CA-C | -5.96 | 105.27      | 112.48   |
| 1   | M     | 415 | GLU  | N-CA-C | 5.94  | 119.28      | 110.48   |
| 1   | D     | 40  | ASN  | N-CA-C | 5.94  | 120.15      | 113.02   |
| 1   | M     | 269 | PHE  | N-CA-C | 5.94  | 120.81      | 113.50   |
| 1   | P     | 204 | VAL  | N-CA-C | -5.93 | 104.95      | 110.53   |
| 1   | M     | 360 | ARG  | CA-C-N | 5.92  | 125.63      | 119.05   |
| 1   | M     | 360 | ARG  | C-N-CA | 5.92  | 125.63      | 119.05   |
| 1   | G     | 204 | VAL  | N-CA-C | -5.92 | 104.96      | 110.53   |
| 2   | B     | 76  | GLU  | N-CA-C | -5.91 | 106.10      | 113.55   |
| 1   | J     | 269 | PHE  | N-CA-C | 5.88  | 120.74      | 113.50   |
| 2   | E     | 89  | PHE  | CA-C-N | -5.87 | 114.70      | 120.52   |
| 2   | E     | 89  | PHE  | C-N-CA | -5.87 | 114.70      | 120.52   |
| 1   | M     | 204 | VAL  | N-CA-C | -5.85 | 104.81      | 110.72   |
| 1   | M     | 40  | ASN  | N-CA-C | 5.81  | 119.99      | 113.02   |
| 1   | G     | 308 | PHE  | N-CA-C | 5.80  | 118.66      | 108.56   |
| 1   | G     | 40  | ASN  | N-CA-C | 5.80  | 119.98      | 113.02   |
| 1   | D     | 269 | PHE  | N-CA-C | 5.79  | 120.62      | 113.50   |
| 3   | I     | 45  | GLN  | N-CA-C | 5.79  | 123.12      | 110.80   |
| 1   | D     | 9   | TYR  | N-CA-C | 5.78  | 118.39      | 110.24   |
| 1   | A     | 161 | VAL  | N-CA-C | 5.77  | 116.55      | 110.72   |
| 1   | J     | 418 | VAL  | N-CA-C | -5.76 | 103.70      | 110.21   |
| 1   | M     | 222 | ASN  | N-CA-C | -5.76 | 102.00      | 110.52   |
| 1   | A     | 86  | ASN  | N-CA-C | 5.75  | 120.31      | 113.12   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 415 | GLU  | N-CA-C  | 5.73  | 118.96      | 110.48   |
| 1   | D     | 86  | ASN  | N-CA-C  | 5.73  | 120.28      | 113.12   |
| 1   | M     | 163 | THR  | N-CA-C  | -5.72 | 105.56      | 112.54   |
| 1   | J     | 369 | LEU  | N-CA-C  | -5.72 | 105.13      | 111.36   |
| 1   | P     | 40  | ASN  | N-CA-C  | 5.71  | 119.87      | 113.02   |
| 1   | A     | 241 | THR  | N-CA-C  | 5.70  | 118.54      | 109.65   |
| 1   | G     | 10  | GLU  | CA-C-N  | 5.70  | 125.63      | 119.76   |
| 1   | G     | 10  | GLU  | C-N-CA  | 5.70  | 125.63      | 119.76   |
| 1   | G     | 86  | ASN  | N-CA-C  | 5.70  | 120.24      | 113.12   |
| 1   | D     | 222 | ASN  | N-CA-C  | -5.69 | 102.09      | 110.52   |
| 1   | A     | 222 | ASN  | N-CA-C  | -5.69 | 102.10      | 110.52   |
| 1   | G     | 163 | THR  | N-CA-C  | -5.69 | 105.60      | 112.54   |
| 1   | M     | 161 | VAL  | N-CA-C  | 5.69  | 115.88      | 110.53   |
| 3   | O     | 49  | SER  | N-CA-C  | -5.67 | 100.43      | 109.23   |
| 1   | J     | 40  | ASN  | N-CA-C  | 5.67  | 119.83      | 113.02   |
| 1   | G     | 360 | ARG  | CA-C-N  | 5.67  | 125.34      | 119.05   |
| 1   | G     | 360 | ARG  | C-N-CA  | 5.67  | 125.34      | 119.05   |
| 1   | D     | 161 | VAL  | N-CA-C  | 5.66  | 116.44      | 110.72   |
| 2   | H     | 45  | VAL  | N-CA-C  | 5.65  | 114.10      | 107.77   |
| 1   | J     | 86  | ASN  | N-CA-C  | 5.63  | 120.16      | 113.12   |
| 1   | P     | 269 | PHE  | N-CA-C  | 5.63  | 120.42      | 113.50   |
| 1   | J     | 163 | THR  | N-CA-C  | -5.62 | 105.68      | 112.54   |
| 3   | I     | 44  | VAL  | CA-C-N  | 5.62  | 132.27      | 121.54   |
| 3   | I     | 44  | VAL  | C-N-CA  | 5.62  | 132.27      | 121.54   |
| 1   | G     | 241 | THR  | N-CA-C  | 5.62  | 118.41      | 109.65   |
| 1   | A     | 415 | GLU  | N-CA-C  | 5.61  | 119.06      | 110.20   |
| 1   | P     | 222 | ASN  | N-CA-C  | -5.61 | 102.22      | 110.52   |
| 1   | J     | 360 | ARG  | CA-C-N  | 5.60  | 125.27      | 119.05   |
| 1   | J     | 360 | ARG  | C-N-CA  | 5.60  | 125.27      | 119.05   |
| 1   | J     | 222 | ASN  | N-CA-C  | -5.59 | 102.25      | 110.52   |
| 1   | J     | 241 | THR  | N-CA-C  | 5.58  | 118.35      | 109.65   |
| 2   | H     | 71  | THR  | N-CA-C  | -5.57 | 100.63      | 109.76   |
| 1   | G     | 222 | ASN  | N-CA-C  | -5.56 | 102.29      | 110.52   |
| 1   | G     | 161 | VAL  | N-CA-C  | 5.55  | 116.33      | 110.72   |
| 2   | N     | 187 | PRO  | CA-C-N  | -5.55 | 112.90      | 119.84   |
| 2   | N     | 187 | PRO  | C-N-CA  | -5.55 | 112.90      | 119.84   |
| 1   | J     | 321 | ILE  | CB-CA-C | -5.54 | 104.78      | 112.04   |
| 3   | F     | 49  | SER  | N-CA-C  | -5.54 | 100.65      | 109.23   |
| 1   | M     | 418 | VAL  | N-CA-C  | -5.54 | 103.95      | 110.21   |
| 1   | D     | 163 | THR  | N-CA-C  | -5.52 | 105.80      | 112.54   |
| 1   | A     | 108 | VAL  | CB-CA-C | -5.52 | 103.32      | 112.26   |
| 1   | J     | 251 | LYS  | N-CA-C  | -5.51 | 105.17      | 111.07   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 204 | VAL  | N-CA-C  | -5.51 | 105.15      | 110.72   |
| 2   | H     | 74  | ASP  | N-CA-C  | 5.51  | 118.31      | 110.10   |
| 1   | P     | 241 | THR  | N-CA-C  | 5.51  | 118.24      | 109.65   |
| 2   | N     | 45  | VAL  | N-CA-C  | 5.51  | 113.94      | 107.77   |
| 2   | Q     | 45  | VAL  | N-CA-C  | 5.48  | 113.91      | 107.77   |
| 3   | O     | 159 | ALA  | N-CA-C  | -5.46 | 105.43      | 113.61   |
| 1   | D     | 360 | ARG  | CA-C-N  | 5.45  | 125.10      | 119.05   |
| 1   | D     | 360 | ARG  | C-N-CA  | 5.45  | 125.10      | 119.05   |
| 1   | D     | 280 | TYR  | N-CA-C  | -5.44 | 106.52      | 112.72   |
| 1   | M     | 241 | THR  | N-CA-C  | 5.43  | 118.12      | 109.65   |
| 1   | M     | 369 | LEU  | N-CA-C  | -5.42 | 105.45      | 111.36   |
| 3   | I     | 122 | TRP  | N-CA-C  | 5.42  | 117.83      | 107.75   |
| 3   | R     | 49  | SER  | N-CA-C  | -5.42 | 100.83      | 109.23   |
| 2   | N     | 141 | GLU  | CA-C-N  | 5.42  | 125.96      | 120.38   |
| 2   | N     | 141 | GLU  | C-N-CA  | 5.42  | 125.96      | 120.38   |
| 1   | A     | 360 | ARG  | CA-C-N  | 5.42  | 125.06      | 119.05   |
| 1   | A     | 360 | ARG  | C-N-CA  | 5.42  | 125.06      | 119.05   |
| 1   | A     | 247 | TYR  | N-CA-C  | 5.41  | 117.60      | 111.11   |
| 1   | A     | 204 | VAL  | N-CA-C  | -5.40 | 105.27      | 110.72   |
| 3   | I     | 49  | SER  | N-CA-C  | -5.40 | 100.86      | 109.23   |
| 1   | G     | 369 | LEU  | N-CA-C  | -5.39 | 105.48      | 111.36   |
| 3   | R     | 159 | ALA  | N-CA-C  | -5.37 | 105.55      | 113.61   |
| 1   | J     | 204 | VAL  | N-CA-C  | -5.36 | 105.30      | 110.72   |
| 1   | G     | 114 | ARG  | N-CA-C  | -5.36 | 105.44      | 111.28   |
| 1   | P     | 355 | ARG  | N-CA-C  | 5.36  | 116.98      | 111.03   |
| 1   | A     | 369 | LEU  | N-CA-C  | -5.35 | 105.53      | 111.36   |
| 1   | A     | 416 | LYS  | CA-C-N  | 5.34  | 125.10      | 119.76   |
| 1   | A     | 416 | LYS  | C-N-CA  | 5.34  | 125.10      | 119.76   |
| 1   | D     | 418 | VAL  | N-CA-C  | -5.34 | 104.17      | 110.21   |
| 1   | A     | 114 | ARG  | N-CA-C  | -5.33 | 105.36      | 111.07   |
| 3   | F     | 122 | TRP  | N-CA-C  | 5.33  | 117.66      | 107.75   |
| 1   | P     | 416 | LYS  | CA-C-N  | 5.31  | 125.47      | 119.90   |
| 1   | P     | 416 | LYS  | C-N-CA  | 5.31  | 125.47      | 119.90   |
| 3   | L     | 159 | ALA  | N-CA-C  | -5.31 | 105.65      | 113.61   |
| 1   | P     | 114 | ARG  | N-CA-C  | -5.30 | 105.40      | 111.07   |
| 1   | D     | 247 | TYR  | N-CA-C  | 5.30  | 117.47      | 111.11   |
| 1   | G     | 325 | ILE  | CB-CA-C | -5.29 | 105.11      | 112.04   |
| 1   | J     | 161 | VAL  | N-CA-C  | 5.29  | 116.06      | 110.72   |
| 1   | G     | 280 | TYR  | N-CA-C  | -5.28 | 106.70      | 112.72   |
| 2   | K     | 141 | GLU  | CA-C-N  | 5.28  | 125.82      | 120.38   |
| 2   | K     | 141 | GLU  | C-N-CA  | 5.28  | 125.82      | 120.38   |
| 2   | E     | 141 | GLU  | CA-C-N  | 5.28  | 125.82      | 120.38   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 141 | GLU  | C-N-CA  | 5.28  | 125.82      | 120.38   |
| 3   | C     | 49  | SER  | N-CA-C  | -5.27 | 101.06      | 109.23   |
| 1   | D     | 369 | LEU  | N-CA-C  | -5.26 | 105.62      | 111.36   |
| 1   | M     | 114 | ARG  | N-CA-C  | -5.24 | 105.57      | 111.28   |
| 2   | E     | 103 | MET  | N-CA-C  | 5.23  | 117.38      | 111.11   |
| 1   | J     | 280 | TYR  | N-CA-C  | -5.22 | 106.77      | 112.72   |
| 3   | I     | 175 | LEU  | N-CA-C  | -5.20 | 102.22      | 109.96   |
| 3   | L     | 49  | SER  | N-CA-C  | -5.18 | 101.19      | 109.23   |
| 1   | J     | 247 | TYR  | N-CA-C  | 5.18  | 117.32      | 111.11   |
| 3   | L     | 175 | LEU  | N-CA-C  | -5.17 | 102.25      | 109.96   |
| 1   | D     | 251 | LYS  | N-CA-C  | -5.17 | 105.65      | 111.28   |
| 3   | O     | 57  | VAL  | N-CA-C  | 5.16  | 115.20      | 107.51   |
| 3   | R     | 175 | LEU  | N-CA-C  | -5.15 | 102.29      | 109.96   |
| 1   | G     | 247 | TYR  | N-CA-C  | 5.14  | 117.28      | 111.11   |
| 1   | G     | 106 | ILE  | N-CA-C  | -5.14 | 105.38      | 110.62   |
| 1   | D     | 114 | ARG  | N-CA-C  | -5.14 | 105.58      | 111.07   |
| 1   | M     | 86  | ASN  | N-CA-C  | 5.13  | 119.54      | 113.12   |
| 1   | A     | 106 | ILE  | CB-CA-C | -5.13 | 105.31      | 111.88   |
| 2   | H     | 78  | GLY  | N-CA-C  | -5.13 | 108.15      | 115.64   |
| 1   | P     | 369 | LEU  | N-CA-C  | -5.13 | 105.77      | 111.36   |
| 3   | C     | 159 | ALA  | N-CA-C  | -5.12 | 105.92      | 113.61   |
| 1   | M     | 247 | TYR  | N-CA-C  | 5.12  | 117.25      | 111.11   |
| 1   | A     | 280 | TYR  | N-CA-C  | -5.11 | 106.90      | 112.72   |
| 1   | J     | 114 | ARG  | N-CA-C  | -5.10 | 105.61      | 111.07   |
| 1   | A     | 76  | ALA  | N-CA-C  | 5.09  | 117.22      | 111.11   |
| 2   | E     | 45  | VAL  | N-CA-C  | 5.09  | 113.47      | 107.77   |
| 1   | M     | 280 | TYR  | N-CA-C  | -5.08 | 106.92      | 112.72   |
| 3   | L     | 57  | VAL  | N-CA-C  | 5.07  | 115.07      | 107.51   |
| 1   | P     | 247 | TYR  | N-CA-C  | 5.07  | 117.20      | 111.11   |
| 1   | P     | 86  | ASN  | N-CA-C  | 5.07  | 119.46      | 113.12   |
| 3   | I     | 144 | PHE  | N-CA-C  | 5.07  | 118.94      | 112.26   |
| 1   | P     | 108 | VAL  | N-CA-CB | 5.07  | 118.18      | 110.58   |
| 3   | I     | 159 | ALA  | N-CA-C  | -5.06 | 106.01      | 113.61   |
| 2   | B     | 216 | MET  | N-CA-C  | -5.06 | 105.84      | 111.36   |
| 3   | F     | 159 | ALA  | N-CA-C  | -5.05 | 106.03      | 113.61   |
| 1   | J     | 414 | ILE  | N-CA-C  | 5.05  | 119.43      | 113.22   |
| 1   | P     | 76  | ALA  | N-CA-C  | 5.05  | 117.17      | 111.11   |
| 2   | B     | 45  | VAL  | N-CA-C  | 5.05  | 113.43      | 107.77   |
| 1   | G     | 416 | LYS  | CA-C-N  | 5.04  | 125.20      | 119.90   |
| 1   | G     | 416 | LYS  | C-N-CA  | 5.04  | 125.20      | 119.90   |
| 3   | I     | 57  | VAL  | N-CA-C  | 5.04  | 115.01      | 107.51   |
| 3   | R     | 31  | VAL  | N-CA-C  | 5.04  | 115.26      | 110.53   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | F     | 175 | LEU  | N-CA-C | -5.03 | 102.47      | 109.96   |
| 1   | P     | 161 | VAL  | N-CA-C | 5.01  | 115.78      | 110.72   |
| 3   | C     | 175 | LEU  | N-CA-C | -5.01 | 102.49      | 109.96   |
| 3   | C     | 57  | VAL  | N-CA-C | 5.01  | 114.97      | 107.51   |
| 1   | P     | 418 | VAL  | N-CA-C | -5.01 | 104.55      | 110.21   |
| 1   | D     | 106 | ILE  | N-CA-C | -5.00 | 105.52      | 110.62   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 32  | TYR  | Sidechain |
| 2   | E     | 32  | TYR  | Sidechain |
| 2   | H     | 32  | TYR  | Sidechain |
| 2   | K     | 32  | TYR  | Sidechain |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3440  | 0        | 3428     | 74      | 0            |
| 1   | D     | 3440  | 0        | 3428     | 90      | 0            |
| 1   | G     | 3440  | 0        | 3428     | 96      | 0            |
| 1   | J     | 3440  | 0        | 3428     | 103     | 0            |
| 1   | M     | 3440  | 0        | 3428     | 99      | 0            |
| 1   | P     | 3440  | 0        | 3428     | 82      | 0            |
| 2   | B     | 1953  | 0        | 1848     | 70      | 0            |
| 2   | E     | 1953  | 0        | 1848     | 90      | 0            |
| 2   | H     | 1953  | 0        | 1848     | 74      | 0            |
| 2   | K     | 1953  | 0        | 1848     | 76      | 0            |
| 2   | N     | 1953  | 0        | 1848     | 87      | 0            |
| 2   | Q     | 1953  | 0        | 1848     | 86      | 0            |
| 3   | C     | 1340  | 0        | 1303     | 27      | 0            |
| 3   | F     | 1340  | 0        | 1303     | 28      | 0            |
| 3   | I     | 1340  | 0        | 1303     | 29      | 0            |
| 3   | L     | 1340  | 0        | 1303     | 27      | 0            |
| 3   | O     | 1340  | 0        | 1303     | 28      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | R     | 1340  | 0        | 1303     | 28      | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | H     | 1     | 0        | 0        | 0       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 4   | M     | 1     | 0        | 0        | 0       | 0            |
| 4   | N     | 1     | 0        | 0        | 0       | 0            |
| 4   | Q     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 86    | 0        | 60       | 7       | 0            |
| 5   | B     | 43    | 0        | 30       | 1       | 0            |
| 5   | D     | 86    | 0        | 60       | 9       | 0            |
| 5   | E     | 43    | 0        | 30       | 1       | 0            |
| 5   | G     | 86    | 0        | 60       | 10      | 0            |
| 5   | H     | 43    | 0        | 30       | 1       | 0            |
| 5   | J     | 86    | 0        | 60       | 15      | 0            |
| 5   | K     | 43    | 0        | 30       | 2       | 0            |
| 5   | M     | 86    | 0        | 60       | 9       | 0            |
| 5   | N     | 43    | 0        | 30       | 3       | 0            |
| 5   | P     | 86    | 0        | 60       | 7       | 0            |
| 5   | Q     | 43    | 0        | 30       | 2       | 0            |
| 6   | A     | 37    | 0        | 42       | 0       | 0            |
| 6   | D     | 37    | 0        | 42       | 0       | 0            |
| 6   | G     | 37    | 0        | 42       | 0       | 0            |
| 6   | J     | 37    | 0        | 42       | 1       | 0            |
| 6   | M     | 37    | 0        | 42       | 0       | 0            |
| 6   | P     | 37    | 0        | 42       | 1       | 0            |
| 7   | A     | 45    | 0        | 67       | 6       | 0            |
| 7   | D     | 45    | 0        | 67       | 2       | 0            |
| 7   | G     | 45    | 0        | 67       | 3       | 0            |
| 7   | J     | 45    | 0        | 67       | 1       | 0            |
| 7   | M     | 45    | 0        | 67       | 3       | 0            |
| 7   | P     | 45    | 0        | 67       | 2       | 0            |
| 8   | A     | 23    | 0        | 26       | 2       | 0            |
| 8   | D     | 23    | 0        | 26       | 2       | 0            |
| 8   | G     | 23    | 0        | 26       | 2       | 0            |
| 8   | J     | 23    | 0        | 26       | 1       | 0            |
| 8   | M     | 23    | 0        | 26       | 2       | 0            |
| 8   | P     | 23    | 0        | 26       | 2       | 0            |
| 9   | B     | 20    | 0        | 28       | 1       | 0            |
| 9   | E     | 20    | 0        | 28       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | G     | 20    | 0        | 28       | 2       | 0            |
| 9   | K     | 20    | 0        | 28       | 2       | 0            |
| 9   | N     | 20    | 0        | 28       | 1       | 0            |
| 9   | P     | 20    | 0        | 28       | 2       | 0            |
| 10  | C     | 4     | 0        | 0        | 0       | 0            |
| 10  | F     | 4     | 0        | 0        | 0       | 0            |
| 10  | I     | 4     | 0        | 0        | 0       | 0            |
| 10  | L     | 4     | 0        | 0        | 0       | 0            |
| 10  | O     | 4     | 0        | 0        | 0       | 0            |
| 10  | R     | 4     | 0        | 0        | 0       | 0            |
| 11  | I     | 1     | 0        | 0        | 0       | 0            |
| 11  | R     | 1     | 0        | 0        | 0       | 0            |
| 12  | R     | 1     | 0        | 0        | 0       | 0            |
| 13  | A     | 73    | 0        | 0        | 1       | 0            |
| 13  | B     | 19    | 0        | 0        | 2       | 0            |
| 13  | C     | 47    | 0        | 0        | 0       | 0            |
| 13  | D     | 64    | 0        | 0        | 4       | 0            |
| 13  | E     | 14    | 0        | 0        | 1       | 0            |
| 13  | F     | 36    | 0        | 0        | 0       | 0            |
| 13  | G     | 68    | 0        | 0        | 2       | 0            |
| 13  | H     | 35    | 0        | 0        | 3       | 0            |
| 13  | I     | 42    | 0        | 0        | 0       | 0            |
| 13  | J     | 55    | 0        | 0        | 3       | 0            |
| 13  | K     | 17    | 0        | 0        | 0       | 0            |
| 13  | L     | 42    | 0        | 0        | 1       | 0            |
| 13  | M     | 34    | 0        | 0        | 1       | 0            |
| 13  | N     | 11    | 0        | 0        | 1       | 0            |
| 13  | O     | 41    | 0        | 0        | 1       | 0            |
| 13  | P     | 60    | 0        | 0        | 1       | 0            |
| 13  | Q     | 16    | 0        | 0        | 1       | 0            |
| 13  | R     | 24    | 0        | 0        | 2       | 0            |
| All | All   | 42656 | 0        | 40992    | 1093    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1093) 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:Q:144:LYS:HA  | 2:Q:144:LYS:HZ3  | 1.06                     | 1.14              |
| 2:K:139:PRO:HG3 | 2:K:158:ARG:HH11 | 1.14                     | 1.12              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:77:THR:HG22  | 2:N:79:GLU:H     | 1.25                     | 1.02              |
| 2:K:194:VAL:HB   | 2:K:207:MET:HE3  | 1.42                     | 1.01              |
| 2:Q:144:LYS:HA   | 2:Q:144:LYS:NZ   | 1.75                     | 1.01              |
| 2:B:194:VAL:HB   | 2:B:207:MET:HE3  | 1.42                     | 1.01              |
| 2:B:250:ARG:HD3  | 3:C:12:ARG:HG2   | 1.41                     | 1.01              |
| 2:Q:194:VAL:HB   | 2:Q:207:MET:HE3  | 1.41                     | 1.01              |
| 2:N:194:VAL:HB   | 2:N:207:MET:HE3  | 1.41                     | 1.00              |
| 2:K:74:ASP:HB3   | 2:K:77:THR:HB    | 1.42                     | 0.99              |
| 2:H:194:VAL:HB   | 2:H:207:MET:HE3  | 1.41                     | 0.98              |
| 2:E:194:VAL:HB   | 2:E:207:MET:HE3  | 1.42                     | 0.97              |
| 2:K:144:LYS:O    | 2:K:147:GLU:HG3  | 1.66                     | 0.95              |
| 2:Q:223:LEU:HD21 | 2:Q:227:LYS:HE3  | 1.45                     | 0.95              |
| 2:N:74:ASP:HB3   | 2:N:77:THR:HB    | 1.48                     | 0.94              |
| 1:D:142:THR:HG21 | 5:D:502:HEM:HBB2 | 1.50                     | 0.94              |
| 1:A:195:PHE:HE2  | 1:D:195:PHE:HE2  | 1.18                     | 0.92              |
| 2:E:144:LYS:O    | 2:E:147:GLU:HG3  | 1.71                     | 0.90              |
| 1:M:329:LYS:HE3  | 3:R:131:HIS:O    | 1.70                     | 0.90              |
| 2:H:77:THR:HG22  | 2:H:79:GLU:H     | 1.36                     | 0.89              |
| 2:N:138:PHE:CD2  | 2:N:187:PRO:HG3  | 2.07                     | 0.89              |
| 2:E:236:PHE:HE2  | 3:F:25:VAL:HG12  | 1.37                     | 0.88              |
| 1:M:410:ILE:HG23 | 1:M:414:ILE:HD12 | 1.57                     | 0.87              |
| 1:M:12:ARG:O     | 1:M:17:LYS:HE2   | 1.74                     | 0.86              |
| 1:A:142:THR:HG21 | 5:A:502:HEM:HBB2 | 1.55                     | 0.86              |
| 1:M:195:PHE:HE2  | 1:P:195:PHE:HE2  | 1.20                     | 0.85              |
| 2:K:42:MET:HE1   | 2:K:218:ALA:CB   | 2.07                     | 0.85              |
| 2:N:142:PRO:HG2  | 2:N:150:GLU:OE2  | 1.77                     | 0.85              |
| 2:E:223:LEU:HD21 | 2:E:227:LYS:HE3  | 1.58                     | 0.85              |
| 2:B:250:ARG:HG2  | 3:C:12:ARG:HD3   | 1.58                     | 0.85              |
| 1:J:424:ILE:HG13 | 13:J:1157:HOH:O  | 1.76                     | 0.84              |
| 1:G:195:PHE:HE2  | 1:J:195:PHE:HE2  | 1.22                     | 0.84              |
| 1:G:410:ILE:HG23 | 1:G:414:ILE:HD12 | 1.58                     | 0.84              |
| 1:G:248:PHE:CD1  | 1:G:251:LYS:HD3  | 2.13                     | 0.83              |
| 2:K:139:PRO:HG3  | 2:K:158:ARG:NH1  | 1.92                     | 0.83              |
| 2:Q:149:HIS:CD2  | 2:Q:168:THR:HG21 | 2.13                     | 0.83              |
| 2:E:149:HIS:CD2  | 2:E:168:THR:HG21 | 2.14                     | 0.83              |
| 2:E:236:PHE:CE2  | 3:F:25:VAL:HG12  | 2.14                     | 0.82              |
| 2:N:77:THR:HG22  | 2:N:79:GLU:N     | 1.95                     | 0.82              |
| 1:D:135:ILE:HG21 | 5:D:501:HEM:HAB  | 1.61                     | 0.81              |
| 1:G:9:TYR:HB2    | 1:G:30:TYR:CD2   | 2.14                     | 0.81              |
| 2:E:15:GLY:H     | 9:E:1042:BGL:H5  | 1.46                     | 0.81              |
| 1:D:246:PRO:HG2  | 2:E:251:LEU:HD21 | 1.63                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:138:PHE:CD2  | 2:E:187:PRO:HG3  | 2.18                     | 0.79              |
| 2:K:138:PHE:CD2  | 2:K:187:PRO:HG3  | 2.17                     | 0.79              |
| 1:G:248:PHE:HD1  | 1:G:251:LYS:HD3  | 1.46                     | 0.79              |
| 2:K:149:HIS:CD2  | 2:K:168:THR:HG21 | 2.18                     | 0.79              |
| 2:H:95:GLU:HG2   | 13:H:327:HOH:O   | 1.82                     | 0.78              |
| 2:E:74:ASP:HB3   | 2:E:77:THR:HB    | 1.64                     | 0.78              |
| 2:E:250:ARG:HG3  | 2:E:250:ARG:HH11 | 1.45                     | 0.78              |
| 1:J:4:ILE:N      | 1:J:4:ILE:HD12   | 1.99                     | 0.78              |
| 2:N:74:ASP:CB    | 2:N:77:THR:HB    | 2.14                     | 0.77              |
| 2:Q:77:THR:HG22  | 2:Q:79:GLU:HB2   | 1.65                     | 0.77              |
| 2:K:77:THR:HG22  | 2:K:79:GLU:H     | 1.50                     | 0.77              |
| 3:O:131:HIS:O    | 1:P:329:LYS:HE3  | 1.84                     | 0.77              |
| 2:B:42:MET:HE1   | 2:B:218:ALA:CB   | 2.14                     | 0.76              |
| 2:H:250:ARG:NH1  | 3:I:12:ARG:HB2   | 2.00                     | 0.76              |
| 2:H:77:THR:HG22  | 2:H:79:GLU:N     | 2.00                     | 0.76              |
| 2:N:231:PHE:O    | 2:N:235:MET:HG2  | 1.84                     | 0.76              |
| 2:K:42:MET:HE1   | 2:K:218:ALA:HB1  | 1.67                     | 0.75              |
| 1:P:239:LYS:HE2  | 1:P:425:GLU:OE2  | 1.86                     | 0.75              |
| 1:M:13:THR:O     | 1:M:17:LYS:HG3   | 1.87                     | 0.75              |
| 2:N:183:ILE:HG23 | 2:N:185:MET:H    | 1.52                     | 0.75              |
| 2:H:250:ARG:CZ   | 3:I:12:ARG:HB2   | 2.17                     | 0.75              |
| 1:M:105:PHE:HA   | 1:M:108:VAL:HG22 | 1.69                     | 0.74              |
| 1:G:239:LYS:HE2  | 1:G:425:GLU:OE2  | 1.87                     | 0.74              |
| 1:G:261:LEU:HD11 | 2:H:234:VAL:HG13 | 1.69                     | 0.74              |
| 1:D:12:ARG:O     | 1:D:17:LYS:HE2   | 1.88                     | 0.74              |
| 1:P:9:TYR:HB2    | 1:P:30:TYR:CD2   | 2.23                     | 0.74              |
| 1:M:4:ILE:HD12   | 1:M:4:ILE:H      | 1.53                     | 0.74              |
| 2:N:40:HIS:ND1   | 2:N:97:ALA:HB1   | 2.03                     | 0.73              |
| 1:G:4:ILE:HD12   | 1:G:4:ILE:H      | 1.49                     | 0.73              |
| 1:A:9:TYR:HB2    | 1:A:30:TYR:CD2   | 2.23                     | 0.73              |
| 2:E:77:THR:CG2   | 2:E:79:GLU:HB2   | 2.19                     | 0.73              |
| 2:Q:223:LEU:CD2  | 2:Q:227:LYS:HE3  | 2.18                     | 0.73              |
| 2:Q:138:PHE:CD2  | 2:Q:187:PRO:HG3  | 2.24                     | 0.73              |
| 1:J:4:ILE:HD12   | 1:J:4:ILE:H      | 1.53                     | 0.72              |
| 1:M:91:PHE:CD1   | 2:N:222:LYS:HG2  | 2.24                     | 0.72              |
| 5:M:502:HEM:HMC1 | 5:M:502:HEM:HBC2 | 1.71                     | 0.72              |
| 1:J:428:PHE:CE1  | 2:K:256:LYS:HD2  | 2.24                     | 0.72              |
| 1:D:92:MET:HE1   | 2:E:226:ARG:HG3  | 1.70                     | 0.72              |
| 1:M:9:TYR:HB2    | 1:M:30:TYR:CD2   | 2.24                     | 0.72              |
| 1:D:213:ILE:HA   | 1:D:216:PHE:CE2  | 2.25                     | 0.72              |
| 1:P:44:MET:HE3   | 7:P:1026:LOP:H92 | 1.72                     | 0.72              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:142:THR:HG21 | 5:G:502:HEM:HBB2  | 1.70                     | 0.72              |
| 1:P:213:ILE:HA   | 1:P:216:PHE:CE2   | 2.25                     | 0.72              |
| 1:P:287:ARG:HG2  | 1:P:287:ARG:HH11  | 1.53                     | 0.72              |
| 1:M:213:ILE:HA   | 1:M:216:PHE:CE2   | 2.26                     | 0.71              |
| 1:J:213:ILE:HA   | 1:J:216:PHE:CE2   | 2.25                     | 0.71              |
| 1:A:213:ILE:HA   | 1:A:216:PHE:CE2   | 2.26                     | 0.71              |
| 3:C:47:LEU:HD23  | 3:C:47:LEU:O      | 1.91                     | 0.71              |
| 1:G:213:ILE:HA   | 1:G:216:PHE:CE2   | 2.26                     | 0.70              |
| 2:Q:59:PRO:HD2   | 2:Q:62:GLN:NE2    | 2.06                     | 0.70              |
| 2:N:59:PRO:HD2   | 2:N:62:GLN:NE2    | 2.06                     | 0.70              |
| 1:J:239:LYS:HE2  | 1:J:425:GLU:OE1   | 1.90                     | 0.70              |
| 1:G:130:ILE:HD11 | 1:G:348:TRP:HH2   | 1.57                     | 0.70              |
| 1:G:246:PRO:HG2  | 2:H:251:LEU:HD21  | 1.74                     | 0.70              |
| 1:A:261:LEU:HD11 | 2:B:234:VAL:HG13  | 1.71                     | 0.70              |
| 1:D:261:LEU:HD11 | 2:E:234:VAL:HG13  | 1.73                     | 0.70              |
| 3:C:84:LEU:HD23  | 3:L:84:LEU:HD23   | 1.74                     | 0.70              |
| 1:M:376:ILE:O    | 1:M:380:VAL:HG22  | 1.92                     | 0.70              |
| 3:F:47:LEU:HD23  | 3:F:47:LEU:O      | 1.92                     | 0.69              |
| 2:H:59:PRO:HD2   | 2:H:62:GLN:NE2    | 2.07                     | 0.69              |
| 1:J:428:PHE:CZ   | 2:K:256:LYS:HB2   | 2.27                     | 0.69              |
| 2:N:194:VAL:HB   | 2:N:207:MET:CE    | 2.21                     | 0.69              |
| 1:P:130:ILE:HD11 | 1:P:348:TRP:HH2   | 1.57                     | 0.69              |
| 2:K:59:PRO:HD2   | 2:K:62:GLN:NE2    | 2.06                     | 0.69              |
| 1:M:269:PHE:HB3  | 9:N:1045:BGL:H1'2 | 1.75                     | 0.69              |
| 1:A:130:ILE:HD11 | 1:A:348:TRP:HH2   | 1.56                     | 0.69              |
| 2:E:59:PRO:HD2   | 2:E:62:GLN:NE2    | 2.07                     | 0.69              |
| 1:J:130:ILE:HD11 | 1:J:348:TRP:HH2   | 1.57                     | 0.69              |
| 3:F:112:GLN:H    | 3:F:112:GLN:NE2   | 1.91                     | 0.69              |
| 1:M:8:HIS:CD2    | 1:M:8:HIS:H       | 2.09                     | 0.69              |
| 1:A:287:ARG:HG2  | 1:A:287:ARG:HH11  | 1.57                     | 0.69              |
| 2:B:59:PRO:HD2   | 2:B:62:GLN:NE2    | 2.07                     | 0.69              |
| 1:P:91:PHE:CD1   | 2:Q:222:LYS:HG2   | 2.28                     | 0.69              |
| 2:E:77:THR:HG22  | 2:E:79:GLU:H      | 1.58                     | 0.69              |
| 5:A:501:HEM:HMC2 | 5:A:501:HEM:HBC2  | 1.75                     | 0.68              |
| 2:E:42:MET:HE1   | 2:E:218:ALA:CB    | 2.23                     | 0.68              |
| 1:A:374:PHE:HD2  | 7:A:1021:LOP:H321 | 1.57                     | 0.68              |
| 2:N:40:HIS:CE1   | 2:N:97:ALA:HB1    | 2.28                     | 0.68              |
| 1:A:376:ILE:O    | 1:A:380:VAL:HG22  | 1.93                     | 0.68              |
| 1:D:130:ILE:HD11 | 1:D:348:TRP:HH2   | 1.57                     | 0.68              |
| 1:J:376:ILE:O    | 1:J:380:VAL:HG22  | 1.92                     | 0.68              |
| 1:P:261:LEU:HD11 | 2:Q:234:VAL:HG13  | 1.76                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:P:376:ILE:O    | 1:P:380:VAL:HG22  | 1.92                     | 0.68              |
| 1:D:376:ILE:O    | 1:D:380:VAL:HG22  | 1.93                     | 0.68              |
| 1:G:376:ILE:O    | 1:G:380:VAL:HG22  | 1.93                     | 0.68              |
| 1:A:92:MET:HE1   | 2:B:226:ARG:HG3   | 1.74                     | 0.68              |
| 2:K:49:SER:HA    | 2:K:52:GLU:HG3    | 1.76                     | 0.68              |
| 3:O:118:GLU:CD   | 3:O:118:GLU:H     | 2.02                     | 0.68              |
| 1:M:130:ILE:HD11 | 1:M:348:TRP:HH2   | 1.57                     | 0.68              |
| 1:A:105:PHE:HA   | 1:A:108:VAL:HG22  | 1.76                     | 0.67              |
| 3:C:70:LYS:HE3   | 1:D:184:PRO:O     | 1.95                     | 0.67              |
| 1:J:104:PHE:O    | 1:J:108:VAL:HG22  | 1.94                     | 0.67              |
| 1:G:103:LEU:HD13 | 7:G:1023:LOP:H211 | 1.76                     | 0.67              |
| 2:H:250:ARG:CZ   | 3:I:12:ARG:CB     | 2.72                     | 0.67              |
| 1:M:230:ARG:HA   | 13:M:528:HOH:O    | 1.94                     | 0.67              |
| 1:P:43:TRP:CZ3   | 1:P:251:LYS:HE3   | 2.30                     | 0.67              |
| 2:B:74:ASP:HB3   | 2:B:77:THR:HB     | 1.76                     | 0.66              |
| 1:M:118:TYR:OH   | 7:M:1025:LOP:H31  | 1.96                     | 0.66              |
| 1:J:62:GLY:C     | 5:J:502:HEM:HAC   | 2.20                     | 0.66              |
| 2:N:138:PHE:HD2  | 2:N:187:PRO:HG3   | 1.56                     | 0.66              |
| 2:Q:194:VAL:HB   | 2:Q:207:MET:CE    | 2.22                     | 0.66              |
| 1:A:246:PRO:HG2  | 2:B:251:LEU:HD21  | 1.76                     | 0.66              |
| 1:M:261:LEU:HD11 | 2:N:234:VAL:HG13  | 1.78                     | 0.66              |
| 3:O:118:GLU:CD   | 3:O:118:GLU:N     | 2.54                     | 0.66              |
| 2:E:77:THR:HG22  | 2:E:79:GLU:N      | 2.11                     | 0.65              |
| 3:L:112:GLN:H    | 3:L:112:GLN:NE2   | 1.93                     | 0.65              |
| 1:M:142:THR:HG21 | 5:M:502:HEM:HBB2  | 1.76                     | 0.65              |
| 1:A:125:ARG:CZ   | 1:A:222:ASN:HB2   | 2.25                     | 0.65              |
| 2:N:224:MET:O    | 2:N:228:GLN:HG3   | 1.95                     | 0.65              |
| 1:D:39:ARG:HH12  | 2:E:255:VAL:CG1   | 2.09                     | 0.65              |
| 2:K:105:LYS:HD3  | 2:K:220:GLU:HG2   | 1.78                     | 0.65              |
| 2:K:194:VAL:HB   | 2:K:207:MET:CE    | 2.23                     | 0.65              |
| 1:J:199:TYR:HA   | 5:J:502:HEM:HBC2  | 1.78                     | 0.65              |
| 2:Q:20:PHE:HB3   | 2:Q:25:LEU:HD11   | 1.78                     | 0.65              |
| 2:B:26:GLN:HG2   | 2:B:58:LEU:HD21   | 1.79                     | 0.65              |
| 2:H:20:PHE:HB3   | 2:H:25:LEU:HD11   | 1.79                     | 0.65              |
| 1:M:39:ARG:HG2   | 1:M:242:VAL:HG13  | 1.79                     | 0.65              |
| 1:D:39:ARG:HG2   | 1:D:242:VAL:HG13  | 1.78                     | 0.65              |
| 2:E:26:GLN:HG2   | 2:E:58:LEU:HD21   | 1.79                     | 0.65              |
| 1:J:24:PRO:HA    | 13:J:1105:HOH:O   | 1.96                     | 0.65              |
| 1:P:39:ARG:HG2   | 1:P:242:VAL:HG13  | 1.78                     | 0.65              |
| 3:R:112:GLN:H    | 3:R:112:GLN:NE2   | 1.95                     | 0.65              |
| 1:J:91:PHE:CE2   | 1:J:92:MET:HE2    | 2.32                     | 0.65              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:K:26:GLN:HG2   | 2:K:58:LEU:HD21   | 1.79                     | 0.65              |
| 1:M:92:MET:HE1   | 2:N:226:ARG:HG3   | 1.79                     | 0.64              |
| 3:C:112:GLN:H    | 3:C:112:GLN:NE2   | 1.95                     | 0.64              |
| 1:G:105:PHE:HA   | 1:G:108:VAL:HG22  | 1.78                     | 0.64              |
| 1:J:105:PHE:HA   | 1:J:108:VAL:HG23  | 1.78                     | 0.64              |
| 2:Q:128:PRO:HG2  | 2:Q:129:GLU:OE1   | 1.98                     | 0.64              |
| 2:H:74:ASP:HB3   | 2:H:77:THR:HB     | 1.80                     | 0.64              |
| 2:K:20:PHE:HB3   | 2:K:25:LEU:HD11   | 1.80                     | 0.64              |
| 1:M:105:PHE:HA   | 1:M:108:VAL:CG2   | 2.26                     | 0.64              |
| 1:J:180:LEU:HD22 | 6:J:1004:SMA:H26  | 1.78                     | 0.64              |
| 2:N:20:PHE:HB3   | 2:N:25:LEU:HD11   | 1.78                     | 0.64              |
| 2:N:26:GLN:HG2   | 2:N:58:LEU:HD21   | 1.80                     | 0.64              |
| 1:D:103:LEU:HD13 | 7:D:1022:LOP:H201 | 1.79                     | 0.64              |
| 2:H:194:VAL:HB   | 2:H:207:MET:CE    | 2.23                     | 0.64              |
| 2:H:26:GLN:HG2   | 2:H:58:LEU:HD21   | 1.80                     | 0.64              |
| 1:P:217:HIS:NE2  | 8:P:1106:UQ2:O4   | 2.31                     | 0.64              |
| 2:Q:61:ASP:HA    | 2:Q:64:ARG:NH1    | 2.12                     | 0.64              |
| 3:I:112:GLN:H    | 3:I:112:GLN:NE2   | 1.96                     | 0.64              |
| 1:G:39:ARG:HG2   | 1:G:242:VAL:HG13  | 1.78                     | 0.64              |
| 1:A:33:ILE:HG13  | 1:A:245:TRP:HB2   | 1.79                     | 0.64              |
| 2:Q:26:GLN:HG2   | 2:Q:58:LEU:HD21   | 1.80                     | 0.63              |
| 1:J:125:ARG:CZ   | 1:J:222:ASN:HB2   | 2.28                     | 0.63              |
| 1:J:428:PHE:HZ   | 2:K:256:LYS:HB2   | 1.63                     | 0.63              |
| 1:J:39:ARG:HG2   | 1:J:242:VAL:HG13  | 1.78                     | 0.63              |
| 1:P:246:PRO:HG2  | 2:Q:251:LEU:HD21  | 1.80                     | 0.63              |
| 1:A:39:ARG:HG2   | 1:A:242:VAL:HG13  | 1.79                     | 0.63              |
| 1:D:33:ILE:HG13  | 1:D:245:TRP:HB2   | 1.79                     | 0.63              |
| 1:G:33:ILE:HG13  | 1:G:245:TRP:HB2   | 1.80                     | 0.63              |
| 2:K:142:PRO:HG2  | 2:K:150:GLU:OE2   | 1.98                     | 0.63              |
| 2:E:250:ARG:HD3  | 3:F:12:ARG:HB3    | 1.80                     | 0.63              |
| 2:E:20:PHE:HB3   | 2:E:25:LEU:HD11   | 1.81                     | 0.63              |
| 1:P:33:ILE:HG13  | 1:P:245:TRP:HB2   | 1.81                     | 0.63              |
| 2:H:142:PRO:HG2  | 2:H:150:GLU:OE2   | 1.98                     | 0.63              |
| 3:I:131:HIS:O    | 1:J:329:LYS:HE3   | 1.99                     | 0.63              |
| 2:K:66:TYR:O     | 2:K:69:GLN:HG2    | 1.98                     | 0.63              |
| 1:P:39:ARG:HH12  | 2:Q:255:VAL:CG1   | 2.11                     | 0.62              |
| 1:M:117:TYR:CE2  | 7:M:1025:LOP:H32  | 2.34                     | 0.62              |
| 1:G:39:ARG:HH12  | 2:H:255:VAL:CG1   | 2.11                     | 0.62              |
| 1:J:33:ILE:HG13  | 1:J:245:TRP:HB2   | 1.80                     | 0.62              |
| 1:M:132:GLY:C    | 5:M:501:HEM:HBC2  | 2.25                     | 0.62              |
| 1:J:103:LEU:HD13 | 7:J:1024:LOP:H211 | 1.82                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:269:PHE:HB3  | 9:G:1043:BGL:H1'2 | 1.81                     | 0.62              |
| 1:J:4:ILE:H      | 1:J:4:ILE:CD1     | 2.12                     | 0.62              |
| 2:B:20:PHE:HB3   | 2:B:25:LEU:HD11   | 1.81                     | 0.62              |
| 1:D:43:TRP:CZ3   | 1:D:251:LYS:HG2   | 2.35                     | 0.62              |
| 1:D:269:PHE:HB3  | 9:E:1042:BGL:H1'2 | 1.80                     | 0.62              |
| 2:B:194:VAL:HB   | 2:B:207:MET:CE    | 2.24                     | 0.61              |
| 2:K:108:ALA:HA   | 2:K:125:ILE:HG22  | 1.83                     | 0.61              |
| 1:A:374:PHE:CD2  | 7:A:1021:LOP:H321 | 2.35                     | 0.61              |
| 1:G:199:TYR:CD2  | 5:G:502:HEM:HBC1  | 2.35                     | 0.61              |
| 1:D:24:PRO:HA    | 13:D:1103:HOH:O   | 2.01                     | 0.61              |
| 1:D:10:GLU:OE2   | 1:D:11:PRO:HD2    | 2.00                     | 0.61              |
| 1:M:33:ILE:HG13  | 1:M:245:TRP:HB2   | 1.81                     | 0.61              |
| 3:O:47:LEU:HD23  | 3:O:47:LEU:O      | 2.00                     | 0.61              |
| 2:E:72:VAL:HG12  | 2:E:73:THR:N      | 2.16                     | 0.61              |
| 2:N:171:ASP:OD2  | 2:N:175:VAL:HB    | 2.01                     | 0.61              |
| 2:B:167:ASP:OD1  | 2:B:167:ASP:N     | 2.28                     | 0.61              |
| 3:C:83:GLU:OE1   | 3:C:83:GLU:HA     | 2.00                     | 0.61              |
| 2:H:256:LYS:O    | 2:H:256:LYS:HG2   | 2.00                     | 0.61              |
| 2:K:189:LEU:O    | 2:K:190:MET:HB2   | 2.00                     | 0.60              |
| 1:P:105:PHE:HA   | 1:P:108:VAL:HG22  | 1.82                     | 0.60              |
| 1:A:39:ARG:HH12  | 2:B:255:VAL:CG1   | 2.15                     | 0.60              |
| 2:B:129:GLU:OE1  | 2:B:129:GLU:N     | 2.27                     | 0.60              |
| 2:N:142:PRO:CG   | 2:N:150:GLU:OE2   | 2.49                     | 0.60              |
| 3:O:112:GLN:H    | 3:O:112:GLN:NE2   | 1.99                     | 0.60              |
| 2:B:149:HIS:CD2  | 2:B:168:THR:HG21  | 2.37                     | 0.60              |
| 1:G:306:ARG:HG3  | 13:G:1156:HOH:O   | 2.01                     | 0.60              |
| 3:L:80:ALA:O     | 3:L:84:LEU:HG     | 2.01                     | 0.60              |
| 2:B:250:ARG:HD3  | 3:C:12:ARG:CG     | 2.26                     | 0.60              |
| 2:N:71:THR:CG2   | 2:N:80:ASP:HB3    | 2.32                     | 0.59              |
| 2:H:77:THR:HG21  | 2:H:79:GLU:HB2    | 1.83                     | 0.59              |
| 1:A:103:LEU:HD13 | 7:A:1021:LOP:H211 | 1.84                     | 0.59              |
| 1:J:425:GLU:HG3  | 1:J:429:ASN:HD21  | 1.67                     | 0.59              |
| 1:P:406:VAL:O    | 1:P:409:PRO:HD2   | 2.01                     | 0.59              |
| 1:A:287:ARG:HG2  | 1:A:287:ARG:NH1   | 2.16                     | 0.59              |
| 2:B:56:PRO:HD2   | 13:B:1044:HOH:O   | 2.01                     | 0.59              |
| 2:E:223:LEU:CD2  | 2:E:227:LYS:HE3   | 2.30                     | 0.59              |
| 2:Q:129:GLU:OE1  | 2:Q:129:GLU:N     | 2.36                     | 0.59              |
| 2:K:77:THR:HG22  | 2:K:79:GLU:N      | 2.16                     | 0.59              |
| 2:E:144:LYS:HE2  | 2:E:144:LYS:HA    | 1.84                     | 0.59              |
| 1:J:144:PHE:HD1  | 13:J:1113:HOH:O   | 1.86                     | 0.58              |
| 2:Q:77:THR:CG2   | 2:Q:79:GLU:HB2    | 2.33                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:406:VAL:O    | 1:G:409:PRO:HD2   | 2.02                     | 0.58              |
| 1:M:221:ASN:HD21 | 8:M:1105:UQ2:H3M1 | 1.68                     | 0.58              |
| 1:M:4:ILE:HD12   | 1:M:4:ILE:N       | 2.18                     | 0.58              |
| 2:Q:77:THR:C     | 2:Q:79:GLU:H      | 2.11                     | 0.58              |
| 3:O:10:THR:HG22  | 3:O:10:THR:O      | 2.04                     | 0.58              |
| 1:A:92:MET:CE    | 2:B:226:ARG:HG3   | 2.33                     | 0.58              |
| 1:D:68:HIS:ND1   | 13:D:1105:HOH:O   | 2.32                     | 0.58              |
| 1:D:91:PHE:CE2   | 1:D:92:MET:HE3    | 2.39                     | 0.58              |
| 1:D:249:ILE:O    | 1:D:253:VAL:HG23  | 2.04                     | 0.58              |
| 3:I:55:SER:HB3   | 3:I:182:THR:OG1   | 2.04                     | 0.58              |
| 3:R:10:THR:O     | 3:R:10:THR:HG22   | 2.04                     | 0.58              |
| 1:A:249:ILE:O    | 1:A:253:VAL:HG23  | 2.04                     | 0.57              |
| 2:E:194:VAL:HB   | 2:E:207:MET:CE    | 2.24                     | 0.57              |
| 1:D:43:TRP:CH2   | 1:D:251:LYS:HG2   | 2.39                     | 0.57              |
| 1:J:351:THR:OG1  | 1:J:412:GLY:HA3   | 2.04                     | 0.57              |
| 2:Q:114:MET:HE3  | 2:Q:114:MET:HA    | 1.85                     | 0.57              |
| 3:L:55:SER:HB3   | 3:L:182:THR:OG1   | 2.04                     | 0.57              |
| 2:N:19:THR:HB    | 2:N:224:MET:HE3   | 1.87                     | 0.57              |
| 3:O:55:SER:HB3   | 3:O:182:THR:OG1   | 2.04                     | 0.57              |
| 3:F:55:SER:HB3   | 3:F:182:THR:OG1   | 2.04                     | 0.57              |
| 1:M:39:ARG:HH12  | 2:N:255:VAL:CG1   | 2.17                     | 0.57              |
| 3:C:55:SER:HB3   | 3:C:182:THR:OG1   | 2.05                     | 0.57              |
| 1:D:91:PHE:HE2   | 1:D:92:MET:HE3    | 1.69                     | 0.57              |
| 3:F:10:THR:HG22  | 3:F:10:THR:O      | 2.04                     | 0.57              |
| 2:K:51:SER:OG    | 2:K:63:VAL:HG21   | 2.05                     | 0.57              |
| 1:D:105:PHE:HA   | 1:D:108:VAL:HG22  | 1.86                     | 0.57              |
| 1:J:105:PHE:HA   | 1:J:108:VAL:CG2   | 2.35                     | 0.57              |
| 1:J:261:LEU:HD11 | 2:K:234:VAL:HG13  | 1.87                     | 0.57              |
| 2:N:71:THR:HG22  | 2:N:80:ASP:HB3    | 1.87                     | 0.57              |
| 1:G:199:TYR:CE2  | 5:G:502:HEM:HBC1  | 2.40                     | 0.57              |
| 2:Q:49:SER:HA    | 2:Q:52:GLU:HG3    | 1.87                     | 0.56              |
| 3:R:55:SER:HB3   | 3:R:182:THR:OG1   | 2.05                     | 0.56              |
| 1:A:114:ARG:C    | 1:A:114:ARG:HD2   | 2.30                     | 0.56              |
| 1:J:114:ARG:HD2  | 1:J:114:ARG:C     | 2.31                     | 0.56              |
| 1:M:411:LEU:O    | 1:M:415:GLU:HG2   | 2.04                     | 0.56              |
| 1:A:5:PRO:HB2    | 1:A:234:LYS:HA    | 1.87                     | 0.56              |
| 3:C:10:THR:O     | 3:C:10:THR:HG22   | 2.05                     | 0.56              |
| 1:D:406:VAL:O    | 1:D:409:PRO:HD2   | 2.05                     | 0.56              |
| 1:G:158:GLY:O    | 1:G:162:ILE:HD12  | 2.04                     | 0.56              |
| 1:G:248:PHE:HA   | 1:G:251:LYS:HG2   | 1.87                     | 0.56              |
| 3:I:10:THR:HG22  | 3:I:10:THR:O      | 2.04                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:L:10:THR:HG22  | 3:L:10:THR:O     | 2.05                     | 0.56              |
| 5:M:502:HEM:HMC1 | 5:M:502:HEM:CBC  | 2.36                     | 0.56              |
| 2:N:138:PHE:CE1  | 2:N:157:ASN:ND2  | 2.73                     | 0.56              |
| 1:P:114:ARG:HD2  | 1:P:114:ARG:C    | 2.31                     | 0.56              |
| 2:H:77:THR:CG2   | 2:H:79:GLU:HB2   | 2.36                     | 0.56              |
| 1:J:5:PRO:HB2    | 1:J:234:LYS:HA   | 1.86                     | 0.56              |
| 1:J:246:PRO:HG2  | 2:K:251:LEU:HD21 | 1.86                     | 0.56              |
| 1:M:125:ARG:CZ   | 1:M:222:ASN:HB2  | 2.35                     | 0.56              |
| 2:Q:72:VAL:HG12  | 2:Q:73:THR:N     | 2.21                     | 0.56              |
| 1:D:217:HIS:NE2  | 8:D:1102:UQ2:O4  | 2.26                     | 0.56              |
| 1:P:351:THR:OG1  | 1:P:412:GLY:HA3  | 2.05                     | 0.56              |
| 1:A:12:ARG:O     | 1:A:17:LYS:HE2   | 2.05                     | 0.56              |
| 1:A:359:TYR:CD2  | 1:A:420:PRO:HB3  | 2.41                     | 0.56              |
| 2:B:145:CYS:O    | 2:B:168:THR:OG1  | 2.21                     | 0.56              |
| 1:M:114:ARG:C    | 1:M:114:ARG:HD2  | 2.31                     | 0.56              |
| 2:N:220:GLU:OE2  | 2:N:226:ARG:NH1  | 2.39                     | 0.56              |
| 1:G:184:PRO:O    | 3:L:70:LYS:HE3   | 2.05                     | 0.56              |
| 2:Q:81:ARG:HG3   | 2:Q:81:ARG:HH11  | 1.70                     | 0.56              |
| 1:G:114:ARG:HD2  | 1:G:114:ARG:C    | 2.30                     | 0.56              |
| 3:C:131:HIS:O    | 1:D:329:LYS:HE3  | 2.06                     | 0.56              |
| 1:P:43:TRP:HZ3   | 1:P:251:LYS:HE3  | 1.69                     | 0.56              |
| 1:D:114:ARG:HD2  | 1:D:114:ARG:C    | 2.31                     | 0.56              |
| 1:G:383:GLN:HE22 | 2:H:115:GLY:HA3  | 1.71                     | 0.56              |
| 1:J:249:ILE:O    | 1:J:253:VAL:HG23 | 2.06                     | 0.55              |
| 2:N:42:MET:HE1   | 2:N:218:ALA:CB   | 2.35                     | 0.55              |
| 1:P:236:GLU:HA   | 1:P:239:LYS:CD   | 2.36                     | 0.55              |
| 1:J:199:TYR:CD2  | 5:J:502:HEM:HBC1 | 2.42                     | 0.55              |
| 1:J:132:GLY:C    | 5:J:501:HEM:HBC2 | 2.31                     | 0.55              |
| 1:D:144:PHE:CD1  | 1:D:162:ILE:HD12 | 2.40                     | 0.55              |
| 2:K:114:MET:O    | 2:K:114:MET:HG2  | 2.05                     | 0.55              |
| 1:A:358:ARG:HH21 | 7:A:1021:LOP:H21 | 1.71                     | 0.55              |
| 1:G:4:ILE:HD12   | 1:G:4:ILE:N      | 2.19                     | 0.55              |
| 1:P:199:TYR:CD2  | 5:P:502:HEM:HBC1 | 2.41                     | 0.55              |
| 2:E:56:PRO:HD2   | 13:E:1045:HOH:O  | 2.06                     | 0.55              |
| 1:A:58:GLN:CB    | 5:A:502:HEM:HAB  | 2.37                     | 0.55              |
| 2:B:250:ARG:CD   | 3:C:12:ARG:HG2   | 2.28                     | 0.55              |
| 1:D:13:THR:HG22  | 1:D:14:GLY:N     | 2.22                     | 0.55              |
| 1:P:287:ARG:HG2  | 1:P:287:ARG:NH1  | 2.21                     | 0.55              |
| 1:A:195:PHE:CE2  | 1:D:195:PHE:HE2  | 2.10                     | 0.55              |
| 2:B:27:ARG:HD2   | 2:B:196:TYR:CE2  | 2.42                     | 0.55              |
| 2:Q:246:LEU:O    | 2:Q:250:ARG:HG2  | 2.07                     | 0.55              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:92:MET:CE    | 2:E:226:ARG:HG3   | 2.35                     | 0.55              |
| 1:M:246:PRO:HG2  | 2:N:251:LEU:HD21  | 1.88                     | 0.54              |
| 1:P:244:PHE:CE1  | 8:P:1106:UQ2:H2M2 | 2.42                     | 0.54              |
| 3:R:89:GLN:O     | 3:R:92:GLN:HB2    | 2.07                     | 0.54              |
| 2:Q:66:TYR:CE1   | 2:Q:70:PHE:HE2    | 2.24                     | 0.54              |
| 1:D:359:TYR:CD2  | 1:D:420:PRO:HB3   | 2.43                     | 0.54              |
| 2:E:169:CYS:O    | 2:E:177:THR:HB    | 2.06                     | 0.54              |
| 2:E:142:PRO:HG2  | 2:E:150:GLU:OE2   | 2.07                     | 0.54              |
| 2:H:146:ALA:O    | 2:H:148:GLY:N     | 2.41                     | 0.54              |
| 1:J:226:GLY:HA2  | 1:J:355:ARG:HD2   | 1.89                     | 0.54              |
| 1:M:249:ILE:O    | 1:M:253:VAL:HG23  | 2.07                     | 0.54              |
| 1:P:406:VAL:C    | 1:P:409:PRO:HD2   | 2.33                     | 0.54              |
| 2:B:141:GLU:O    | 2:B:141:GLU:HG3   | 2.07                     | 0.54              |
| 1:D:13:THR:HG22  | 1:D:14:GLY:H      | 1.72                     | 0.54              |
| 2:E:250:ARG:CD   | 3:F:12:ARG:HB3    | 2.36                     | 0.54              |
| 1:G:185:ALA:HB2  | 3:L:70:LYS:HG3    | 1.87                     | 0.54              |
| 1:G:249:ILE:O    | 1:G:253:VAL:HG23  | 2.06                     | 0.54              |
| 1:P:269:PHE:HB3  | 9:P:1046:BGL:H1'2 | 1.89                     | 0.54              |
| 2:Q:169:CYS:O    | 2:Q:177:THR:HB    | 2.08                     | 0.54              |
| 2:B:42:MET:CE    | 2:B:218:ALA:CB    | 2.85                     | 0.54              |
| 2:B:169:CYS:O    | 2:B:177:THR:HB    | 2.08                     | 0.54              |
| 1:M:362:MET:CB   | 1:M:411:LEU:HD21  | 2.38                     | 0.54              |
| 1:A:5:PRO:HB3    | 1:A:234:LYS:HG2   | 1.90                     | 0.54              |
| 1:A:13:THR:HG22  | 1:A:14:GLY:N      | 2.22                     | 0.54              |
| 2:N:128:PRO:HG2  | 2:N:129:GLU:OE1   | 2.08                     | 0.54              |
| 1:G:13:THR:HG22  | 1:G:14:GLY:H      | 1.73                     | 0.54              |
| 1:M:8:HIS:CD2    | 1:M:8:HIS:N       | 2.73                     | 0.54              |
| 1:M:122:LYS:O    | 1:M:123:ALA:C     | 2.51                     | 0.54              |
| 1:P:249:ILE:O    | 1:P:253:VAL:HG23  | 2.07                     | 0.54              |
| 2:Q:236:PHE:CE1  | 3:R:25:VAL:CG1    | 2.90                     | 0.54              |
| 2:E:66:TYR:O     | 2:E:69:GLN:HG2    | 2.07                     | 0.54              |
| 1:A:195:PHE:HE2  | 1:D:195:PHE:CE2   | 2.10                     | 0.53              |
| 2:B:128:PRO:HG2  | 2:B:129:GLU:OE1   | 2.08                     | 0.53              |
| 1:D:346:VAL:HG12 | 1:D:347:PRO:HD3   | 1.90                     | 0.53              |
| 1:A:13:THR:O     | 1:A:17:LYS:HG3    | 2.08                     | 0.53              |
| 2:B:149:HIS:CE1  | 2:B:168:THR:HG21  | 2.43                     | 0.53              |
| 1:G:13:THR:HG22  | 1:G:14:GLY:N      | 2.23                     | 0.53              |
| 2:N:146:ALA:O    | 2:N:148:GLY:N     | 2.40                     | 0.53              |
| 3:O:90:LEU:HD11  | 3:O:108:GLU:HB3   | 1.90                     | 0.53              |
| 1:P:112:ILE:HG12 | 5:P:501:HEM:HAC   | 1.90                     | 0.53              |
| 1:A:217:HIS:NE2  | 8:A:1101:UQ2:O4   | 2.40                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:146:ALA:O    | 2:K:148:GLY:N    | 2.41                     | 0.53              |
| 1:M:13:THR:HG22  | 1:M:14:GLY:N     | 2.24                     | 0.53              |
| 1:M:234:LYS:O    | 1:M:238:GLN:HG3  | 2.09                     | 0.53              |
| 2:Q:146:ALA:O    | 2:Q:148:GLY:N    | 2.41                     | 0.53              |
| 1:A:13:THR:HG22  | 1:A:14:GLY:H     | 1.72                     | 0.53              |
| 1:J:13:THR:HG22  | 1:J:14:GLY:N     | 2.23                     | 0.53              |
| 2:B:49:SER:HA    | 2:B:52:GLU:HG3   | 1.89                     | 0.53              |
| 2:B:146:ALA:O    | 2:B:148:GLY:N    | 2.41                     | 0.53              |
| 2:E:66:TYR:CE1   | 2:E:70:PHE:HE2   | 2.26                     | 0.53              |
| 1:M:346:VAL:HG12 | 1:M:347:PRO:HD3  | 1.91                     | 0.53              |
| 1:M:362:MET:HB2  | 1:M:411:LEU:HD21 | 1.91                     | 0.53              |
| 2:E:81:ARG:HG3   | 2:E:81:ARG:HH11  | 1.74                     | 0.53              |
| 1:G:58:GLN:CB    | 5:G:502:HEM:HAB  | 2.38                     | 0.53              |
| 1:J:13:THR:HG22  | 1:J:14:GLY:H     | 1.73                     | 0.53              |
| 2:Q:144:LYS:HZ3  | 2:Q:144:LYS:CA   | 1.97                     | 0.53              |
| 1:A:184:PRO:O    | 3:F:70:LYS:HE3   | 2.08                     | 0.53              |
| 1:D:39:ARG:NH1   | 2:E:255:VAL:CG1  | 2.72                     | 0.53              |
| 1:G:33:ILE:HG13  | 1:G:245:TRP:CB   | 2.39                     | 0.53              |
| 2:N:169:CYS:O    | 2:N:177:THR:HB   | 2.08                     | 0.53              |
| 1:P:199:TYR:CE2  | 5:P:502:HEM:HBC1 | 2.44                     | 0.53              |
| 2:Q:142:PRO:HB3  | 2:Q:150:GLU:OE2  | 2.09                     | 0.53              |
| 1:D:9:TYR:HB2    | 1:D:30:TYR:CD2   | 2.44                     | 0.52              |
| 1:D:199:TYR:CZ   | 5:D:502:HEM:HBC1 | 2.43                     | 0.52              |
| 1:J:428:PHE:CZ   | 2:K:256:LYS:HD2  | 2.43                     | 0.52              |
| 2:K:169:CYS:O    | 2:K:177:THR:HB   | 2.09                     | 0.52              |
| 2:E:40:HIS:ND1   | 2:E:97:ALA:HB1   | 2.23                     | 0.52              |
| 2:H:128:PRO:HG2  | 2:H:129:GLU:OE1  | 2.09                     | 0.52              |
| 1:J:346:VAL:HG12 | 1:J:347:PRO:HD3  | 1.90                     | 0.52              |
| 2:K:77:THR:HG22  | 2:K:79:GLU:CB    | 2.40                     | 0.52              |
| 1:P:13:THR:HG22  | 1:P:14:GLY:N     | 2.23                     | 0.52              |
| 1:P:33:ILE:HG13  | 1:P:245:TRP:CB   | 2.39                     | 0.52              |
| 2:B:220:GLU:OE2  | 2:B:226:ARG:NH1  | 2.43                     | 0.52              |
| 2:E:189:LEU:O    | 2:E:190:MET:HB2  | 2.10                     | 0.52              |
| 1:J:234:LYS:O    | 1:J:238:GLN:HG3  | 2.09                     | 0.52              |
| 1:M:13:THR:HG22  | 1:M:14:GLY:H     | 1.74                     | 0.52              |
| 1:M:352:SER:HB2  | 1:M:415:GLU:OE2  | 2.09                     | 0.52              |
| 1:A:33:ILE:HG13  | 1:A:245:TRP:CB   | 2.39                     | 0.52              |
| 2:E:146:ALA:O    | 2:E:148:GLY:N    | 2.43                     | 0.52              |
| 2:K:74:ASP:HB3   | 2:K:77:THR:CB    | 2.29                     | 0.52              |
| 1:P:346:VAL:HG12 | 1:P:347:PRO:HD3  | 1.90                     | 0.52              |
| 2:B:77:THR:C     | 2:B:79:GLU:H     | 2.16                     | 0.52              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:205:HIS:ND1  | 2:B:205:HIS:C     | 2.68                     | 0.52              |
| 3:C:84:LEU:CD2   | 3:L:84:LEU:HD23   | 2.39                     | 0.52              |
| 1:D:33:ILE:HG13  | 1:D:245:TRP:CB    | 2.39                     | 0.52              |
| 1:G:144:PHE:CD1  | 1:G:162:ILE:HD13  | 2.43                     | 0.52              |
| 1:G:217:HIS:NE2  | 8:G:1103:UQ2:O4   | 2.36                     | 0.52              |
| 1:J:199:TYR:CE2  | 5:J:502:HEM:HBC1  | 2.45                     | 0.52              |
| 1:M:33:ILE:HG13  | 1:M:245:TRP:CB    | 2.39                     | 0.52              |
| 3:C:70:LYS:HG3   | 1:D:185:ALA:HB2   | 1.92                     | 0.52              |
| 1:D:150:PRO:HG3  | 5:D:502:HEM:O2D   | 2.10                     | 0.52              |
| 2:E:74:ASP:CB    | 2:E:77:THR:HB     | 2.35                     | 0.52              |
| 1:J:229:VAL:HG22 | 1:J:424:ILE:HD12  | 1.92                     | 0.52              |
| 3:O:80:ALA:O     | 3:O:84:LEU:HG     | 2.09                     | 0.52              |
| 1:P:32:THR:HG23  | 1:P:217:HIS:HE1   | 1.74                     | 0.52              |
| 2:B:171:ASP:OD1  | 2:B:173:ASN:N     | 2.37                     | 0.52              |
| 2:E:250:ARG:CZ   | 3:F:12:ARG:HG2    | 2.40                     | 0.52              |
| 1:J:269:PHE:HB3  | 9:K:1044:BGL:H1'2 | 1.92                     | 0.52              |
| 2:K:185:MET:HB2  | 5:K:301:HEM:C1D   | 2.45                     | 0.52              |
| 1:P:13:THR:HG22  | 1:P:14:GLY:H      | 1.74                     | 0.52              |
| 1:G:346:VAL:HG12 | 1:G:347:PRO:HD3   | 1.91                     | 0.52              |
| 2:K:42:MET:CE    | 2:K:218:ALA:HB1   | 2.38                     | 0.52              |
| 1:M:236:GLU:HA   | 1:M:239:LYS:CD    | 2.40                     | 0.52              |
| 1:M:236:GLU:HA   | 1:M:239:LYS:HD3   | 1.92                     | 0.52              |
| 1:M:58:GLN:CB    | 5:M:502:HEM:HAB   | 2.39                     | 0.52              |
| 1:P:39:ARG:NH1   | 2:Q:255:VAL:CG1   | 2.72                     | 0.52              |
| 1:A:346:VAL:HG12 | 1:A:347:PRO:HD3   | 1.91                     | 0.51              |
| 2:E:77:THR:C     | 2:E:79:GLU:H      | 2.17                     | 0.51              |
| 1:G:195:PHE:CE2  | 1:J:195:PHE:HE2   | 2.13                     | 0.51              |
| 2:H:114:MET:O    | 2:H:114:MET:HG2   | 2.10                     | 0.51              |
| 1:J:33:ILE:HG13  | 1:J:245:TRP:CB    | 2.39                     | 0.51              |
| 2:N:160:PHE:CE2  | 2:N:183:ILE:HG13  | 2.44                     | 0.51              |
| 2:N:205:HIS:ND1  | 2:N:205:HIS:C     | 2.69                     | 0.51              |
| 1:A:154:MET:HE2  | 1:A:154:MET:HA    | 1.93                     | 0.51              |
| 2:E:77:THR:HG22  | 2:E:79:GLU:HB2    | 1.92                     | 0.51              |
| 1:J:142:THR:HG21 | 5:J:502:HEM:HBB2  | 1.92                     | 0.51              |
| 2:E:205:HIS:ND1  | 2:E:205:HIS:C     | 2.68                     | 0.51              |
| 2:H:205:HIS:ND1  | 2:H:205:HIS:C     | 2.69                     | 0.51              |
| 2:B:224:MET:O    | 2:B:228:GLN:HG3   | 2.11                     | 0.51              |
| 1:G:125:ARG:NE   | 1:G:222:ASN:HB2   | 2.25                     | 0.51              |
| 2:H:250:ARG:CZ   | 3:I:12:ARG:HB3    | 2.40                     | 0.51              |
| 2:E:42:MET:CE    | 2:E:218:ALA:CB    | 2.89                     | 0.51              |
| 1:G:132:GLY:C    | 5:G:501:HEM:HBC2  | 2.35                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:D:501:HEM:HBB2 | 5:D:501:HEM:CMB  | 2.41                     | 0.51              |
| 2:H:169:CYS:O    | 2:H:177:THR:HB   | 2.11                     | 0.51              |
| 2:K:40:HIS:HE1   | 2:K:98:PRO:HD2   | 1.76                     | 0.51              |
| 1:G:125:ARG:HD2  | 13:G:1118:HOH:O  | 2.11                     | 0.50              |
| 2:Q:66:TYR:CE1   | 2:Q:70:PHE:CE2   | 3.00                     | 0.50              |
| 2:H:220:GLU:OE2  | 2:H:226:ARG:NH1  | 2.44                     | 0.50              |
| 2:H:250:ARG:NH1  | 3:I:12:ARG:CB    | 2.73                     | 0.50              |
| 1:J:39:ARG:HH12  | 2:K:255:VAL:CG1  | 2.25                     | 0.50              |
| 1:M:133:MET:N    | 5:M:501:HEM:HBC2 | 2.27                     | 0.50              |
| 1:G:5:PRO:HB3    | 1:G:234:LYS:HG2  | 1.93                     | 0.50              |
| 1:A:383:GLN:HE22 | 2:B:115:GLY:HA3  | 1.76                     | 0.50              |
| 1:G:154:MET:HA   | 1:G:154:MET:HE2  | 1.94                     | 0.50              |
| 1:D:91:PHE:CD1   | 2:E:222:LYS:HG2  | 2.46                     | 0.50              |
| 2:Q:205:HIS:ND1  | 2:Q:205:HIS:C    | 2.69                     | 0.50              |
| 2:B:108:ALA:HA   | 2:B:125:ILE:HG22 | 1.93                     | 0.50              |
| 1:G:92:MET:HE1   | 2:H:226:ARG:HG3  | 1.92                     | 0.50              |
| 2:K:205:HIS:ND1  | 2:K:205:HIS:C    | 2.68                     | 0.50              |
| 2:N:176:LYS:O    | 2:N:176:LYS:HD3  | 2.11                     | 0.50              |
| 3:C:57:VAL:HG22  | 3:C:63:LEU:HD13  | 1.94                     | 0.50              |
| 2:E:66:TYR:CE1   | 2:E:70:PHE:CE2   | 2.99                     | 0.50              |
| 1:P:94:ARG:C     | 1:P:94:ARG:HD3   | 2.37                     | 0.50              |
| 1:P:312:VAL:HG12 | 1:P:314:VAL:HG12 | 1.94                     | 0.50              |
| 3:I:70:LYS:HE3   | 1:J:185:ALA:HB2  | 1.92                     | 0.50              |
| 1:M:125:ARG:NH1  | 1:M:222:ASN:HB2  | 2.27                     | 0.50              |
| 2:N:149:HIS:CD2  | 2:N:168:THR:HG21 | 2.46                     | 0.50              |
| 2:Q:236:PHE:CE1  | 3:R:25:VAL:HG12  | 2.46                     | 0.50              |
| 1:D:92:MET:HE1   | 2:E:226:ARG:CG   | 2.40                     | 0.50              |
| 2:E:42:MET:CE    | 2:E:218:ALA:HB1  | 2.42                     | 0.50              |
| 2:H:149:HIS:CE1  | 2:H:168:THR:HG21 | 2.47                     | 0.50              |
| 1:P:11:PRO:HB2   | 1:P:17:LYS:HG2   | 1.94                     | 0.50              |
| 1:G:236:GLU:HA   | 1:G:239:LYS:HG3  | 1.92                     | 0.49              |
| 2:H:154:PHE:HB3  | 2:H:182:TRP:HB3  | 1.94                     | 0.49              |
| 3:L:157:ASP:HB2  | 13:L:505:HOH:O   | 2.12                     | 0.49              |
| 1:A:266:ILE:HD12 | 1:A:270:MET:HE2  | 1.94                     | 0.49              |
| 2:E:40:HIS:CE1   | 2:E:97:ALA:HB1   | 2.47                     | 0.49              |
| 2:Q:220:GLU:OE2  | 2:Q:226:ARG:NH1  | 2.45                     | 0.49              |
| 3:R:70:LYS:HB2   | 3:R:70:LYS:NZ    | 2.27                     | 0.49              |
| 2:B:171:ASP:OD1  | 2:B:171:ASP:C    | 2.56                     | 0.49              |
| 1:G:5:PRO:CB     | 1:G:234:LYS:HG2  | 2.42                     | 0.49              |
| 2:H:76:GLU:O     | 2:H:77:THR:C     | 2.55                     | 0.49              |
| 2:K:234:VAL:HG12 | 2:K:235:MET:HE2  | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:128:THR:HG21 | 5:P:501:HEM:HBD1 | 1.94                     | 0.49              |
| 1:J:236:GLU:HA   | 1:J:239:LYS:CD   | 2.41                     | 0.49              |
| 2:K:236:PHE:CE1  | 3:L:25:VAL:HG12  | 2.47                     | 0.49              |
| 2:N:143:PRO:HG3  | 2:N:178:THR:CG2  | 2.42                     | 0.49              |
| 1:P:248:PHE:CD1  | 1:P:251:LYS:HD3  | 2.48                     | 0.49              |
| 1:P:354:VAL:HG21 | 1:P:417:PRO:CB   | 2.42                     | 0.49              |
| 3:C:59:PRO:HD3   | 3:C:76:ARG:NH1   | 2.28                     | 0.49              |
| 2:K:154:PHE:HB3  | 2:K:182:TRP:HB3  | 1.94                     | 0.49              |
| 2:N:149:HIS:CG   | 2:N:168:THR:HG21 | 2.47                     | 0.49              |
| 2:Q:151:PRO:HD2  | 2:Q:182:TRP:CD1  | 2.47                     | 0.49              |
| 1:D:43:TRP:HA    | 1:D:43:TRP:CE3   | 2.48                     | 0.49              |
| 1:M:235:ALA:O    | 1:M:239:LYS:HG3  | 2.13                     | 0.49              |
| 2:N:183:ILE:HG23 | 2:N:185:MET:N    | 2.24                     | 0.49              |
| 3:F:57:VAL:HG22  | 3:F:63:LEU:HD13  | 1.95                     | 0.49              |
| 1:G:266:ILE:HD12 | 1:G:270:MET:HE2  | 1.95                     | 0.49              |
| 3:R:59:PRO:HD3   | 3:R:76:ARG:NH1   | 2.28                     | 0.49              |
| 3:F:118:GLU:CD   | 3:F:118:GLU:N    | 2.70                     | 0.49              |
| 1:M:92:MET:CE    | 2:N:226:ARG:HG3  | 2.42                     | 0.49              |
| 1:J:266:ILE:HD12 | 1:J:270:MET:HE2  | 1.95                     | 0.49              |
| 2:K:49:SER:HA    | 2:K:52:GLU:CG    | 2.43                     | 0.49              |
| 1:G:362:MET:N    | 1:G:415:GLU:OE2  | 2.45                     | 0.49              |
| 2:K:231:PHE:O    | 2:K:235:MET:HG2  | 2.13                     | 0.49              |
| 1:A:92:MET:HE1   | 2:B:226:ARG:CG   | 2.41                     | 0.48              |
| 1:D:39:ARG:HH12  | 2:E:255:VAL:HG12 | 1.76                     | 0.48              |
| 1:P:32:THR:HG23  | 1:P:217:HIS:CE1  | 2.48                     | 0.48              |
| 1:D:102:SER:O    | 1:D:106:ILE:HG13 | 2.13                     | 0.48              |
| 2:H:250:ARG:NH1  | 3:I:16:TYR:CZ    | 2.81                     | 0.48              |
| 1:M:406:VAL:O    | 1:M:409:PRO:HD2  | 2.12                     | 0.48              |
| 1:D:4:ILE:HD12   | 1:D:4:ILE:N      | 2.28                     | 0.48              |
| 2:N:197:ALA:C    | 2:N:199:GLY:H    | 2.22                     | 0.48              |
| 3:I:59:PRO:HD3   | 3:I:76:ARG:NH1   | 2.28                     | 0.48              |
| 2:K:145:CYS:O    | 2:K:168:THR:OG1  | 2.28                     | 0.48              |
| 1:P:132:GLY:C    | 5:P:501:HEM:HBC2 | 2.38                     | 0.48              |
| 2:Q:130:TYR:OH   | 5:Q:301:HEM:O2A  | 2.17                     | 0.48              |
| 3:R:57:VAL:HG22  | 3:R:63:LEU:HD13  | 1.94                     | 0.48              |
| 1:D:154:MET:HE2  | 1:D:154:MET:HA   | 1.94                     | 0.48              |
| 1:D:266:ILE:HD12 | 1:D:270:MET:HE2  | 1.94                     | 0.48              |
| 1:G:125:ARG:CZ   | 1:G:222:ASN:HB2  | 2.43                     | 0.48              |
| 1:G:406:VAL:C    | 1:G:409:PRO:HD2  | 2.38                     | 0.48              |
| 9:G:1043:BGL:H5  | 2:H:15:GLY:H     | 1.77                     | 0.48              |
| 2:N:72:VAL:O     | 2:N:80:ASP:HA    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:184:ALA:HB3  | 5:N:301:HEM:HBD2 | 1.95                     | 0.48              |
| 2:B:149:HIS:NE2  | 2:B:168:THR:HG21 | 2.28                     | 0.48              |
| 3:F:47:LEU:O     | 3:F:47:LEU:CD2   | 2.61                     | 0.48              |
| 1:G:39:ARG:NH1   | 2:H:255:VAL:CG1  | 2.76                     | 0.48              |
| 1:J:154:MET:HE2  | 1:J:154:MET:HA   | 1.96                     | 0.48              |
| 1:G:58:GLN:HB3   | 5:G:502:HEM:HAB  | 1.95                     | 0.48              |
| 1:G:105:PHE:HA   | 1:G:108:VAL:CG2  | 2.44                     | 0.48              |
| 1:J:91:PHE:HE2   | 1:J:92:MET:CE    | 2.26                     | 0.48              |
| 1:J:355:ARG:HG3  | 1:J:355:ARG:HH11 | 1.79                     | 0.48              |
| 3:L:57:VAL:HG22  | 3:L:63:LEU:HD13  | 1.94                     | 0.48              |
| 2:N:154:PHE:HB3  | 2:N:182:TRP:HB3  | 1.95                     | 0.48              |
| 3:F:90:LEU:HD11  | 3:F:108:GLU:HB3  | 1.95                     | 0.48              |
| 1:M:51:LEU:HB3   | 5:M:501:HEM:HMB1 | 1.96                     | 0.48              |
| 2:N:42:MET:CE    | 2:N:218:ALA:CB   | 2.91                     | 0.48              |
| 2:Q:73:THR:HG23  | 2:Q:80:ASP:OD1   | 2.13                     | 0.48              |
| 1:G:312:VAL:HG12 | 1:G:314:VAL:HG12 | 1.96                     | 0.48              |
| 1:M:346:VAL:CG1  | 1:M:347:PRO:HD3  | 2.44                     | 0.48              |
| 1:P:91:PHE:CE2   | 1:P:92:MET:HE3   | 2.48                     | 0.48              |
| 2:E:72:VAL:CG1   | 2:E:73:THR:N     | 2.76                     | 0.48              |
| 3:I:57:VAL:HG22  | 3:I:63:LEU:HD13  | 1.95                     | 0.48              |
| 3:L:59:PRO:HD3   | 3:L:76:ARG:NH1   | 2.29                     | 0.48              |
| 3:L:90:LEU:HD11  | 3:L:108:GLU:HB3  | 1.96                     | 0.48              |
| 1:M:266:ILE:HD12 | 1:M:270:MET:HE2  | 1.96                     | 0.48              |
| 2:N:74:ASP:CG    | 2:N:77:THR:HB    | 2.39                     | 0.48              |
| 2:N:108:ALA:HA   | 2:N:125:ILE:O    | 2.14                     | 0.48              |
| 2:Q:185:MET:HB2  | 5:Q:301:HEM:C1D  | 2.49                     | 0.48              |
| 2:Q:197:ALA:C    | 2:Q:199:GLY:H    | 2.21                     | 0.48              |
| 1:D:43:TRP:O     | 1:D:46:ILE:HG12  | 2.14                     | 0.47              |
| 1:J:51:LEU:HB3   | 5:J:501:HEM:HMB1 | 1.96                     | 0.47              |
| 3:O:59:PRO:HD3   | 3:O:76:ARG:NH1   | 2.29                     | 0.47              |
| 2:Q:81:ARG:HG3   | 2:Q:81:ARG:NH1   | 2.29                     | 0.47              |
| 2:Q:141:GLU:H    | 2:Q:141:GLU:HG2  | 1.49                     | 0.47              |
| 1:A:236:GLU:HA   | 1:A:239:LYS:HD3  | 1.97                     | 0.47              |
| 1:G:346:VAL:CG1  | 1:G:347:PRO:HD3  | 2.44                     | 0.47              |
| 2:K:42:MET:HE2   | 2:K:101:SER:HA   | 1.95                     | 0.47              |
| 1:M:4:ILE:H      | 1:M:4:ILE:CD1    | 2.24                     | 0.47              |
| 1:M:425:GLU:O    | 1:M:429:ASN:ND2  | 2.47                     | 0.47              |
| 1:P:43:TRP:HA    | 1:P:43:TRP:CE3   | 2.49                     | 0.47              |
| 1:D:246:PRO:CG   | 2:E:251:LEU:HD21 | 2.41                     | 0.47              |
| 2:E:142:PRO:CG   | 2:E:150:GLU:OE2  | 2.62                     | 0.47              |
| 3:F:59:PRO:HD3   | 3:F:76:ARG:NH1   | 2.30                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:248:PHE:CE1  | 1:G:251:LYS:HD3   | 2.48                     | 0.47              |
| 3:I:66:LYS:HE2   | 3:I:69:GLY:HA2    | 1.96                     | 0.47              |
| 2:K:197:ALA:C    | 2:K:199:GLY:H     | 2.23                     | 0.47              |
| 1:M:6:HIS:ND1    | 1:M:6:HIS:C       | 2.71                     | 0.47              |
| 1:P:346:VAL:CG1  | 1:P:347:PRO:HD3   | 2.44                     | 0.47              |
| 1:A:346:VAL:CG1  | 1:A:347:PRO:HD3   | 2.45                     | 0.47              |
| 2:B:42:MET:CE    | 2:B:218:ALA:HB1   | 2.45                     | 0.47              |
| 2:E:40:HIS:HE1   | 2:E:98:PRO:HD2    | 1.79                     | 0.47              |
| 3:I:84:LEU:O     | 3:I:88:VAL:HG23   | 2.14                     | 0.47              |
| 1:J:91:PHE:CE2   | 1:J:92:MET:CE     | 2.97                     | 0.47              |
| 2:K:220:GLU:OE2  | 2:K:226:ARG:NH1   | 2.48                     | 0.47              |
| 1:M:43:TRP:CZ3   | 1:M:251:LYS:HE2   | 2.50                     | 0.47              |
| 1:M:154:MET:HE2  | 1:M:154:MET:HA    | 1.95                     | 0.47              |
| 3:O:57:VAL:HG22  | 3:O:63:LEU:HD13   | 1.95                     | 0.47              |
| 2:Q:19:THR:CG2   | 2:Q:224:MET:HE3   | 2.45                     | 0.47              |
| 3:R:62:GLN:NE2   | 3:R:73:PHE:CD1    | 2.83                     | 0.47              |
| 1:A:360:ARG:O    | 1:A:364:LYS:HG3   | 2.14                     | 0.47              |
| 1:M:10:GLU:HA    | 1:M:11:PRO:HD3    | 1.70                     | 0.47              |
| 2:N:103:MET:C    | 2:N:105:LYS:H     | 2.21                     | 0.47              |
| 1:P:177:GLN:NE2  | 13:P:611:HOH:O    | 2.40                     | 0.47              |
| 1:P:266:ILE:HD12 | 1:P:270:MET:HE2   | 1.96                     | 0.47              |
| 1:A:43:TRP:CZ3   | 1:A:251:LYS:HE3   | 2.50                     | 0.47              |
| 1:D:346:VAL:CG1  | 1:D:347:PRO:HD3   | 2.44                     | 0.47              |
| 1:J:407:ILE:O    | 1:J:411:LEU:HG    | 2.14                     | 0.47              |
| 1:M:113:PHE:HB3  | 7:M:1025:LOP:H261 | 1.95                     | 0.47              |
| 2:Q:236:PHE:CE1  | 3:R:25:VAL:HG11   | 2.49                     | 0.47              |
| 1:A:199:TYR:CD2  | 5:A:502:HEM:HBC1  | 2.50                     | 0.47              |
| 1:G:39:ARG:HD3   | 1:G:428:PHE:CD2   | 2.50                     | 0.47              |
| 1:J:217:HIS:NE2  | 8:J:1104:UQ2:O4   | 2.46                     | 0.47              |
| 1:J:346:VAL:CG1  | 1:J:347:PRO:HD3   | 2.44                     | 0.47              |
| 3:O:47:LEU:HD23  | 3:O:47:LEU:C      | 2.39                     | 0.47              |
| 1:A:118:TYR:OH   | 7:A:1021:LOP:H32  | 2.15                     | 0.47              |
| 1:D:423:THR:OG1  | 1:D:426:GLU:HB2   | 2.14                     | 0.47              |
| 2:N:157:ASN:O    | 2:N:180:GLY:HA3   | 2.15                     | 0.47              |
| 1:J:128:THR:HG21 | 5:J:501:HEM:HBD1  | 1.97                     | 0.47              |
| 1:M:92:MET:CE    | 1:M:92:MET:HA     | 2.45                     | 0.47              |
| 1:M:195:PHE:HE2  | 1:P:195:PHE:CE2   | 2.12                     | 0.47              |
| 2:Q:157:ASN:O    | 2:Q:180:GLY:HA3   | 2.15                     | 0.47              |
| 2:Q:226:ARG:HD3  | 13:Q:672:HOH:O    | 2.14                     | 0.47              |
| 1:A:123:ALA:O    | 1:A:355:ARG:NH1   | 2.48                     | 0.47              |
| 5:A:501:HEM:HMC2 | 5:A:501:HEM:CBC   | 2.43                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:43:TRP:HA    | 1:G:43:TRP:CE3    | 2.50                     | 0.47              |
| 2:E:185:MET:HB2  | 5:E:301:HEM:C1D   | 2.50                     | 0.46              |
| 2:K:77:THR:HG22  | 2:K:79:GLU:HG3    | 1.97                     | 0.46              |
| 3:L:66:LYS:HD3   | 3:L:69:GLY:HA2    | 1.96                     | 0.46              |
| 1:M:30:TYR:HA    | 1:M:33:ILE:HG22   | 1.97                     | 0.46              |
| 3:O:47:LEU:HG    | 3:O:68:LEU:HD21   | 1.97                     | 0.46              |
| 1:D:406:VAL:C    | 1:D:409:PRO:HD2   | 2.40                     | 0.46              |
| 2:E:76:GLU:O     | 2:E:77:THR:C      | 2.57                     | 0.46              |
| 1:G:30:TYR:HA    | 1:G:33:ILE:HG22   | 1.98                     | 0.46              |
| 1:J:30:TYR:HA    | 1:J:33:ILE:HG22   | 1.97                     | 0.46              |
| 1:M:106:ILE:HG13 | 1:M:296:TRP:CH2   | 2.50                     | 0.46              |
| 1:M:410:ILE:HG23 | 1:M:414:ILE:CD1   | 2.37                     | 0.46              |
| 2:Q:145:CYS:O    | 2:Q:168:THR:OG1   | 2.26                     | 0.46              |
| 1:A:39:ARG:NH1   | 2:B:255:VAL:CG1   | 2.79                     | 0.46              |
| 1:A:234:LYS:O    | 1:A:238:GLN:HG3   | 2.16                     | 0.46              |
| 2:B:147:GLU:OE1  | 2:B:147:GLU:HA    | 2.14                     | 0.46              |
| 1:M:49:VAL:HG21  | 1:M:252:ASP:OD2   | 2.15                     | 0.46              |
| 2:N:81:ARG:NH1   | 2:N:84:LYS:HG3    | 2.30                     | 0.46              |
| 1:P:122:LYS:O    | 1:P:123:ALA:C     | 2.58                     | 0.46              |
| 9:P:1046:BGL:H5  | 2:Q:15:GLY:H      | 1.81                     | 0.46              |
| 3:R:39:ASN:HB3   | 13:R:676:HOH:O    | 2.14                     | 0.46              |
| 1:D:30:TYR:HA    | 1:D:33:ILE:HG22   | 1.98                     | 0.46              |
| 1:D:269:PHE:HB3  | 9:E:1042:BGL:O1   | 2.15                     | 0.46              |
| 2:N:155:TYR:CZ   | 2:N:186:PRO:HB3   | 2.50                     | 0.46              |
| 3:O:58:GLU:N     | 3:O:58:GLU:CD     | 2.74                     | 0.46              |
| 1:A:30:TYR:HA    | 1:A:33:ILE:HG22   | 1.98                     | 0.46              |
| 2:B:155:TYR:CZ   | 2:B:186:PRO:HB3   | 2.51                     | 0.46              |
| 3:I:58:GLU:N     | 3:I:58:GLU:CD     | 2.73                     | 0.46              |
| 1:J:354:VAL:HG21 | 1:J:417:PRO:CB    | 2.46                     | 0.46              |
| 1:J:414:ILE:O    | 1:J:414:ILE:CG2   | 2.62                     | 0.46              |
| 2:Q:154:PHE:C    | 2:Q:155:TYR:CD1   | 2.94                     | 0.46              |
| 1:A:122:LYS:O    | 1:A:123:ALA:C     | 2.59                     | 0.46              |
| 2:B:165:VAL:CG1  | 2:B:169:CYS:HB2   | 2.46                     | 0.46              |
| 1:D:4:ILE:O      | 1:D:6:HIS:HD2     | 1.99                     | 0.46              |
| 1:D:51:LEU:CD2   | 1:D:108:VAL:HG13  | 2.46                     | 0.46              |
| 1:G:244:PHE:CE1  | 8:G:1103:UQ2:H2M2 | 2.51                     | 0.46              |
| 2:H:165:VAL:CG1  | 2:H:169:CYS:HB2   | 2.45                     | 0.46              |
| 2:K:155:TYR:CZ   | 2:K:186:PRO:HB3   | 2.51                     | 0.46              |
| 1:M:359:TYR:CD2  | 1:M:420:PRO:HB3   | 2.51                     | 0.46              |
| 2:B:90:PRO:HA    | 13:B:1046:HOH:O   | 2.15                     | 0.46              |
| 1:G:111:HIS:CD2  | 5:G:501:HEM:NC    | 2.84                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:234:LYS:O    | 1:G:238:GLN:HG3   | 2.15                     | 0.46              |
| 2:Q:154:PHE:HB3  | 2:Q:182:TRP:HB3   | 1.98                     | 0.46              |
| 2:Q:223:LEU:HD21 | 2:Q:227:LYS:CE    | 2.32                     | 0.46              |
| 3:R:58:GLU:CD    | 3:R:58:GLU:N      | 2.73                     | 0.46              |
| 2:E:144:LYS:HE2  | 2:E:144:LYS:CA    | 2.46                     | 0.46              |
| 1:G:43:TRP:CZ3   | 1:G:251:LYS:HE3   | 2.49                     | 0.46              |
| 2:H:113:PRO:O    | 2:H:114:MET:HB3   | 2.16                     | 0.46              |
| 3:I:131:HIS:O    | 1:J:329:LYS:CE    | 2.64                     | 0.46              |
| 1:J:236:GLU:HA   | 1:J:239:LYS:HD3   | 1.98                     | 0.46              |
| 1:J:362:MET:HE1  | 1:J:414:ILE:HG22  | 1.97                     | 0.46              |
| 2:K:77:THR:HG22  | 2:K:79:GLU:CG     | 2.46                     | 0.46              |
| 2:K:157:ASN:O    | 2:K:180:GLY:HA3   | 2.16                     | 0.46              |
| 2:K:246:LEU:O    | 2:K:250:ARG:HG2   | 2.16                     | 0.46              |
| 3:L:58:GLU:N     | 3:L:58:GLU:CD     | 2.73                     | 0.46              |
| 1:M:58:GLN:HB3   | 5:M:502:HEM:HAB   | 1.96                     | 0.46              |
| 1:P:154:MET:HE2  | 1:P:154:MET:HA    | 1.97                     | 0.46              |
| 2:Q:72:VAL:CG1   | 2:Q:73:THR:N      | 2.79                     | 0.46              |
| 3:F:58:GLU:CD    | 3:F:58:GLU:N      | 2.74                     | 0.46              |
| 2:H:149:HIS:N    | 2:H:149:HIS:CD2   | 2.83                     | 0.46              |
| 1:J:122:LYS:O    | 1:J:123:ALA:C     | 2.59                     | 0.46              |
| 2:K:77:THR:CG2   | 2:K:79:GLU:HB2    | 2.46                     | 0.46              |
| 2:Q:27:ARG:HD2   | 2:Q:196:TYR:CE2   | 2.51                     | 0.46              |
| 3:C:90:LEU:HB2   | 2:H:172:ALA:HB1   | 1.98                     | 0.45              |
| 1:P:30:TYR:HA    | 1:P:33:ILE:HG22   | 1.98                     | 0.45              |
| 2:E:155:TYR:CZ   | 2:E:186:PRO:HB3   | 2.51                     | 0.45              |
| 2:H:155:TYR:CZ   | 2:H:186:PRO:HB3   | 2.51                     | 0.45              |
| 2:H:197:ALA:C    | 2:H:199:GLY:H     | 2.23                     | 0.45              |
| 1:J:291:HIS:O    | 1:J:293:VAL:HG23  | 2.16                     | 0.45              |
| 1:J:322:SER:O    | 1:J:323:PHE:HB2   | 2.16                     | 0.45              |
| 1:P:291:HIS:O    | 1:P:293:VAL:HG23  | 2.16                     | 0.45              |
| 2:Q:155:TYR:CZ   | 2:Q:186:PRO:HB3   | 2.51                     | 0.45              |
| 1:A:244:PHE:CE1  | 8:A:1101:UQ2:H2M3 | 2.51                     | 0.45              |
| 1:A:291:HIS:O    | 1:A:293:VAL:HG23  | 2.16                     | 0.45              |
| 2:B:154:PHE:C    | 2:B:155:TYR:CD1   | 2.94                     | 0.45              |
| 3:C:58:GLU:CD    | 3:C:58:GLU:N      | 2.73                     | 0.45              |
| 2:E:40:HIS:HB3   | 2:E:100:LEU:HG    | 1.98                     | 0.45              |
| 2:E:145:CYS:O    | 2:E:168:THR:OG1   | 2.27                     | 0.45              |
| 2:N:154:PHE:C    | 2:N:155:TYR:CD1   | 2.94                     | 0.45              |
| 2:Q:77:THR:C     | 2:Q:79:GLU:N      | 2.73                     | 0.45              |
| 2:B:77:THR:HG22  | 2:B:79:GLU:CG     | 2.47                     | 0.45              |
| 2:E:42:MET:HE1   | 2:E:218:ALA:HB2   | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:250:ARG:HG3  | 2:E:250:ARG:NH1  | 2.23                     | 0.45              |
| 2:E:250:ARG:NH2  | 3:F:15:LEU:HD22  | 2.31                     | 0.45              |
| 1:G:125:ARG:HH21 | 1:G:221:ASN:C    | 2.23                     | 0.45              |
| 2:H:250:ARG:NH1  | 3:I:16:TYR:CE1   | 2.84                     | 0.45              |
| 1:M:150:PRO:HG3  | 5:M:502:HEM:O2D  | 2.16                     | 0.45              |
| 2:N:152:ASP:C    | 2:N:152:ASP:OD1  | 2.59                     | 0.45              |
| 2:Q:236:PHE:HE1  | 3:R:25:VAL:HG11  | 1.81                     | 0.45              |
| 1:A:58:GLN:HB3   | 5:A:502:HEM:HAB  | 1.98                     | 0.45              |
| 2:B:197:ALA:C    | 2:B:199:GLY:H    | 2.24                     | 0.45              |
| 2:E:141:GLU:O    | 2:E:141:GLU:HG3  | 2.16                     | 0.45              |
| 2:E:157:ASN:O    | 2:E:180:GLY:HA3  | 2.16                     | 0.45              |
| 1:G:418:VAL:CG1  | 1:G:419:ALA:N    | 2.80                     | 0.45              |
| 2:E:146:ALA:O    | 2:E:147:GLU:C    | 2.59                     | 0.45              |
| 2:E:154:PHE:C    | 2:E:155:TYR:CD1  | 2.94                     | 0.45              |
| 2:E:197:ALA:C    | 2:E:199:GLY:H    | 2.23                     | 0.45              |
| 1:G:23:LEU:HD13  | 1:J:215:ALA:HA   | 1.98                     | 0.45              |
| 1:G:428:PHE:CE1  | 2:H:256:LYS:HD3  | 2.51                     | 0.45              |
| 2:H:157:ASN:O    | 2:H:180:GLY:HA3  | 2.16                     | 0.45              |
| 2:H:185:MET:HB2  | 5:H:301:HEM:C1D  | 2.52                     | 0.45              |
| 2:H:203:SER:O    | 2:H:204:VAL:C    | 2.60                     | 0.45              |
| 1:J:209:VAL:HG22 | 5:J:501:HEM:HBB2 | 1.98                     | 0.45              |
| 2:K:154:PHE:C    | 2:K:155:TYR:CD1  | 2.94                     | 0.45              |
| 1:M:291:HIS:O    | 1:M:293:VAL:HG23 | 2.16                     | 0.45              |
| 2:N:48:ARG:HB3   | 2:N:85:PRO:O     | 2.17                     | 0.45              |
| 2:B:77:THR:HG22  | 2:B:79:GLU:HB2   | 1.99                     | 0.45              |
| 2:E:203:SER:O    | 2:E:204:VAL:C    | 2.60                     | 0.45              |
| 2:H:68:THR:HG23  | 2:H:82:GLU:OE1   | 2.16                     | 0.45              |
| 1:J:6:HIS:ND1    | 1:J:6:HIS:C      | 2.75                     | 0.45              |
| 3:L:118:GLU:N    | 3:L:118:GLU:CD   | 2.75                     | 0.45              |
| 1:M:415:GLU:O    | 1:M:417:PRO:HD3  | 2.17                     | 0.45              |
| 2:N:77:THR:CG2   | 2:N:79:GLU:HB2   | 2.46                     | 0.45              |
| 2:N:250:ARG:HH11 | 3:O:12:ARG:HA    | 1.80                     | 0.45              |
| 1:P:118:TYR:OH   | 7:P:1026:LOP:H32 | 2.17                     | 0.45              |
| 2:Q:42:MET:HE2   | 2:Q:218:ALA:HB1  | 1.99                     | 0.45              |
| 1:D:51:LEU:HD21  | 1:D:108:VAL:HG13 | 1.98                     | 0.45              |
| 2:H:48:ARG:HB3   | 2:H:85:PRO:O     | 2.17                     | 0.45              |
| 1:P:162:ILE:CG2  | 6:P:1006:SMA:H21 | 2.46                     | 0.45              |
| 3:R:142:GLY:HA3  | 13:R:691:HOH:O   | 2.16                     | 0.45              |
| 2:B:157:ASN:O    | 2:B:180:GLY:HA3  | 2.17                     | 0.45              |
| 1:G:13:THR:O     | 1:G:17:LYS:HG3   | 2.17                     | 0.45              |
| 1:G:291:HIS:O    | 1:G:293:VAL:HG23 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:154:PHE:C    | 2:H:155:TYR:CD1   | 2.95                     | 0.45              |
| 2:Q:19:THR:HB    | 2:Q:224:MET:HE3   | 1.98                     | 0.45              |
| 1:D:44:MET:HE3   | 7:D:1022:LOP:H92  | 1.99                     | 0.45              |
| 2:E:250:ARG:HH11 | 2:E:250:ARG:CG    | 2.19                     | 0.45              |
| 1:G:118:TYR:OH   | 7:G:1023:LOP:H32  | 2.15                     | 0.45              |
| 2:N:51:SER:OG    | 2:N:63:VAL:HG21   | 2.17                     | 0.45              |
| 1:D:291:HIS:O    | 1:D:293:VAL:HG23  | 2.16                     | 0.44              |
| 1:G:47:TRP:CZ2   | 1:G:110:LEU:HD13  | 2.53                     | 0.44              |
| 2:K:203:SER:O    | 2:K:204:VAL:C     | 2.60                     | 0.44              |
| 1:P:102:SER:O    | 1:P:106:ILE:HG13  | 2.16                     | 0.44              |
| 1:G:121:TYR:HB3  | 1:G:129:TRP:CE3   | 2.53                     | 0.44              |
| 1:G:416:LYS:HA   | 1:G:416:LYS:HD3   | 1.63                     | 0.44              |
| 1:D:47:TRP:CZ2   | 1:D:110:LEU:HD13  | 2.53                     | 0.44              |
| 1:G:106:ILE:HD12 | 7:G:1023:LOP:H212 | 1.99                     | 0.44              |
| 2:H:235:MET:HA   | 2:H:235:MET:HE2   | 1.99                     | 0.44              |
| 2:K:144:LYS:C    | 2:K:147:GLU:HG3   | 2.38                     | 0.44              |
| 2:K:171:ASP:CG   | 2:K:172:ALA:N     | 2.75                     | 0.44              |
| 1:A:418:VAL:CG1  | 1:A:419:ALA:N     | 2.80                     | 0.44              |
| 2:B:223:LEU:CD2  | 2:B:227:LYS:HD2   | 2.46                     | 0.44              |
| 2:H:138:PHE:CD2  | 2:H:187:PRO:HG3   | 2.51                     | 0.44              |
| 3:I:14:PHE:O     | 3:I:17:TYR:HB3    | 2.17                     | 0.44              |
| 1:J:130:ILE:HD11 | 1:J:348:TRP:CH2   | 2.46                     | 0.44              |
| 1:J:209:VAL:CG2  | 5:J:501:HEM:HBB2  | 2.48                     | 0.44              |
| 2:N:203:SER:O    | 2:N:204:VAL:C     | 2.61                     | 0.44              |
| 3:R:140:VAL:O    | 3:R:140:VAL:HG12  | 2.16                     | 0.44              |
| 1:A:47:TRP:CZ2   | 1:A:110:LEU:HD13  | 2.53                     | 0.44              |
| 1:G:428:PHE:CZ   | 2:H:256:LYS:HB3   | 2.52                     | 0.44              |
| 2:H:146:ALA:O    | 2:H:147:GLU:C     | 2.60                     | 0.44              |
| 1:J:406:VAL:O    | 1:J:409:PRO:HD2   | 2.18                     | 0.44              |
| 1:M:39:ARG:NH1   | 2:N:255:VAL:CG1   | 2.80                     | 0.44              |
| 1:P:427:ASP:O    | 1:P:430:ALA:HB3   | 2.18                     | 0.44              |
| 2:Q:17:PHE:CE1   | 2:Q:231:PHE:CZ    | 3.04                     | 0.44              |
| 2:K:236:PHE:HE1  | 3:L:25:VAL:CG1    | 2.30                     | 0.44              |
| 1:A:121:TYR:HB3  | 1:A:129:TRP:CE3   | 2.52                     | 0.44              |
| 1:A:125:ARG:HH21 | 1:A:221:ASN:C     | 2.26                     | 0.44              |
| 1:G:133:MET:SD   | 5:G:501:HEM:HBC1  | 2.58                     | 0.44              |
| 2:K:146:ALA:O    | 2:K:147:GLU:C     | 2.60                     | 0.44              |
| 3:O:47:LEU:O     | 3:O:47:LEU:CD2    | 2.64                     | 0.44              |
| 2:Q:48:ARG:HB3   | 2:Q:85:PRO:O      | 2.17                     | 0.44              |
| 1:A:8:HIS:CD2    | 1:A:8:HIS:H       | 2.36                     | 0.44              |
| 2:B:113:PRO:HD2  | 2:B:118:ILE:HB    | 1.99                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:203:SER:O    | 2:B:204:VAL:C     | 2.59                     | 0.44              |
| 1:D:49:VAL:HG23  | 8:D:1102:UQ2:H2M3 | 1.99                     | 0.44              |
| 2:K:144:LYS:HA   | 2:K:147:GLU:HG3   | 1.99                     | 0.44              |
| 3:L:143:ASP:OD2  | 3:L:164:LYS:NZ    | 2.51                     | 0.44              |
| 1:M:387:PHE:CE1  | 1:M:388:PRO:HB3   | 2.53                     | 0.44              |
| 2:Q:74:ASP:HB3   | 2:Q:77:THR:HB     | 2.00                     | 0.44              |
| 2:B:19:THR:HB    | 2:B:224:MET:HE3   | 2.00                     | 0.43              |
| 1:D:121:TYR:HB3  | 1:D:129:TRP:CE3   | 2.53                     | 0.43              |
| 2:H:222:LYS:HB2  | 13:H:347:HOH:O    | 2.18                     | 0.43              |
| 1:M:425:GLU:HG2  | 1:M:429:ASN:HD21  | 1.82                     | 0.43              |
| 1:A:106:ILE:HD12 | 7:A:1021:LOP:H212 | 1.99                     | 0.43              |
| 2:B:15:GLY:H     | 9:B:1041:BGL:H1   | 1.82                     | 0.43              |
| 2:E:113:PRO:HD2  | 2:E:118:ILE:HB    | 2.00                     | 0.43              |
| 1:G:132:GLY:O    | 5:G:501:HEM:HMC3  | 2.18                     | 0.43              |
| 3:I:12:ARG:H     | 3:I:12:ARG:HG2    | 1.60                     | 0.43              |
| 1:J:226:GLY:CA   | 1:J:355:ARG:HD2   | 2.49                     | 0.43              |
| 2:N:111:HIS:HE1  | 13:N:552:HOH:O    | 2.00                     | 0.43              |
| 1:P:10:GLU:HA    | 1:P:11:PRO:HD3    | 1.69                     | 0.43              |
| 1:P:248:PHE:HD1  | 1:P:251:LYS:HD3   | 1.82                     | 0.43              |
| 2:Q:146:ALA:O    | 2:Q:147:GLU:C     | 2.60                     | 0.43              |
| 3:R:77:ARG:HB3   | 3:R:81:ASP:HB2    | 2.00                     | 0.43              |
| 1:G:92:MET:CE    | 1:G:92:MET:HA     | 2.47                     | 0.43              |
| 2:H:223:LEU:HD21 | 2:H:227:LYS:CE    | 2.49                     | 0.43              |
| 1:J:43:TRP:HE3   | 1:J:43:TRP:HA     | 1.83                     | 0.43              |
| 3:L:118:GLU:CD   | 3:L:118:GLU:H     | 2.27                     | 0.43              |
| 2:B:146:ALA:O    | 2:B:147:GLU:C     | 2.59                     | 0.43              |
| 2:E:34:GLU:OE1   | 2:E:194:VAL:HG22  | 2.19                     | 0.43              |
| 1:J:262:VAL:HG13 | 9:K:1044:BGL:H8'1 | 1.99                     | 0.43              |
| 2:K:48:ARG:HB3   | 2:K:85:PRO:O      | 2.17                     | 0.43              |
| 1:M:195:PHE:CE2  | 1:P:195:PHE:HE2   | 2.12                     | 0.43              |
| 2:N:146:ALA:O    | 2:N:147:GLU:C     | 2.61                     | 0.43              |
| 1:P:105:PHE:HA   | 1:P:108:VAL:CG2   | 2.48                     | 0.43              |
| 5:P:502:HEM:CBC  | 5:P:502:HEM:HHD   | 2.48                     | 0.43              |
| 2:B:144:LYS:O    | 2:B:145:CYS:C     | 2.61                     | 0.43              |
| 3:C:84:LEU:HD23  | 3:C:84:LEU:HA     | 1.81                     | 0.43              |
| 1:D:355:ARG:CD   | 13:D:1155:HOH:O   | 2.66                     | 0.43              |
| 3:I:179:ILE:HD13 | 3:I:179:ILE:HA    | 1.74                     | 0.43              |
| 2:K:40:HIS:HB3   | 2:K:100:LEU:HG    | 2.00                     | 0.43              |
| 2:K:141:GLU:HA   | 2:K:142:PRO:HD3   | 1.76                     | 0.43              |
| 1:P:43:TRP:HA    | 1:P:43:TRP:HE3    | 1.84                     | 0.43              |
| 3:R:10:THR:O     | 3:R:14:PHE:HB3    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:R:62:GLN:NE2    | 3:R:73:PHE:CG     | 2.87                     | 0.43              |
| 2:H:141:GLU:HG2   | 13:H:338:HOH:O    | 2.19                     | 0.43              |
| 2:N:149:HIS:CD2   | 2:N:168:THR:OG1   | 2.70                     | 0.43              |
| 3:O:140:VAL:O     | 3:O:140:VAL:HG12  | 2.17                     | 0.43              |
| 1:P:359:TYR:CD2   | 1:P:420:PRO:HB3   | 2.53                     | 0.43              |
| 2:H:77:THR:HG23   | 2:H:79:GLU:OE2    | 2.19                     | 0.43              |
| 1:J:43:TRP:HA     | 1:J:43:TRP:CE3    | 2.54                     | 0.43              |
| 8:M:1105:UQ2:H3M3 | 8:M:1105:UQ2:H2M2 | 2.01                     | 0.43              |
| 1:P:47:TRP:CZ2    | 1:P:110:LEU:HD13  | 2.53                     | 0.43              |
| 2:Q:144:LYS:NZ    | 2:Q:147:GLU:OE1   | 2.51                     | 0.43              |
| 1:A:105:PHE:HA    | 1:A:108:VAL:CG2   | 2.45                     | 0.43              |
| 2:B:34:GLU:OE1    | 2:B:194:VAL:HG22  | 2.18                     | 0.43              |
| 2:B:155:TYR:CD1   | 2:B:155:TYR:N     | 2.87                     | 0.43              |
| 1:J:359:TYR:CD2   | 1:J:420:PRO:HB3   | 2.54                     | 0.43              |
| 2:K:155:TYR:CD1   | 2:K:155:TYR:N     | 2.87                     | 0.43              |
| 2:K:165:VAL:CG1   | 2:K:169:CYS:HB2   | 2.48                     | 0.43              |
| 1:M:427:ASP:O     | 1:M:430:ALA:HB3   | 2.18                     | 0.43              |
| 1:P:92:MET:HA     | 1:P:92:MET:HE2    | 2.01                     | 0.43              |
| 1:P:360:ARG:O     | 1:P:364:LYS:HG3   | 2.19                     | 0.43              |
| 1:A:45:TRP:CZ3    | 1:A:224:PRO:HG3   | 2.53                     | 0.43              |
| 3:C:14:PHE:O      | 3:C:17:TYR:HB3    | 2.18                     | 0.43              |
| 2:E:144:LYS:HD3   | 2:E:147:GLU:OE2   | 2.18                     | 0.43              |
| 2:E:220:GLU:OE2   | 2:E:226:ARG:NH1   | 2.52                     | 0.43              |
| 1:G:45:TRP:CZ3    | 1:G:224:PRO:HG3   | 2.54                     | 0.43              |
| 2:H:155:TYR:CD1   | 2:H:155:TYR:N     | 2.87                     | 0.43              |
| 1:J:47:TRP:CZ2    | 1:J:110:LEU:HD13  | 2.53                     | 0.43              |
| 1:J:121:TYR:HB3   | 1:J:129:TRP:CE3   | 2.53                     | 0.43              |
| 2:K:113:PRO:HD2   | 2:K:118:ILE:HB    | 2.01                     | 0.43              |
| 3:L:77:ARG:HB3    | 3:L:81:ASP:HB2    | 2.01                     | 0.43              |
| 2:N:74:ASP:C      | 2:N:76:GLU:H      | 2.27                     | 0.43              |
| 1:P:45:TRP:CZ3    | 1:P:224:PRO:HG3   | 2.54                     | 0.43              |
| 1:A:406:VAL:O     | 1:A:409:PRO:HD2   | 2.19                     | 0.43              |
| 1:G:306:ARG:NH2   | 1:G:383:GLN:O     | 2.40                     | 0.43              |
| 1:J:45:TRP:CZ3    | 1:J:224:PRO:HG3   | 2.54                     | 0.43              |
| 1:J:111:HIS:CD2   | 5:J:501:HEM:NC    | 2.87                     | 0.43              |
| 1:M:47:TRP:CZ2    | 1:M:110:LEU:HD13  | 2.53                     | 0.43              |
| 2:N:34:GLU:OE1    | 2:N:194:VAL:HG22  | 2.19                     | 0.43              |
| 3:R:59:PRO:HD3    | 3:R:76:ARG:HH11   | 1.83                     | 0.43              |
| 1:A:140:MET:HE1   | 1:A:340:ILE:HD13  | 2.01                     | 0.42              |
| 1:D:428:PHE:CZ    | 2:E:256:LYS:HB2   | 2.53                     | 0.42              |
| 5:D:501:HEM:HBC2  | 5:D:501:HEM:HMC2  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:155:TYR:CD1  | 2:E:155:TYR:N    | 2.86                     | 0.42              |
| 2:K:107:ARG:HH21 | 5:K:301:HEM:CGA  | 2.32                     | 0.42              |
| 3:L:59:PRO:HD3   | 3:L:76:ARG:HH11  | 1.84                     | 0.42              |
| 1:M:10:GLU:OE2   | 1:M:11:PRO:HD2   | 2.19                     | 0.42              |
| 1:M:350:ASP:HB2  | 1:M:408:LEU:HD13 | 2.01                     | 0.42              |
| 3:O:44:VAL:C     | 3:O:46:ALA:H     | 2.27                     | 0.42              |
| 2:B:48:ARG:HB3   | 2:B:85:PRO:O     | 2.19                     | 0.42              |
| 3:C:59:PRO:HD3   | 3:C:76:ARG:HH11  | 1.84                     | 0.42              |
| 3:C:138:GLY:O    | 3:C:141:SER:OG   | 2.32                     | 0.42              |
| 1:D:79:SER:O     | 1:D:83:ILE:HG13  | 2.20                     | 0.42              |
| 2:H:34:GLU:OE1   | 2:H:194:VAL:HG22 | 2.19                     | 0.42              |
| 2:N:42:MET:HE2   | 2:N:218:ALA:HB1  | 2.00                     | 0.42              |
| 2:Q:34:GLU:OE1   | 2:Q:194:VAL:HG22 | 2.19                     | 0.42              |
| 2:Q:42:MET:CE    | 2:Q:218:ALA:CB   | 2.97                     | 0.42              |
| 2:Q:171:ASP:OD1  | 2:Q:171:ASP:C    | 2.61                     | 0.42              |
| 1:A:79:SER:O     | 1:A:83:ILE:HG13  | 2.19                     | 0.42              |
| 1:D:133:MET:SD   | 5:D:501:HEM:HBC1 | 2.59                     | 0.42              |
| 1:G:91:PHE:CD1   | 2:H:222:LYS:HG2  | 2.54                     | 0.42              |
| 1:M:123:ALA:O    | 1:M:355:ARG:NH1  | 2.53                     | 0.42              |
| 2:N:189:LEU:C    | 2:N:204:VAL:HG22 | 2.44                     | 0.42              |
| 3:R:124:VAL:O    | 3:R:173:ILE:HG23 | 2.19                     | 0.42              |
| 2:B:185:MET:HB2  | 5:B:301:HEM:C1D  | 2.54                     | 0.42              |
| 1:J:112:ILE:HG12 | 5:J:501:HEM:HAC  | 2.00                     | 0.42              |
| 2:K:34:GLU:OE1   | 2:K:194:VAL:HG22 | 2.19                     | 0.42              |
| 1:M:394:LEU:HD23 | 1:M:394:LEU:HA   | 1.89                     | 0.42              |
| 3:R:179:ILE:HD13 | 3:R:179:ILE:HA   | 1.74                     | 0.42              |
| 2:B:42:MET:HE1   | 2:B:218:ALA:HB2  | 1.98                     | 0.42              |
| 1:D:236:GLU:HA   | 1:D:239:LYS:HD2  | 2.02                     | 0.42              |
| 1:G:387:PHE:CD1  | 1:G:387:PHE:C    | 2.98                     | 0.42              |
| 2:H:113:PRO:HD2  | 2:H:118:ILE:HB   | 2.00                     | 0.42              |
| 3:L:124:VAL:O    | 3:L:173:ILE:HG23 | 2.20                     | 0.42              |
| 3:C:126:TRP:C    | 3:C:128:VAL:H    | 2.28                     | 0.42              |
| 1:M:121:TYR:HB3  | 1:M:129:TRP:CE3  | 2.54                     | 0.42              |
| 3:C:179:ILE:CG1  | 3:C:185:GLN:HE21 | 2.33                     | 0.42              |
| 1:D:45:TRP:CZ3   | 1:D:224:PRO:HG3  | 2.54                     | 0.42              |
| 2:E:236:PHE:CE2  | 3:F:25:VAL:CG1   | 2.95                     | 0.42              |
| 1:G:394:LEU:HD23 | 1:G:394:LEU:HA   | 1.89                     | 0.42              |
| 3:I:126:TRP:C    | 3:I:128:VAL:H    | 2.27                     | 0.42              |
| 1:J:418:VAL:CG1  | 1:J:419:ALA:N    | 2.83                     | 0.42              |
| 2:Q:183:ILE:HG12 | 2:Q:185:MET:H    | 1.85                     | 0.42              |
| 1:D:39:ARG:NH1   | 2:E:255:VAL:HG12 | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:140:MET:HE1  | 1:D:340:ILE:HD13 | 2.00                     | 0.42              |
| 1:G:140:MET:HE1  | 1:G:340:ILE:HD13 | 2.02                     | 0.42              |
| 3:I:59:PRO:HD3   | 3:I:76:ARG:HH11  | 1.84                     | 0.42              |
| 1:J:4:ILE:HA     | 1:J:5:PRO:HD3    | 1.88                     | 0.42              |
| 2:N:68:THR:HG23  | 2:N:82:GLU:HB3   | 2.01                     | 0.42              |
| 2:N:155:TYR:CD1  | 2:N:155:TYR:N    | 2.87                     | 0.42              |
| 2:N:250:ARG:NH1  | 3:O:12:ARG:HA    | 2.33                     | 0.42              |
| 1:P:37:THR:O     | 1:P:38:PRO:C     | 2.62                     | 0.42              |
| 1:P:121:TYR:HB3  | 1:P:129:TRP:CE3  | 2.54                     | 0.42              |
| 2:Q:42:MET:HE1   | 2:Q:218:ALA:CB   | 2.49                     | 0.42              |
| 2:Q:155:TYR:CD1  | 2:Q:155:TYR:N    | 2.87                     | 0.42              |
| 3:R:179:ILE:CG1  | 3:R:185:GLN:HE21 | 2.33                     | 0.42              |
| 1:G:92:MET:CE    | 2:H:226:ARG:HG3  | 2.50                     | 0.42              |
| 1:G:359:TYR:CD2  | 1:G:420:PRO:HB3  | 2.55                     | 0.42              |
| 1:J:108:VAL:HG21 | 1:J:139:MET:HE1  | 2.02                     | 0.42              |
| 1:M:105:PHE:O    | 1:M:108:VAL:HG23 | 2.20                     | 0.42              |
| 1:M:215:ALA:HA   | 1:P:23:LEU:HD13  | 2.01                     | 0.42              |
| 1:M:239:LYS:HE2  | 1:M:425:GLU:OE2  | 2.20                     | 0.42              |
| 2:N:94:LEU:HD22  | 5:N:301:HEM:HAC  | 2.01                     | 0.42              |
| 1:P:234:LYS:O    | 1:P:238:GLN:HG3  | 2.19                     | 0.42              |
| 2:Q:165:VAL:CG1  | 2:Q:169:CYS:HB2  | 2.50                     | 0.42              |
| 1:A:291:HIS:CE1  | 2:B:2:GLY:HA2    | 2.54                     | 0.42              |
| 1:D:92:MET:HA    | 1:D:92:MET:HE2   | 2.02                     | 0.42              |
| 1:D:364:LYS:O    | 1:D:368:TRP:HD1  | 2.02                     | 0.42              |
| 2:E:30:GLN:HG2   | 2:E:34:GLU:OE2   | 2.20                     | 0.42              |
| 2:E:250:ARG:NH1  | 2:E:250:ARG:CG   | 2.82                     | 0.42              |
| 3:F:13:ASP:O     | 3:F:17:TYR:HD2   | 2.02                     | 0.42              |
| 3:F:77:ARG:HB3   | 3:F:81:ASP:HB2   | 2.01                     | 0.42              |
| 1:G:102:SER:O    | 1:G:106:ILE:HG13 | 2.20                     | 0.42              |
| 2:H:145:CYS:O    | 2:H:168:THR:OG1  | 2.28                     | 0.42              |
| 3:I:77:ARG:HB3   | 3:I:81:ASP:HB2   | 2.01                     | 0.42              |
| 1:J:108:VAL:CG2  | 1:J:139:MET:HE1  | 2.50                     | 0.42              |
| 2:K:72:VAL:CG1   | 2:K:73:THR:N     | 2.83                     | 0.42              |
| 3:L:179:ILE:HD13 | 3:L:179:ILE:HA   | 1.74                     | 0.42              |
| 1:M:45:TRP:CZ3   | 1:M:224:PRO:HG3  | 2.54                     | 0.42              |
| 1:M:262:VAL:O    | 1:M:266:ILE:HG12 | 2.20                     | 0.42              |
| 1:M:362:MET:HB3  | 1:M:411:LEU:HD21 | 2.02                     | 0.42              |
| 2:N:143:PRO:HG3  | 2:N:178:THR:HG21 | 2.02                     | 0.42              |
| 2:Q:42:MET:HE3   | 2:Q:215:LEU:CD2  | 2.50                     | 0.42              |
| 3:L:179:ILE:CG1  | 3:L:185:GLN:HE21 | 2.33                     | 0.41              |
| 1:M:239:LYS:HB3  | 1:M:425:GLU:OE2  | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:314:VAL:H    | 1:M:314:VAL:HG23 | 1.63                     | 0.41              |
| 2:N:20:PHE:CB    | 2:N:25:LEU:HD11  | 2.48                     | 0.41              |
| 3:R:126:TRP:C    | 3:R:128:VAL:H    | 2.28                     | 0.41              |
| 1:A:355:ARG:HD3  | 13:A:1122:HOH:O  | 2.19                     | 0.41              |
| 2:B:40:HIS:HB3   | 2:B:100:LEU:HG   | 2.02                     | 0.41              |
| 3:C:77:ARG:HB3   | 3:C:81:ASP:HB2   | 2.02                     | 0.41              |
| 2:E:48:ARG:HB3   | 2:E:85:PRO:O     | 2.19                     | 0.41              |
| 2:E:154:PHE:HB3  | 2:E:182:TRP:HB3  | 2.01                     | 0.41              |
| 3:F:124:VAL:O    | 3:F:173:ILE:HG23 | 2.20                     | 0.41              |
| 1:G:39:ARG:HH12  | 2:H:255:VAL:HG12 | 1.82                     | 0.41              |
| 2:H:141:GLU:HA   | 2:H:142:PRO:HD3  | 1.87                     | 0.41              |
| 3:I:89:GLN:O     | 3:I:90:LEU:C     | 2.63                     | 0.41              |
| 1:M:34:MET:O     | 1:M:35:ILE:C     | 2.63                     | 0.41              |
| 2:N:160:PHE:CG   | 2:N:183:ILE:HD12 | 2.55                     | 0.41              |
| 3:O:44:VAL:O     | 3:O:46:ALA:N     | 2.53                     | 0.41              |
| 1:P:394:LEU:HA   | 1:P:394:LEU:HD23 | 1.89                     | 0.41              |
| 2:B:19:THR:CG2   | 2:B:224:MET:HE3  | 2.50                     | 0.41              |
| 1:D:135:ILE:CG2  | 5:D:501:HEM:HAB  | 2.42                     | 0.41              |
| 1:D:261:LEU:CD1  | 2:E:234:VAL:HG13 | 2.46                     | 0.41              |
| 2:H:171:ASP:C    | 2:H:171:ASP:OD1  | 2.62                     | 0.41              |
| 3:I:124:VAL:O    | 3:I:173:ILE:HG23 | 2.19                     | 0.41              |
| 2:K:48:ARG:HG3   | 2:K:48:ARG:HH11  | 1.86                     | 0.41              |
| 2:N:94:LEU:CD2   | 5:N:301:HEM:HAC  | 2.49                     | 0.41              |
| 1:A:111:HIS:CD2  | 5:A:501:HEM:NC   | 2.89                     | 0.41              |
| 1:D:233:SER:O    | 1:D:234:LYS:C    | 2.62                     | 0.41              |
| 1:D:394:LEU:HD23 | 1:D:394:LEU:HA   | 1.90                     | 0.41              |
| 1:D:408:LEU:HD23 | 1:D:408:LEU:HA   | 1.89                     | 0.41              |
| 3:I:162:ILE:HD11 | 3:I:164:LYS:O    | 2.21                     | 0.41              |
| 1:M:92:MET:HA    | 1:M:92:MET:HE3   | 2.01                     | 0.41              |
| 1:M:322:SER:O    | 1:M:325:ILE:HD12 | 2.21                     | 0.41              |
| 2:N:42:MET:HE1   | 2:N:218:ALA:HB2  | 2.03                     | 0.41              |
| 2:N:113:PRO:HD2  | 2:N:118:ILE:HB   | 2.02                     | 0.41              |
| 3:O:124:VAL:O    | 3:O:173:ILE:HG23 | 2.20                     | 0.41              |
| 1:P:408:LEU:HD23 | 1:P:408:LEU:HA   | 1.91                     | 0.41              |
| 2:Q:20:PHE:CB    | 2:Q:25:LEU:HD11  | 2.48                     | 0.41              |
| 2:Q:203:SER:O    | 2:Q:204:VAL:C    | 2.60                     | 0.41              |
| 3:C:47:LEU:O     | 3:C:47:LEU:CD2   | 2.63                     | 0.41              |
| 2:E:189:LEU:O    | 2:E:190:MET:CB   | 2.68                     | 0.41              |
| 2:H:30:GLN:HG2   | 2:H:34:GLU:OE2   | 2.20                     | 0.41              |
| 1:J:140:MET:HE1  | 1:J:340:ILE:HD13 | 2.01                     | 0.41              |
| 2:N:176:LYS:HG2  | 2:N:178:THR:O    | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:77:ARG:HB3   | 3:O:81:ASP:HB2   | 2.01                     | 0.41              |
| 1:P:132:GLY:HA3  | 5:P:501:HEM:HBC2 | 2.02                     | 0.41              |
| 2:Q:149:HIS:CG   | 2:Q:168:THR:HG21 | 2.53                     | 0.41              |
| 1:D:306:ARG:HG3  | 13:D:1150:HOH:O  | 2.19                     | 0.41              |
| 1:J:10:GLU:HA    | 1:J:11:PRO:HD3   | 1.87                     | 0.41              |
| 1:J:262:VAL:O    | 1:J:266:ILE:HG12 | 2.21                     | 0.41              |
| 2:K:30:GLN:HG2   | 2:K:34:GLU:OE2   | 2.21                     | 0.41              |
| 2:N:143:PRO:HG3  | 2:N:178:THR:HG22 | 2.03                     | 0.41              |
| 2:Q:48:ARG:HH11  | 2:Q:48:ARG:HG3   | 1.86                     | 0.41              |
| 3:R:70:LYS:HB2   | 3:R:70:LYS:HZ3   | 1.84                     | 0.41              |
| 1:J:199:TYR:CG   | 5:J:502:HEM:HBC1 | 2.56                     | 0.41              |
| 1:J:250:ILE:HD12 | 2:K:251:LEU:CD2  | 2.51                     | 0.41              |
| 3:O:162:ILE:HD11 | 3:O:164:LYS:O    | 2.20                     | 0.41              |
| 1:P:354:VAL:HG21 | 1:P:417:PRO:HB2  | 2.03                     | 0.41              |
| 2:Q:30:GLN:HG2   | 2:Q:34:GLU:OE2   | 2.21                     | 0.41              |
| 2:Q:223:LEU:HD23 | 2:Q:223:LEU:C    | 2.45                     | 0.41              |
| 2:Q:242:VAL:O    | 2:Q:246:LEU:HG   | 2.21                     | 0.41              |
| 1:A:239:LYS:HE2  | 1:A:425:GLU:OE1  | 2.21                     | 0.41              |
| 1:D:122:LYS:O    | 1:D:123:ALA:C    | 2.64                     | 0.41              |
| 3:F:126:TRP:C    | 3:F:128:VAL:H    | 2.29                     | 0.41              |
| 1:G:51:LEU:HB3   | 5:G:501:HEM:HMB1 | 2.03                     | 0.41              |
| 1:J:37:THR:O     | 1:J:38:PRO:C     | 2.63                     | 0.41              |
| 1:J:43:TRP:CZ3   | 1:J:251:LYS:HD3  | 2.55                     | 0.41              |
| 1:J:64:VAL:HG11  | 1:J:93:LEU:HD13  | 2.02                     | 0.41              |
| 1:J:133:MET:N    | 5:J:501:HEM:HBC2 | 2.36                     | 0.41              |
| 2:N:48:ARG:HH11  | 2:N:48:ARG:HG3   | 1.86                     | 0.41              |
| 3:O:54:VAL:O     | 3:O:54:VAL:HG13  | 2.20                     | 0.41              |
| 1:A:130:ILE:HD11 | 1:A:348:TRP:CH2  | 2.46                     | 0.41              |
| 2:B:30:GLN:HG2   | 2:B:34:GLU:OE2   | 2.20                     | 0.41              |
| 2:B:77:THR:HG22  | 2:B:79:GLU:HG3   | 2.02                     | 0.41              |
| 3:C:124:VAL:O    | 3:C:173:ILE:HG23 | 2.21                     | 0.41              |
| 1:D:37:THR:O     | 1:D:38:PRO:C     | 2.64                     | 0.41              |
| 1:D:132:GLY:C    | 5:D:501:HEM:HBC2 | 2.46                     | 0.41              |
| 1:D:250:ILE:HD12 | 2:E:251:LEU:CD2  | 2.50                     | 0.41              |
| 2:H:129:GLU:OE1  | 2:H:129:GLU:N    | 2.42                     | 0.41              |
| 2:H:223:LEU:HD21 | 2:H:227:LYS:HE3  | 2.03                     | 0.41              |
| 1:J:51:LEU:HD13  | 5:J:501:HEM:C3B  | 2.55                     | 0.41              |
| 2:K:19:THR:HB    | 2:K:224:MET:HE3  | 2.03                     | 0.41              |
| 2:K:189:LEU:O    | 2:K:190:MET:CB   | 2.69                     | 0.41              |
| 3:L:171:LEU:HA   | 3:L:172:PRO:HD3  | 1.95                     | 0.41              |
| 1:M:37:THR:O     | 1:M:38:PRO:C     | 2.62                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:64:VAL:HG11  | 1:M:93:LEU:HD13  | 2.03                     | 0.41              |
| 1:M:75:LEU:O     | 1:M:79:SER:HB3   | 2.21                     | 0.41              |
| 2:N:40:HIS:HB3   | 2:N:100:LEU:HG   | 2.02                     | 0.41              |
| 2:N:103:MET:C    | 2:N:105:LYS:N    | 2.78                     | 0.41              |
| 1:P:130:ILE:HD11 | 1:P:348:TRP:CH2  | 2.47                     | 0.41              |
| 1:A:193:ARG:NH1  | 3:F:38:MET:HG2   | 2.36                     | 0.41              |
| 2:B:77:THR:HG22  | 2:B:79:GLU:CB    | 2.51                     | 0.41              |
| 2:E:61:ASP:OD1   | 2:E:61:ASP:N     | 2.53                     | 0.41              |
| 3:F:54:VAL:O     | 3:F:54:VAL:HG13  | 2.20                     | 0.41              |
| 1:G:75:LEU:O     | 1:G:79:SER:HB3   | 2.21                     | 0.41              |
| 2:H:74:ASP:CB    | 2:H:77:THR:HB    | 2.51                     | 0.41              |
| 3:I:179:ILE:CG1  | 3:I:185:GLN:HE21 | 2.33                     | 0.41              |
| 1:J:425:GLU:HG3  | 1:J:429:ASN:ND2  | 2.33                     | 0.41              |
| 2:N:242:VAL:O    | 2:N:246:LEU:HG   | 2.21                     | 0.41              |
| 1:P:43:TRP:O     | 1:P:46:ILE:HG12  | 2.20                     | 0.41              |
| 1:P:287:ARG:NH1  | 1:P:287:ARG:CG   | 2.83                     | 0.41              |
| 2:Q:53:PRO:HA    | 2:Q:57:GLU:CD    | 2.46                     | 0.41              |
| 2:Q:113:PRO:HD2  | 2:Q:118:ILE:HB   | 2.03                     | 0.41              |
| 1:A:64:VAL:HG11  | 1:A:93:LEU:HD13  | 2.02                     | 0.40              |
| 2:B:154:PHE:HB3  | 2:B:182:TRP:HB3  | 2.03                     | 0.40              |
| 1:D:236:GLU:O    | 1:D:239:LYS:HB2  | 2.20                     | 0.40              |
| 1:G:37:THR:O     | 1:G:38:PRO:C     | 2.63                     | 0.40              |
| 1:G:43:TRP:O     | 1:G:46:ILE:HG12  | 2.22                     | 0.40              |
| 2:H:40:HIS:HB3   | 2:H:100:LEU:HG   | 2.03                     | 0.40              |
| 2:H:250:ARG:NH2  | 3:I:12:ARG:HB2   | 2.35                     | 0.40              |
| 1:M:106:ILE:HG13 | 1:M:296:TRP:CZ2  | 2.56                     | 0.40              |
| 3:O:59:PRO:HD3   | 3:O:76:ARG:HH11  | 1.85                     | 0.40              |
| 3:O:93:LEU:HB3   | 13:O:574:HOH:O   | 2.20                     | 0.40              |
| 3:O:179:ILE:CG1  | 3:O:185:GLN:HE21 | 2.33                     | 0.40              |
| 2:Q:108:ALA:HA   | 2:Q:125:ILE:O    | 2.20                     | 0.40              |
| 3:R:156:TYR:HA   | 3:R:161:ARG:O    | 2.21                     | 0.40              |
| 1:D:64:VAL:HG11  | 1:D:93:LEU:HD13  | 2.02                     | 0.40              |
| 2:E:234:VAL:HG12 | 2:E:235:MET:HE2  | 2.01                     | 0.40              |
| 3:F:59:PRO:HD3   | 3:F:76:ARG:HH11  | 1.86                     | 0.40              |
| 1:M:140:MET:HE1  | 1:M:340:ILE:HD13 | 2.03                     | 0.40              |
| 1:M:286:LEU:HD21 | 3:R:66:LYS:HB2   | 2.04                     | 0.40              |
| 2:Q:143:PRO:HG3  | 2:Q:178:THR:CG2  | 2.52                     | 0.40              |
| 1:D:75:LEU:O     | 1:D:79:SER:HB3   | 2.21                     | 0.40              |
| 3:F:155:HIS:CD2  | 3:F:164:LYS:HD3  | 2.56                     | 0.40              |
| 3:F:179:ILE:CG1  | 3:F:185:GLN:HE21 | 2.33                     | 0.40              |
| 1:G:79:SER:O     | 1:G:83:ILE:HG13  | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:130:ILE:HD11 | 1:G:348:TRP:CH2  | 2.46                     | 0.40              |
| 1:G:261:LEU:CD1  | 2:H:234:VAL:HG13 | 2.44                     | 0.40              |
| 2:H:176:LYS:NZ   | 2:H:178:THR:O    | 2.53                     | 0.40              |
| 1:J:43:TRP:HH2   | 1:J:251:LYS:HG2  | 1.86                     | 0.40              |
| 2:N:30:GLN:HG2   | 2:N:34:GLU:OE2   | 2.21                     | 0.40              |
| 3:O:70:LYS:HB3   | 3:O:71:PRO:HD2   | 2.02                     | 0.40              |
| 1:A:394:LEU:HD23 | 1:A:394:LEU:HA   | 1.90                     | 0.40              |
| 2:B:113:PRO:O    | 2:B:114:MET:HB2  | 2.21                     | 0.40              |
| 2:Q:65:ALA:O     | 2:Q:68:THR:HB    | 2.22                     | 0.40              |
| 1:D:414:ILE:O    | 1:D:414:ILE:HG23 | 2.22                     | 0.40              |
| 2:E:141:GLU:HA   | 2:E:142:PRO:HD3  | 1.77                     | 0.40              |
| 2:E:171:ASP:OD1  | 2:E:171:ASP:C    | 2.64                     | 0.40              |
| 2:E:250:ARG:HD3  | 3:F:12:ARG:CG    | 2.51                     | 0.40              |
| 1:J:394:LEU:HD23 | 1:J:394:LEU:HA   | 1.90                     | 0.40              |
| 1:J:423:THR:OG1  | 1:J:426:GLU:HB2  | 2.22                     | 0.40              |
| 2:K:113:PRO:O    | 2:K:114:MET:HB3  | 2.21                     | 0.40              |
| 2:K:137:GLY:O    | 2:K:139:PRO:HD3  | 2.20                     | 0.40              |
| 3:L:100:ASN:HA   | 3:L:173:ILE:HB   | 2.03                     | 0.40              |
| 3:L:126:TRP:C    | 3:L:128:VAL:H    | 2.28                     | 0.40              |
| 2:N:40:HIS:HD1   | 2:N:97:ALA:HB1   | 1.83                     | 0.40              |
| 2:N:65:ALA:O     | 2:N:68:THR:HB    | 2.22                     | 0.40              |
| 2:N:105:LYS:C    | 2:N:107:ARG:H    | 2.29                     | 0.40              |
| 1:P:75:LEU:O     | 1:P:79:SER:HB3   | 2.21                     | 0.40              |
| 1:P:140:MET:HE1  | 1:P:340:ILE:HD13 | 2.03                     | 0.40              |
| 2:Q:141:GLU:HA   | 2:Q:142:PRO:HD3  | 1.88                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |
|-----|-------|---------------|-----------|---------|----------|-------------|
| 1   | A     | 426/445 (96%) | 412 (97%) | 14 (3%) | 0        | 100 100     |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | D     | 426/445 (96%)   | 413 (97%)  | 13 (3%)  | 0        | 100         | 100 |
| 1   | G     | 426/445 (96%)   | 412 (97%)  | 14 (3%)  | 0        | 100         | 100 |
| 1   | J     | 426/445 (96%)   | 407 (96%)  | 18 (4%)  | 1 (0%)   | 43          | 58  |
| 1   | M     | 426/445 (96%)   | 407 (96%)  | 19 (4%)  | 0        | 100         | 100 |
| 1   | P     | 426/445 (96%)   | 408 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 2   | B     | 254/269 (94%)   | 233 (92%)  | 18 (7%)  | 3 (1%)   | 10          | 16  |
| 2   | E     | 254/269 (94%)   | 231 (91%)  | 20 (8%)  | 3 (1%)   | 10          | 16  |
| 2   | H     | 254/269 (94%)   | 233 (92%)  | 18 (7%)  | 3 (1%)   | 10          | 16  |
| 2   | K     | 254/269 (94%)   | 231 (91%)  | 18 (7%)  | 5 (2%)   | 6           | 7   |
| 2   | N     | 254/269 (94%)   | 229 (90%)  | 20 (8%)  | 5 (2%)   | 6           | 7   |
| 2   | Q     | 254/269 (94%)   | 231 (91%)  | 21 (8%)  | 2 (1%)   | 16          | 25  |
| 3   | C     | 177/187 (95%)   | 163 (92%)  | 13 (7%)  | 1 (1%)   | 21          | 32  |
| 3   | F     | 177/187 (95%)   | 161 (91%)  | 15 (8%)  | 1 (1%)   | 21          | 32  |
| 3   | I     | 177/187 (95%)   | 162 (92%)  | 12 (7%)  | 3 (2%)   | 7           | 10  |
| 3   | L     | 177/187 (95%)   | 161 (91%)  | 14 (8%)  | 2 (1%)   | 11          | 18  |
| 3   | O     | 177/187 (95%)   | 162 (92%)  | 12 (7%)  | 3 (2%)   | 7           | 10  |
| 3   | R     | 177/187 (95%)   | 161 (91%)  | 15 (8%)  | 1 (1%)   | 21          | 32  |
| All | All   | 5142/5406 (95%) | 4817 (94%) | 292 (6%) | 33 (1%)  | 21          | 32  |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 147 | GLU  |
| 2   | E     | 147 | GLU  |
| 2   | E     | 190 | MET  |
| 2   | H     | 77  | THR  |
| 2   | H     | 147 | GLU  |
| 2   | K     | 147 | GLU  |
| 2   | K     | 190 | MET  |
| 2   | N     | 147 | GLU  |
| 2   | Q     | 147 | GLU  |
| 2   | B     | 198 | ASP  |
| 2   | E     | 198 | ASP  |
| 2   | H     | 198 | ASP  |
| 2   | K     | 198 | ASP  |
| 2   | N     | 198 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Q     | 198 | ASP  |
| 2   | B     | 190 | MET  |
| 3   | C     | 109 | ALA  |
| 3   | F     | 109 | ALA  |
| 3   | I     | 109 | ALA  |
| 1   | J     | 43  | TRP  |
| 3   | L     | 109 | ALA  |
| 2   | N     | 75  | GLU  |
| 3   | O     | 109 | ALA  |
| 3   | R     | 109 | ALA  |
| 3   | I     | 45  | GLN  |
| 2   | K     | 145 | CYS  |
| 3   | O     | 45  | GLN  |
| 2   | N     | 104 | ALA  |
| 3   | O     | 90  | LEU  |
| 3   | I     | 140 | VAL  |
| 2   | K     | 255 | VAL  |
| 2   | N     | 255 | VAL  |
| 3   | L     | 140 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 353/366 (96%) | 342 (97%) | 11 (3%)  | 35          | 57 |
| 1   | D     | 353/366 (96%) | 345 (98%) | 8 (2%)   | 44          | 66 |
| 1   | G     | 353/366 (96%) | 345 (98%) | 8 (2%)   | 44          | 66 |
| 1   | J     | 353/366 (96%) | 342 (97%) | 11 (3%)  | 35          | 57 |
| 1   | M     | 353/366 (96%) | 343 (97%) | 10 (3%)  | 38          | 60 |
| 1   | P     | 353/366 (96%) | 345 (98%) | 8 (2%)   | 44          | 66 |
| 2   | B     | 203/215 (94%) | 191 (94%) | 12 (6%)  | 18          | 31 |
| 2   | E     | 203/215 (94%) | 191 (94%) | 12 (6%)  | 18          | 31 |
| 2   | H     | 203/215 (94%) | 196 (97%) | 7 (3%)   | 32          | 54 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 2   | K     | 203/215 (94%)   | 192 (95%)  | 11 (5%)  | 20          | 35 |
| 2   | N     | 203/215 (94%)   | 193 (95%)  | 10 (5%)  | 22          | 39 |
| 2   | Q     | 203/215 (94%)   | 189 (93%)  | 14 (7%)  | 14          | 24 |
| 3   | C     | 138/144 (96%)   | 131 (95%)  | 7 (5%)   | 21          | 37 |
| 3   | F     | 138/144 (96%)   | 129 (94%)  | 9 (6%)   | 15          | 27 |
| 3   | I     | 138/144 (96%)   | 129 (94%)  | 9 (6%)   | 15          | 27 |
| 3   | L     | 138/144 (96%)   | 130 (94%)  | 8 (6%)   | 18          | 32 |
| 3   | O     | 138/144 (96%)   | 128 (93%)  | 10 (7%)  | 13          | 23 |
| 3   | R     | 138/144 (96%)   | 130 (94%)  | 8 (6%)   | 18          | 32 |
| All | All   | 4164/4350 (96%) | 3991 (96%) | 173 (4%) | 26          | 45 |

All (173) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | ASP  |
| 1   | A     | 79  | SER  |
| 1   | A     | 92  | MET  |
| 1   | A     | 108 | VAL  |
| 1   | A     | 137 | LEU  |
| 1   | A     | 217 | HIS  |
| 1   | A     | 246 | PRO  |
| 1   | A     | 314 | VAL  |
| 1   | A     | 380 | VAL  |
| 1   | A     | 385 | THR  |
| 1   | A     | 414 | ILE  |
| 2   | B     | 61  | ASP  |
| 2   | B     | 73  | THR  |
| 2   | B     | 95  | GLU  |
| 2   | B     | 136 | THR  |
| 2   | B     | 147 | GLU  |
| 2   | B     | 149 | HIS  |
| 2   | B     | 167 | ASP  |
| 2   | B     | 168 | THR  |
| 2   | B     | 177 | THR  |
| 2   | B     | 188 | PRO  |
| 2   | B     | 194 | VAL  |
| 2   | B     | 205 | HIS  |
| 3   | C     | 47  | LEU  |
| 3   | C     | 63  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 65  | VAL  |
| 3   | C     | 72  | ILE  |
| 3   | C     | 112 | GLN  |
| 3   | C     | 174 | PRO  |
| 3   | C     | 179 | ILE  |
| 1   | D     | 7   | ASP  |
| 1   | D     | 10  | GLU  |
| 1   | D     | 79  | SER  |
| 1   | D     | 92  | MET  |
| 1   | D     | 246 | PRO  |
| 1   | D     | 380 | VAL  |
| 1   | D     | 385 | THR  |
| 1   | D     | 414 | ILE  |
| 2   | E     | 43  | LYS  |
| 2   | E     | 61  | ASP  |
| 2   | E     | 76  | GLU  |
| 2   | E     | 82  | GLU  |
| 2   | E     | 136 | THR  |
| 2   | E     | 141 | GLU  |
| 2   | E     | 152 | ASP  |
| 2   | E     | 168 | THR  |
| 2   | E     | 177 | THR  |
| 2   | E     | 194 | VAL  |
| 2   | E     | 195 | GLU  |
| 2   | E     | 205 | HIS  |
| 3   | F     | 47  | LEU  |
| 3   | F     | 63  | LEU  |
| 3   | F     | 65  | VAL  |
| 3   | F     | 72  | ILE  |
| 3   | F     | 112 | GLN  |
| 3   | F     | 118 | GLU  |
| 3   | F     | 174 | PRO  |
| 3   | F     | 177 | LYS  |
| 3   | F     | 179 | ILE  |
| 1   | G     | 4   | ILE  |
| 1   | G     | 79  | SER  |
| 1   | G     | 92  | MET  |
| 1   | G     | 108 | VAL  |
| 1   | G     | 246 | PRO  |
| 1   | G     | 380 | VAL  |
| 1   | G     | 385 | THR  |
| 1   | G     | 421 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 136 | THR  |
| 2   | H     | 147 | GLU  |
| 2   | H     | 149 | HIS  |
| 2   | H     | 168 | THR  |
| 2   | H     | 177 | THR  |
| 2   | H     | 194 | VAL  |
| 2   | H     | 205 | HIS  |
| 3   | I     | 47  | LEU  |
| 3   | I     | 63  | LEU  |
| 3   | I     | 65  | VAL  |
| 3   | I     | 72  | ILE  |
| 3   | I     | 83  | GLU  |
| 3   | I     | 90  | LEU  |
| 3   | I     | 112 | GLN  |
| 3   | I     | 174 | PRO  |
| 3   | I     | 179 | ILE  |
| 1   | J     | 4   | ILE  |
| 1   | J     | 43  | TRP  |
| 1   | J     | 79  | SER  |
| 1   | J     | 108 | VAL  |
| 1   | J     | 162 | ILE  |
| 1   | J     | 217 | HIS  |
| 1   | J     | 246 | PRO  |
| 1   | J     | 380 | VAL  |
| 1   | J     | 385 | THR  |
| 1   | J     | 418 | VAL  |
| 1   | J     | 425 | GLU  |
| 2   | K     | 52  | GLU  |
| 2   | K     | 72  | VAL  |
| 2   | K     | 136 | THR  |
| 2   | K     | 149 | HIS  |
| 2   | K     | 168 | THR  |
| 2   | K     | 171 | ASP  |
| 2   | K     | 177 | THR  |
| 2   | K     | 181 | SER  |
| 2   | K     | 194 | VAL  |
| 2   | K     | 195 | GLU  |
| 2   | K     | 205 | HIS  |
| 3   | L     | 47  | LEU  |
| 3   | L     | 63  | LEU  |
| 3   | L     | 65  | VAL  |
| 3   | L     | 66  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L     | 72  | ILE  |
| 3   | L     | 112 | GLN  |
| 3   | L     | 174 | PRO  |
| 3   | L     | 179 | ILE  |
| 1   | M     | 8   | HIS  |
| 1   | M     | 79  | SER  |
| 1   | M     | 92  | MET  |
| 1   | M     | 108 | VAL  |
| 1   | M     | 162 | ILE  |
| 1   | M     | 246 | PRO  |
| 1   | M     | 287 | ARG  |
| 1   | M     | 314 | VAL  |
| 1   | M     | 380 | VAL  |
| 1   | M     | 385 | THR  |
| 2   | N     | 72  | VAL  |
| 2   | N     | 77  | THR  |
| 2   | N     | 136 | THR  |
| 2   | N     | 149 | HIS  |
| 2   | N     | 167 | ASP  |
| 2   | N     | 168 | THR  |
| 2   | N     | 176 | LYS  |
| 2   | N     | 177 | THR  |
| 2   | N     | 194 | VAL  |
| 2   | N     | 205 | HIS  |
| 3   | O     | 14  | PHE  |
| 3   | O     | 17  | TYR  |
| 3   | O     | 47  | LEU  |
| 3   | O     | 63  | LEU  |
| 3   | O     | 65  | VAL  |
| 3   | O     | 70  | LYS  |
| 3   | O     | 72  | ILE  |
| 3   | O     | 112 | GLN  |
| 3   | O     | 174 | PRO  |
| 3   | O     | 179 | ILE  |
| 1   | P     | 10  | GLU  |
| 1   | P     | 79  | SER  |
| 1   | P     | 92  | MET  |
| 1   | P     | 108 | VAL  |
| 1   | P     | 246 | PRO  |
| 1   | P     | 380 | VAL  |
| 1   | P     | 418 | VAL  |
| 1   | P     | 421 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | Q     | 14  | GLU  |
| 2   | Q     | 43  | LYS  |
| 2   | Q     | 71  | THR  |
| 2   | Q     | 73  | THR  |
| 2   | Q     | 76  | GLU  |
| 2   | Q     | 80  | ASP  |
| 2   | Q     | 136 | THR  |
| 2   | Q     | 144 | LYS  |
| 2   | Q     | 158 | ARG  |
| 2   | Q     | 168 | THR  |
| 2   | Q     | 177 | THR  |
| 2   | Q     | 194 | VAL  |
| 2   | Q     | 195 | GLU  |
| 2   | Q     | 205 | HIS  |
| 3   | R     | 47  | LEU  |
| 3   | R     | 63  | LEU  |
| 3   | R     | 65  | VAL  |
| 3   | R     | 72  | ILE  |
| 3   | R     | 92  | GLN  |
| 3   | R     | 112 | GLN  |
| 3   | R     | 174 | PRO  |
| 3   | R     | 179 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 6   | HIS  |
| 1   | A     | 8   | HIS  |
| 1   | A     | 383 | GLN  |
| 1   | A     | 429 | ASN  |
| 2   | B     | 22  | GLN  |
| 2   | B     | 23  | HIS  |
| 2   | B     | 62  | GLN  |
| 2   | B     | 149 | HIS  |
| 2   | B     | 161 | GLN  |
| 2   | B     | 228 | GLN  |
| 3   | C     | 36  | ASN  |
| 3   | C     | 39  | ASN  |
| 3   | C     | 89  | GLN  |
| 3   | C     | 112 | GLN  |
| 3   | C     | 185 | GLN  |
| 1   | D     | 6   | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 383 | GLN  |
| 2   | E     | 5   | HIS  |
| 2   | E     | 22  | GLN  |
| 2   | E     | 23  | HIS  |
| 2   | E     | 62  | GLN  |
| 2   | E     | 149 | HIS  |
| 2   | E     | 228 | GLN  |
| 3   | F     | 36  | ASN  |
| 3   | F     | 45  | GLN  |
| 3   | F     | 89  | GLN  |
| 3   | F     | 112 | GLN  |
| 3   | F     | 185 | GLN  |
| 1   | G     | 383 | GLN  |
| 2   | H     | 22  | GLN  |
| 2   | H     | 23  | HIS  |
| 2   | H     | 62  | GLN  |
| 2   | H     | 149 | HIS  |
| 3   | I     | 36  | ASN  |
| 3   | I     | 39  | ASN  |
| 3   | I     | 112 | GLN  |
| 3   | I     | 185 | GLN  |
| 1   | J     | 177 | GLN  |
| 1   | J     | 221 | ASN  |
| 1   | J     | 383 | GLN  |
| 1   | J     | 429 | ASN  |
| 2   | K     | 22  | GLN  |
| 2   | K     | 62  | GLN  |
| 2   | K     | 149 | HIS  |
| 2   | K     | 228 | GLN  |
| 3   | L     | 36  | ASN  |
| 3   | L     | 39  | ASN  |
| 3   | L     | 112 | GLN  |
| 3   | L     | 185 | GLN  |
| 1   | M     | 8   | HIS  |
| 1   | M     | 174 | HIS  |
| 1   | M     | 177 | GLN  |
| 1   | M     | 221 | ASN  |
| 1   | M     | 291 | HIS  |
| 1   | M     | 383 | GLN  |
| 1   | M     | 429 | ASN  |
| 2   | N     | 22  | GLN  |
| 2   | N     | 23  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 62  | GLN  |
| 2   | N     | 149 | HIS  |
| 2   | N     | 228 | GLN  |
| 2   | N     | 248 | ASN  |
| 3   | O     | 36  | ASN  |
| 3   | O     | 39  | ASN  |
| 3   | O     | 112 | GLN  |
| 3   | O     | 185 | GLN  |
| 1   | P     | 8   | HIS  |
| 1   | P     | 221 | ASN  |
| 1   | P     | 291 | HIS  |
| 1   | P     | 383 | GLN  |
| 2   | Q     | 22  | GLN  |
| 2   | Q     | 62  | GLN  |
| 2   | Q     | 149 | HIS  |
| 3   | R     | 36  | ASN  |
| 3   | R     | 39  | ASN  |
| 3   | R     | 45  | GLN  |
| 3   | R     | 112 | GLN  |
| 3   | R     | 185 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 12 are monoatomic - leaving 48 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 |
| 8   | UQ2  | D     | 1102 | -    | 23,23,23     | 1.44 | 5 (21%)  | 30,31,31    | 1.17 | 2 (6%)   |
| 5   | HEM  | M     | 502  | 1    | 50,50,50     | 1.27 | 4 (8%)   | 67,82,82    | 1.00 | 3 (4%)   |
| 5   | HEM  | B     | 301  | 2    | 50,50,50     | 1.36 | 4 (8%)   | 67,82,82    | 1.05 | 3 (4%)   |
| 5   | HEM  | J     | 501  | 1    | 50,50,50     | 1.32 | 4 (8%)   | 67,82,82    | 1.03 | 3 (4%)   |
| 6   | SMA  | J     | 1004 | -    | 38,38,38     | 1.99 | 9 (23%)  | 47,52,52    | 1.72 | 9 (19%)  |
| 9   | BGL  | N     | 1045 | -    | 20,20,20     | 1.33 | 1 (5%)   | 24,25,25    | 0.73 | 0        |
| 10  | FES  | C     | 200  | 3    | 0,4,4        | -    | -        | -           | -    | -        |
| 5   | HEM  | D     | 501  | 1    | 50,50,50     | 1.24 | 2 (4%)   | 67,82,82    | 1.03 | 3 (4%)   |
| 5   | HEM  | G     | 502  | 1    | 50,50,50     | 1.33 | 4 (8%)   | 67,82,82    | 1.05 | 3 (4%)   |
| 5   | HEM  | E     | 301  | 2    | 50,50,50     | 1.29 | 4 (8%)   | 67,82,82    | 1.04 | 3 (4%)   |
| 5   | HEM  | D     | 502  | 1    | 50,50,50     | 1.23 | 4 (8%)   | 67,82,82    | 1.02 | 3 (4%)   |
| 10  | FES  | R     | 200  | 3    | 0,4,4        | -    | -        | -           | -    | -        |
| 9   | BGL  | P     | 1046 | -    | 20,20,20     | 1.18 | 1 (5%)   | 24,25,25    | 0.92 | 1 (4%)   |
| 5   | HEM  | A     | 502  | 1    | 50,50,50     | 1.31 | 3 (6%)   | 67,82,82    | 1.04 | 3 (4%)   |
| 10  | FES  | L     | 200  | 3    | 0,4,4        | -    | -        | -           | -    | -        |
| 8   | UQ2  | G     | 1103 | -    | 23,23,23     | 1.52 | 5 (21%)  | 30,31,31    | 1.09 | 1 (3%)   |
| 6   | SMA  | G     | 1003 | -    | 38,38,38     | 2.08 | 10 (26%) | 47,52,52    | 1.82 | 11 (23%) |
| 5   | HEM  | M     | 501  | 1    | 50,50,50     | 1.24 | 4 (8%)   | 67,82,82    | 1.01 | 3 (4%)   |
| 5   | HEM  | Q     | 301  | 2    | 50,50,50     | 1.30 | 3 (6%)   | 67,82,82    | 1.04 | 3 (4%)   |
| 6   | SMA  | A     | 1001 | -    | 38,38,38     | 2.12 | 10 (26%) | 47,52,52    | 1.91 | 14 (29%) |
| 8   | UQ2  | M     | 1105 | -    | 23,23,23     | 1.54 | 5 (21%)  | 30,31,31    | 1.16 | 3 (10%)  |
| 8   | UQ2  | J     | 1104 | -    | 23,23,23     | 1.31 | 4 (17%)  | 30,31,31    | 1.19 | 3 (10%)  |
| 8   | UQ2  | P     | 1106 | -    | 23,23,23     | 1.63 | 5 (21%)  | 30,31,31    | 1.22 | 5 (16%)  |
| 10  | FES  | O     | 200  | 3    | 0,4,4        | -    | -        | -           | -    | -        |
| 5   | HEM  | P     | 502  | 1    | 50,50,50     | 1.25 | 3 (6%)   | 67,82,82    | 1.03 | 4 (5%)   |
| 7   | LOP  | A     | 1021 | -    | 44,44,44     | 0.63 | 0        | 47,49,49    | 1.17 | 6 (12%)  |
| 10  | FES  | I     | 200  | 3    | 0,4,4        | -    | -        | -           | -    | -        |
| 9   | BGL  | E     | 1042 | -    | 20,20,20     | 1.03 | 1 (5%)   | 24,25,25    | 0.95 | 1 (4%)   |
| 9   | BGL  | B     | 1041 | -    | 20,20,20     | 1.05 | 1 (5%)   | 24,25,25    | 0.87 | 1 (4%)   |
| 5   | HEM  | P     | 501  | 1    | 50,50,50     | 1.27 | 4 (8%)   | 67,82,82    | 1.04 | 3 (4%)   |
| 5   | HEM  | J     | 502  | 1    | 50,50,50     | 1.34 | 4 (8%)   | 67,82,82    | 1.05 | 3 (4%)   |
| 7   | LOP  | J     | 1024 | -    | 44,44,44     | 0.65 | 0        | 47,49,49    | 1.24 | 6 (12%)  |
| 9   | BGL  | K     | 1044 | -    | 20,20,20     | 1.00 | 1 (5%)   | 24,25,25    | 1.11 | 2 (8%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | SMA  | P     | 1006 | -    | 38,38,38     | 2.03 | 9 (23%)  | 47,52,52    | 2.09 | 14 (29%) |
| 6   | SMA  | D     | 1002 | -    | 38,38,38     | 2.00 | 9 (23%)  | 47,52,52    | 1.89 | 12 (25%) |
| 6   | SMA  | M     | 1005 | -    | 38,38,38     | 2.07 | 9 (23%)  | 47,52,52    | 1.89 | 10 (21%) |
| 5   | HEM  | A     | 501  | 1    | 50,50,50     | 1.27 | 3 (6%)   | 67,82,82    | 1.02 | 3 (4%)   |
| 7   | LOP  | P     | 1026 | -    | 44,44,44     | 0.62 | 0        | 47,49,49    | 1.18 | 5 (10%)  |
| 8   | UQ2  | A     | 1101 | -    | 23,23,23     | 1.57 | 6 (26%)  | 30,31,31    | 1.19 | 2 (6%)   |
| 10  | FES  | F     | 200  | 3    | 0,4,4        | -    | -        | -           | -    | -        |
| 7   | LOP  | G     | 1023 | -    | 44,44,44     | 0.72 | 0        | 47,49,49    | 1.16 | 4 (8%)   |
| 5   | HEM  | N     | 301  | 2    | 50,50,50     | 1.34 | 3 (6%)   | 67,82,82    | 1.10 | 3 (4%)   |
| 5   | HEM  | K     | 301  | 2    | 50,50,50     | 1.33 | 3 (6%)   | 67,82,82    | 1.07 | 3 (4%)   |
| 7   | LOP  | M     | 1025 | -    | 44,44,44     | 0.70 | 0        | 47,49,49    | 1.16 | 3 (6%)   |
| 5   | HEM  | H     | 301  | 2    | 50,50,50     | 1.29 | 3 (6%)   | 67,82,82    | 1.11 | 3 (4%)   |
| 5   | HEM  | G     | 501  | 1    | 50,50,50     | 1.29 | 4 (8%)   | 67,82,82    | 1.01 | 3 (4%)   |
| 7   | LOP  | D     | 1022 | -    | 44,44,44     | 0.71 | 0        | 47,49,49    | 1.17 | 5 (10%)  |
| 9   | BGL  | G     | 1043 | -    | 20,20,20     | 1.32 | 1 (5%)   | 24,25,25    | 0.75 | 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   |
|-----|------|-------|------|------|---------|------------|---------|
| 8   | UQ2  | D     | 1102 | -    | -       | 2/15/39/39 | 0/1/1/1 |
| 5   | HEM  | M     | 502  | 1    | -       | 7/14/54/54 | -       |
| 5   | HEM  | B     | 301  | 2    | -       | 8/14/54/54 | -       |
| 5   | HEM  | J     | 501  | 1    | -       | 4/14/54/54 | -       |
| 6   | SMA  | J     | 1004 | -    | -       | 2/34/34/34 | 0/2/2/2 |
| 9   | BGL  | N     | 1045 | -    | -       | 0/11/31/31 | 0/1/1/1 |
| 10  | FES  | C     | 200  | 3    | -       | -          | 0/1/1/1 |
| 5   | HEM  | D     | 501  | 1    | -       | 3/14/54/54 | -       |
| 5   | HEM  | G     | 502  | 1    | -       | 9/14/54/54 | -       |
| 5   | HEM  | E     | 301  | 2    | -       | 9/14/54/54 | -       |
| 5   | HEM  | D     | 502  | 1    | -       | 8/14/54/54 | -       |
| 10  | FES  | R     | 200  | 3    | -       | -          | 0/1/1/1 |
| 9   | BGL  | P     | 1046 | -    | -       | 0/11/31/31 | 0/1/1/1 |
| 5   | HEM  | A     | 502  | 1    | -       | 7/14/54/54 | -       |
| 10  | FES  | L     | 200  | 3    | -       | -          | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 8   | UQ2  | G     | 1103 | -    | -       | 5/15/39/39  | 0/1/1/1 |
| 6   | SMA  | G     | 1003 | -    | -       | 5/34/34/34  | 0/2/2/2 |
| 5   | HEM  | M     | 501  | 1    | -       | 6/14/54/54  | -       |
| 5   | HEM  | Q     | 301  | 2    | -       | 7/14/54/54  | -       |
| 6   | SMA  | A     | 1001 | -    | -       | 5/34/34/34  | 0/2/2/2 |
| 8   | UQ2  | M     | 1105 | -    | -       | 2/15/39/39  | 0/1/1/1 |
| 8   | UQ2  | J     | 1104 | -    | -       | 0/15/39/39  | 0/1/1/1 |
| 8   | UQ2  | P     | 1106 | -    | -       | 4/15/39/39  | 0/1/1/1 |
| 10  | FES  | O     | 200  | 3    | -       | -           | 0/1/1/1 |
| 5   | HEM  | P     | 502  | 1    | -       | 5/14/54/54  | -       |
| 7   | LOP  | A     | 1021 | -    | -       | 12/48/48/48 | -       |
| 10  | FES  | I     | 200  | 3    | -       | -           | 0/1/1/1 |
| 9   | BGL  | E     | 1042 | -    | -       | 0/11/31/31  | 0/1/1/1 |
| 9   | BGL  | B     | 1041 | -    | -       | 0/11/31/31  | 0/1/1/1 |
| 5   | HEM  | P     | 501  | 1    | -       | 6/14/54/54  | -       |
| 5   | HEM  | J     | 502  | 1    | -       | 8/14/54/54  | -       |
| 7   | LOP  | J     | 1024 | -    | -       | 10/48/48/48 | -       |
| 9   | BGL  | K     | 1044 | -    | -       | 0/11/31/31  | 0/1/1/1 |
| 6   | SMA  | P     | 1006 | -    | -       | 7/34/34/34  | 0/2/2/2 |
| 6   | SMA  | D     | 1002 | -    | -       | 6/34/34/34  | 0/2/2/2 |
| 6   | SMA  | M     | 1005 | -    | -       | 8/34/34/34  | 0/2/2/2 |
| 5   | HEM  | A     | 501  | 1    | -       | 3/14/54/54  | -       |
| 7   | LOP  | P     | 1026 | -    | -       | 8/48/48/48  | -       |
| 8   | UQ2  | A     | 1101 | -    | -       | 6/15/39/39  | 0/1/1/1 |
| 10  | FES  | F     | 200  | 3    | -       | -           | 0/1/1/1 |
| 7   | LOP  | G     | 1023 | -    | -       | 11/48/48/48 | -       |
| 5   | HEM  | N     | 301  | 2    | -       | 8/14/54/54  | -       |
| 5   | HEM  | K     | 301  | 2    | -       | 8/14/54/54  | -       |
| 7   | LOP  | M     | 1025 | -    | -       | 4/48/48/48  | -       |
| 5   | HEM  | H     | 301  | 2    | -       | 8/14/54/54  | -       |
| 5   | HEM  | G     | 501  | 1    | -       | 6/14/54/54  | -       |
| 7   | LOP  | D     | 1022 | -    | -       | 4/48/48/48  | -       |
| 9   | BGL  | G     | 1043 | -    | -       | 0/11/31/31  | 0/1/1/1 |

All (155) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 6   | G     | 1003 | SMA  | O5-C5   | 7.24 | 1.48        | 1.37     |
| 6   | A     | 1001 | SMA  | O5-C5   | 6.96 | 1.48        | 1.37     |
| 6   | J     | 1004 | SMA  | O5-C5   | 6.64 | 1.47        | 1.37     |
| 6   | D     | 1002 | SMA  | O5-C5   | 6.55 | 1.47        | 1.37     |
| 6   | M     | 1005 | SMA  | O7-C7   | 6.53 | 1.47        | 1.37     |
| 6   | A     | 1001 | SMA  | O7-C7   | 6.40 | 1.47        | 1.37     |
| 6   | M     | 1005 | SMA  | O5-C5   | 6.17 | 1.47        | 1.37     |
| 6   | P     | 1006 | SMA  | O5-C5   | 6.05 | 1.47        | 1.37     |
| 6   | J     | 1004 | SMA  | O7-C7   | 5.77 | 1.46        | 1.37     |
| 6   | G     | 1003 | SMA  | O7-C7   | 5.43 | 1.46        | 1.37     |
| 6   | P     | 1006 | SMA  | O7-C7   | 5.23 | 1.45        | 1.37     |
| 5   | K     | 301  | HEM  | CBB-CAB | 5.14 | 1.55        | 1.30     |
| 6   | D     | 1002 | SMA  | O7-C7   | 5.06 | 1.45        | 1.37     |
| 5   | H     | 301  | HEM  | CBB-CAB | 5.01 | 1.54        | 1.30     |
| 5   | B     | 301  | HEM  | CBC-CAC | 4.99 | 1.54        | 1.30     |
| 5   | Q     | 301  | HEM  | CBB-CAB | 4.95 | 1.54        | 1.30     |
| 5   | H     | 301  | HEM  | CBC-CAC | 4.95 | 1.54        | 1.30     |
| 5   | N     | 301  | HEM  | CBB-CAB | 4.89 | 1.53        | 1.30     |
| 5   | E     | 301  | HEM  | CBB-CAB | 4.89 | 1.53        | 1.30     |
| 5   | B     | 301  | HEM  | CBB-CAB | 4.88 | 1.53        | 1.30     |
| 5   | Q     | 301  | HEM  | CBC-CAC | 4.87 | 1.53        | 1.30     |
| 5   | K     | 301  | HEM  | CBC-CAC | 4.87 | 1.53        | 1.30     |
| 5   | N     | 301  | HEM  | CBC-CAC | 4.87 | 1.53        | 1.30     |
| 5   | E     | 301  | HEM  | CBC-CAC | 4.79 | 1.53        | 1.30     |
| 5   | G     | 501  | HEM  | CBC-CAC | 4.76 | 1.53        | 1.30     |
| 5   | P     | 502  | HEM  | CBB-CAB | 4.76 | 1.53        | 1.30     |
| 5   | D     | 501  | HEM  | CBC-CAC | 4.72 | 1.53        | 1.30     |
| 5   | A     | 501  | HEM  | CBB-CAB | 4.69 | 1.52        | 1.30     |
| 5   | J     | 502  | HEM  | CBB-CAB | 4.66 | 1.52        | 1.30     |
| 5   | J     | 501  | HEM  | CBC-CAC | 4.66 | 1.52        | 1.30     |
| 5   | A     | 501  | HEM  | CBC-CAC | 4.59 | 1.52        | 1.30     |
| 5   | J     | 501  | HEM  | CBB-CAB | 4.58 | 1.52        | 1.30     |
| 5   | P     | 501  | HEM  | CBB-CAB | 4.56 | 1.52        | 1.30     |
| 5   | M     | 502  | HEM  | CBC-CAC | 4.55 | 1.52        | 1.30     |
| 5   | A     | 502  | HEM  | CBB-CAB | 4.55 | 1.52        | 1.30     |
| 5   | G     | 501  | HEM  | CBB-CAB | 4.54 | 1.52        | 1.30     |
| 5   | A     | 502  | HEM  | CBC-CAC | 4.54 | 1.52        | 1.30     |
| 5   | D     | 501  | HEM  | CBB-CAB | 4.53 | 1.52        | 1.30     |
| 5   | M     | 501  | HEM  | CBC-CAC | 4.52 | 1.52        | 1.30     |
| 5   | M     | 501  | HEM  | CBB-CAB | 4.50 | 1.52        | 1.30     |
| 5   | P     | 501  | HEM  | CBC-CAC | 4.49 | 1.52        | 1.30     |
| 5   | G     | 502  | HEM  | CBB-CAB | 4.49 | 1.51        | 1.30     |
| 5   | D     | 502  | HEM  | CBB-CAB | 4.46 | 1.51        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | G     | 1043 | BGL  | C1-C2   | 4.45  | 1.56        | 1.52     |
| 5   | M     | 502  | HEM  | CBB-CAB | 4.44  | 1.51        | 1.30     |
| 5   | D     | 502  | HEM  | CBC-CAC | 4.35  | 1.51        | 1.30     |
| 9   | N     | 1045 | BGL  | C1-C2   | 4.31  | 1.56        | 1.52     |
| 5   | P     | 502  | HEM  | CBC-CAC | 4.30  | 1.51        | 1.30     |
| 5   | G     | 502  | HEM  | CBC-CAC | 4.15  | 1.50        | 1.30     |
| 5   | J     | 502  | HEM  | CAC-C3C | -4.08 | 1.36        | 1.47     |
| 8   | G     | 1103 | UQ2  | C6-C5   | 3.91  | 1.42        | 1.35     |
| 8   | P     | 1106 | UQ2  | C6-C5   | 3.89  | 1.42        | 1.35     |
| 6   | A     | 1001 | SMA  | O8-C8   | 3.87  | 1.45        | 1.36     |
| 5   | J     | 502  | HEM  | CBC-CAC | 3.77  | 1.48        | 1.30     |
| 9   | P     | 1046 | BGL  | C1-C2   | 3.66  | 1.55        | 1.52     |
| 6   | P     | 1006 | SMA  | C3-C4   | -3.64 | 1.39        | 1.47     |
| 9   | B     | 1041 | BGL  | C1-C2   | 3.56  | 1.55        | 1.52     |
| 8   | M     | 1105 | UQ2  | C6-C5   | 3.52  | 1.41        | 1.35     |
| 8   | M     | 1105 | UQ2  | C7-C8   | 3.50  | 1.56        | 1.50     |
| 8   | A     | 1101 | UQ2  | C7-C8   | 3.46  | 1.56        | 1.50     |
| 6   | M     | 1005 | SMA  | O8-C8   | 3.41  | 1.44        | 1.36     |
| 9   | E     | 1042 | BGL  | C1-C2   | 3.41  | 1.55        | 1.52     |
| 6   | D     | 1002 | SMA  | C7-C8   | -3.35 | 1.35        | 1.40     |
| 6   | D     | 1002 | SMA  | O8-C8   | 3.35  | 1.44        | 1.36     |
| 6   | P     | 1006 | SMA  | O8-C8   | 3.32  | 1.44        | 1.36     |
| 6   | J     | 1004 | SMA  | O8-C8   | 3.27  | 1.44        | 1.36     |
| 8   | D     | 1102 | UQ2  | C6-C5   | 3.26  | 1.41        | 1.35     |
| 8   | P     | 1106 | UQ2  | C7-C8   | 3.25  | 1.55        | 1.50     |
| 8   | P     | 1106 | UQ2  | C7-C6   | 3.25  | 1.57        | 1.51     |
| 6   | G     | 1003 | SMA  | O8-C8   | 3.23  | 1.44        | 1.36     |
| 8   | A     | 1101 | UQ2  | C6-C5   | 3.22  | 1.41        | 1.35     |
| 5   | G     | 502  | HEM  | CAC-C3C | -3.16 | 1.38        | 1.47     |
| 8   | G     | 1103 | UQ2  | C7-C8   | 3.16  | 1.55        | 1.50     |
| 5   | N     | 301  | HEM  | CAC-C3C | -3.15 | 1.39        | 1.47     |
| 6   | P     | 1006 | SMA  | C7-C8   | -2.99 | 1.36        | 1.40     |
| 6   | P     | 1006 | SMA  | C4A-C4  | -2.94 | 1.39        | 1.46     |
| 8   | D     | 1102 | UQ2  | C7-C8   | 2.91  | 1.55        | 1.50     |
| 8   | J     | 1104 | UQ2  | C6-C5   | 2.85  | 1.40        | 1.35     |
| 5   | A     | 502  | HEM  | CAB-C3B | -2.84 | 1.39        | 1.47     |
| 6   | D     | 1002 | SMA  | C4A-C4  | -2.84 | 1.39        | 1.46     |
| 5   | J     | 501  | HEM  | CAB-C3B | -2.82 | 1.39        | 1.47     |
| 8   | J     | 1104 | UQ2  | C7-C8   | 2.82  | 1.55        | 1.50     |
| 6   | A     | 1001 | SMA  | C3-C4   | -2.82 | 1.41        | 1.47     |
| 5   | M     | 502  | HEM  | CAB-C3B | -2.80 | 1.39        | 1.47     |
| 5   | B     | 301  | HEM  | CAC-C3C | -2.77 | 1.40        | 1.47     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6   | D     | 1002 | SMA  | C3-C2   | 2.75  | 1.39        | 1.34     |
| 9   | K     | 1044 | BGL  | C1-C2   | 2.69  | 1.55        | 1.52     |
| 6   | J     | 1004 | SMA  | C3-C4   | -2.64 | 1.41        | 1.47     |
| 6   | M     | 1005 | SMA  | C3-C4   | -2.63 | 1.41        | 1.47     |
| 8   | D     | 1102 | UQ2  | O3-C3   | 2.62  | 1.43        | 1.36     |
| 6   | J     | 1004 | SMA  | C7-C8   | -2.58 | 1.36        | 1.40     |
| 8   | G     | 1103 | UQ2  | O3-C3   | 2.58  | 1.43        | 1.36     |
| 5   | P     | 502  | HEM  | CAC-C3C | -2.56 | 1.40        | 1.47     |
| 8   | A     | 1101 | UQ2  | O2-C2   | 2.56  | 1.42        | 1.36     |
| 6   | G     | 1003 | SMA  | C7-C8   | -2.56 | 1.37        | 1.40     |
| 6   | M     | 1005 | SMA  | C20-C19 | 2.56  | 1.35        | 1.33     |
| 8   | G     | 1103 | UQ2  | O2-C2   | 2.55  | 1.42        | 1.36     |
| 6   | D     | 1002 | SMA  | C3-C4   | -2.55 | 1.41        | 1.47     |
| 6   | G     | 1003 | SMA  | C20-C19 | 2.54  | 1.35        | 1.33     |
| 8   | M     | 1105 | UQ2  | C7-C6   | 2.53  | 1.56        | 1.51     |
| 6   | A     | 1001 | SMA  | C4A-C4  | -2.53 | 1.40        | 1.46     |
| 6   | G     | 1003 | SMA  | C4A-C4  | -2.52 | 1.40        | 1.46     |
| 5   | Q     | 301  | HEM  | CAB-C3B | -2.49 | 1.40        | 1.47     |
| 6   | D     | 1002 | SMA  | O5-C5M  | 2.49  | 1.49        | 1.42     |
| 8   | P     | 1106 | UQ2  | O3-C3   | 2.47  | 1.42        | 1.36     |
| 5   | A     | 501  | HEM  | CAB-C3B | -2.47 | 1.40        | 1.47     |
| 6   | J     | 1004 | SMA  | C4A-C4  | -2.45 | 1.40        | 1.46     |
| 6   | M     | 1005 | SMA  | O1-C2   | 2.44  | 1.39        | 1.36     |
| 5   | B     | 301  | HEM  | CAB-C3B | -2.44 | 1.40        | 1.47     |
| 6   | G     | 1003 | SMA  | C3-C4   | -2.42 | 1.42        | 1.47     |
| 5   | D     | 502  | HEM  | CAC-C3C | -2.41 | 1.40        | 1.47     |
| 6   | D     | 1002 | SMA  | O12-C12 | 2.40  | 1.48        | 1.42     |
| 5   | J     | 502  | HEM  | CAB-C3B | -2.40 | 1.41        | 1.47     |
| 8   | G     | 1103 | UQ2  | C7-C6   | 2.39  | 1.55        | 1.51     |
| 6   | M     | 1005 | SMA  | C7-C8   | -2.39 | 1.37        | 1.40     |
| 5   | M     | 501  | HEM  | CAC-C3C | -2.38 | 1.41        | 1.47     |
| 6   | A     | 1001 | SMA  | C20-C19 | 2.38  | 1.35        | 1.33     |
| 8   | D     | 1102 | UQ2  | O2-C2   | 2.38  | 1.42        | 1.36     |
| 5   | E     | 301  | HEM  | CAC-C3C | -2.37 | 1.41        | 1.47     |
| 6   | P     | 1006 | SMA  | O12-C12 | 2.37  | 1.48        | 1.42     |
| 5   | M     | 501  | HEM  | CAB-C3B | -2.36 | 1.41        | 1.47     |
| 6   | A     | 1001 | SMA  | C7-C8   | -2.35 | 1.37        | 1.40     |
| 6   | A     | 1001 | SMA  | C3-C2   | 2.34  | 1.39        | 1.34     |
| 8   | M     | 1105 | UQ2  | O3-C3   | 2.34  | 1.42        | 1.36     |
| 8   | A     | 1101 | UQ2  | C7-C6   | 2.33  | 1.55        | 1.51     |
| 8   | P     | 1106 | UQ2  | O2-C2   | 2.30  | 1.42        | 1.36     |
| 6   | J     | 1004 | SMA  | C3-C2   | 2.29  | 1.39        | 1.34     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 5   | P     | 501  | HEM  | CAC-C3C | -2.26 | 1.41        | 1.47     |
| 6   | G     | 1003 | SMA  | C8-C8A  | -2.25 | 1.36        | 1.39     |
| 5   | M     | 502  | HEM  | CAC-C3C | -2.24 | 1.41        | 1.47     |
| 6   | G     | 1003 | SMA  | O12-C12 | 2.23  | 1.48        | 1.42     |
| 5   | H     | 301  | HEM  | CAC-C3C | -2.22 | 1.41        | 1.47     |
| 8   | J     | 1104 | UQ2  | O3-C3   | 2.21  | 1.42        | 1.36     |
| 5   | G     | 502  | HEM  | CAB-C3B | -2.21 | 1.41        | 1.47     |
| 5   | D     | 502  | HEM  | CAB-C3B | -2.20 | 1.41        | 1.47     |
| 6   | M     | 1005 | SMA  | C4A-C4  | -2.17 | 1.41        | 1.46     |
| 5   | P     | 501  | HEM  | CAB-C3B | -2.17 | 1.41        | 1.47     |
| 6   | M     | 1005 | SMA  | C3-C2   | 2.16  | 1.38        | 1.34     |
| 6   | A     | 1001 | SMA  | C24-C13 | 2.15  | 1.57        | 1.53     |
| 6   | P     | 1006 | SMA  | O5-C5M  | 2.14  | 1.48        | 1.42     |
| 5   | K     | 301  | HEM  | CAC-C3C | -2.14 | 1.41        | 1.47     |
| 8   | M     | 1105 | UQ2  | C8-C9   | 2.12  | 1.38        | 1.33     |
| 5   | J     | 501  | HEM  | CAC-C3C | -2.10 | 1.41        | 1.47     |
| 5   | G     | 501  | HEM  | CAB-C3B | -2.08 | 1.41        | 1.47     |
| 5   | E     | 301  | HEM  | CAB-C3B | -2.08 | 1.41        | 1.47     |
| 8   | J     | 1104 | UQ2  | O2-C2   | 2.07  | 1.41        | 1.36     |
| 6   | G     | 1003 | SMA  | C3-C2   | 2.06  | 1.38        | 1.34     |
| 8   | A     | 1101 | UQ2  | C8-C9   | 2.06  | 1.37        | 1.33     |
| 5   | G     | 501  | HEM  | CAC-C3C | -2.06 | 1.41        | 1.47     |
| 8   | A     | 1101 | UQ2  | O3-C3   | 2.06  | 1.41        | 1.36     |
| 6   | J     | 1004 | SMA  | O5-C5M  | 2.05  | 1.48        | 1.42     |
| 6   | J     | 1004 | SMA  | C8-C8A  | -2.03 | 1.36        | 1.39     |
| 6   | A     | 1001 | SMA  | C8-C8A  | -2.01 | 1.36        | 1.39     |
| 8   | D     | 1102 | UQ2  | C7-C6   | 2.00  | 1.55        | 1.51     |
| 6   | P     | 1006 | SMA  | O1-C2   | 2.00  | 1.39        | 1.36     |

All (175) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | P     | 1006 | SMA  | C14-C15-C16 | 6.09  | 138.23      | 125.88   |
| 6   | P     | 1006 | SMA  | O7-C7-C8    | 4.96  | 119.71      | 114.53   |
| 6   | M     | 1005 | SMA  | C5M-O5-C5   | -4.94 | 110.27      | 117.51   |
| 6   | A     | 1001 | SMA  | O5-C5-C4A   | 4.79  | 122.63      | 115.84   |
| 6   | A     | 1001 | SMA  | O7-C7-C8    | 4.55  | 119.29      | 114.53   |
| 6   | D     | 1002 | SMA  | O5-C5-C4A   | 4.43  | 122.12      | 115.84   |
| 6   | M     | 1005 | SMA  | O5-C5-C4A   | 4.35  | 122.01      | 115.84   |
| 6   | G     | 1003 | SMA  | O5-C5-C4A   | 4.24  | 121.85      | 115.84   |
| 6   | G     | 1003 | SMA  | O1-C2-C9    | 4.14  | 118.91      | 110.12   |
| 6   | M     | 1005 | SMA  | O7-C7-C8    | 4.14  | 118.86      | 114.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | P     | 1006 | SMA  | O1-C2-C9    | 4.08  | 118.78      | 110.12   |
| 6   | A     | 1001 | SMA  | O1-C2-C9    | 4.04  | 118.69      | 110.12   |
| 6   | D     | 1002 | SMA  | C5M-O5-C5   | -4.02 | 111.61      | 117.51   |
| 6   | J     | 1004 | SMA  | O5-C5-C4A   | 4.01  | 121.53      | 115.84   |
| 6   | P     | 1006 | SMA  | O5-C5-C4A   | 3.94  | 121.43      | 115.84   |
| 6   | M     | 1005 | SMA  | O1-C2-C9    | 3.92  | 118.43      | 110.12   |
| 6   | P     | 1006 | SMA  | C5M-O5-C5   | -3.91 | 111.78      | 117.51   |
| 6   | J     | 1004 | SMA  | C5M-O5-C5   | -3.90 | 111.79      | 117.51   |
| 6   | J     | 1004 | SMA  | O7-C7-C8    | 3.89  | 118.60      | 114.53   |
| 6   | J     | 1004 | SMA  | C9-C10-C11  | -3.86 | 107.25      | 114.46   |
| 5   | J     | 502  | HEM  | CBC-CAC-C3C | -3.84 | 108.32      | 127.53   |
| 6   | D     | 1002 | SMA  | O1-C2-C9    | 3.84  | 118.27      | 110.12   |
| 6   | G     | 1003 | SMA  | O7-C7-C8    | 3.79  | 118.49      | 114.53   |
| 6   | J     | 1004 | SMA  | O1-C2-C9    | 3.77  | 118.12      | 110.12   |
| 6   | D     | 1002 | SMA  | O7-C7-C8    | 3.73  | 118.43      | 114.53   |
| 7   | J     | 1024 | LOP  | O5-C6-C7    | 3.70  | 119.49      | 111.48   |
| 6   | A     | 1001 | SMA  | O5-C5-C6    | -3.69 | 117.72      | 124.08   |
| 5   | G     | 502  | HEM  | CBC-CAC-C3C | -3.66 | 109.25      | 127.53   |
| 6   | A     | 1001 | SMA  | C5M-O5-C5   | -3.65 | 112.16      | 117.51   |
| 6   | G     | 1003 | SMA  | C5M-O5-C5   | -3.54 | 112.31      | 117.51   |
| 6   | G     | 1003 | SMA  | C14-C15-C16 | 3.54  | 133.06      | 125.88   |
| 5   | K     | 301  | HEM  | CBB-CAB-C3B | -3.54 | 109.86      | 127.53   |
| 5   | H     | 301  | HEM  | CBB-CAB-C3B | -3.53 | 109.87      | 127.53   |
| 5   | H     | 301  | HEM  | C3B-C4B-NB  | 3.51  | 111.99      | 109.47   |
| 5   | E     | 301  | HEM  | CBB-CAB-C3B | -3.50 | 110.04      | 127.53   |
| 5   | B     | 301  | HEM  | CBB-CAB-C3B | -3.50 | 110.06      | 127.53   |
| 5   | J     | 501  | HEM  | CBB-CAB-C3B | -3.47 | 110.16      | 127.53   |
| 5   | D     | 502  | HEM  | CBB-CAB-C3B | -3.47 | 110.17      | 127.53   |
| 9   | K     | 1044 | BGL  | C1'-O2-C2   | -3.47 | 106.31      | 114.02   |
| 5   | N     | 301  | HEM  | CBC-CAC-C3C | -3.47 | 110.20      | 127.53   |
| 5   | Q     | 301  | HEM  | CBB-CAB-C3B | -3.46 | 110.24      | 127.53   |
| 5   | B     | 301  | HEM  | CBC-CAC-C3C | -3.45 | 110.31      | 127.53   |
| 5   | A     | 502  | HEM  | CBB-CAB-C3B | -3.43 | 110.38      | 127.53   |
| 5   | P     | 501  | HEM  | CBC-CAC-C3C | -3.42 | 110.45      | 127.53   |
| 5   | N     | 301  | HEM  | CBB-CAB-C3B | -3.41 | 110.46      | 127.53   |
| 5   | K     | 301  | HEM  | CBC-CAC-C3C | -3.41 | 110.47      | 127.53   |
| 5   | H     | 301  | HEM  | CBC-CAC-C3C | -3.40 | 110.54      | 127.53   |
| 5   | J     | 501  | HEM  | CBC-CAC-C3C | -3.37 | 110.67      | 127.53   |
| 5   | E     | 301  | HEM  | CBC-CAC-C3C | -3.37 | 110.68      | 127.53   |
| 5   | Q     | 301  | HEM  | CBC-CAC-C3C | -3.37 | 110.68      | 127.53   |
| 5   | M     | 501  | HEM  | CBB-CAB-C3B | -3.37 | 110.71      | 127.53   |
| 5   | A     | 502  | HEM  | CBC-CAC-C3C | -3.36 | 110.72      | 127.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | M     | 502  | HEM  | CBB-CAB-C3B | -3.36 | 110.74      | 127.53   |
| 5   | G     | 502  | HEM  | CBB-CAB-C3B | -3.36 | 110.75      | 127.53   |
| 6   | D     | 1002 | SMA  | C17-C18-C19 | -3.35 | 117.17      | 126.36   |
| 5   | G     | 501  | HEM  | CBC-CAC-C3C | -3.34 | 110.81      | 127.53   |
| 5   | M     | 501  | HEM  | CBC-CAC-C3C | -3.31 | 110.98      | 127.53   |
| 5   | G     | 501  | HEM  | CBB-CAB-C3B | -3.30 | 111.02      | 127.53   |
| 5   | J     | 502  | HEM  | CBB-CAB-C3B | -3.28 | 111.13      | 127.53   |
| 5   | P     | 501  | HEM  | CBB-CAB-C3B | -3.28 | 111.14      | 127.53   |
| 5   | M     | 502  | HEM  | CBC-CAC-C3C | -3.28 | 111.15      | 127.53   |
| 5   | P     | 502  | HEM  | CBC-CAC-C3C | -3.28 | 111.15      | 127.53   |
| 5   | A     | 501  | HEM  | CBB-CAB-C3B | -3.23 | 111.39      | 127.53   |
| 6   | D     | 1002 | SMA  | C9-C10-C11  | -3.21 | 108.47      | 114.46   |
| 5   | D     | 502  | HEM  | CBC-CAC-C3C | -3.21 | 111.51      | 127.53   |
| 5   | P     | 502  | HEM  | CBB-CAB-C3B | -3.20 | 111.54      | 127.53   |
| 5   | D     | 501  | HEM  | CBC-CAC-C3C | -3.17 | 111.70      | 127.53   |
| 5   | A     | 501  | HEM  | CBC-CAC-C3C | -3.13 | 111.88      | 127.53   |
| 6   | A     | 1001 | SMA  | C9-C10-C11  | -3.13 | 108.61      | 114.46   |
| 5   | D     | 501  | HEM  | CBB-CAB-C3B | -3.12 | 111.92      | 127.53   |
| 7   | A     | 1021 | LOP  | O5-C6-C7    | 3.03  | 118.03      | 111.48   |
| 5   | N     | 301  | HEM  | C3B-C4B-NB  | 3.01  | 111.63      | 109.47   |
| 9   | P     | 1046 | BGL  | C1'-O2-C2   | -3.01 | 107.34      | 114.02   |
| 6   | D     | 1002 | SMA  | O5-C5-C6    | -2.99 | 118.94      | 124.08   |
| 6   | P     | 1006 | SMA  | C7M-O7-C7   | -2.98 | 113.14      | 117.51   |
| 7   | G     | 1023 | LOP  | O5-C6-C7    | 2.98  | 117.93      | 111.48   |
| 6   | P     | 1006 | SMA  | C9-C10-C11  | -2.97 | 108.92      | 114.46   |
| 6   | G     | 1003 | SMA  | C9-C10-C11  | -2.94 | 108.97      | 114.46   |
| 7   | G     | 1023 | LOP  | C19-C18-C17 | -2.94 | 99.52       | 114.37   |
| 6   | M     | 1005 | SMA  | O5-C5-C6    | -2.93 | 119.02      | 124.08   |
| 5   | G     | 502  | HEM  | C3B-C4B-NB  | 2.93  | 111.57      | 109.47   |
| 7   | M     | 1025 | LOP  | O5-C6-C7    | 2.91  | 117.77      | 111.48   |
| 6   | M     | 1005 | SMA  | C17-C18-C19 | -2.90 | 118.41      | 126.36   |
| 7   | D     | 1022 | LOP  | O5-C6-C7    | 2.87  | 117.69      | 111.48   |
| 9   | E     | 1042 | BGL  | C1'-O2-C2   | -2.87 | 107.65      | 114.02   |
| 6   | D     | 1002 | SMA  | C14-C15-C16 | 2.86  | 131.68      | 125.88   |
| 6   | M     | 1005 | SMA  | C7M-O7-C7   | -2.85 | 113.33      | 117.51   |
| 7   | D     | 1022 | LOP  | C27-C26-C25 | -2.84 | 102.69      | 113.13   |
| 8   | A     | 1101 | UQ2  | C10-C9-C11  | 2.84  | 120.15      | 115.23   |
| 6   | M     | 1005 | SMA  | C14-C15-C16 | 2.83  | 131.62      | 125.88   |
| 7   | A     | 1021 | LOP  | C19-C18-C17 | -2.82 | 100.09      | 114.37   |
| 5   | E     | 301  | HEM  | C3B-C4B-NB  | 2.80  | 111.48      | 109.47   |
| 5   | P     | 501  | HEM  | C3B-C4B-NB  | 2.79  | 111.47      | 109.47   |
| 6   | P     | 1006 | SMA  | C13-C14-C15 | 2.78  | 118.13      | 112.11   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | M     | 502  | HEM  | C3B-C4B-NB  | 2.78  | 111.46      | 109.47   |
| 5   | G     | 501  | HEM  | C3B-C4B-NB  | 2.78  | 111.46      | 109.47   |
| 7   | J     | 1024 | LOP  | O6-C24-C25  | 2.77  | 120.29      | 111.83   |
| 5   | D     | 501  | HEM  | C3B-C4B-NB  | 2.75  | 111.44      | 109.47   |
| 5   | J     | 502  | HEM  | C3B-C4B-NB  | 2.74  | 111.43      | 109.47   |
| 5   | B     | 301  | HEM  | C3B-C4B-NB  | 2.72  | 111.42      | 109.47   |
| 6   | G     | 1003 | SMA  | O1-C2-C3    | -2.72 | 119.42      | 121.81   |
| 6   | D     | 1002 | SMA  | O1-C2-C3    | -2.71 | 119.43      | 121.81   |
| 6   | D     | 1002 | SMA  | C7M-O7-C7   | -2.70 | 113.55      | 117.51   |
| 7   | P     | 1026 | LOP  | C9-C8-C7    | -2.70 | 103.22      | 113.13   |
| 5   | P     | 502  | HEM  | C3B-C4B-NB  | 2.69  | 111.40      | 109.47   |
| 7   | G     | 1023 | LOP  | C21-C20-C19 | -2.67 | 100.87      | 114.37   |
| 6   | A     | 1001 | SMA  | O1-C2-C3    | -2.66 | 119.48      | 121.81   |
| 7   | P     | 1026 | LOP  | C27-C26-C25 | -2.65 | 103.37      | 113.13   |
| 6   | J     | 1004 | SMA  | C7M-O7-C7   | -2.64 | 113.65      | 117.51   |
| 6   | G     | 1003 | SMA  | C7M-O7-C7   | -2.62 | 113.67      | 117.51   |
| 7   | G     | 1023 | LOP  | O6-C24-C25  | 2.61  | 119.79      | 111.83   |
| 5   | M     | 501  | HEM  | C3B-C4B-NB  | 2.61  | 111.34      | 109.47   |
| 5   | Q     | 301  | HEM  | C3B-C4B-NB  | 2.61  | 111.34      | 109.47   |
| 5   | K     | 301  | HEM  | C3B-C4B-NB  | 2.59  | 111.33      | 109.47   |
| 6   | A     | 1001 | SMA  | C7M-O7-C7   | -2.57 | 113.75      | 117.51   |
| 6   | M     | 1005 | SMA  | O1-C2-C3    | -2.56 | 119.56      | 121.81   |
| 9   | B     | 1041 | BGL  | C1'-O2-C2   | -2.56 | 108.33      | 114.02   |
| 5   | A     | 501  | HEM  | C3B-C4B-NB  | 2.56  | 111.31      | 109.47   |
| 8   | P     | 1106 | UQ2  | C8-C7-C6    | 2.54  | 118.35      | 112.08   |
| 6   | P     | 1006 | SMA  | O5-C5-C6    | -2.54 | 119.69      | 124.08   |
| 8   | J     | 1104 | UQ2  | C10-C9-C11  | 2.54  | 119.64      | 115.23   |
| 8   | A     | 1101 | UQ2  | C7-C8-C9    | -2.54 | 122.46      | 126.83   |
| 6   | G     | 1003 | SMA  | C26-C19-C18 | 2.53  | 121.96      | 118.09   |
| 6   | G     | 1003 | SMA  | O5-C5-C6    | -2.53 | 119.72      | 124.08   |
| 6   | J     | 1004 | SMA  | O1-C2-C3    | -2.53 | 119.59      | 121.81   |
| 6   | J     | 1004 | SMA  | C17-C18-C19 | -2.53 | 119.44      | 126.36   |
| 7   | M     | 1025 | LOP  | C21-C20-C19 | -2.53 | 101.60      | 114.37   |
| 7   | M     | 1025 | LOP  | C19-C18-C17 | -2.51 | 101.67      | 114.37   |
| 7   | D     | 1022 | LOP  | O6-C24-C25  | 2.50  | 119.46      | 111.83   |
| 5   | J     | 501  | HEM  | C3B-C4B-NB  | 2.50  | 111.26      | 109.47   |
| 7   | D     | 1022 | LOP  | C19-C18-C17 | -2.48 | 101.81      | 114.37   |
| 6   | P     | 1006 | SMA  | C26-C19-C18 | 2.47  | 121.86      | 118.09   |
| 7   | P     | 1026 | LOP  | O5-C6-C7    | 2.47  | 116.82      | 111.48   |
| 8   | M     | 1105 | UQ2  | C10-C9-C11  | 2.46  | 119.49      | 115.23   |
| 5   | A     | 502  | HEM  | C3B-C4B-NB  | 2.44  | 111.22      | 109.47   |
| 8   | D     | 1102 | UQ2  | C10-C9-C11  | 2.42  | 119.43      | 115.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 7   | A     | 1021 | LOP  | C21-C20-C19 | -2.41 | 102.16      | 114.37   |
| 7   | P     | 1026 | LOP  | O6-C24-C25  | 2.41  | 119.17      | 111.83   |
| 8   | J     | 1104 | UQ2  | C7-C6-C5    | -2.40 | 120.78      | 124.89   |
| 7   | J     | 1024 | LOP  | C19-C18-C17 | -2.38 | 102.34      | 114.37   |
| 6   | J     | 1004 | SMA  | O5-C5-C6    | -2.37 | 119.99      | 124.08   |
| 6   | P     | 1006 | SMA  | O7-C7-C6    | -2.36 | 120.01      | 124.08   |
| 8   | M     | 1105 | UQ2  | C7-C8-C9    | -2.31 | 122.84      | 126.83   |
| 9   | K     | 1044 | BGL  | C3'-C2'-C1' | -2.31 | 103.43      | 113.47   |
| 6   | P     | 1006 | SMA  | C17-C18-C19 | -2.28 | 120.11      | 126.36   |
| 6   | M     | 1005 | SMA  | C9-C10-C11  | -2.26 | 110.24      | 114.46   |
| 8   | P     | 1106 | UQ2  | C10-C9-C11  | 2.23  | 119.10      | 115.23   |
| 7   | A     | 1021 | LOP  | C31-C30-C29 | -2.23 | 103.10      | 114.37   |
| 8   | D     | 1102 | UQ2  | C7-C8-C9    | -2.21 | 123.02      | 126.83   |
| 6   | D     | 1002 | SMA  | C26-C19-C18 | 2.21  | 121.46      | 118.09   |
| 7   | A     | 1021 | LOP  | C29-C28-C27 | -2.21 | 103.21      | 114.37   |
| 7   | J     | 1024 | LOP  | C21-C20-C19 | -2.20 | 103.25      | 114.37   |
| 6   | G     | 1003 | SMA  | C17-C18-C19 | -2.19 | 120.34      | 126.36   |
| 7   | J     | 1024 | LOP  | C29-C28-C27 | -2.18 | 103.35      | 114.37   |
| 8   | J     | 1104 | UQ2  | CM5-C5-C6   | -2.17 | 120.88      | 124.45   |
| 5   | P     | 502  | HEM  | CAC-C3C-C4C | 2.17  | 130.00      | 124.82   |
| 5   | D     | 502  | HEM  | C3B-C4B-NB  | 2.16  | 111.02      | 109.47   |
| 6   | A     | 1001 | SMA  | C17-C18-C19 | -2.15 | 120.46      | 126.36   |
| 6   | A     | 1001 | SMA  | C13-C14-C15 | -2.15 | 107.48      | 112.11   |
| 6   | P     | 1006 | SMA  | O1-C2-C3    | -2.14 | 119.93      | 121.81   |
| 6   | A     | 1001 | SMA  | C3M-C3-C2   | -2.13 | 120.12      | 123.28   |
| 8   | P     | 1106 | UQ2  | C5-C6-C1    | -2.12 | 117.56      | 119.62   |
| 6   | D     | 1002 | SMA  | C3M-C3-C2   | -2.12 | 120.14      | 123.28   |
| 7   | P     | 1026 | LOP  | C19-C18-C17 | -2.12 | 103.67      | 114.37   |
| 6   | A     | 1001 | SMA  | C3M-C3-C4   | 2.10  | 120.54      | 116.68   |
| 8   | G     | 1103 | UQ2  | C7-C8-C9    | -2.09 | 123.22      | 126.83   |
| 6   | P     | 1006 | SMA  | C17-C16-C15 | -2.09 | 110.32      | 124.25   |
| 6   | A     | 1001 | SMA  | C14-C15-C16 | -2.08 | 121.67      | 125.88   |
| 8   | P     | 1106 | UQ2  | C7-C8-C9    | -2.08 | 123.25      | 126.83   |
| 6   | A     | 1001 | SMA  | C16-C17-C18 | -2.08 | 119.74      | 124.65   |
| 7   | J     | 1024 | LOP  | C27-C26-C25 | -2.06 | 105.55      | 113.13   |
| 7   | A     | 1021 | LOP  | O6-C24-C25  | 2.06  | 118.12      | 111.83   |
| 8   | M     | 1105 | UQ2  | C8-C7-C6    | 2.04  | 117.12      | 112.08   |
| 7   | D     | 1022 | LOP  | P1-O1-C2    | -2.03 | 111.57      | 121.26   |
| 8   | P     | 1106 | UQ2  | C3-C4-C5    | 2.03  | 122.11      | 118.10   |

There are no chirality outliers.

All (221) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | A     | 502  | HEM  | C2B-C3B-CAB-CBB |
| 5   | A     | 502  | HEM  | C4B-C3B-CAB-CBB |
| 5   | D     | 502  | HEM  | C2B-C3B-CAB-CBB |
| 5   | D     | 502  | HEM  | C4B-C3B-CAB-CBB |
| 5   | E     | 301  | HEM  | C2C-C3C-CAC-CBC |
| 5   | G     | 502  | HEM  | C2B-C3B-CAB-CBB |
| 5   | J     | 501  | HEM  | C2B-C3B-CAB-CBB |
| 5   | J     | 501  | HEM  | C2C-C3C-CAC-CBC |
| 5   | J     | 501  | HEM  | C4C-C3C-CAC-CBC |
| 5   | J     | 502  | HEM  | C2B-C3B-CAB-CBB |
| 5   | J     | 502  | HEM  | C2C-C3C-CAC-CBC |
| 5   | K     | 301  | HEM  | C2C-C3C-CAC-CBC |
| 5   | M     | 501  | HEM  | C2B-C3B-CAB-CBB |
| 5   | M     | 501  | HEM  | C2C-C3C-CAC-CBC |
| 5   | M     | 502  | HEM  | C2B-C3B-CAB-CBB |
| 5   | N     | 301  | HEM  | C2C-C3C-CAC-CBC |
| 5   | P     | 501  | HEM  | C2C-C3C-CAC-CBC |
| 5   | P     | 501  | HEM  | C4C-C3C-CAC-CBC |
| 6   | G     | 1003 | SMA  | C13-C14-C15-C16 |
| 6   | M     | 1005 | SMA  | C13-C14-C15-C16 |
| 6   | P     | 1006 | SMA  | C13-C14-C15-C16 |
| 7   | A     | 1021 | LOP  | C2-O1-P1-O2     |
| 7   | A     | 1021 | LOP  | C2-O1-P1-O3     |
| 7   | A     | 1021 | LOP  | C2-O1-P1-O4     |
| 7   | G     | 1023 | LOP  | C2-O1-P1-O2     |
| 7   | G     | 1023 | LOP  | C2-O1-P1-O3     |
| 7   | G     | 1023 | LOP  | C2-O1-P1-O4     |
| 7   | J     | 1024 | LOP  | C2-O1-P1-O2     |
| 7   | J     | 1024 | LOP  | C2-O1-P1-O3     |
| 7   | J     | 1024 | LOP  | C3-O2-P1-O1     |
| 7   | J     | 1024 | LOP  | C3-O2-P1-O3     |
| 7   | P     | 1026 | LOP  | C2-O1-P1-O2     |
| 7   | P     | 1026 | LOP  | C2-O1-P1-O3     |
| 7   | P     | 1026 | LOP  | C2-O1-P1-O4     |
| 8   | P     | 1106 | UQ2  | C1-C6-C7-C8     |
| 8   | A     | 1101 | UQ2  | C9-C11-C12-C13  |
| 8   | G     | 1103 | UQ2  | C9-C11-C12-C13  |
| 8   | A     | 1101 | UQ2  | C12-C11-C9-C8   |
| 6   | G     | 1003 | SMA  | C9-C10-C11-C22  |
| 6   | M     | 1005 | SMA  | C6-C5-O5-C5M    |
| 7   | G     | 1023 | LOP  | O5-C4-C5-O6     |
| 6   | M     | 1005 | SMA  | C4A-C5-O5-C5M   |
| 6   | A     | 1001 | SMA  | C4A-C5-O5-C5M   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | A     | 1001 | SMA  | C6-C5-O5-C5M    |
| 6   | P     | 1006 | SMA  | C9-C10-C11-C22  |
| 6   | A     | 1001 | SMA  | C9-C10-C11-C22  |
| 6   | P     | 1006 | SMA  | C8-C7-O7-C7M    |
| 6   | M     | 1005 | SMA  | C11-C10-C9-C2   |
| 6   | J     | 1004 | SMA  | C6-C5-O5-C5M    |
| 6   | D     | 1002 | SMA  | C9-C10-C11-C22  |
| 8   | P     | 1106 | UQ2  | C5-C6-C7-C8     |
| 8   | A     | 1101 | UQ2  | C12-C11-C9-C10  |
| 5   | E     | 301  | HEM  | C2B-C3B-CAB-CBB |
| 5   | G     | 501  | HEM  | C2B-C3B-CAB-CBB |
| 5   | G     | 501  | HEM  | C2C-C3C-CAC-CBC |
| 5   | G     | 502  | HEM  | C2C-C3C-CAC-CBC |
| 5   | H     | 301  | HEM  | C2C-C3C-CAC-CBC |
| 5   | N     | 301  | HEM  | C2B-C3B-CAB-CBB |
| 5   | P     | 501  | HEM  | C2B-C3B-CAB-CBB |
| 5   | Q     | 301  | HEM  | C2C-C3C-CAC-CBC |
| 5   | G     | 502  | HEM  | C4B-C3B-CAB-CBB |
| 5   | J     | 501  | HEM  | C4B-C3B-CAB-CBB |
| 5   | J     | 502  | HEM  | C4C-C3C-CAC-CBC |
| 5   | M     | 501  | HEM  | C4B-C3B-CAB-CBB |
| 5   | M     | 501  | HEM  | C4C-C3C-CAC-CBC |
| 5   | M     | 502  | HEM  | C4B-C3B-CAB-CBB |
| 7   | G     | 1023 | LOP  | C3-C4-C5-O6     |
| 6   | J     | 1004 | SMA  | C4A-C5-O5-C5M   |
| 7   | G     | 1023 | LOP  | O2-C3-C4-O5     |
| 7   | G     | 1023 | LOP  | C17-C18-C19-C20 |
| 6   | M     | 1005 | SMA  | C9-C10-C11-C22  |
| 7   | A     | 1021 | LOP  | C17-C18-C19-C20 |
| 7   | J     | 1024 | LOP  | C17-C18-C19-C20 |
| 6   | D     | 1002 | SMA  | C11-C10-C9-C2   |
| 6   | D     | 1002 | SMA  | O14-C14-C15-C16 |
| 7   | D     | 1022 | LOP  | C17-C18-C19-C20 |
| 7   | A     | 1021 | LOP  | O5-C4-C5-O6     |
| 8   | P     | 1106 | UQ2  | C9-C11-C12-C13  |
| 5   | A     | 501  | HEM  | C2B-C3B-CAB-CBB |
| 5   | B     | 301  | HEM  | C2B-C3B-CAB-CBB |
| 5   | B     | 301  | HEM  | C2C-C3C-CAC-CBC |
| 5   | D     | 501  | HEM  | C2C-C3C-CAC-CBC |
| 5   | H     | 301  | HEM  | C2B-C3B-CAB-CBB |
| 5   | K     | 301  | HEM  | C2B-C3B-CAB-CBB |
| 5   | Q     | 301  | HEM  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 6   | A     | 1001 | SMA  | C15-C14-O14-C25 |
| 8   | D     | 1102 | UQ2  | C4-C3-O3-CM3    |
| 8   | P     | 1106 | UQ2  | C4-C3-O3-CM3    |
| 5   | E     | 301  | HEM  | C4B-C3B-CAB-CBB |
| 5   | G     | 502  | HEM  | C4C-C3C-CAC-CBC |
| 5   | K     | 301  | HEM  | C4C-C3C-CAC-CBC |
| 5   | N     | 301  | HEM  | C4B-C3B-CAB-CBB |
| 5   | N     | 301  | HEM  | C4C-C3C-CAC-CBC |
| 8   | A     | 1101 | UQ2  | C1-C6-C7-C8     |
| 8   | G     | 1103 | UQ2  | C1-C6-C7-C8     |
| 8   | M     | 1105 | UQ2  | C1-C6-C7-C8     |
| 6   | D     | 1002 | SMA  | C13-C14-C15-C16 |
| 6   | P     | 1006 | SMA  | C6-C7-O7-C7M    |
| 7   | G     | 1023 | LOP  | O2-C3-C4-C5     |
| 7   | A     | 1021 | LOP  | C3-C4-C5-O6     |
| 6   | D     | 1002 | SMA  | C4A-C5-O5-C5M   |
| 6   | G     | 1003 | SMA  | O14-C14-C15-C16 |
| 6   | M     | 1005 | SMA  | O14-C14-C15-C16 |
| 8   | A     | 1101 | UQ2  | C1-C2-O2-CM2    |
| 6   | P     | 1006 | SMA  | C6-C5-O5-C5M    |
| 7   | J     | 1024 | LOP  | C3-O2-P1-O4     |
| 7   | M     | 1025 | LOP  | C3-O2-P1-O4     |
| 6   | D     | 1002 | SMA  | C6-C5-O5-C5M    |
| 8   | G     | 1103 | UQ2  | C4-C3-O3-CM3    |
| 7   | M     | 1025 | LOP  | C14-C15-C16-C17 |
| 8   | G     | 1103 | UQ2  | C5-C6-C7-C8     |
| 8   | A     | 1101 | UQ2  | C3-C2-O2-CM2    |
| 5   | B     | 301  | HEM  | C4B-C3B-CAB-CBB |
| 5   | E     | 301  | HEM  | C4C-C3C-CAC-CBC |
| 5   | H     | 301  | HEM  | C4B-C3B-CAB-CBB |
| 5   | J     | 502  | HEM  | C4B-C3B-CAB-CBB |
| 5   | K     | 301  | HEM  | C4B-C3B-CAB-CBB |
| 5   | Q     | 301  | HEM  | C4C-C3C-CAC-CBC |
| 6   | P     | 1006 | SMA  | C4A-C5-O5-C5M   |
| 5   | K     | 301  | HEM  | CAA-CBA-CGA-O2A |
| 6   | M     | 1005 | SMA  | C24-C13-C14-C15 |
| 5   | E     | 301  | HEM  | CAD-CBD-CGD-O2D |
| 5   | B     | 301  | HEM  | CAD-CBD-CGD-O1D |
| 5   | J     | 502  | HEM  | CAA-CBA-CGA-O1A |
| 5   | D     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 5   | J     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 5   | M     | 502  | HEM  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 8   | G     | 1103 | UQ2  | C2-C3-O3-CM3    |
| 5   | B     | 301  | HEM  | CAD-CBD-CGD-O2D |
| 5   | G     | 501  | HEM  | CAA-CBA-CGA-O1A |
| 5   | A     | 501  | HEM  | CAA-CBA-CGA-O2A |
| 5   | A     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 5   | D     | 501  | HEM  | CAA-CBA-CGA-O1A |
| 5   | E     | 301  | HEM  | CAA-CBA-CGA-O2A |
| 5   | P     | 502  | HEM  | CAA-CBA-CGA-O1A |
| 5   | D     | 502  | HEM  | C3D-CAD-CBD-CGD |
| 5   | M     | 502  | HEM  | C3D-CAD-CBD-CGD |
| 5   | E     | 301  | HEM  | CAD-CBD-CGD-O1D |
| 5   | M     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 7   | J     | 1024 | LOP  | O5-C4-C5-O6     |
| 5   | D     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 5   | G     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 5   | H     | 301  | HEM  | CAA-CBA-CGA-O2A |
| 5   | K     | 301  | HEM  | CAA-CBA-CGA-O1A |
| 5   | A     | 501  | HEM  | CAA-CBA-CGA-O1A |
| 5   | J     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 5   | M     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 5   | Q     | 301  | HEM  | CAA-CBA-CGA-O2A |
| 7   | P     | 1026 | LOP  | C17-C18-C19-C20 |
| 5   | P     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 5   | A     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 5   | D     | 501  | HEM  | CAA-CBA-CGA-O2A |
| 5   | M     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 5   | D     | 502  | HEM  | CAA-CBA-CGA-O1A |
| 5   | G     | 502  | HEM  | C3D-CAD-CBD-CGD |
| 7   | P     | 1026 | LOP  | C27-C28-C29-C30 |
| 5   | D     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 5   | E     | 301  | HEM  | CAA-CBA-CGA-O1A |
| 5   | H     | 301  | HEM  | CAD-CBD-CGD-O2D |
| 5   | B     | 301  | HEM  | CAA-CBA-CGA-O2A |
| 5   | M     | 501  | HEM  | CAA-CBA-CGA-O2A |
| 6   | P     | 1006 | SMA  | C11-C10-C9-C2   |
| 5   | G     | 501  | HEM  | CAA-CBA-CGA-O2A |
| 5   | J     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 7   | P     | 1026 | LOP  | C14-C15-C16-C17 |
| 5   | G     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 7   | A     | 1021 | LOP  | C12-C13-C14-C15 |
| 5   | K     | 301  | HEM  | CAD-CBD-CGD-O2D |
| 5   | Q     | 301  | HEM  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 7   | D     | 1022 | LOP  | C15-C16-C17-C18 |
| 5   | M     | 501  | HEM  | CAA-CBA-CGA-O1A |
| 5   | N     | 301  | HEM  | CAD-CBD-CGD-O2D |
| 5   | E     | 301  | HEM  | C4D-C3D-CAD-CBD |
| 5   | D     | 502  | HEM  | C2C-C3C-CAC-CBC |
| 5   | P     | 502  | HEM  | C2B-C3B-CAB-CBB |
| 5   | H     | 301  | HEM  | CAA-CBA-CGA-O1A |
| 7   | D     | 1022 | LOP  | C14-C15-C16-C17 |
| 7   | G     | 1023 | LOP  | C12-C13-C14-C15 |
| 7   | M     | 1025 | LOP  | C12-C13-C14-C15 |
| 7   | P     | 1026 | LOP  | C12-C13-C14-C15 |
| 5   | B     | 301  | HEM  | CAA-CBA-CGA-O1A |
| 5   | P     | 502  | HEM  | CAD-CBD-CGD-O1D |
| 5   | H     | 301  | HEM  | CAD-CBD-CGD-O1D |
| 5   | P     | 502  | HEM  | CAD-CBD-CGD-O2D |
| 5   | G     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 5   | G     | 502  | HEM  | CAA-CBA-CGA-O1A |
| 5   | N     | 301  | HEM  | CAD-CBD-CGD-O1D |
| 5   | K     | 301  | HEM  | CAD-CBD-CGD-O1D |
| 5   | A     | 502  | HEM  | C4C-C3C-CAC-CBC |
| 5   | B     | 301  | HEM  | C4C-C3C-CAC-CBC |
| 5   | G     | 501  | HEM  | C4B-C3B-CAB-CBB |
| 5   | G     | 501  | HEM  | C4C-C3C-CAC-CBC |
| 5   | H     | 301  | HEM  | C4C-C3C-CAC-CBC |
| 5   | P     | 501  | HEM  | C4B-C3B-CAB-CBB |
| 5   | Q     | 301  | HEM  | C4B-C3B-CAB-CBB |
| 5   | A     | 502  | HEM  | CAA-CBA-CGA-O2A |
| 5   | A     | 502  | HEM  | CAA-CBA-CGA-O1A |
| 7   | J     | 1024 | LOP  | C12-C13-C14-C15 |
| 7   | J     | 1024 | LOP  | C14-C15-C16-C17 |
| 7   | A     | 1021 | LOP  | O2-C3-C4-C5     |
| 8   | D     | 1102 | UQ2  | C2-C3-O3-CM3    |
| 7   | D     | 1022 | LOP  | C12-C13-C14-C15 |
| 7   | P     | 1026 | LOP  | C30-C31-C32-C33 |
| 6   | M     | 1005 | SMA  | C24-C13-C14-O14 |
| 5   | P     | 501  | HEM  | CAA-CBA-CGA-O1A |
| 5   | P     | 501  | HEM  | CAA-CBA-CGA-O2A |
| 7   | A     | 1021 | LOP  | O6-C24-C25-C26  |
| 7   | A     | 1021 | LOP  | O5-C6-C7-C8     |
| 7   | G     | 1023 | LOP  | O5-C6-C7-C8     |
| 6   | G     | 1003 | SMA  | C11-C10-C9-C2   |
| 6   | G     | 1003 | SMA  | C4A-C5-O5-C5M   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 5   | N     | 301  | HEM  | CAA-CBA-CGA-O2A |
| 7   | M     | 1025 | LOP  | O6-C24-C25-C26  |
| 8   | M     | 1105 | UQ2  | C4-C3-O3-CM3    |
| 7   | G     | 1023 | LOP  | O7-C6-C7-C8     |
| 5   | N     | 301  | HEM  | CAA-CBA-CGA-O1A |
| 7   | A     | 1021 | LOP  | C14-C15-C16-C17 |
| 7   | A     | 1021 | LOP  | O8-C24-C25-C26  |
| 6   | A     | 1001 | SMA  | C11-C10-C9-C2   |
| 5   | Q     | 301  | HEM  | CAD-CBD-CGD-O2D |
| 7   | J     | 1024 | LOP  | O6-C24-C25-C26  |

There are no ring outliers.

38 monomers are involved in 108 short contacts:

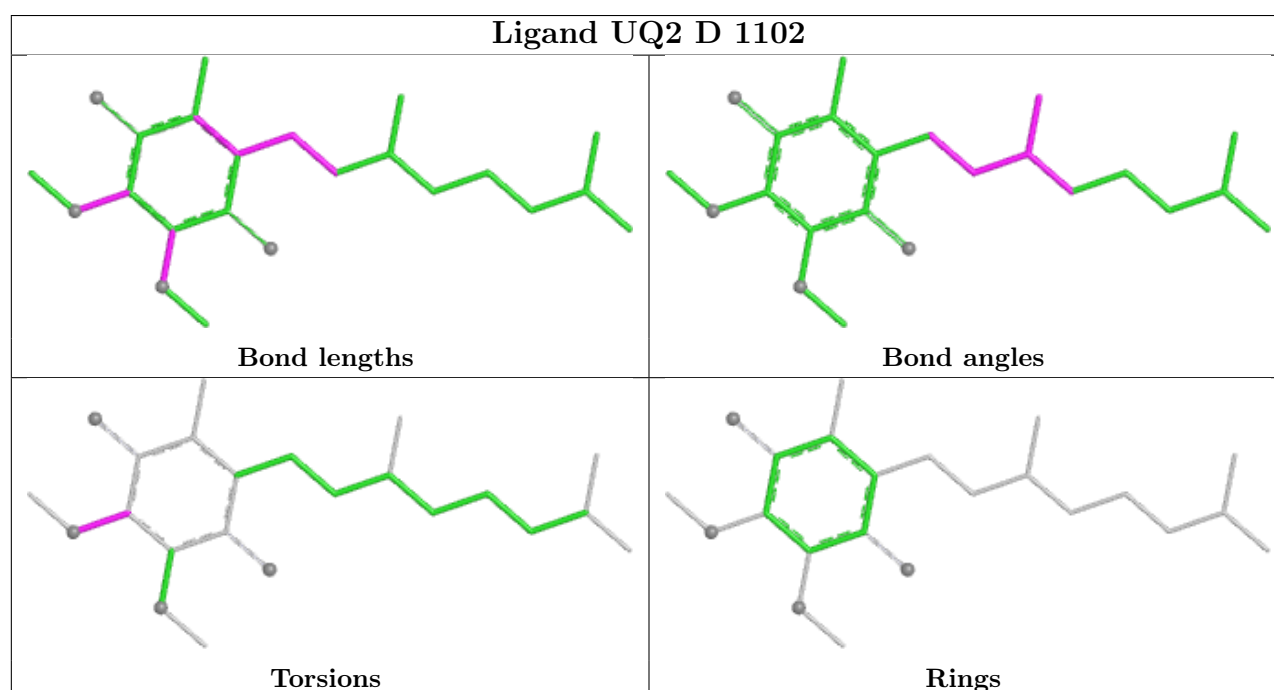
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 8   | D     | 1102 | UQ2  | 2       | 0            |
| 5   | M     | 502  | HEM  | 6       | 0            |
| 5   | B     | 301  | HEM  | 1       | 0            |
| 5   | J     | 501  | HEM  | 9       | 0            |
| 6   | J     | 1004 | SMA  | 1       | 0            |
| 9   | N     | 1045 | BGL  | 1       | 0            |
| 5   | D     | 501  | HEM  | 6       | 0            |
| 5   | G     | 502  | HEM  | 5       | 0            |
| 5   | E     | 301  | HEM  | 1       | 0            |
| 5   | D     | 502  | HEM  | 3       | 0            |
| 9   | P     | 1046 | BGL  | 2       | 0            |
| 5   | A     | 502  | HEM  | 4       | 0            |
| 8   | G     | 1103 | UQ2  | 2       | 0            |
| 5   | M     | 501  | HEM  | 3       | 0            |
| 5   | Q     | 301  | HEM  | 2       | 0            |
| 8   | M     | 1105 | UQ2  | 2       | 0            |
| 8   | J     | 1104 | UQ2  | 1       | 0            |
| 8   | P     | 1106 | UQ2  | 2       | 0            |
| 5   | P     | 502  | HEM  | 3       | 0            |
| 7   | A     | 1021 | LOP  | 6       | 0            |
| 9   | E     | 1042 | BGL  | 3       | 0            |
| 9   | B     | 1041 | BGL  | 1       | 0            |
| 5   | P     | 501  | HEM  | 4       | 0            |
| 5   | J     | 502  | HEM  | 6       | 0            |
| 7   | J     | 1024 | LOP  | 1       | 0            |
| 9   | K     | 1044 | BGL  | 2       | 0            |
| 6   | P     | 1006 | SMA  | 1       | 0            |

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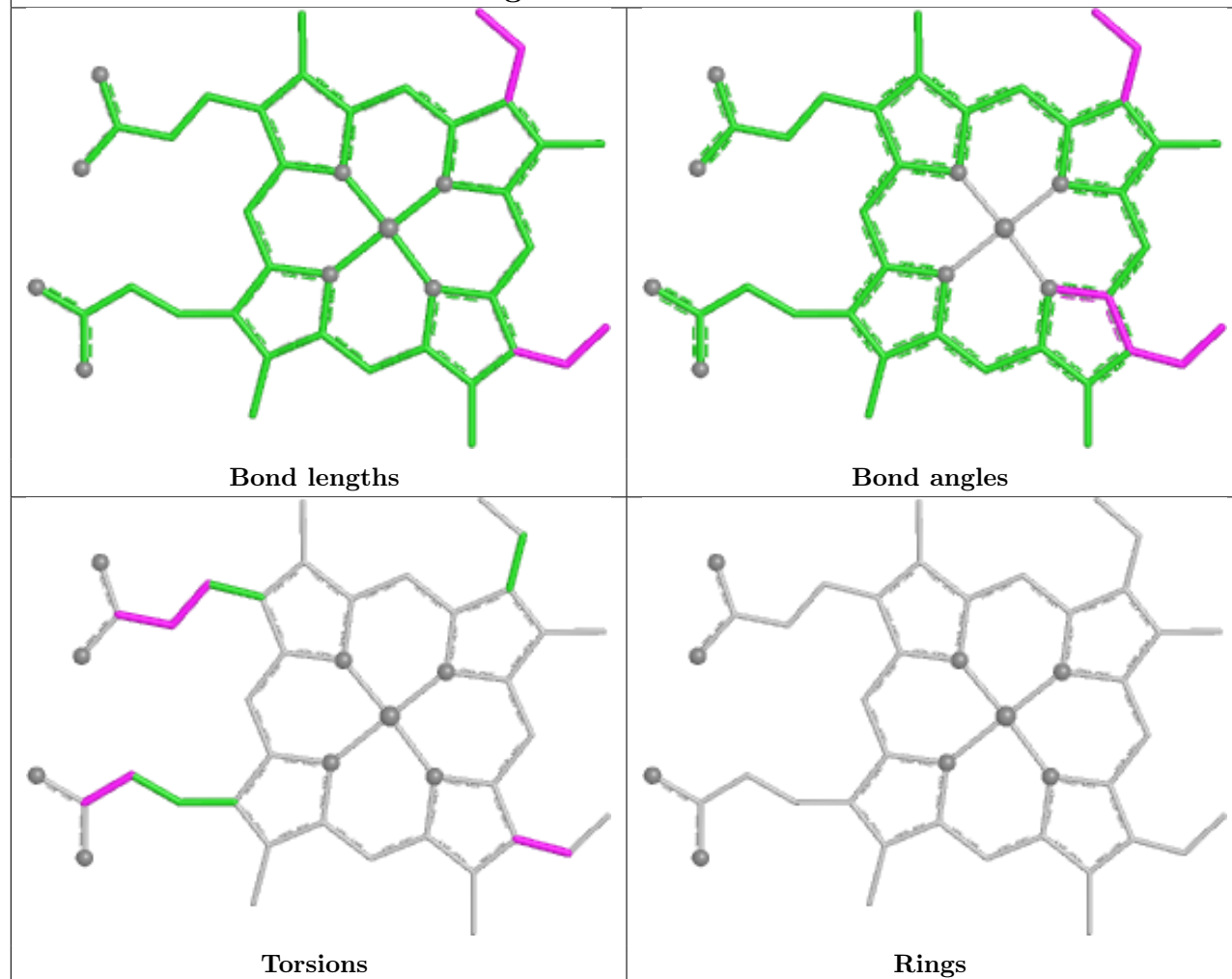
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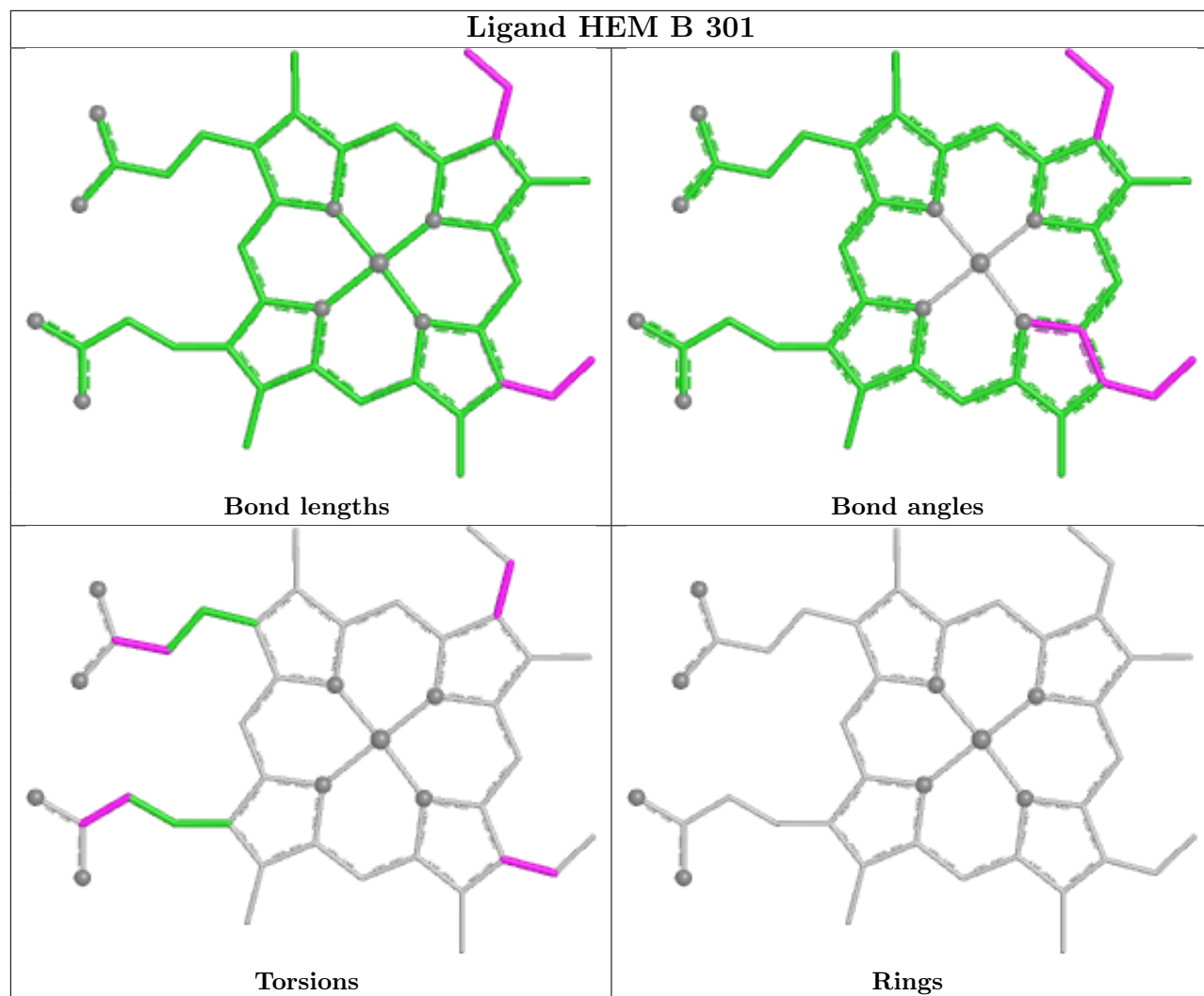
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | A     | 501  | HEM  | 3       | 0            |
| 7   | P     | 1026 | LOP  | 2       | 0            |
| 8   | A     | 1101 | UQ2  | 2       | 0            |
| 7   | G     | 1023 | LOP  | 3       | 0            |
| 5   | N     | 301  | HEM  | 3       | 0            |
| 5   | K     | 301  | HEM  | 2       | 0            |
| 7   | M     | 1025 | LOP  | 3       | 0            |
| 5   | H     | 301  | HEM  | 1       | 0            |
| 5   | G     | 501  | HEM  | 5       | 0            |
| 7   | D     | 1022 | LOP  | 2       | 0            |
| 9   | G     | 1043 | BGL  | 2       | 0            |

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

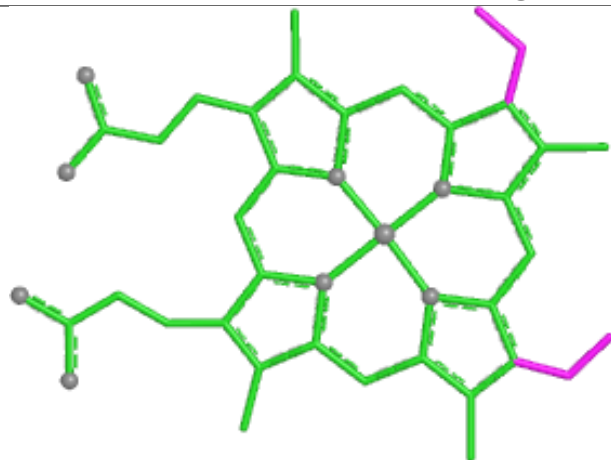


## Ligand HEM M 502

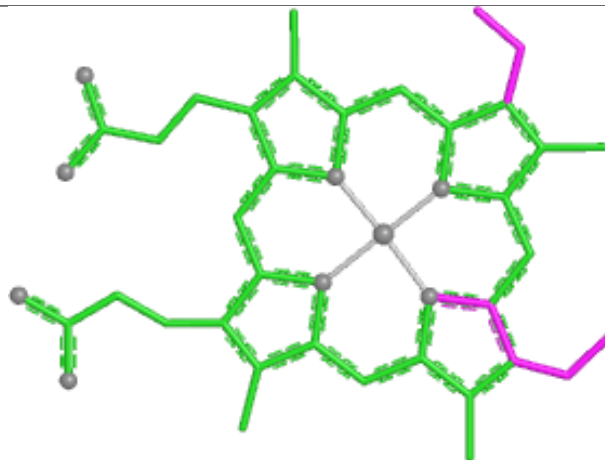




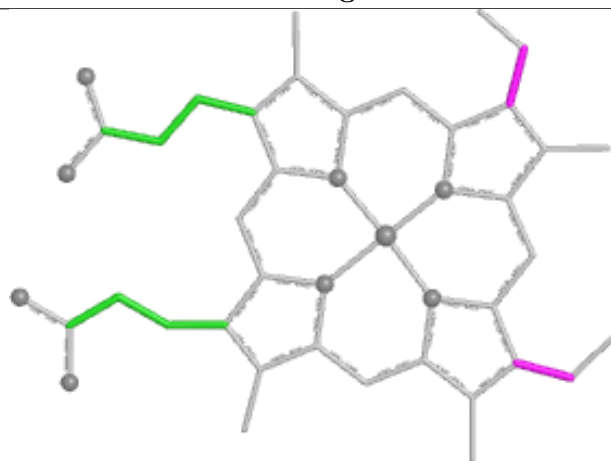
## Ligand HEM J 501



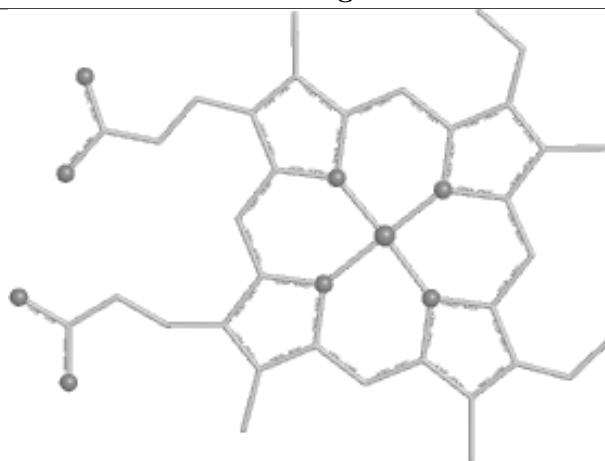
Bond lengths



Bond angles

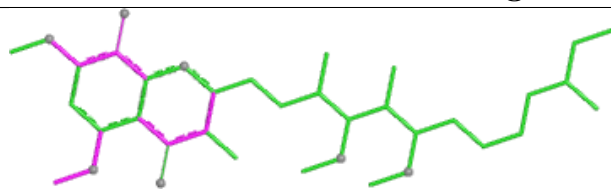


Torsions

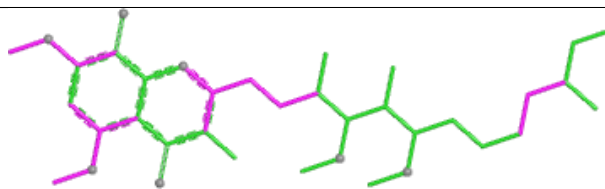


Rings

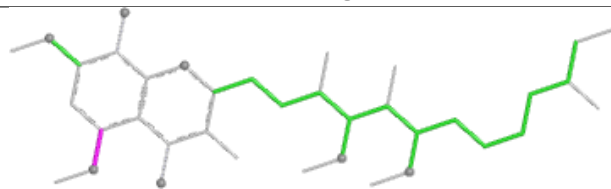
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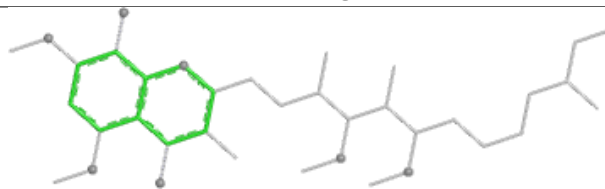
Bond lengths



Bond angles

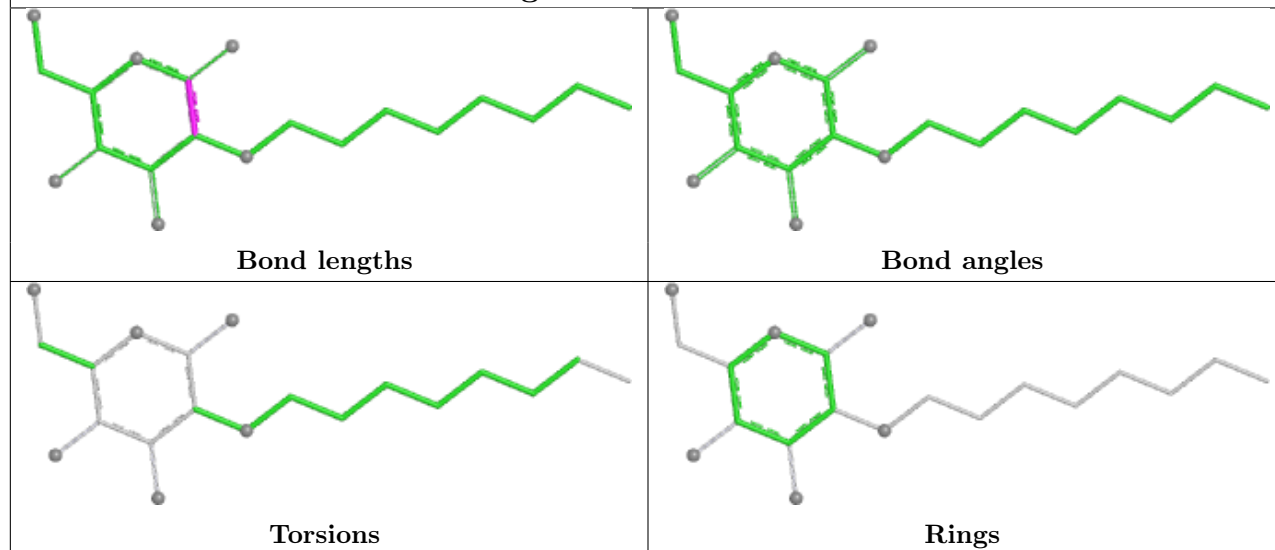


Torsions

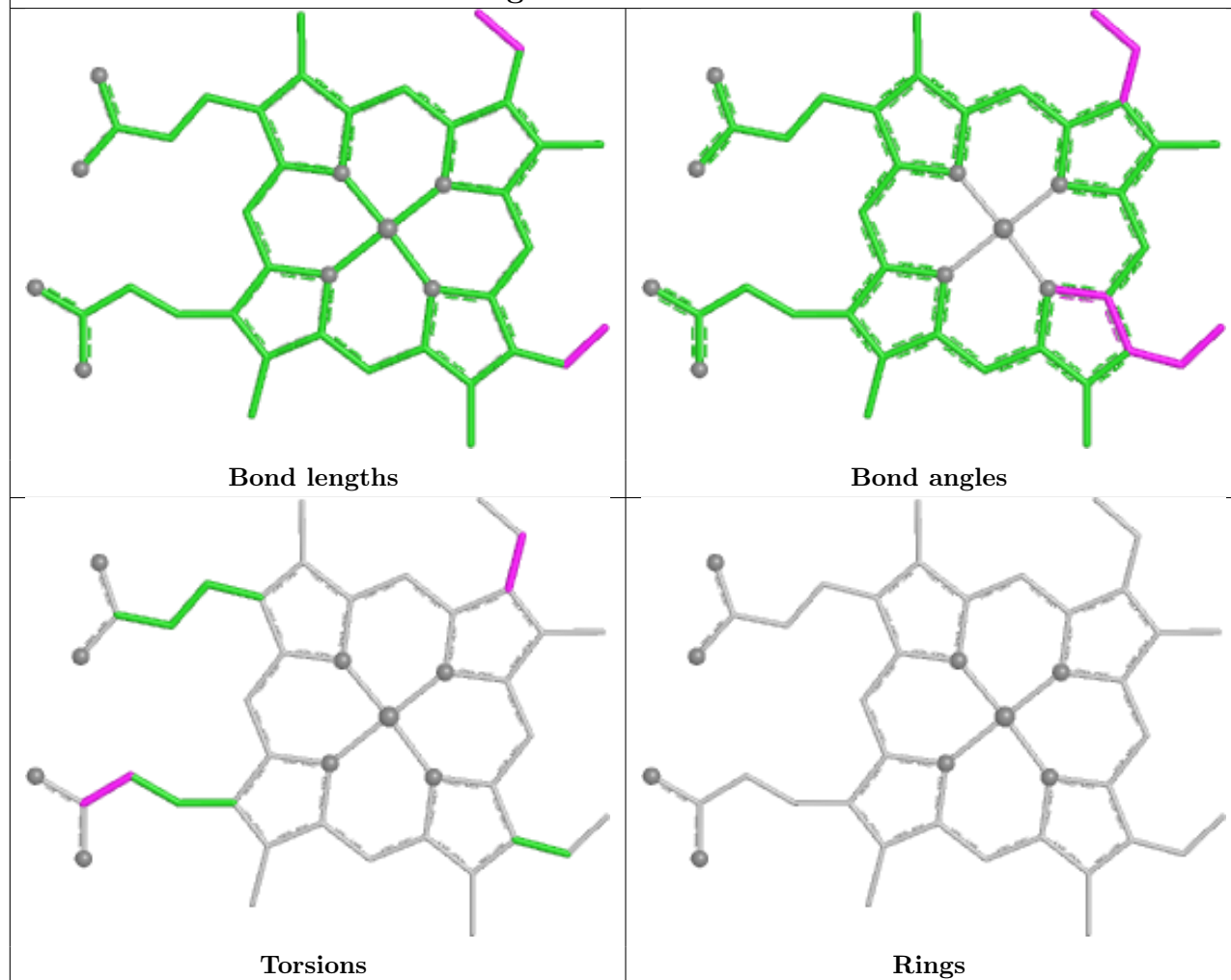


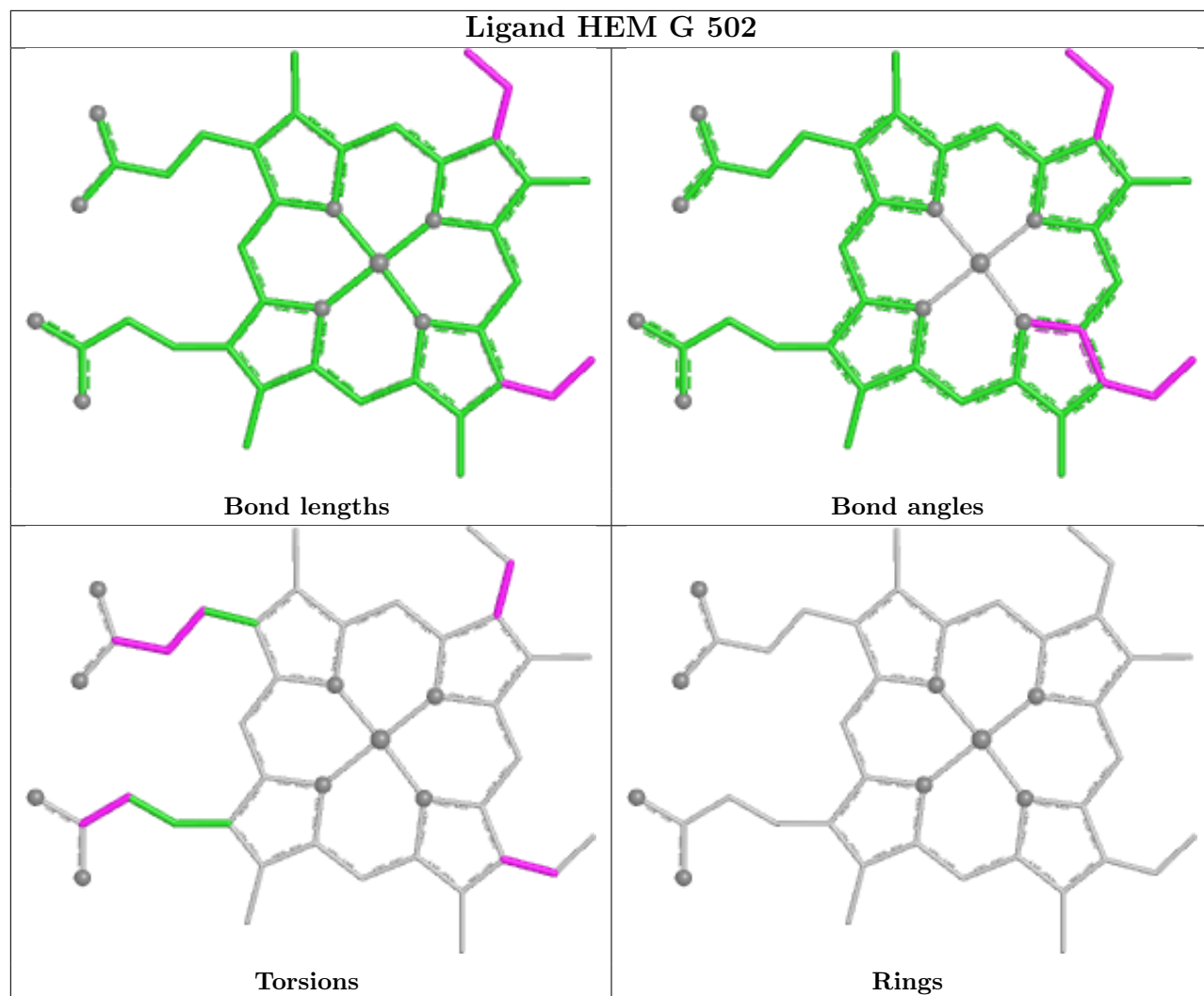
Rings

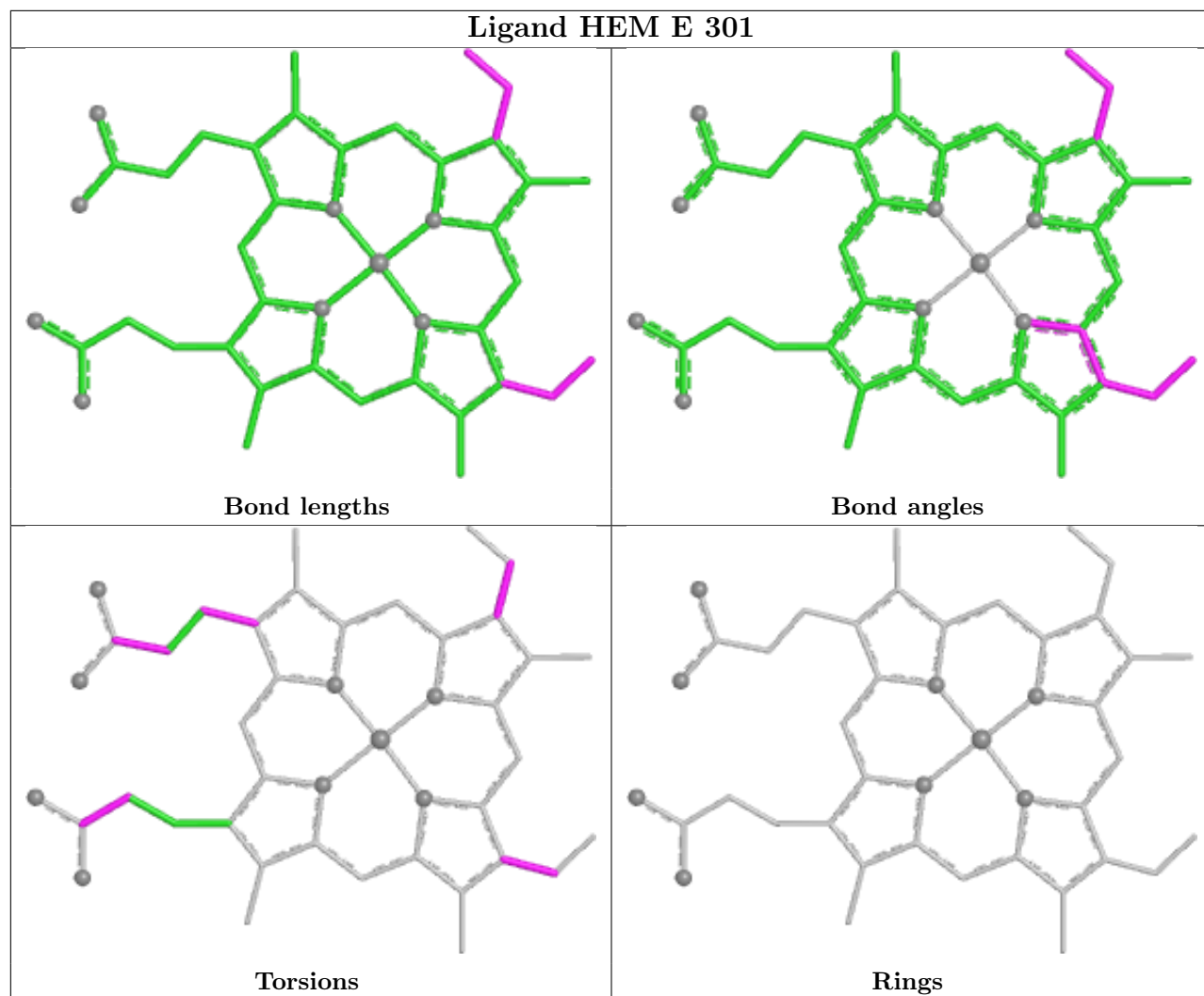
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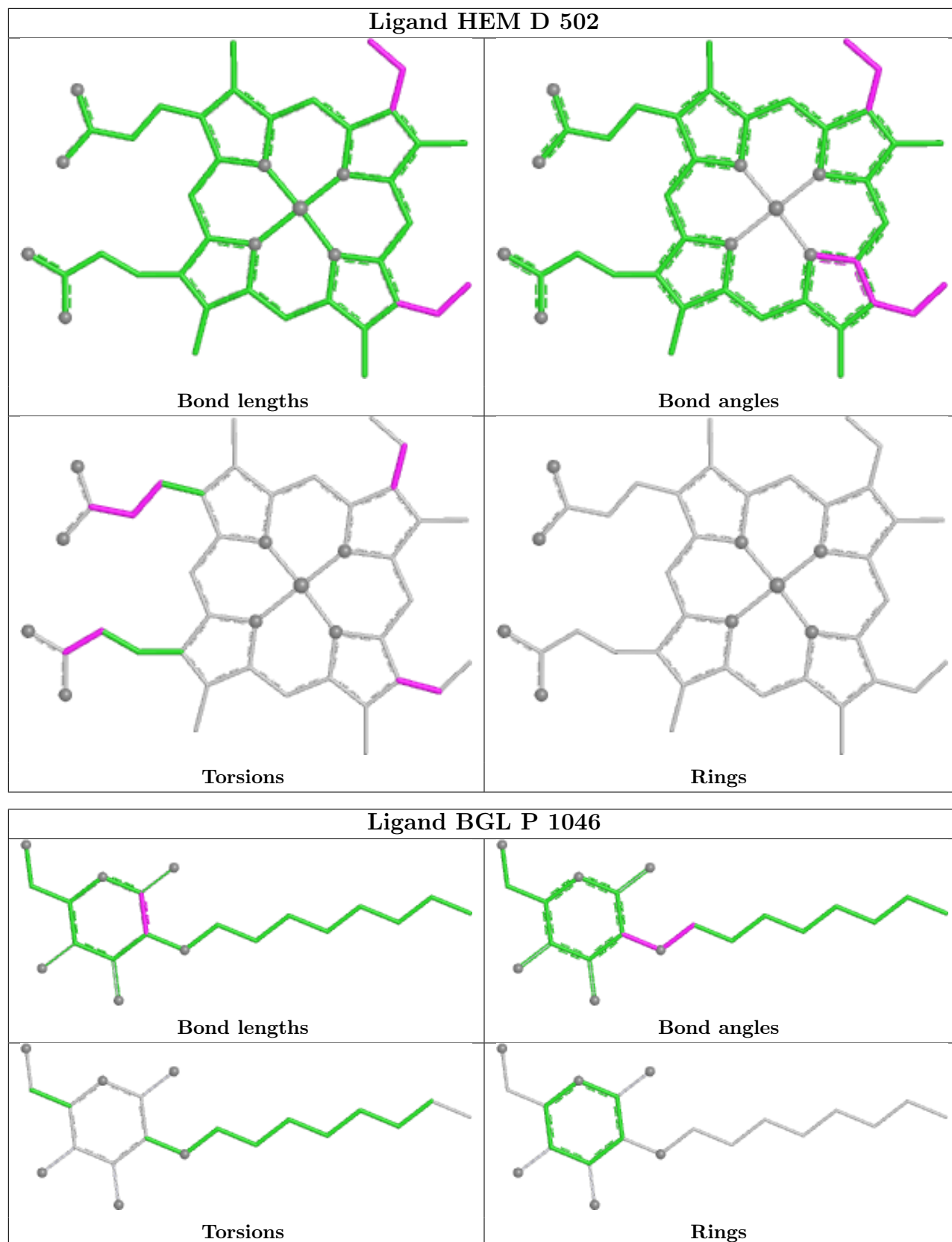


## Ligand HEM D 501

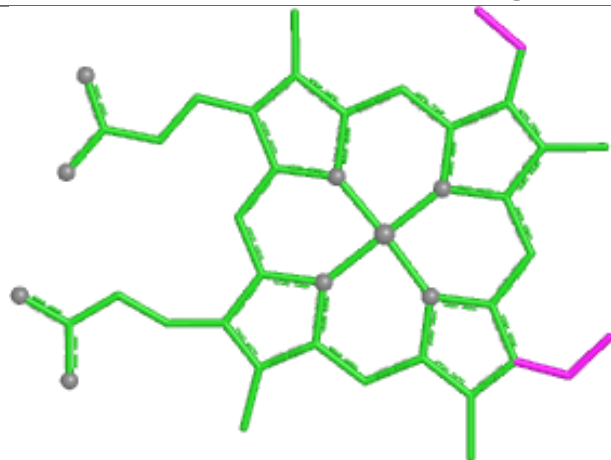




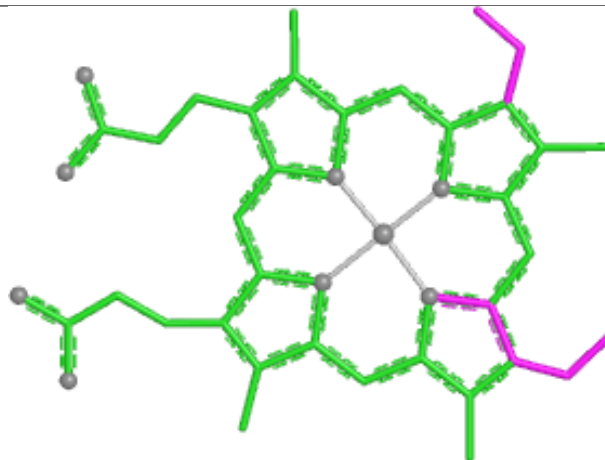




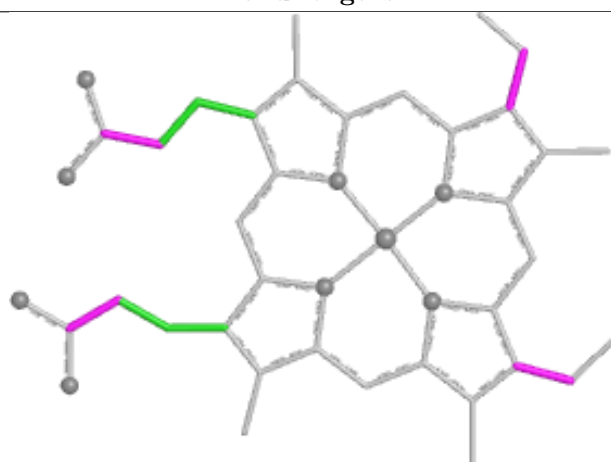
## Ligand HEM A 502



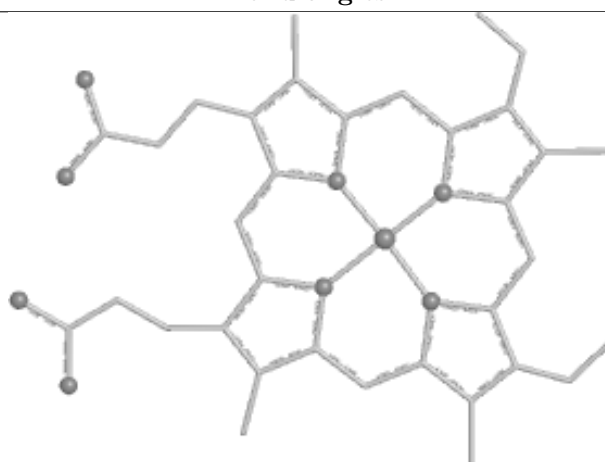
Bond lengths



Bond angles

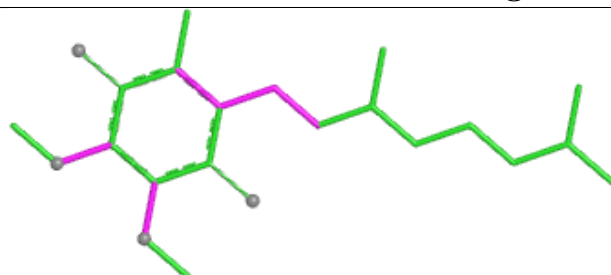


Torsions

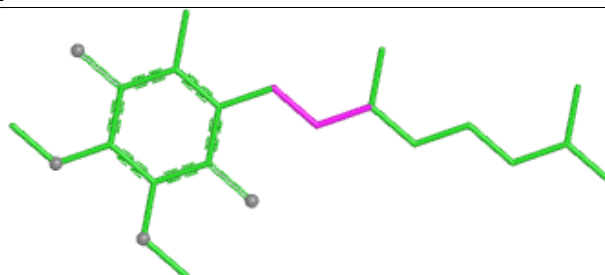


Rings

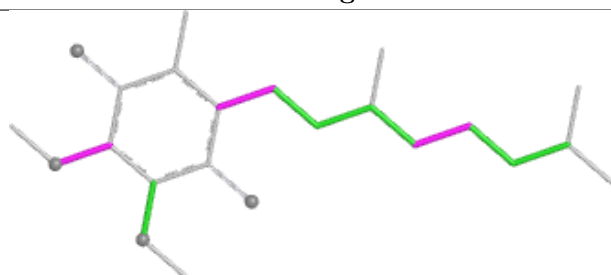
## Ligand UQ2 G 1103



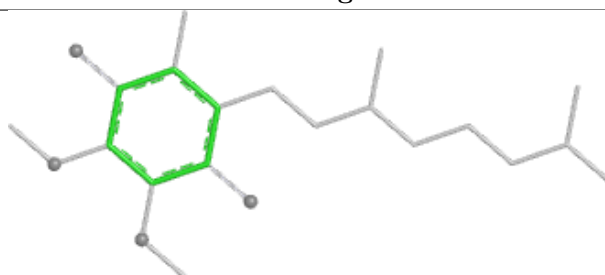
Bond lengths



Bond angles

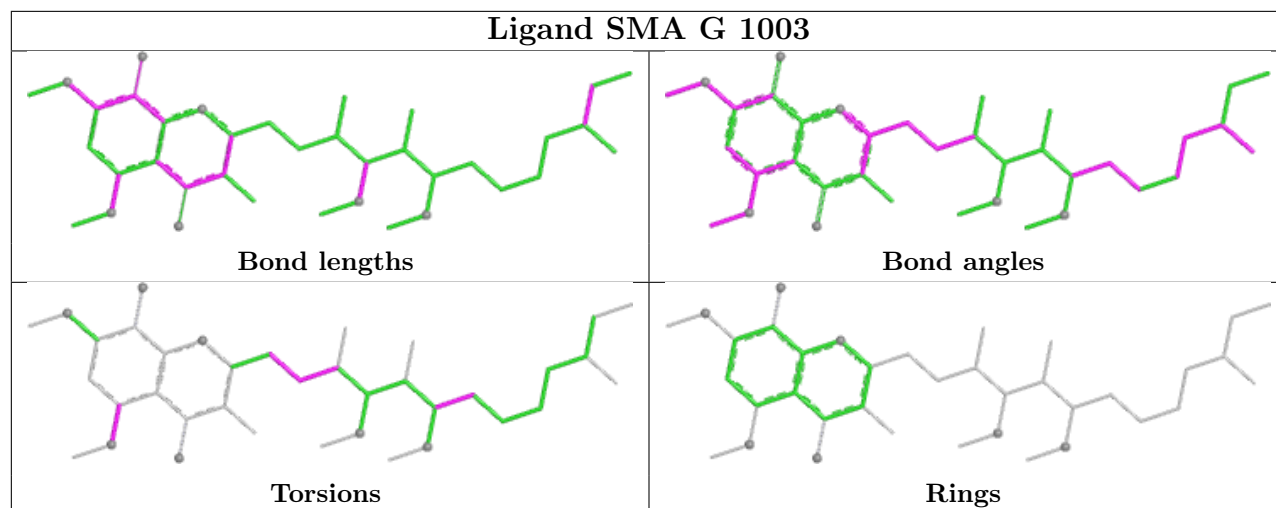


Torsions

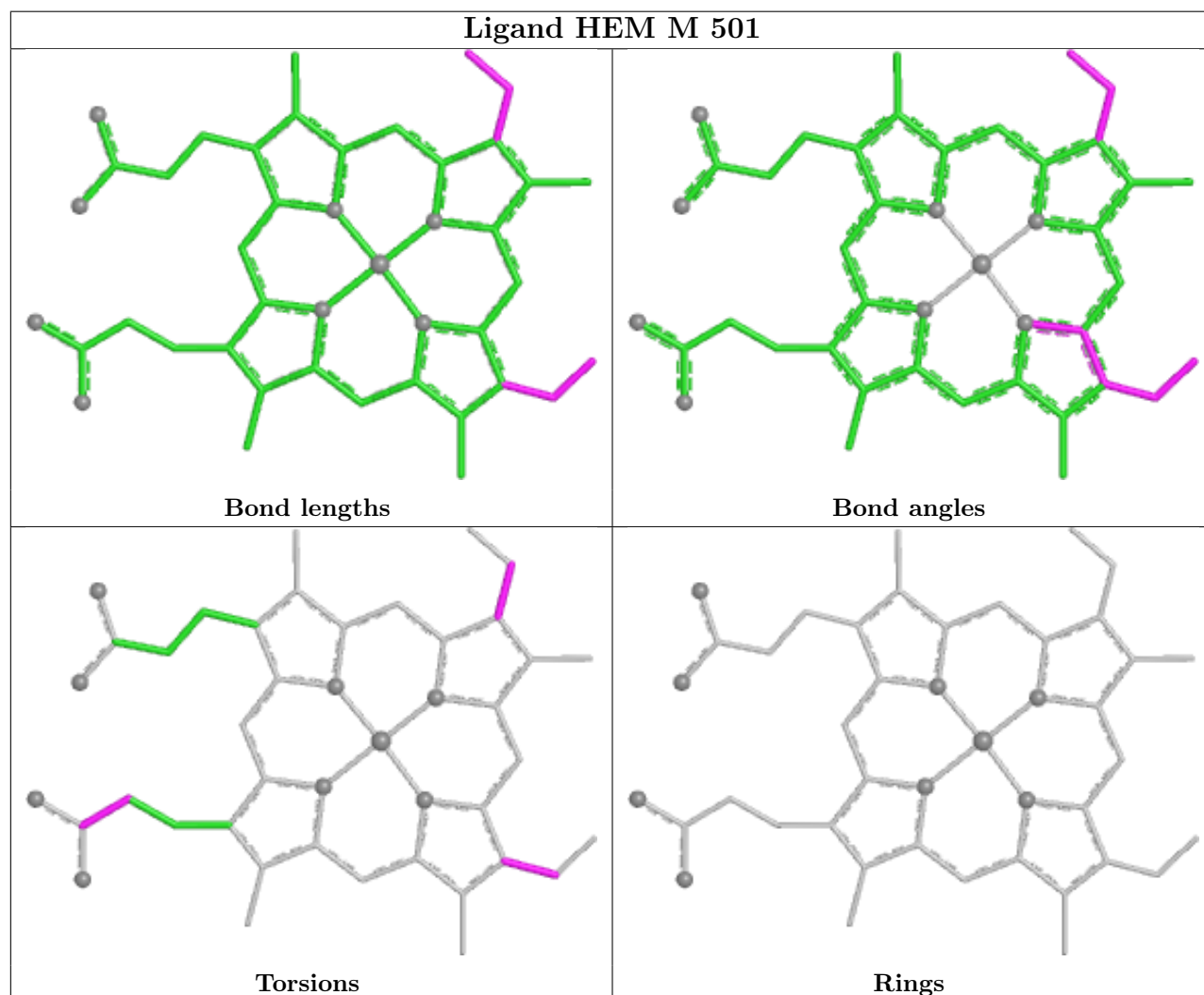


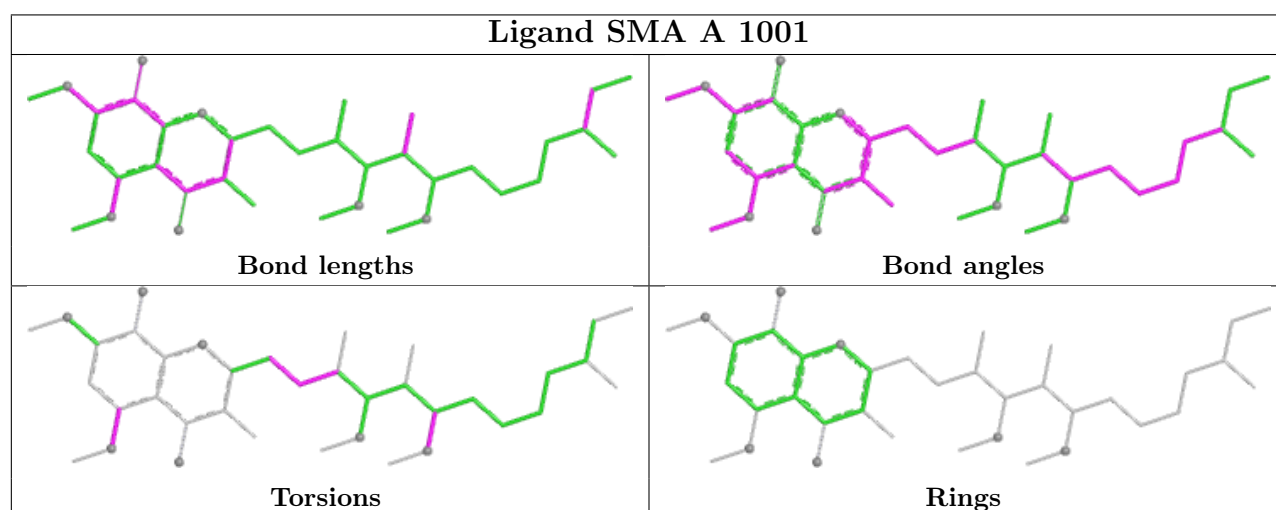
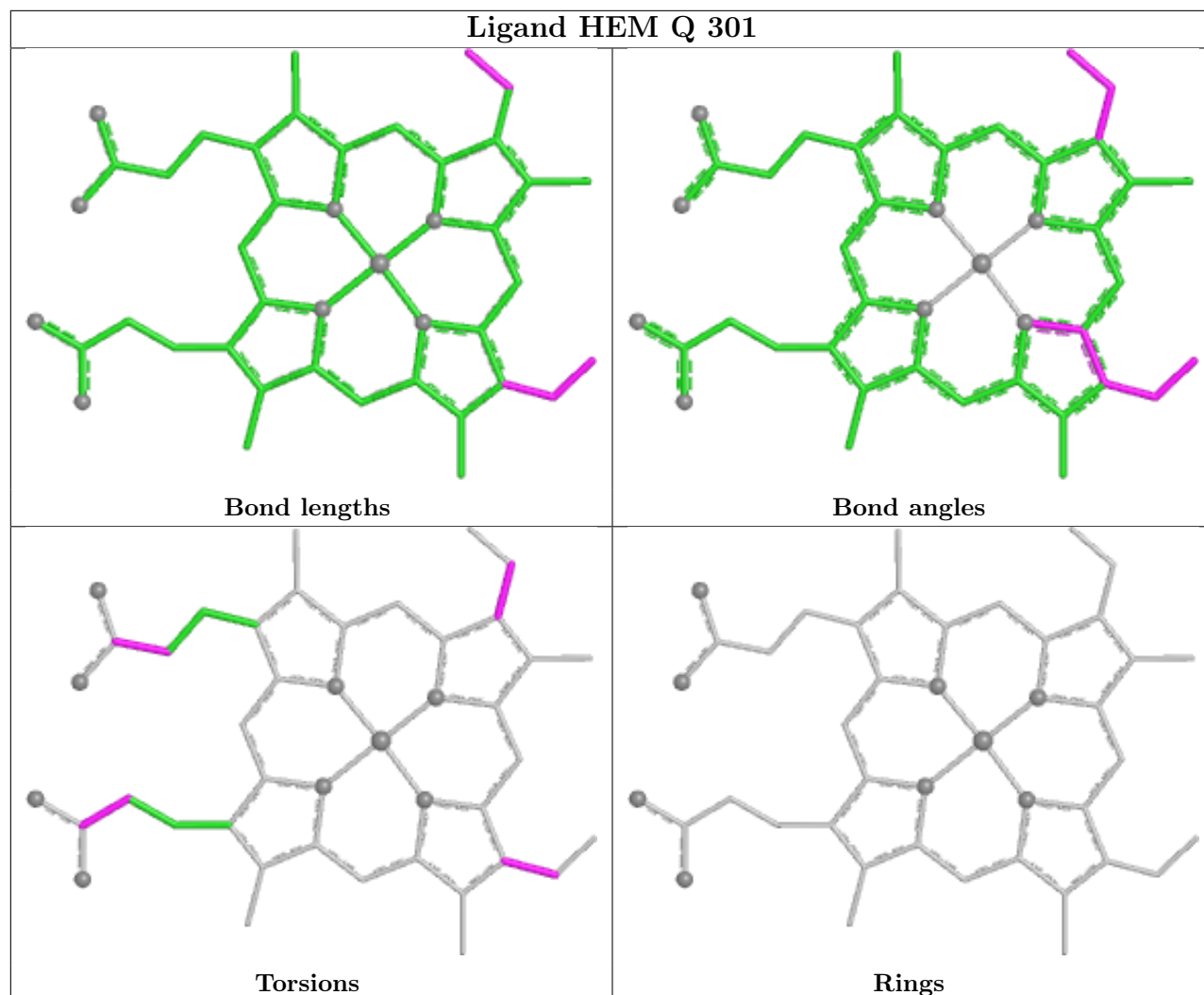
Rings

## Ligand SMA G 1003

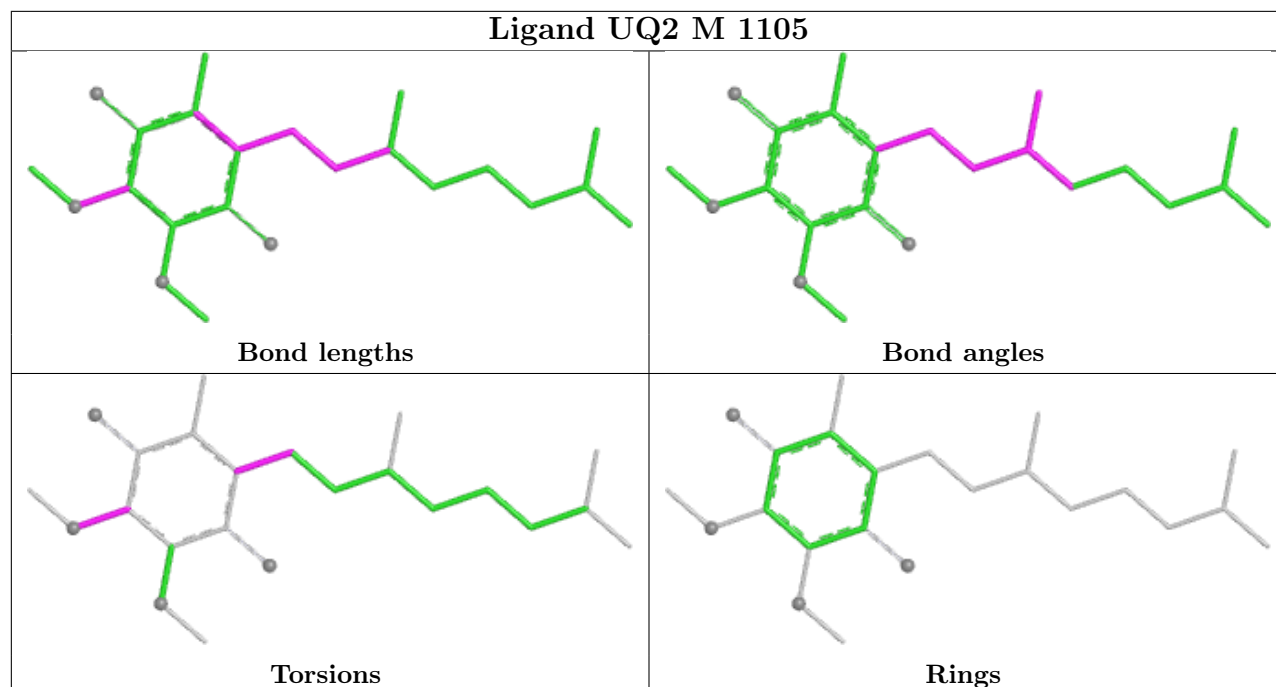


## Ligand HEM M 501

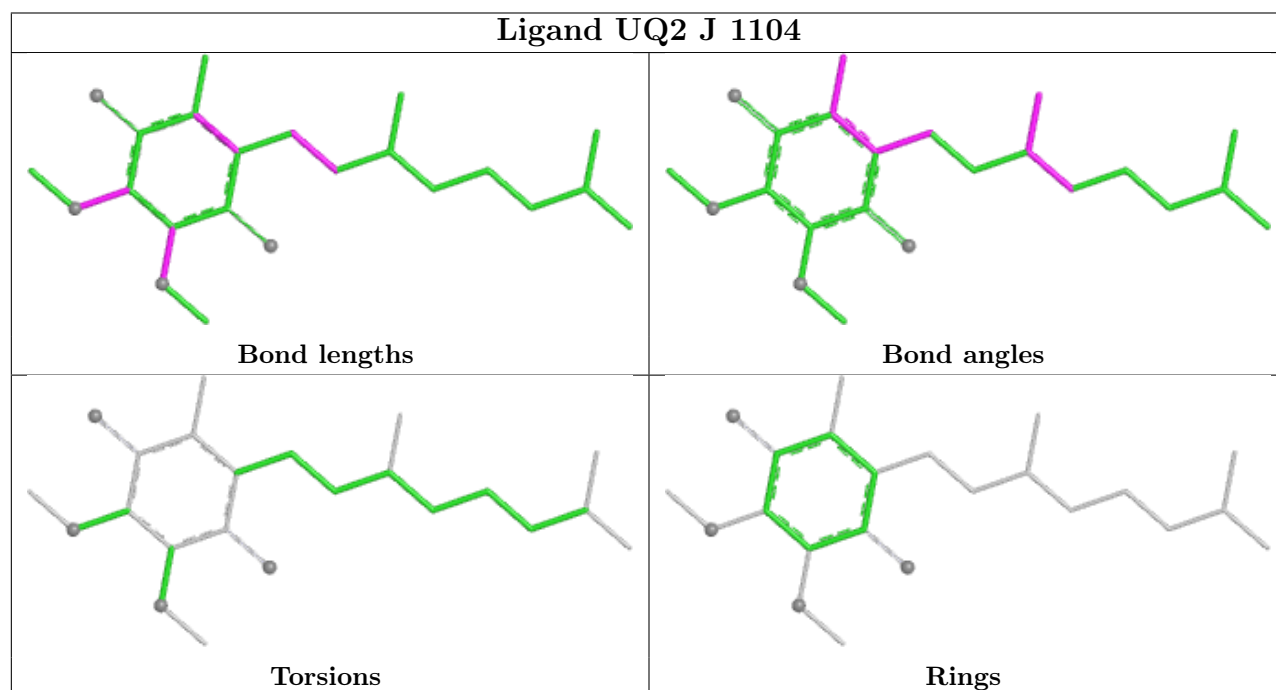




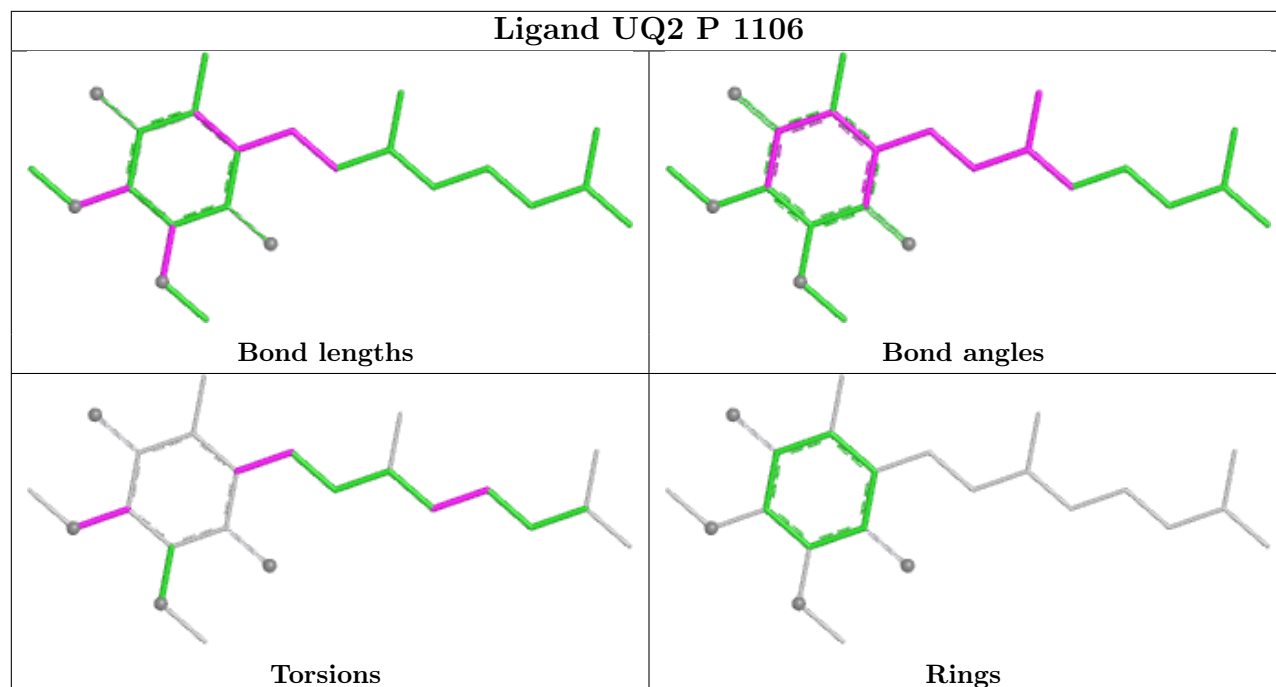
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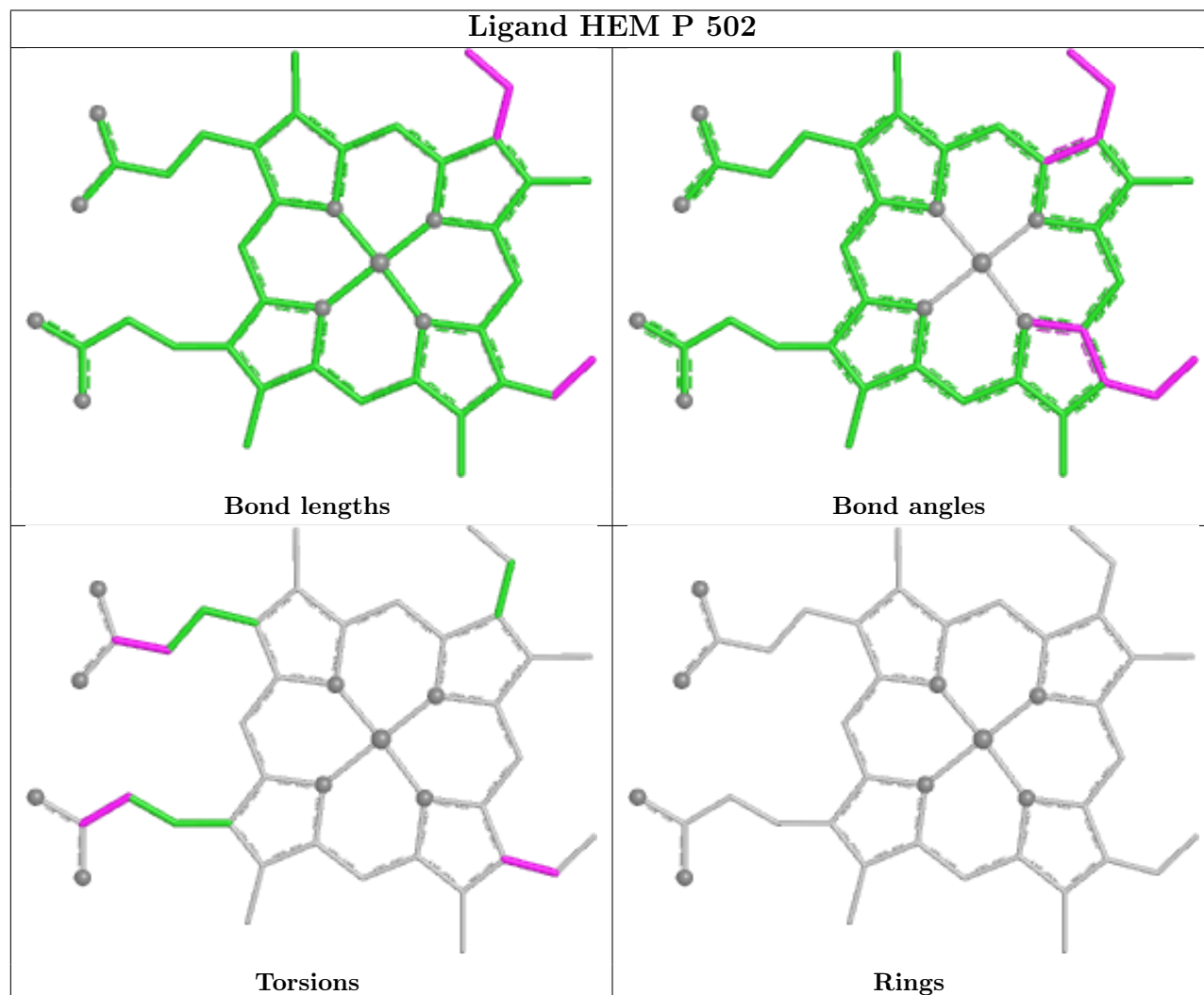
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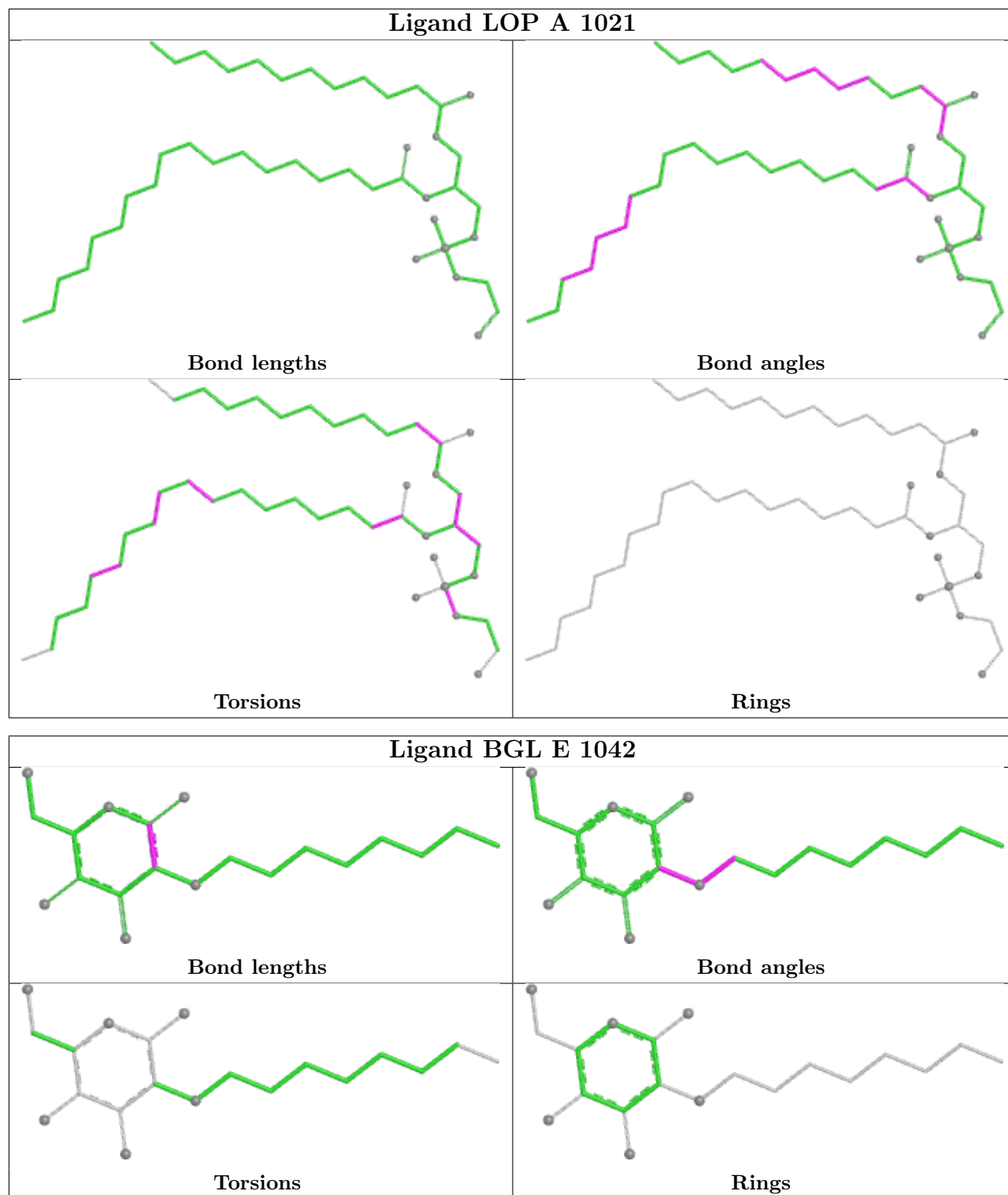


## Ligand UQ2 P 1106

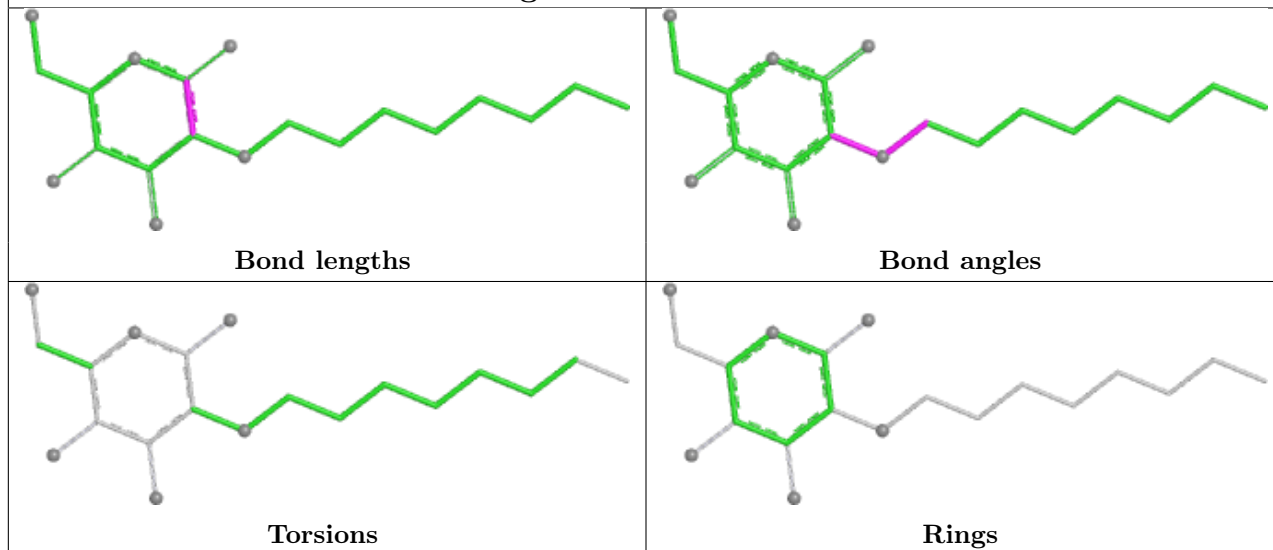


## Ligand HEM P 502

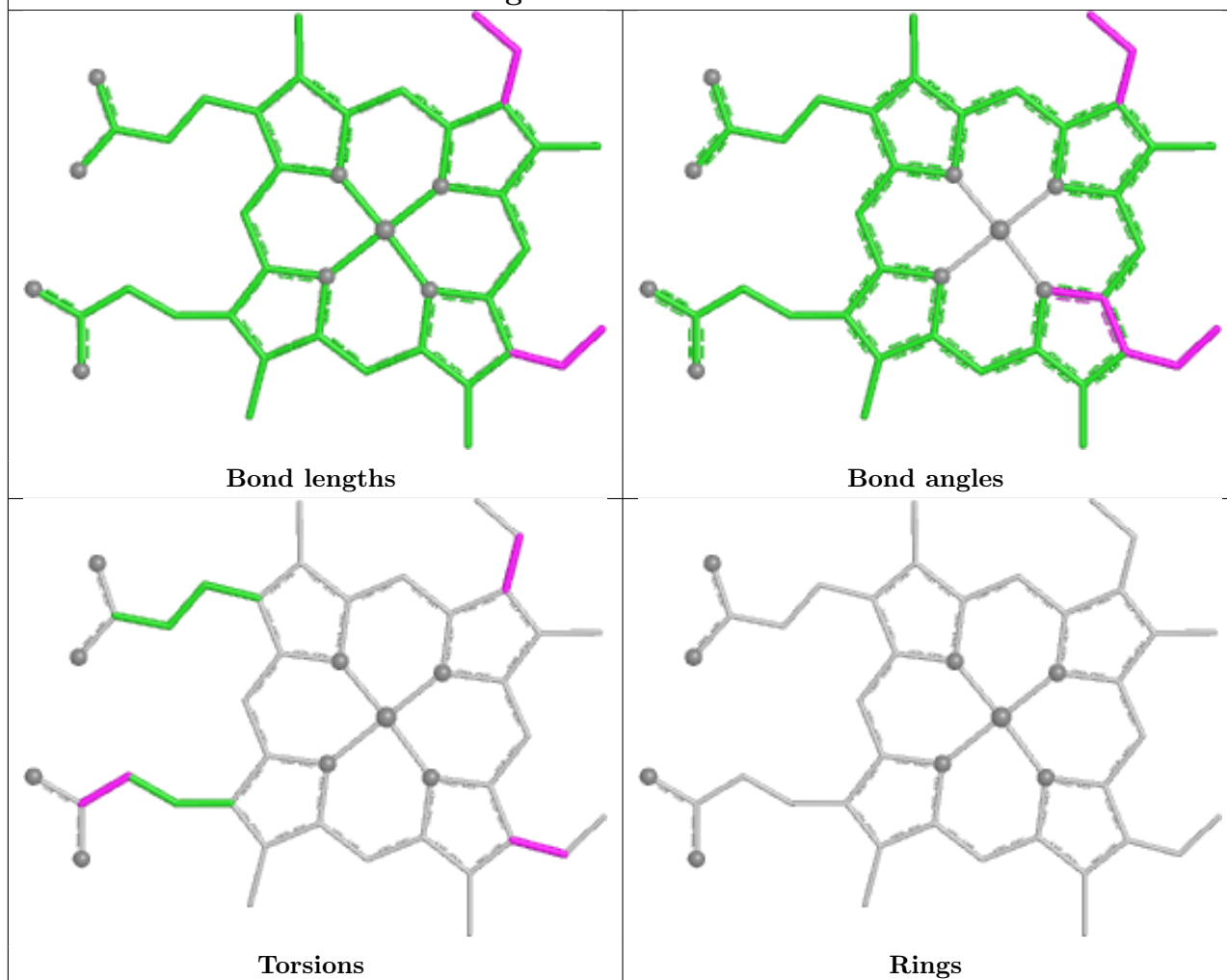


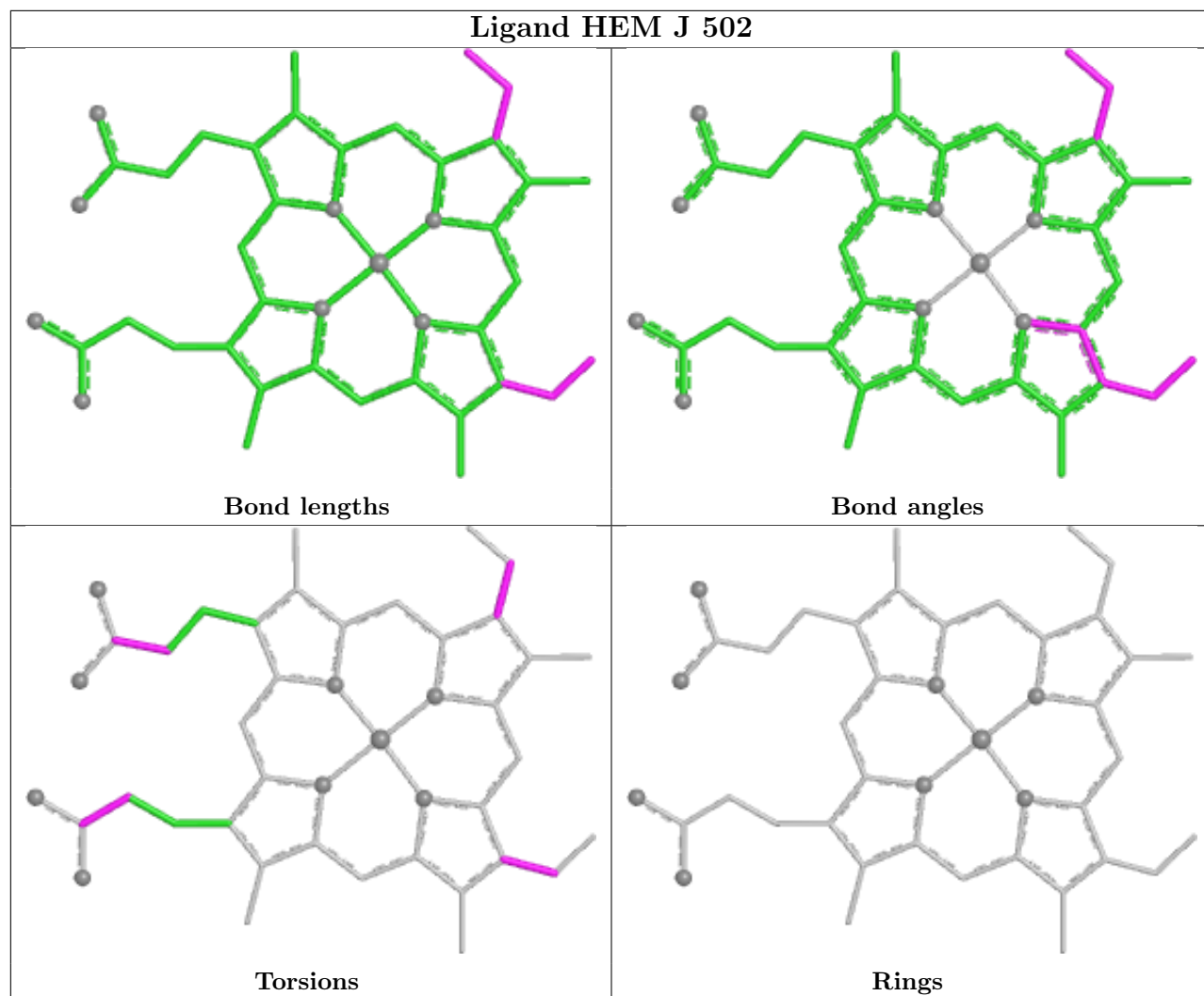


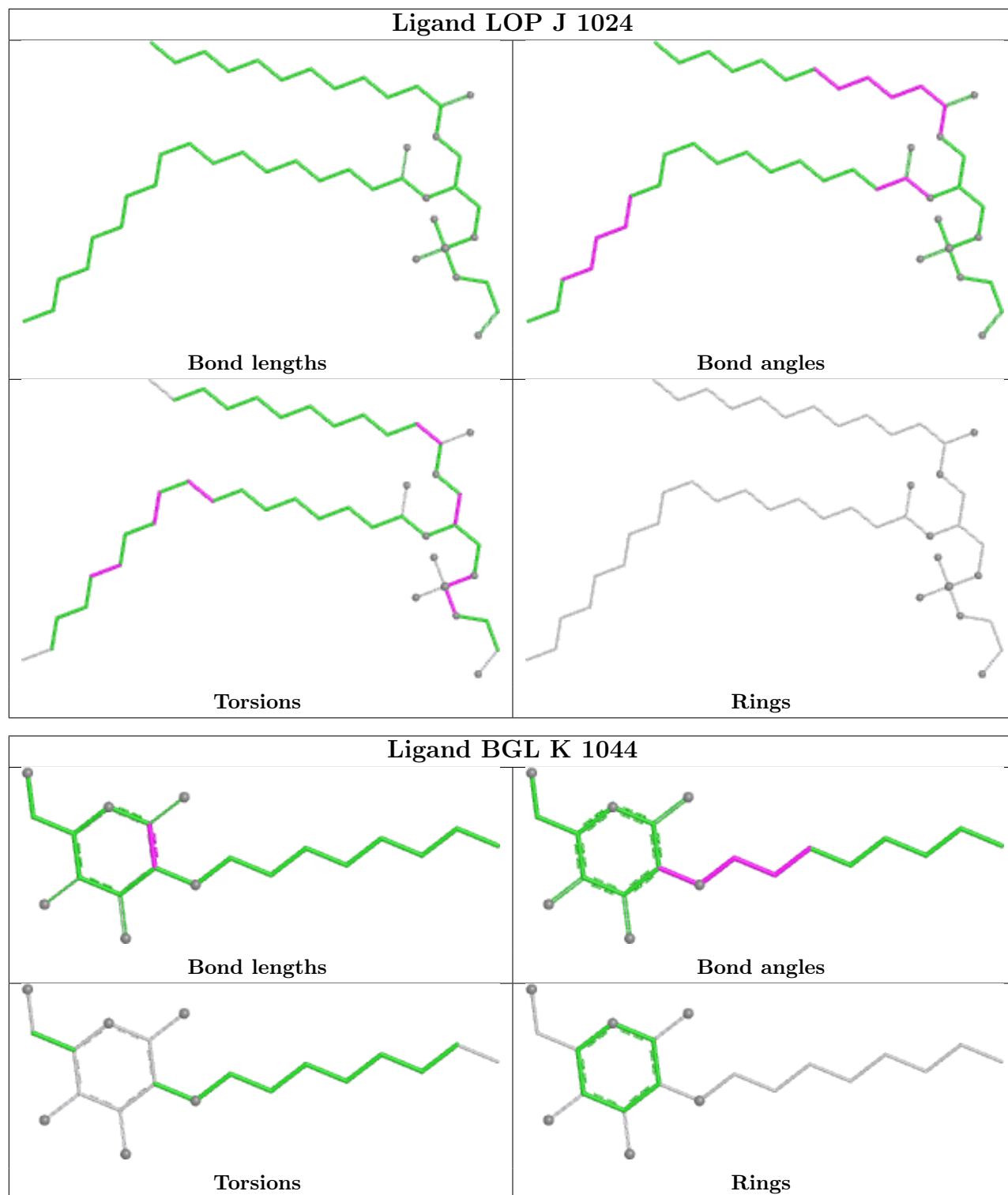
## Ligand BGL B 1041

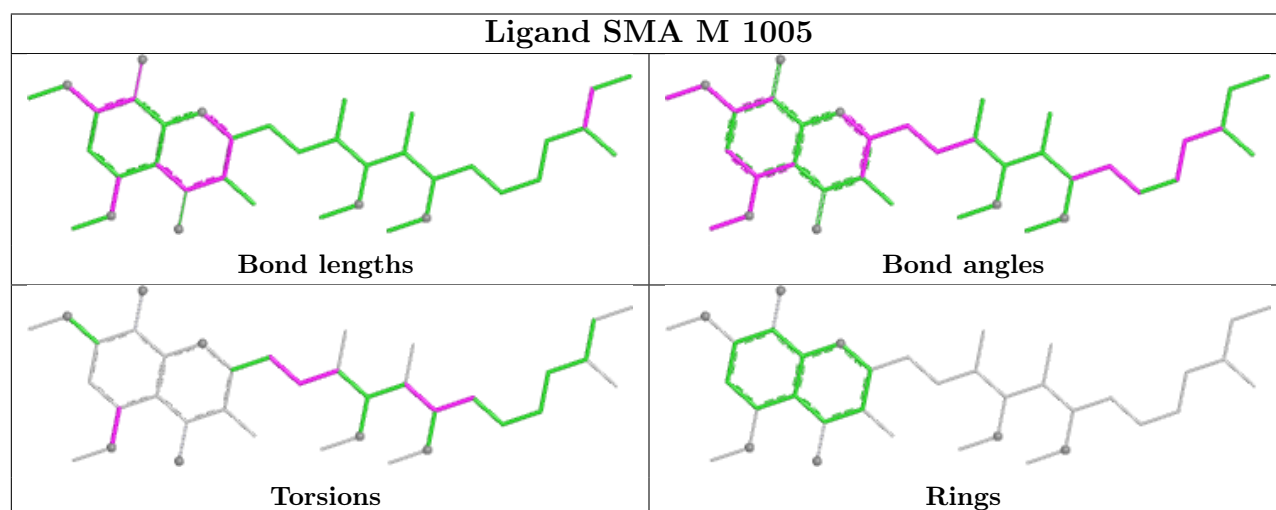
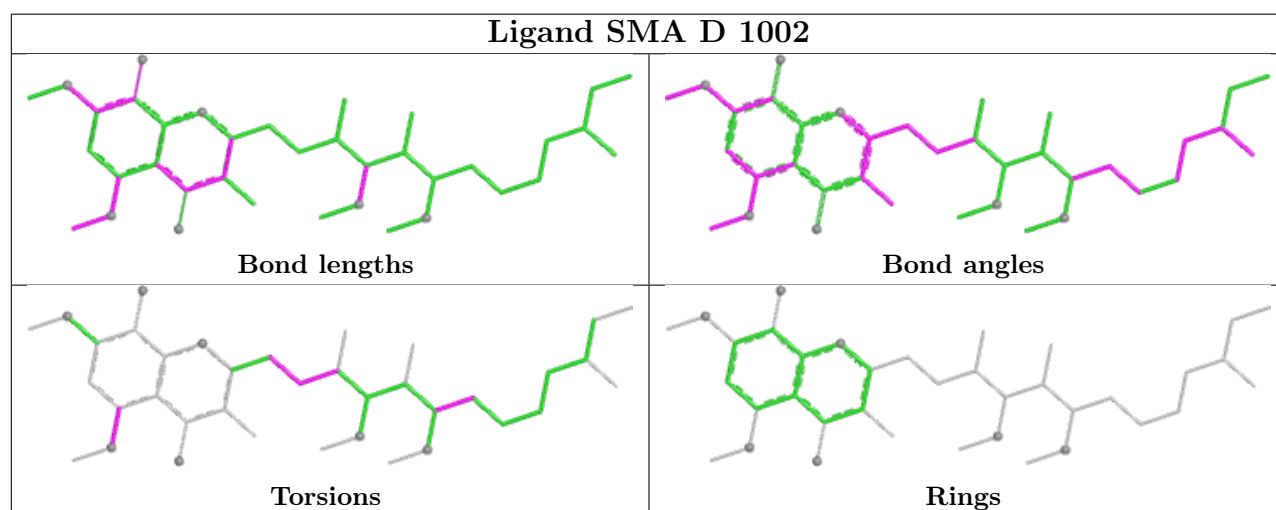
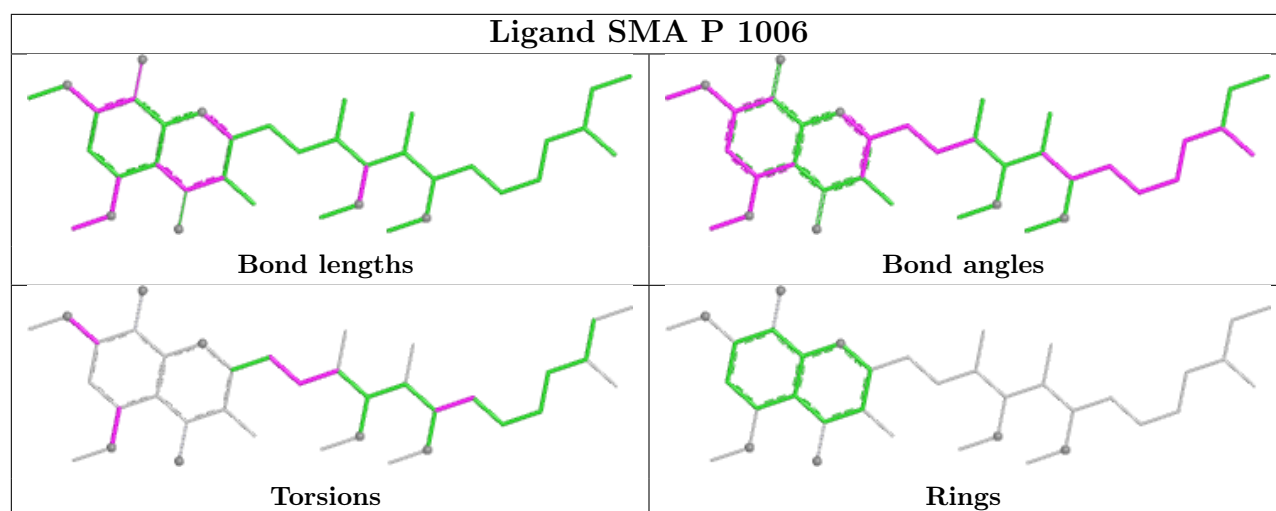


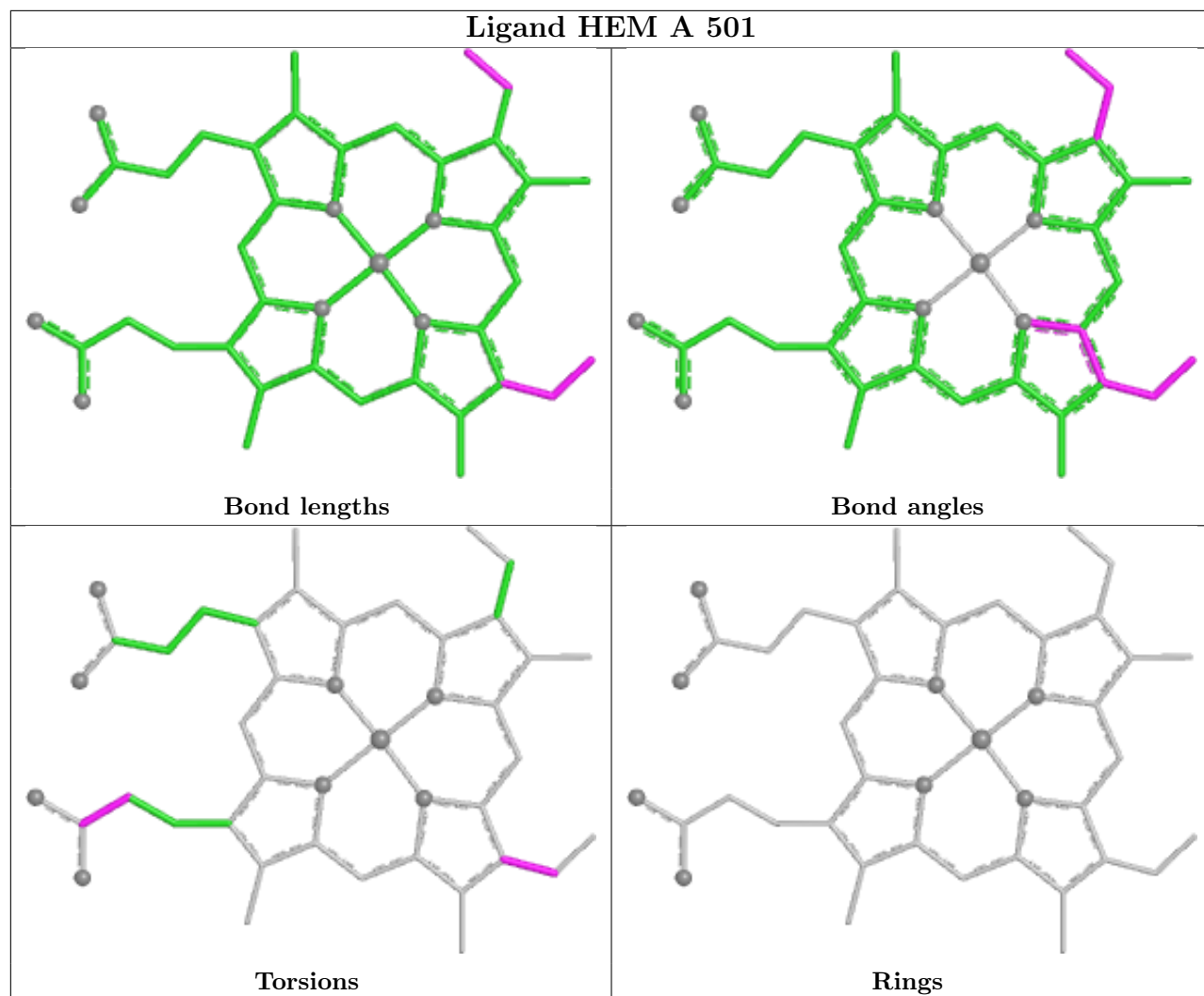
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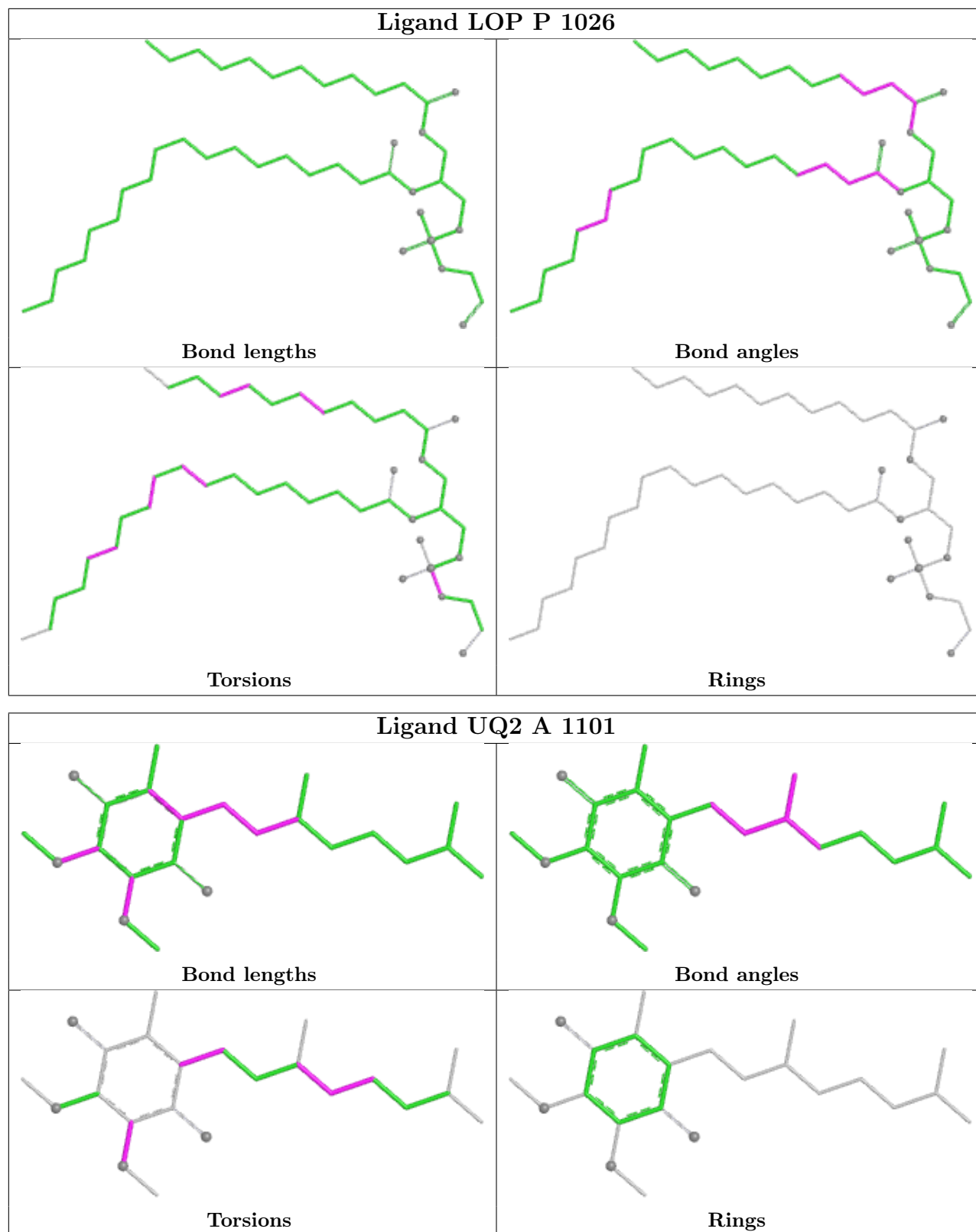


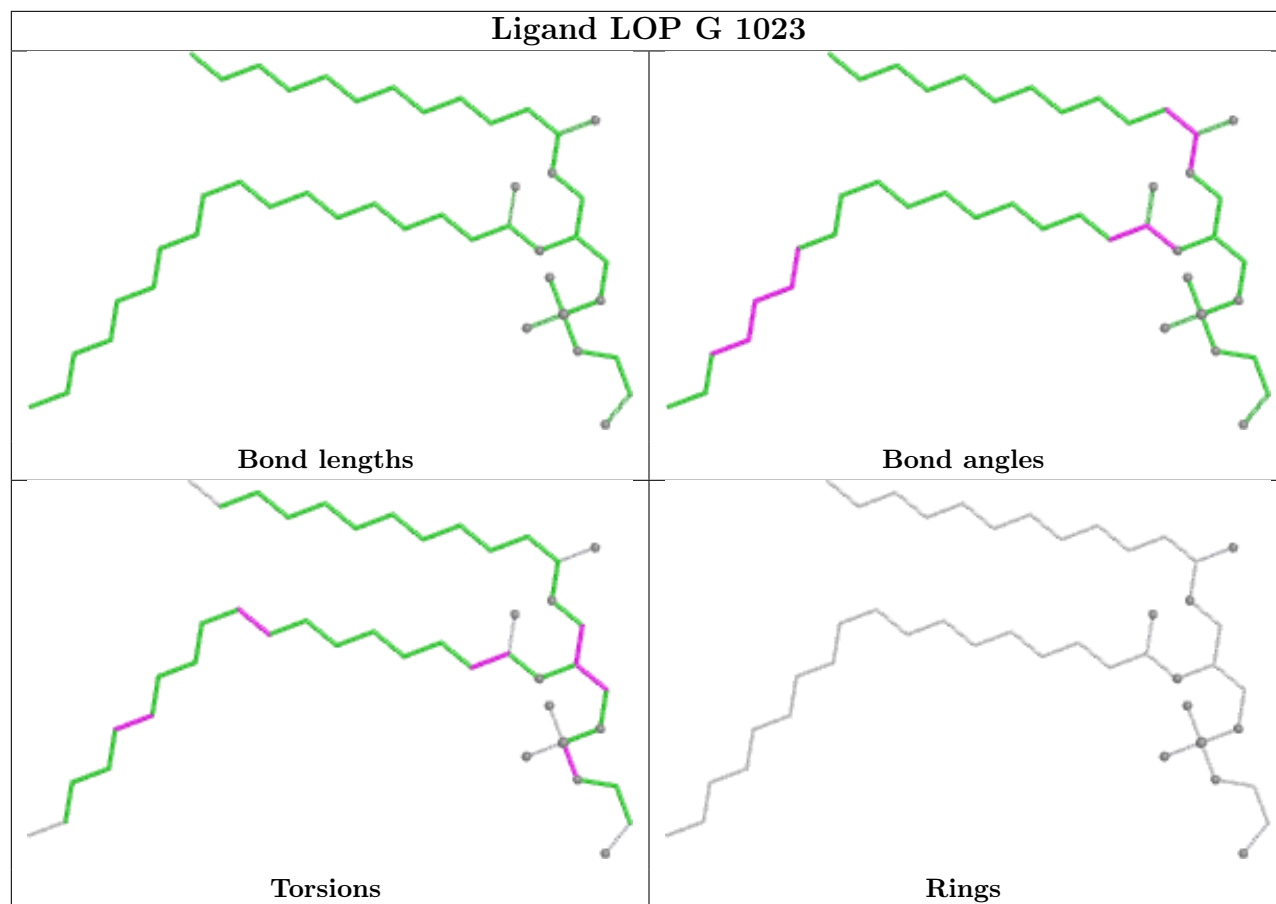


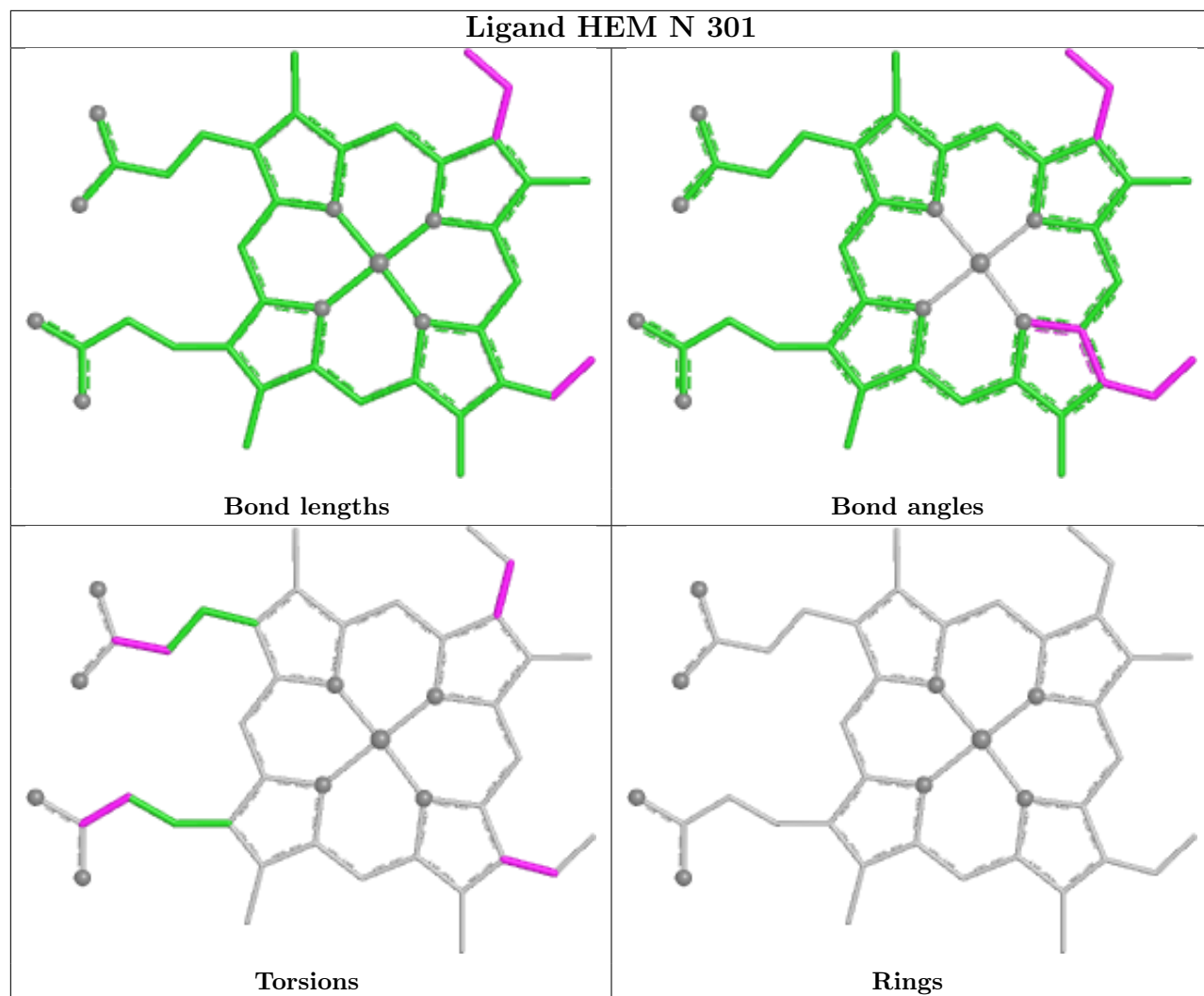


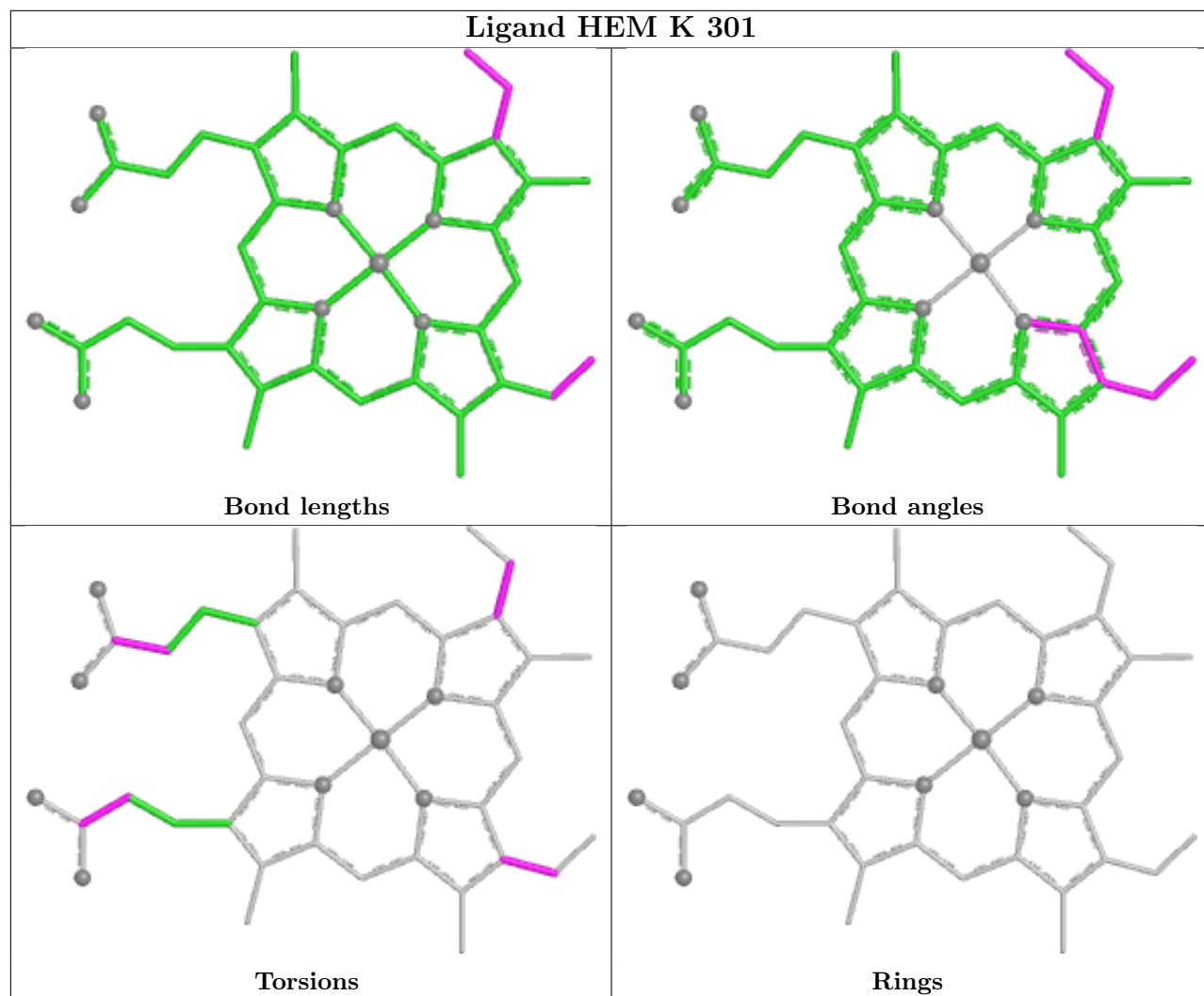


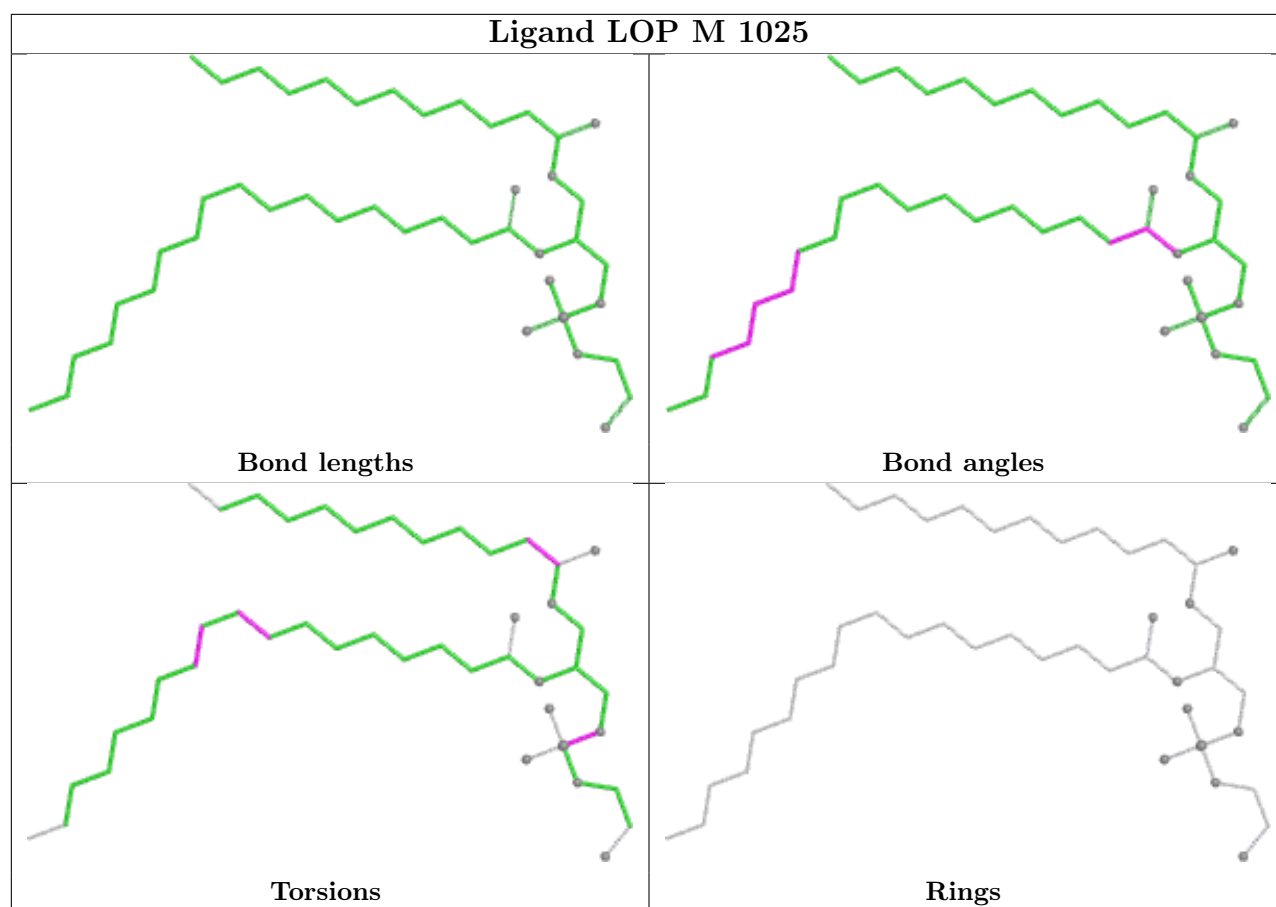


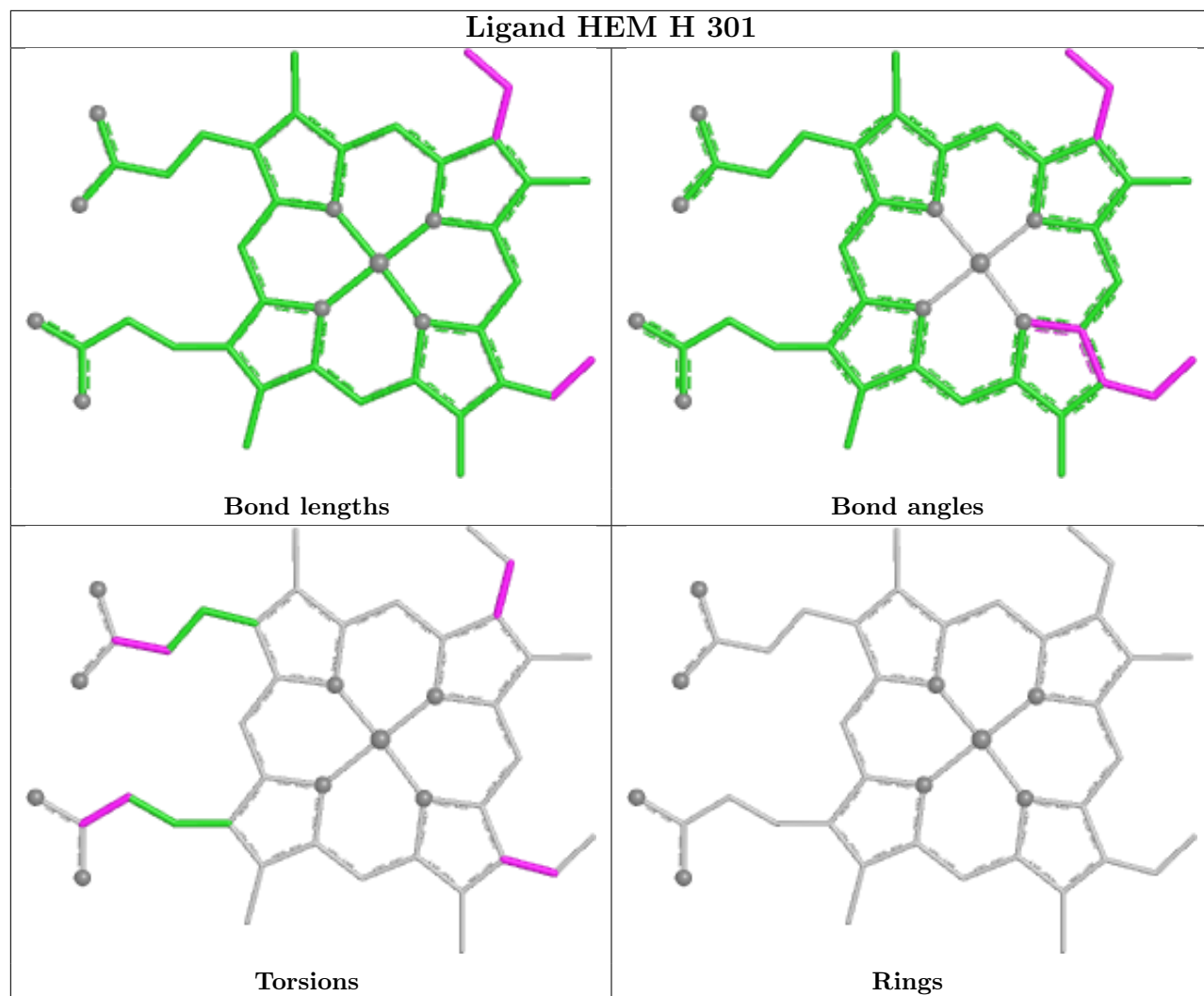


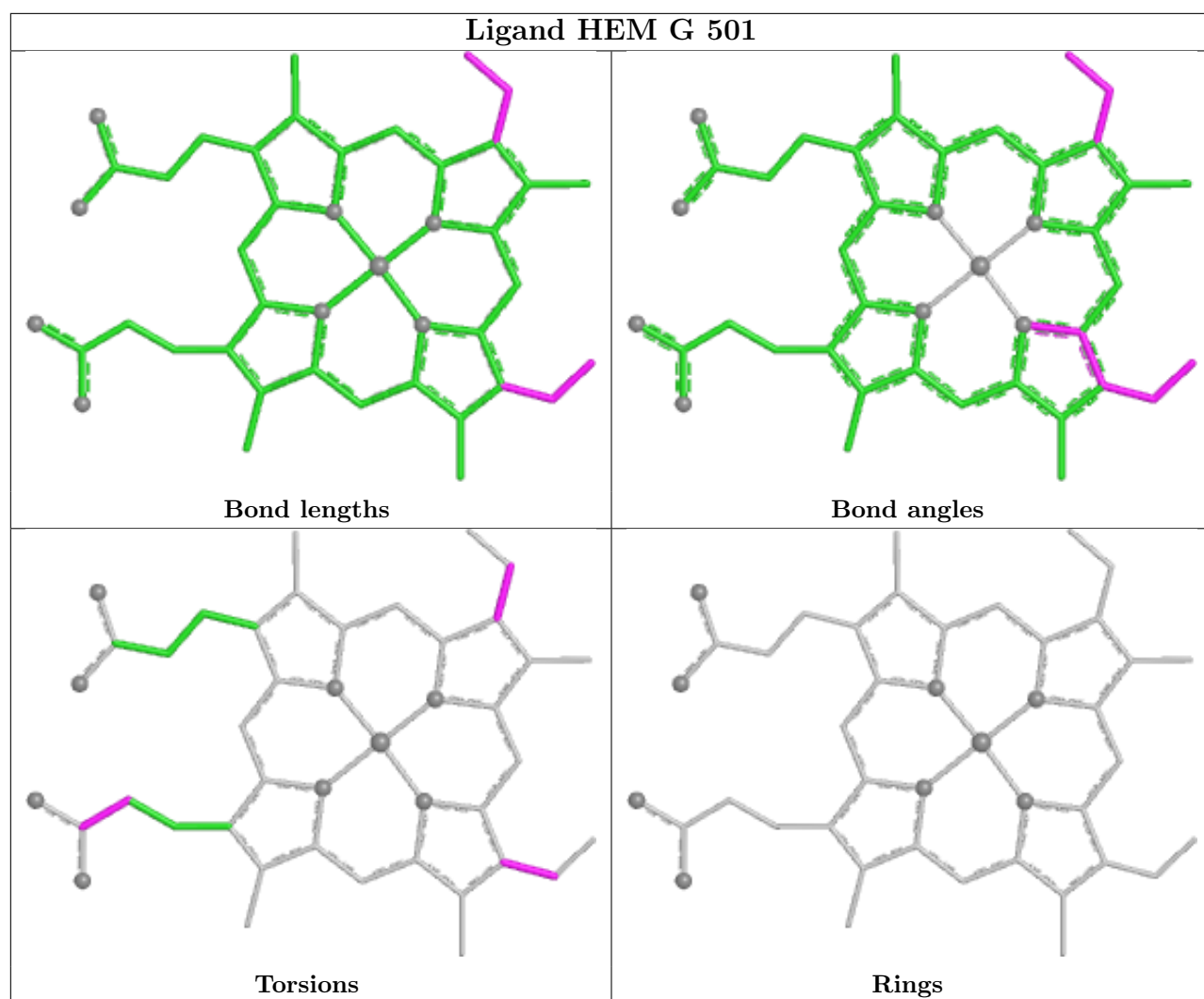


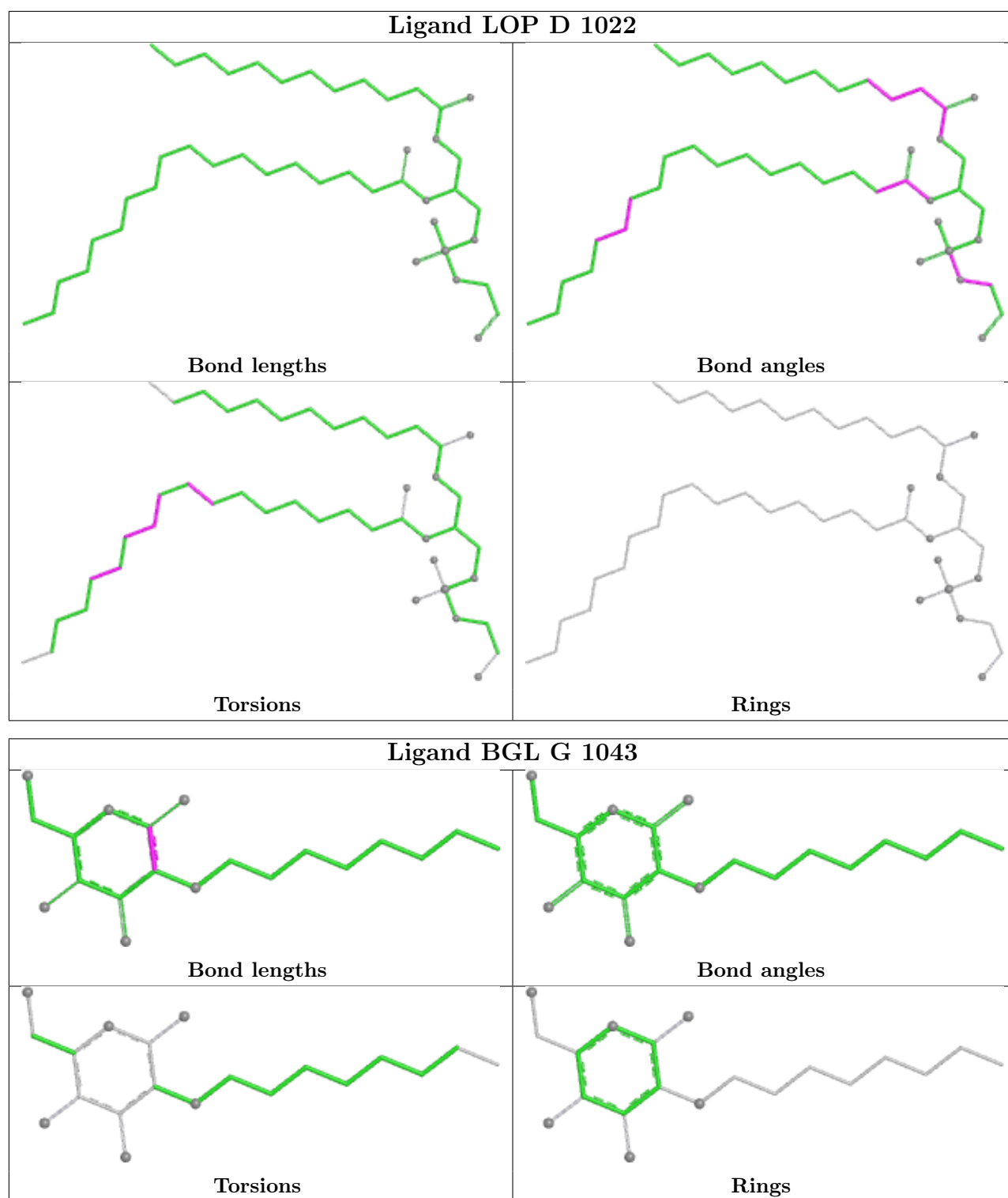












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 428/445 (96%)   | -0.02  | 4 (0%) 81 78   | 35, 53, 90, 117       | 0     |
| 1   | D     | 428/445 (96%)   | 0.04   | 4 (0%) 81 78   | 35, 53, 93, 124       | 0     |
| 1   | G     | 428/445 (96%)   | 0.20   | 8 (1%) 66 62   | 35, 56, 100, 124      | 0     |
| 1   | J     | 428/445 (96%)   | 0.39   | 15 (3%) 47 43  | 36, 62, 101, 125      | 0     |
| 1   | M     | 428/445 (96%)   | 0.41   | 9 (2%) 63 59   | 38, 67, 107, 130      | 0     |
| 1   | P     | 428/445 (96%)   | 0.18   | 9 (2%) 63 59   | 35, 56, 100, 127      | 0     |
| 2   | B     | 256/269 (95%)   | 0.62   | 12 (4%) 36 32  | 47, 78, 112, 134      | 0     |
| 2   | E     | 256/269 (95%)   | 0.72   | 20 (7%) 19 15  | 50, 80, 117, 133      | 0     |
| 2   | H     | 256/269 (95%)   | 0.58   | 18 (7%) 22 19  | 40, 72, 113, 135      | 0     |
| 2   | K     | 256/269 (95%)   | 0.91   | 33 (12%) 7 5   | 49, 87, 120, 136      | 0     |
| 2   | N     | 256/269 (95%)   | 1.12   | 39 (15%) 5 4   | 59, 95, 121, 135      | 0     |
| 2   | Q     | 256/269 (95%)   | 0.90   | 24 (9%) 14 11  | 51, 87, 119, 134      | 0     |
| 3   | C     | 179/187 (95%)   | 0.25   | 6 (3%) 48 44   | 37, 59, 101, 139      | 0     |
| 3   | F     | 179/187 (95%)   | 0.26   | 4 (2%) 62 58   | 38, 63, 102, 140      | 0     |
| 3   | I     | 179/187 (95%)   | 0.29   | 5 (2%) 55 51   | 41, 58, 105, 139      | 0     |
| 3   | L     | 179/187 (95%)   | 0.29   | 12 (6%) 24 20  | 37, 59, 104, 139      | 0     |
| 3   | O     | 179/187 (95%)   | 0.34   | 7 (3%) 43 39   | 34, 64, 108, 138      | 0     |
| 3   | R     | 179/187 (95%)   | 0.65   | 7 (3%) 43 39   | 46, 70, 108, 138      | 0     |
| All | All   | 5178/5406 (95%) | 0.41   | 236 (4%) 37 33 | 34, 66, 112, 140      | 0     |

All (236) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 109 | GLY  | 5.6  |
| 3   | I     | 47  | LEU  | 4.5  |
| 2   | K     | 172 | ALA  | 4.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | B     | 121 | LEU  | 4.4  |
| 2   | H     | 115 | GLY  | 4.3  |
| 2   | N     | 109 | GLY  | 4.3  |
| 3   | L     | 12  | ARG  | 4.3  |
| 2   | H     | 1   | ALA  | 4.2  |
| 2   | N     | 202 | ALA  | 4.1  |
| 3   | F     | 9   | GLY  | 4.1  |
| 3   | L     | 9   | GLY  | 4.0  |
| 3   | C     | 47  | LEU  | 4.0  |
| 2   | K     | 124 | GLY  | 4.0  |
| 2   | H     | 114 | MET  | 3.9  |
| 2   | K     | 114 | MET  | 3.9  |
| 1   | J     | 311 | ASP  | 3.9  |
| 2   | N     | 110 | PHE  | 3.9  |
| 2   | N     | 169 | CYS  | 3.8  |
| 3   | F     | 47  | LEU  | 3.8  |
| 1   | M     | 354 | VAL  | 3.8  |
| 3   | I     | 46  | ALA  | 3.8  |
| 1   | J     | 413 | ALA  | 3.8  |
| 2   | E     | 110 | PHE  | 3.7  |
| 2   | H     | 256 | LYS  | 3.7  |
| 3   | L     | 47  | LEU  | 3.6  |
| 2   | K     | 110 | PHE  | 3.6  |
| 3   | L     | 15  | LEU  | 3.6  |
| 2   | N     | 125 | ILE  | 3.6  |
| 2   | K     | 196 | TYR  | 3.5  |
| 2   | K     | 169 | CYS  | 3.5  |
| 3   | O     | 9   | GLY  | 3.5  |
| 2   | E     | 3   | GLY  | 3.5  |
| 2   | Q     | 110 | PHE  | 3.5  |
| 1   | G     | 3   | GLY  | 3.4  |
| 2   | N     | 179 | ALA  | 3.4  |
| 2   | Q     | 123 | ASN  | 3.4  |
| 2   | N     | 151 | PRO  | 3.4  |
| 2   | N     | 178 | THR  | 3.4  |
| 1   | A     | 30  | TYR  | 3.3  |
| 3   | L     | 14  | PHE  | 3.3  |
| 2   | E     | 115 | GLY  | 3.3  |
| 3   | C     | 9   | GLY  | 3.3  |
| 2   | N     | 164 | SER  | 3.3  |
| 2   | K     | 151 | PRO  | 3.3  |
| 1   | J     | 430 | ALA  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 2   | GLY  | 3.2  |
| 2   | H     | 145 | CYS  | 3.2  |
| 3   | I     | 9   | GLY  | 3.1  |
| 1   | M     | 6   | HIS  | 3.1  |
| 1   | A     | 311 | ASP  | 3.1  |
| 2   | Q     | 251 | LEU  | 3.1  |
| 2   | E     | 4   | GLY  | 3.1  |
| 3   | F     | 12  | ARG  | 3.1  |
| 2   | H     | 3   | GLY  | 3.1  |
| 2   | K     | 121 | LEU  | 3.0  |
| 1   | G     | 311 | ASP  | 3.0  |
| 2   | N     | 115 | GLY  | 3.0  |
| 2   | K     | 256 | LYS  | 3.0  |
| 2   | K     | 120 | GLN  | 3.0  |
| 2   | K     | 125 | ILE  | 3.0  |
| 1   | M     | 3   | GLY  | 3.0  |
| 2   | K     | 115 | GLY  | 3.0  |
| 2   | K     | 118 | ILE  | 2.9  |
| 2   | N     | 6   | VAL  | 2.9  |
| 2   | N     | 1   | ALA  | 2.9  |
| 2   | N     | 121 | LEU  | 2.9  |
| 1   | P     | 3   | GLY  | 2.9  |
| 2   | B     | 118 | ILE  | 2.9  |
| 3   | I     | 10  | THR  | 2.9  |
| 3   | L     | 10  | THR  | 2.9  |
| 2   | B     | 110 | PHE  | 2.9  |
| 2   | Q     | 115 | GLY  | 2.9  |
| 3   | L     | 181 | GLU  | 2.9  |
| 2   | B     | 145 | CYS  | 2.9  |
| 2   | Q     | 145 | CYS  | 2.9  |
| 2   | K     | 175 | VAL  | 2.9  |
| 1   | D     | 311 | ASP  | 2.9  |
| 2   | Q     | 6   | VAL  | 2.9  |
| 3   | C     | 10  | THR  | 2.9  |
| 3   | R     | 47  | LEU  | 2.9  |
| 1   | P     | 311 | ASP  | 2.9  |
| 2   | N     | 190 | MET  | 2.9  |
| 2   | Q     | 242 | VAL  | 2.8  |
| 1   | M     | 311 | ASP  | 2.8  |
| 3   | L     | 46  | ALA  | 2.8  |
| 2   | Q     | 113 | PRO  | 2.8  |
| 2   | K     | 113 | PRO  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 3   | GLY  | 2.7  |
| 2   | K     | 3   | GLY  | 2.7  |
| 2   | N     | 157 | ASN  | 2.7  |
| 3   | O     | 47  | LEU  | 2.7  |
| 1   | G     | 4   | ILE  | 2.7  |
| 2   | N     | 123 | ASN  | 2.7  |
| 2   | Q     | 175 | VAL  | 2.7  |
| 2   | B     | 256 | LYS  | 2.7  |
| 2   | N     | 177 | THR  | 2.7  |
| 2   | H     | 231 | PHE  | 2.7  |
| 2   | H     | 123 | ASN  | 2.7  |
| 2   | Q     | 204 | VAL  | 2.7  |
| 2   | B     | 190 | MET  | 2.7  |
| 2   | B     | 2   | GLY  | 2.7  |
| 2   | K     | 145 | CYS  | 2.7  |
| 2   | E     | 175 | VAL  | 2.7  |
| 2   | B     | 172 | ALA  | 2.7  |
| 1   | G     | 15  | ILE  | 2.6  |
| 2   | N     | 166 | PRO  | 2.6  |
| 2   | E     | 196 | TYR  | 2.6  |
| 2   | E     | 200 | HIS  | 2.6  |
| 1   | P     | 430 | ALA  | 2.6  |
| 1   | G     | 232 | THR  | 2.6  |
| 2   | N     | 182 | TRP  | 2.5  |
| 2   | Q     | 152 | ASP  | 2.5  |
| 1   | J     | 215 | ALA  | 2.5  |
| 3   | L     | 19  | THR  | 2.5  |
| 3   | F     | 16  | TYR  | 2.5  |
| 1   | J     | 216 | PHE  | 2.5  |
| 2   | N     | 172 | ALA  | 2.5  |
| 2   | Q     | 196 | TYR  | 2.5  |
| 1   | D     | 414 | ILE  | 2.5  |
| 2   | N     | 118 | ILE  | 2.5  |
| 2   | N     | 9   | VAL  | 2.5  |
| 2   | N     | 111 | HIS  | 2.5  |
| 1   | D     | 12  | ARG  | 2.5  |
| 2   | B     | 143 | PRO  | 2.5  |
| 1   | J     | 427 | ASP  | 2.5  |
| 1   | P     | 15  | ILE  | 2.5  |
| 3   | O     | 176 | ALA  | 2.5  |
| 2   | E     | 125 | ILE  | 2.4  |
| 2   | N     | 189 | LEU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | Q     | 182 | TRP  | 2.4  |
| 2   | N     | 256 | LYS  | 2.4  |
| 1   | M     | 424 | ILE  | 2.4  |
| 1   | M     | 30  | TYR  | 2.4  |
| 3   | O     | 16  | TYR  | 2.4  |
| 2   | K     | 116 | THR  | 2.4  |
| 2   | E     | 117 | GLY  | 2.4  |
| 3   | I     | 179 | ILE  | 2.4  |
| 3   | R     | 46  | ALA  | 2.4  |
| 2   | B     | 200 | HIS  | 2.4  |
| 2   | Q     | 58  | LEU  | 2.4  |
| 2   | Q     | 1   | ALA  | 2.4  |
| 2   | E     | 18  | GLY  | 2.3  |
| 2   | N     | 137 | GLY  | 2.3  |
| 2   | N     | 4   | GLY  | 2.3  |
| 2   | Q     | 148 | GLY  | 2.3  |
| 2   | E     | 201 | ASP  | 2.3  |
| 1   | A     | 430 | ALA  | 2.3  |
| 1   | G     | 310 | ALA  | 2.3  |
| 2   | E     | 1   | ALA  | 2.3  |
| 2   | Q     | 197 | ALA  | 2.3  |
| 1   | P     | 13  | THR  | 2.3  |
| 2   | K     | 174 | GLY  | 2.3  |
| 1   | M     | 418 | VAL  | 2.3  |
| 2   | E     | 145 | CYS  | 2.3  |
| 1   | J     | 123 | ALA  | 2.3  |
| 3   | O     | 12  | ARG  | 2.3  |
| 1   | P     | 232 | THR  | 2.3  |
| 2   | E     | 199 | GLY  | 2.3  |
| 2   | H     | 60  | GLU  | 2.3  |
| 2   | K     | 166 | PRO  | 2.3  |
| 1   | J     | 310 | ALA  | 2.2  |
| 1   | P     | 30  | TYR  | 2.3  |
| 2   | K     | 1   | ALA  | 2.2  |
| 2   | N     | 200 | HIS  | 2.2  |
| 1   | G     | 414 | ILE  | 2.2  |
| 1   | J     | 15  | ILE  | 2.2  |
| 2   | K     | 192 | ASP  | 2.2  |
| 2   | N     | 20  | PHE  | 2.2  |
| 2   | H     | 6   | VAL  | 2.2  |
| 2   | Q     | 158 | ARG  | 2.2  |
| 2   | K     | 2   | GLY  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | K     | 112 | GLY  | 2.2  |
| 2   | N     | 174 | GLY  | 2.2  |
| 2   | K     | 251 | LEU  | 2.2  |
| 3   | R     | 15  | LEU  | 2.2  |
| 2   | K     | 143 | PRO  | 2.2  |
| 2   | E     | 2   | GLY  | 2.2  |
| 1   | D     | 15  | ILE  | 2.2  |
| 2   | E     | 118 | ILE  | 2.2  |
| 2   | Q     | 10  | PRO  | 2.2  |
| 3   | R     | 14  | PHE  | 2.2  |
| 2   | Q     | 190 | MET  | 2.2  |
| 1   | M     | 183 | GLY  | 2.2  |
| 1   | J     | 240 | ASP  | 2.2  |
| 1   | J     | 252 | ASP  | 2.2  |
| 2   | N     | 16  | PRO  | 2.2  |
| 2   | N     | 165 | VAL  | 2.1  |
| 1   | G     | 430 | ALA  | 2.1  |
| 2   | Q     | 189 | LEU  | 2.1  |
| 3   | R     | 9   | GLY  | 2.1  |
| 3   | L     | 16  | TYR  | 2.1  |
| 3   | C     | 12  | ARG  | 2.1  |
| 2   | Q     | 256 | LYS  | 2.1  |
| 2   | H     | 236 | PHE  | 2.1  |
| 3   | O     | 14  | PHE  | 2.1  |
| 2   | K     | 9   | VAL  | 2.1  |
| 2   | E     | 116 | THR  | 2.1  |
| 3   | O     | 182 | THR  | 2.1  |
| 3   | R     | 10  | THR  | 2.1  |
| 2   | H     | 118 | ILE  | 2.1  |
| 1   | J     | 362 | MET  | 2.1  |
| 2   | K     | 149 | HIS  | 2.1  |
| 3   | R     | 44  | VAL  | 2.1  |
| 2   | K     | 173 | ASN  | 2.1  |
| 2   | H     | 4   | GLY  | 2.1  |
| 2   | H     | 136 | THR  | 2.1  |
| 2   | N     | 124 | GLY  | 2.1  |
| 2   | H     | 196 | TYR  | 2.1  |
| 2   | E     | 6   | VAL  | 2.1  |
| 2   | N     | 138 | PHE  | 2.1  |
| 2   | E     | 251 | LEU  | 2.1  |
| 1   | A     | 183 | GLY  | 2.1  |
| 2   | K     | 78  | GLY  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 4   | ILE  | 2.1  |
| 1   | M     | 15  | ILE  | 2.1  |
| 1   | J     | 121 | TYR  | 2.1  |
| 2   | N     | 196 | TYR  | 2.1  |
| 2   | H     | 22  | GLN  | 2.0  |
| 2   | K     | 204 | VAL  | 2.0  |
| 2   | N     | 11  | PHE  | 2.0  |
| 2   | N     | 38  | ALA  | 2.0  |
| 3   | C     | 11  | ARG  | 2.0  |
| 3   | C     | 48  | ALA  | 2.0  |
| 2   | B     | 4   | GLY  | 2.0  |
| 2   | K     | 109 | GLY  | 2.0  |
| 1   | P     | 11  | PRO  | 2.0  |
| 2   | N     | 194 | VAL  | 2.0  |
| 2   | Q     | 165 | VAL  | 2.0  |
| 3   | L     | 48  | ALA  | 2.0  |
| 2   | B     | 124 | GLY  | 2.0  |
| 2   | Q     | 2   | GLY  | 2.0  |
| 1   | P     | 4   | ILE  | 2.0  |
| 2   | E     | 151 | PRO  | 2.0  |
| 2   | N     | 235 | MET  | 2.0  |
| 3   | L     | 13  | ASP  | 2.0  |
| 2   | K     | 156 | TYR  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 8   | UQ2  | J     | 1104 | 23/23 | 0.57 | 0.27 | 107,115,116,117             | 0     |
| 8   | UQ2  | G     | 1103 | 23/23 | 0.65 | 0.29 | 109,116,117,118             | 0     |
| 8   | UQ2  | A     | 1101 | 23/23 | 0.66 | 0.25 | 102,105,108,109             | 0     |
| 8   | UQ2  | M     | 1105 | 23/23 | 0.68 | 0.26 | 112,123,125,125             | 0     |
| 8   | UQ2  | D     | 1102 | 23/23 | 0.69 | 0.25 | 92,98,107,107               | 0     |
| 8   | UQ2  | P     | 1106 | 23/23 | 0.71 | 0.25 | 101,104,107,108             | 0     |
| 9   | BGL  | N     | 1045 | 20/20 | 0.72 | 0.22 | 107,111,113,114             | 0     |
| 7   | LOP  | M     | 1025 | 45/45 | 0.73 | 0.20 | 89,114,123,123              | 0     |
| 7   | LOP  | J     | 1024 | 45/45 | 0.76 | 0.18 | 93,113,125,126              | 0     |
| 9   | BGL  | B     | 1041 | 20/20 | 0.77 | 0.22 | 87,97,101,102               | 0     |
| 9   | BGL  | K     | 1044 | 20/20 | 0.77 | 0.19 | 95,99,101,101               | 0     |
| 7   | LOP  | G     | 1023 | 45/45 | 0.77 | 0.19 | 88,102,112,113              | 0     |
| 9   | BGL  | P     | 1046 | 20/20 | 0.79 | 0.18 | 87,93,95,95                 | 0     |
| 7   | LOP  | P     | 1026 | 45/45 | 0.80 | 0.18 | 69,95,99,100                | 0     |
| 9   | BGL  | G     | 1043 | 20/20 | 0.82 | 0.21 | 89,91,101,101               | 0     |
| 7   | LOP  | A     | 1021 | 45/45 | 0.84 | 0.16 | 72,86,94,99                 | 0     |
| 9   | BGL  | E     | 1042 | 20/20 | 0.84 | 0.17 | 80,85,102,102               | 0     |
| 7   | LOP  | D     | 1022 | 45/45 | 0.84 | 0.15 | 63,88,98,102                | 0     |
| 4   | SR   | M     | 1019 | 1/1   | 0.87 | 0.07 | 154,154,154,154             | 0     |
| 4   | SR   | Q     | 1016 | 1/1   | 0.88 | 0.08 | 137,137,137,137             | 0     |
| 4   | SR   | A     | 1017 | 1/1   | 0.89 | 0.07 | 114,114,114,114             | 0     |
| 4   | SR   | N     | 1015 | 1/1   | 0.90 | 0.07 | 153,153,153,153             | 0     |
| 4   | SR   | B     | 1011 | 1/1   | 0.91 | 0.06 | 132,132,132,132             | 0     |
| 4   | SR   | K     | 1014 | 1/1   | 0.92 | 0.05 | 145,145,145,145             | 0     |
| 4   | SR   | G     | 1018 | 1/1   | 0.92 | 0.05 | 98,98,98,98                 | 0     |
| 6   | SMA  | D     | 1002 | 37/37 | 0.93 | 0.10 | 39,44,76,78                 | 0     |
| 6   | SMA  | A     | 1001 | 37/37 | 0.94 | 0.08 | 38,47,54,56                 | 0     |
| 6   | SMA  | G     | 1003 | 37/37 | 0.94 | 0.09 | 35,43,60,65                 | 0     |
| 6   | SMA  | M     | 1005 | 37/37 | 0.94 | 0.10 | 56,66,73,73                 | 0     |
| 12  | NA   | R     | 2001 | 1/1   | 0.94 | 0.07 | 62,62,62,62                 | 0     |
| 5   | HEM  | J     | 501  | 43/43 | 0.95 | 0.13 | 67,75,79,81                 | 0     |
| 6   | SMA  | P     | 1006 | 37/37 | 0.95 | 0.09 | 34,45,76,77                 | 0     |
| 11  | CL   | I     | 2004 | 1/1   | 0.95 | 0.08 | 67,67,67,67                 | 0     |
| 11  | CL   | R     | 2005 | 1/1   | 0.95 | 0.14 | 67,67,67,67                 | 0     |
| 6   | SMA  | J     | 1004 | 37/37 | 0.95 | 0.09 | 40,49,79,85                 | 0     |
| 4   | SR   | H     | 1013 | 1/1   | 0.96 | 0.05 | 113,113,113,113             | 0     |
| 4   | SR   | E     | 1012 | 1/1   | 0.96 | 0.06 | 138,138,138,138             | 0     |
| 5   | HEM  | N     | 301  | 43/43 | 0.96 | 0.10 | 65,72,79,84                 | 0     |
| 5   | HEM  | M     | 501  | 43/43 | 0.97 | 0.10 | 63,69,75,78                 | 0     |
| 5   | HEM  | E     | 301  | 43/43 | 0.97 | 0.09 | 53,62,73,76                 | 0     |
| 5   | HEM  | Q     | 301  | 43/43 | 0.97 | 0.08 | 56,65,73,78                 | 0     |

*Continued on next page...*

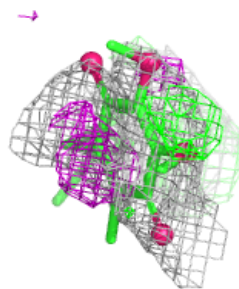
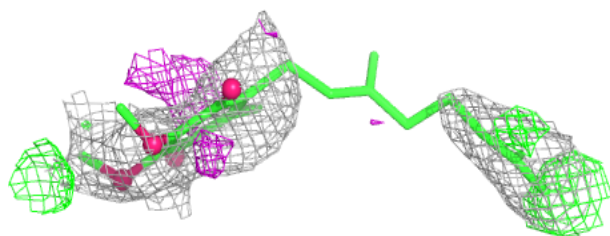
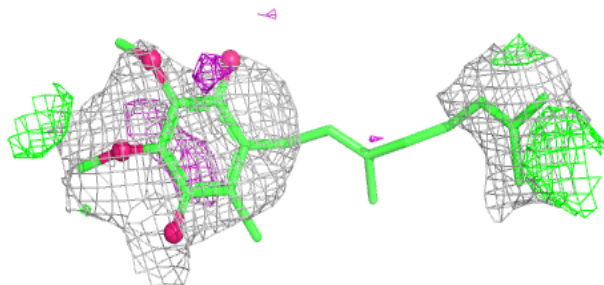
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | HEM  | G     | 501 | 43/43 | 0.97 | 0.09 | 50,59,62,62                 | 0     |
| 5   | HEM  | B     | 301 | 43/43 | 0.97 | 0.09 | 51,56,70,73                 | 0     |
| 5   | HEM  | K     | 301 | 43/43 | 0.97 | 0.09 | 49,55,67,69                 | 0     |
| 5   | HEM  | P     | 501 | 43/43 | 0.98 | 0.08 | 48,54,57,57                 | 0     |
| 5   | HEM  | P     | 502 | 43/43 | 0.98 | 0.08 | 35,40,49,53                 | 0     |
| 5   | HEM  | G     | 502 | 43/43 | 0.98 | 0.09 | 32,36,45,49                 | 0     |
| 5   | HEM  | H     | 301 | 43/43 | 0.98 | 0.07 | 33,42,47,50                 | 0     |
| 5   | HEM  | D     | 501 | 43/43 | 0.98 | 0.08 | 40,48,53,55                 | 0     |
| 5   | HEM  | J     | 502 | 43/43 | 0.98 | 0.07 | 37,41,54,57                 | 0     |
| 5   | HEM  | D     | 502 | 43/43 | 0.98 | 0.08 | 32,37,49,58                 | 0     |
| 10  | FES  | O     | 200 | 4/4   | 0.98 | 0.04 | 42,43,43,43                 | 0     |
| 5   | HEM  | A     | 502 | 43/43 | 0.98 | 0.09 | 32,37,49,49                 | 0     |
| 5   | HEM  | M     | 502 | 43/43 | 0.98 | 0.08 | 47,49,59,63                 | 0     |
| 5   | HEM  | A     | 501 | 43/43 | 0.98 | 0.07 | 43,47,51,53                 | 0     |
| 10  | FES  | C     | 200 | 4/4   | 0.99 | 0.03 | 41,42,42,43                 | 0     |
| 10  | FES  | R     | 200 | 4/4   | 0.99 | 0.04 | 55,57,58,58                 | 0     |
| 10  | FES  | F     | 200 | 4/4   | 0.99 | 0.04 | 43,43,44,45                 | 0     |
| 10  | FES  | I     | 200 | 4/4   | 0.99 | 0.04 | 47,48,48,48                 | 0     |
| 10  | FES  | L     | 200 | 4/4   | 0.99 | 0.04 | 40,41,41,42                 | 0     |

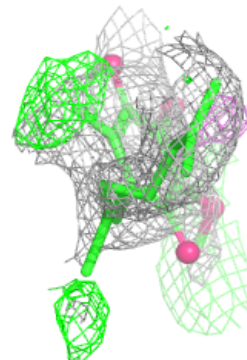
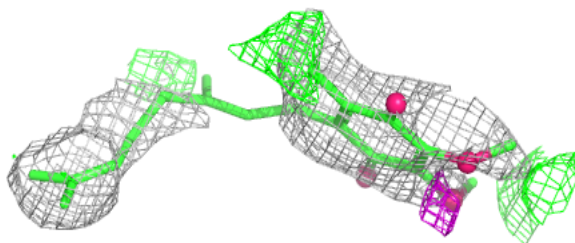
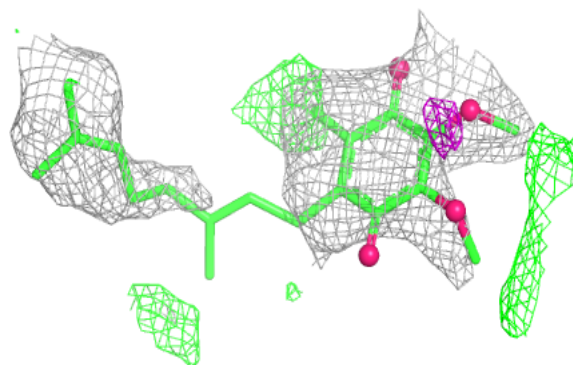
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UQ2 J 1104:**

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

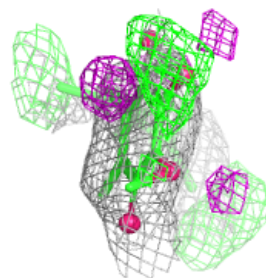
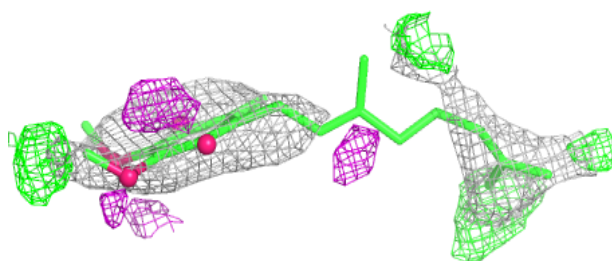
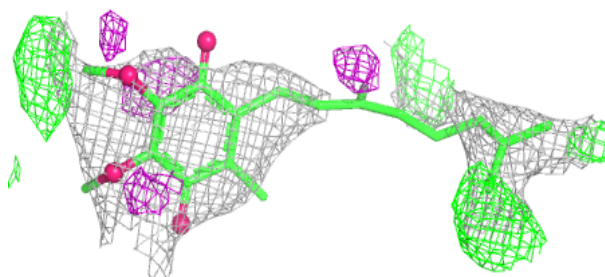
**Electron density around UQ2 G 1103:**

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

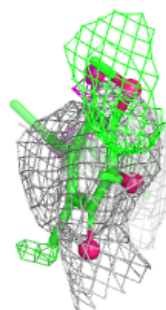
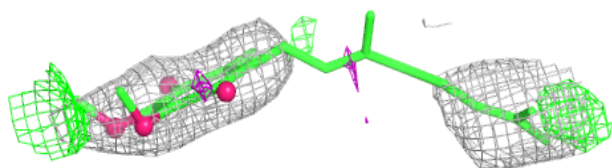
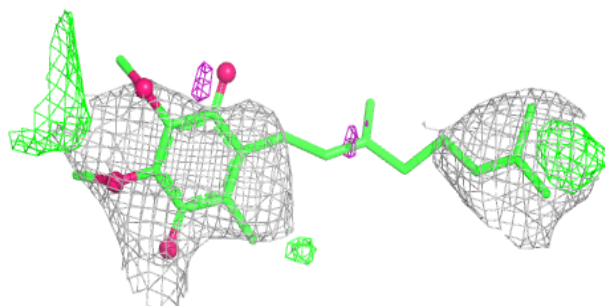


**Electron density around UQ2 A 1101:**

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

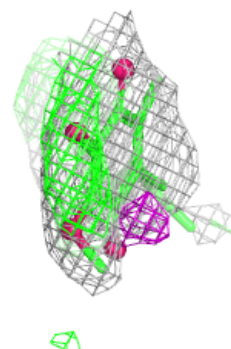
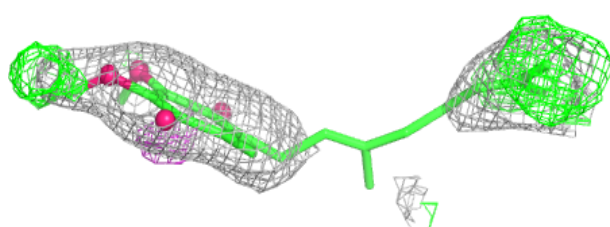
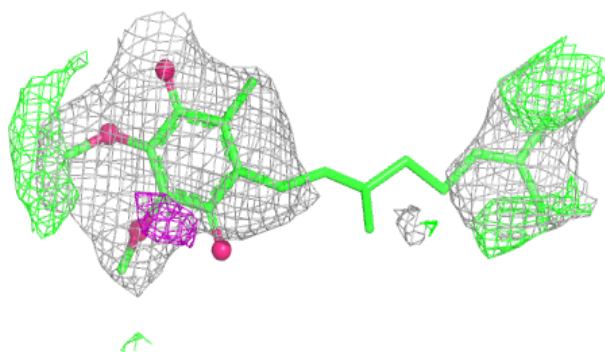
**Electron density around UQ2 M 1105:**

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

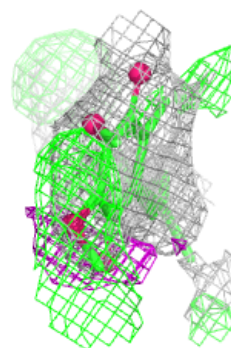
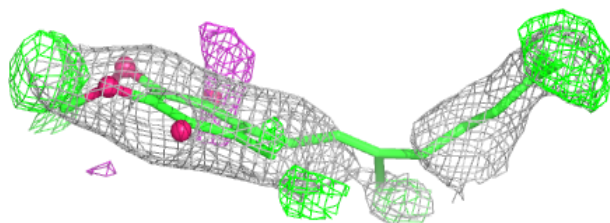
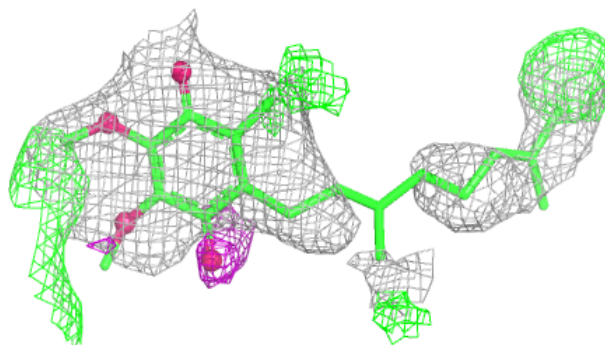


**Electron density around UQ2 D 1102:**

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

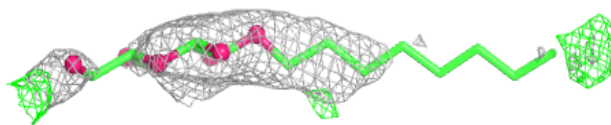
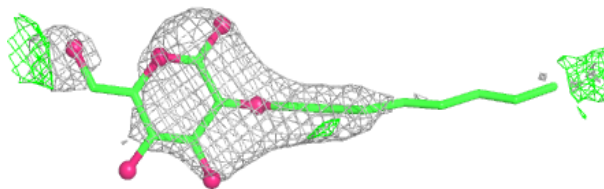
**Electron density around UQ2 P 1106:**

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

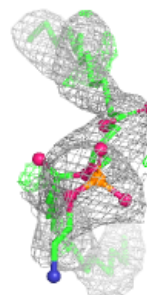
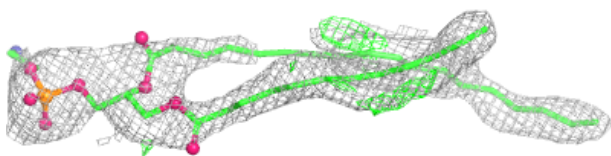
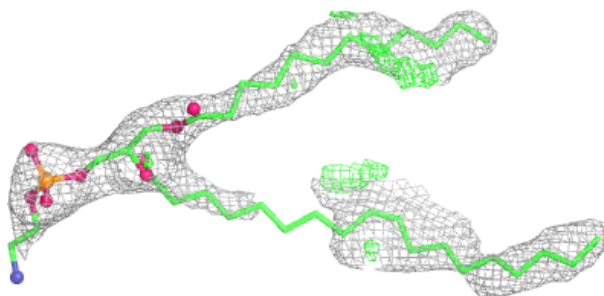


**Electron density around BGL N 1045:**

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

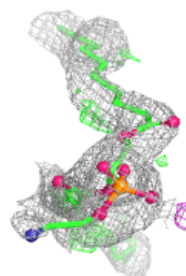
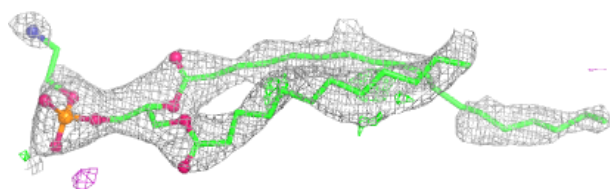
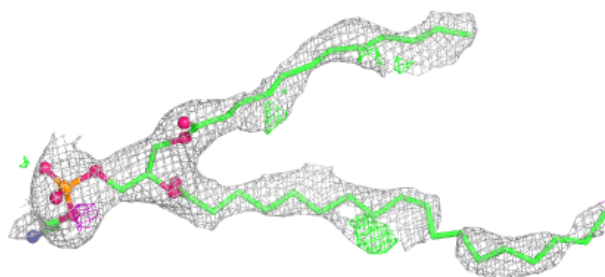
**Electron density around LOP M 1025:**

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

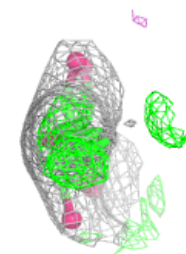
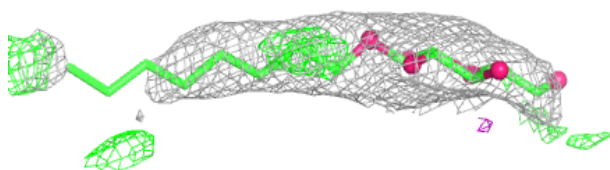
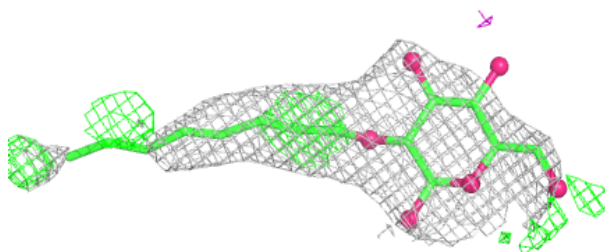


**Electron density around LOP J 1024:**

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

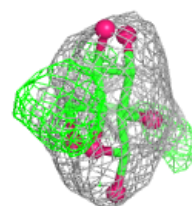
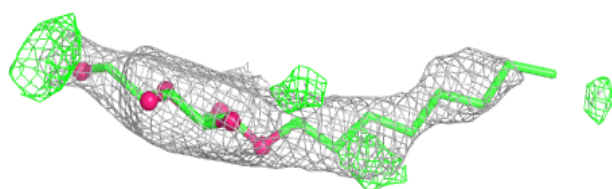
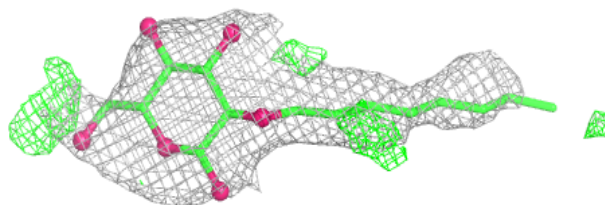
**Electron density around BGL B 1041:**

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

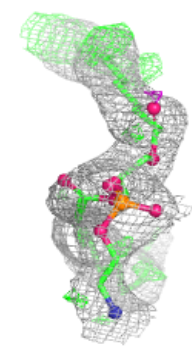
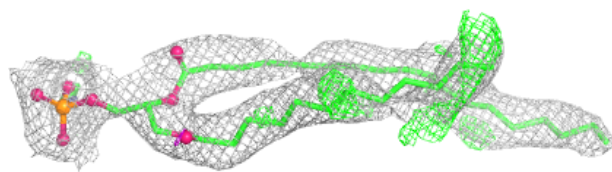
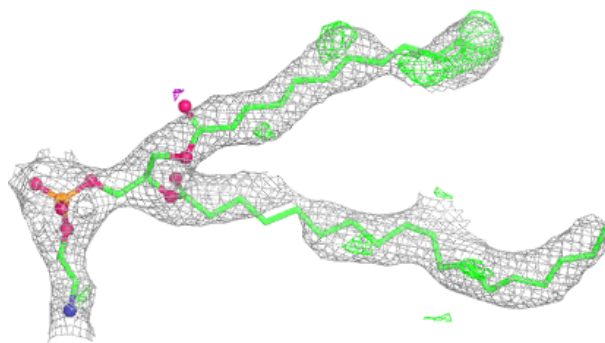


**Electron density around BGL K 1044:**

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

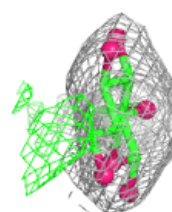
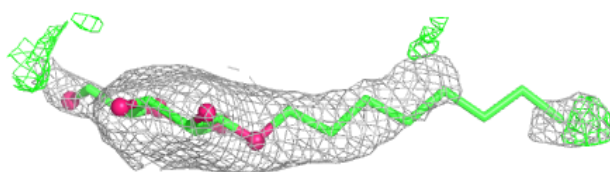
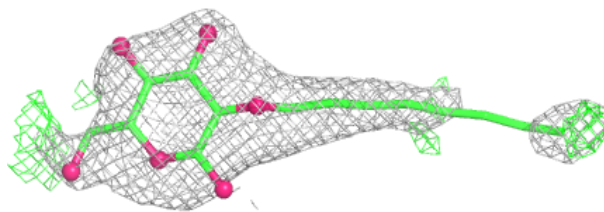
**Electron density around LOP G 1023:**

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

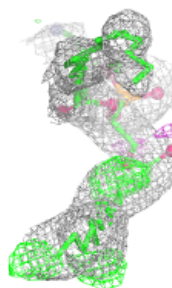
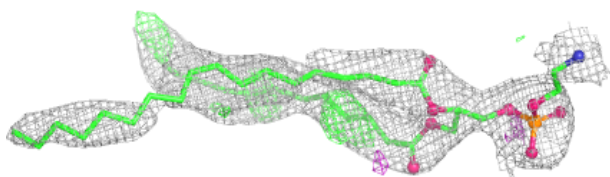
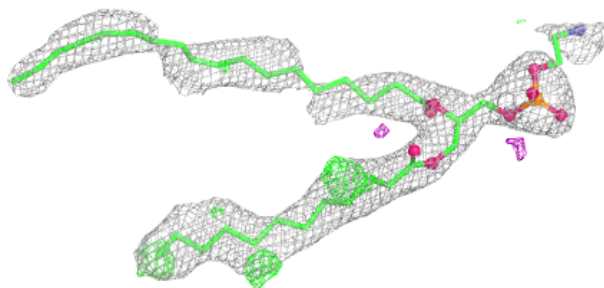


**Electron density around BGL P 1046:**

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

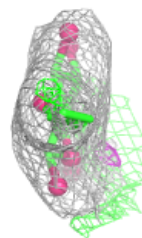
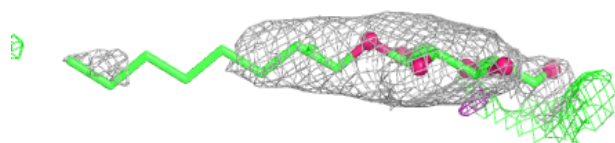
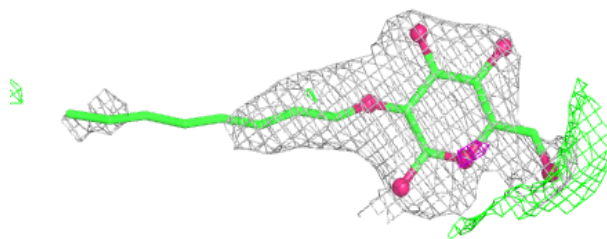
**Electron density around LOP P 1026:**

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

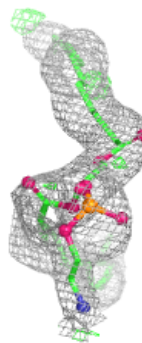
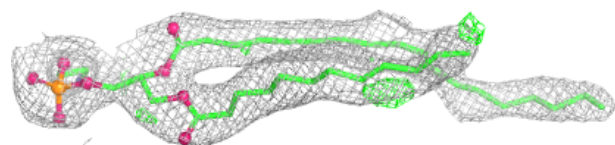
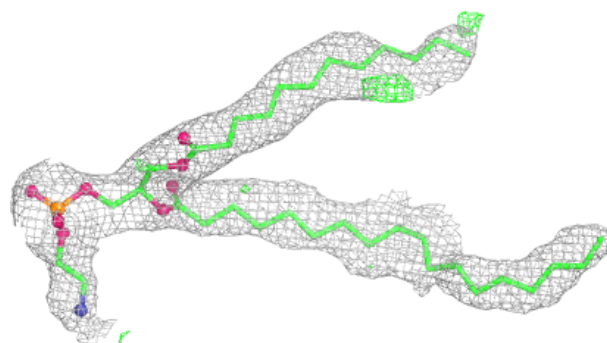


**Electron density around BGL G 1043:**

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

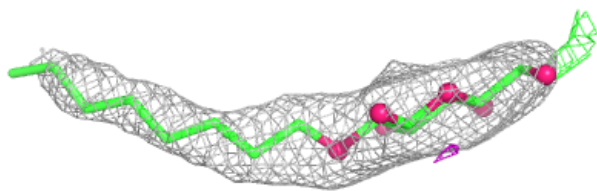
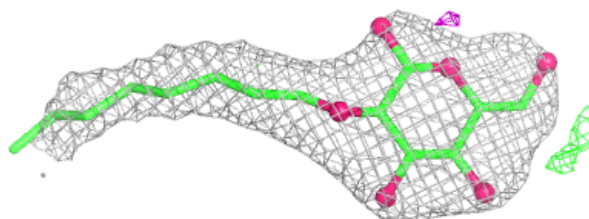
**Electron density around LOP A 1021:**

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

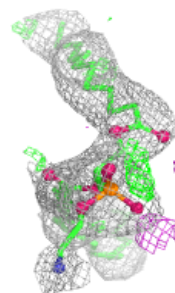
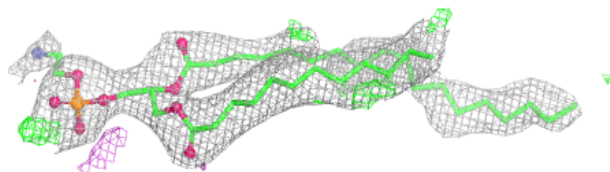
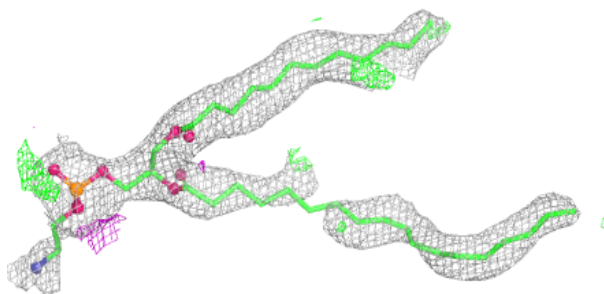


**Electron density around BGL E 1042:**

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

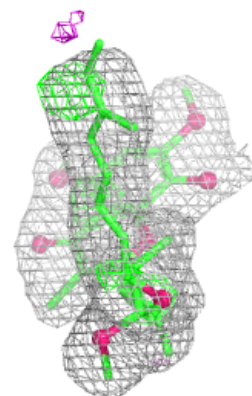
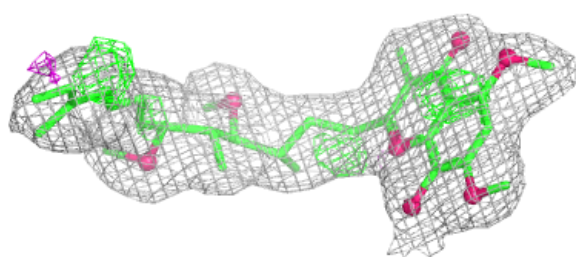
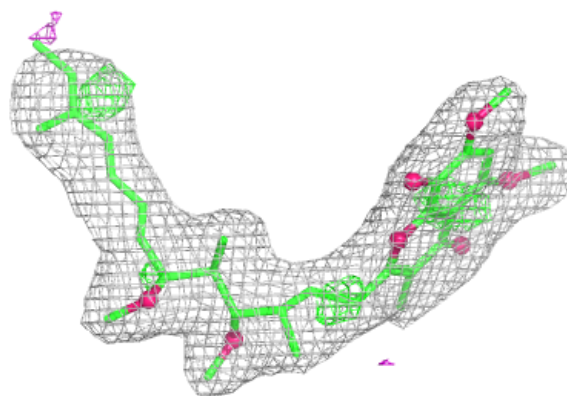
**Electron density around LOP D 1022:**

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

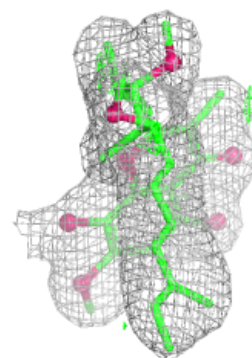
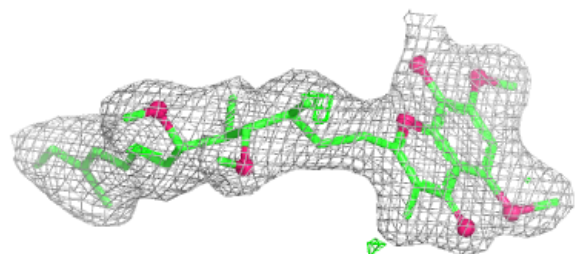
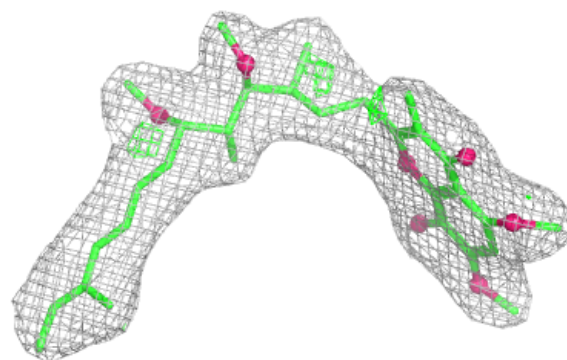


**Electron density around SMA D 1002:**

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

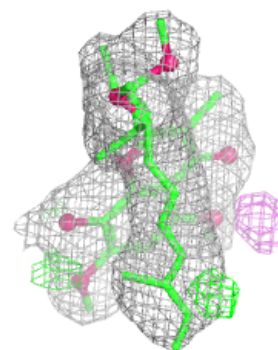
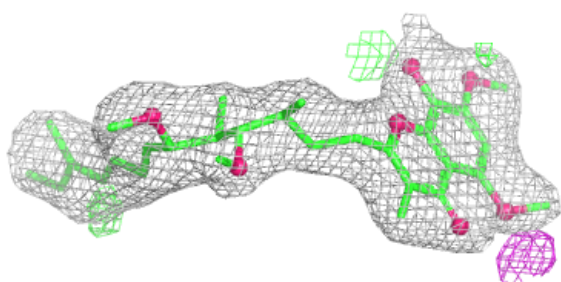
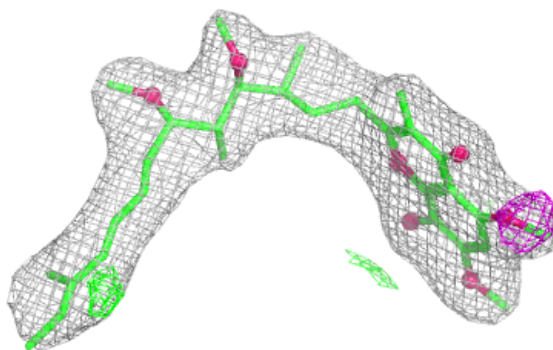
**Electron density around SMA A 1001:**

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

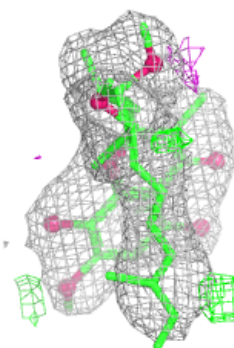
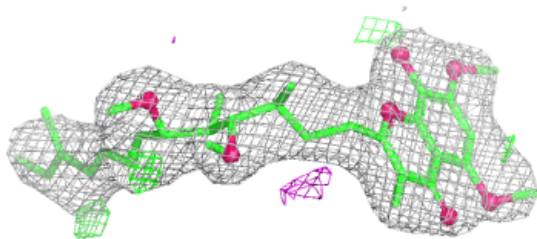
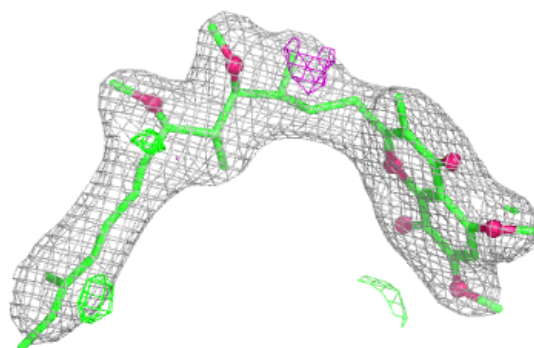


**Electron density around SMA G 1003:**

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

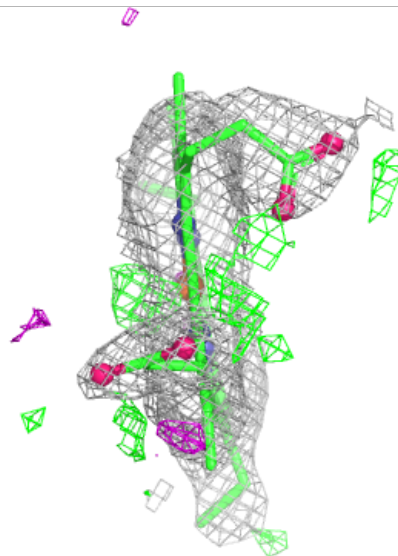
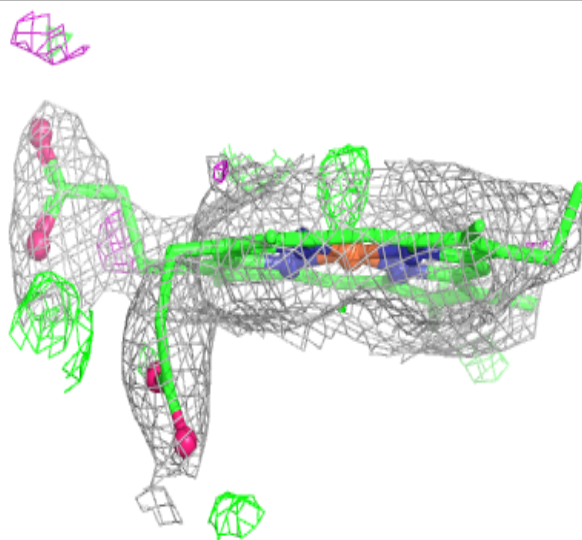
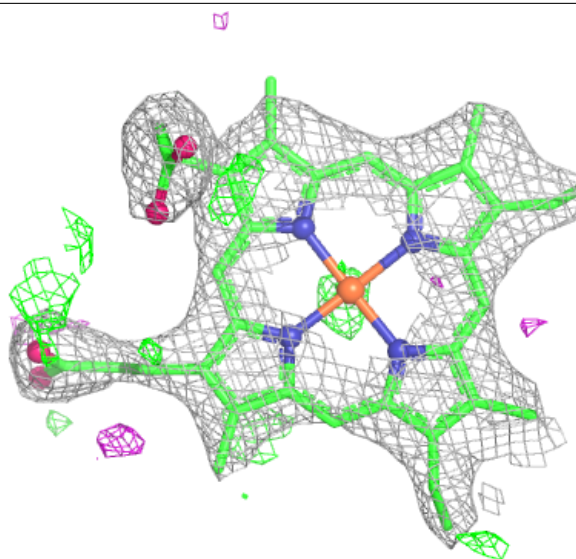
**Electron density around SMA M 1005:**

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



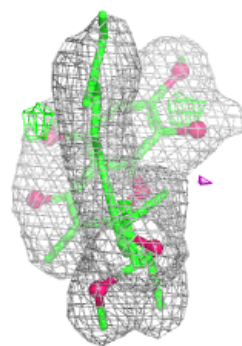
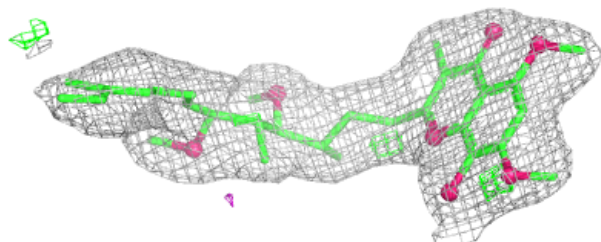
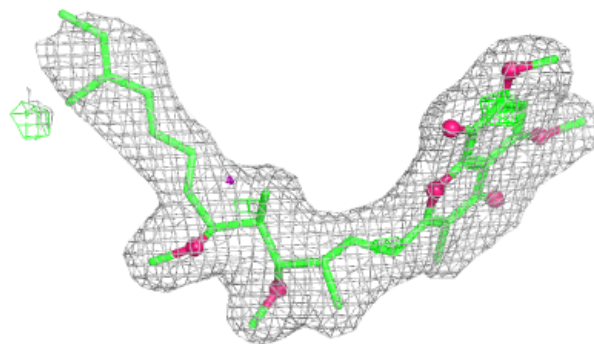
**Electron density around HEM J 501:**

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

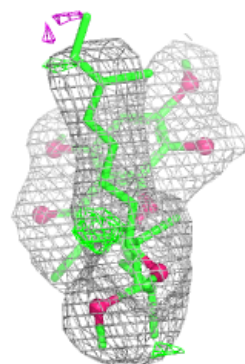
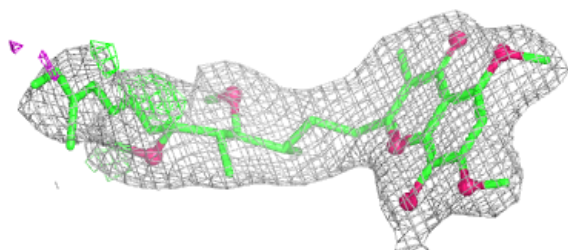
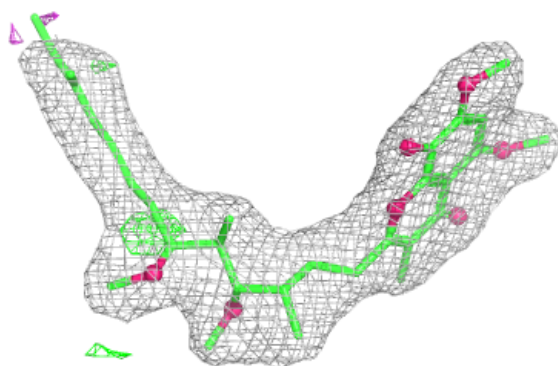


**Electron density around SMA P 1006:**

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

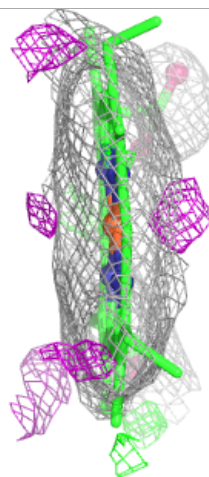
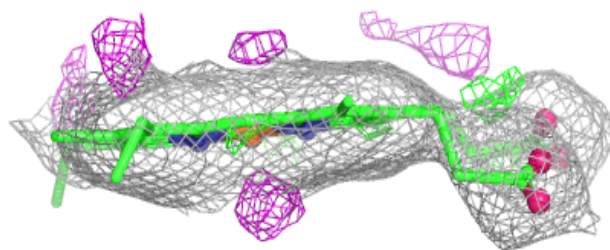
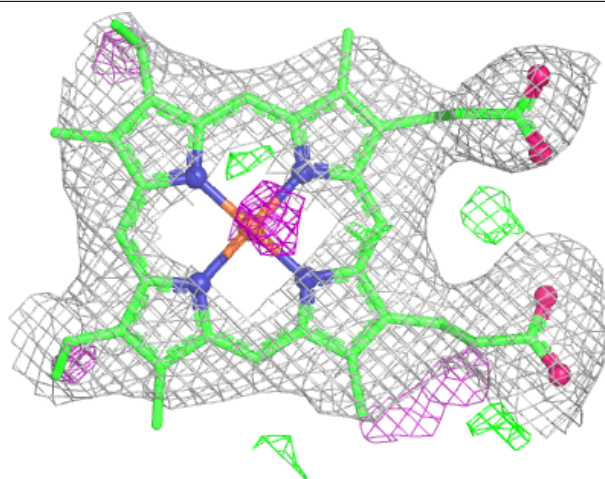
**Electron density around SMA J 1004:**

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



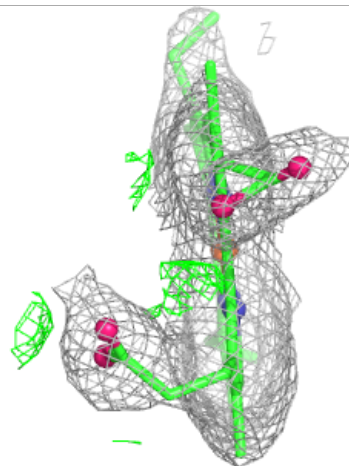
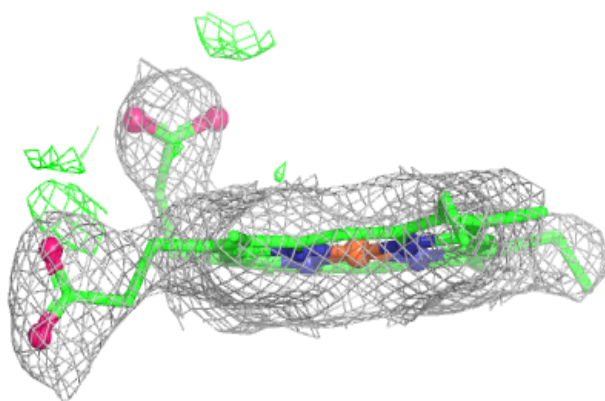
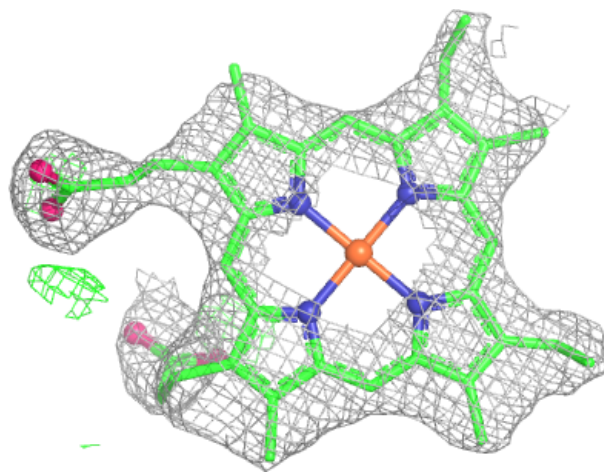
**Electron density around HEM N 301:**

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



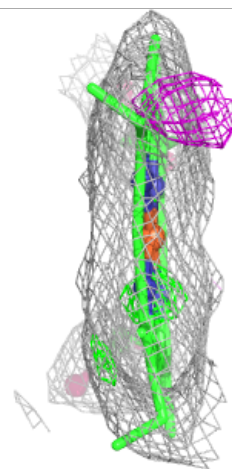
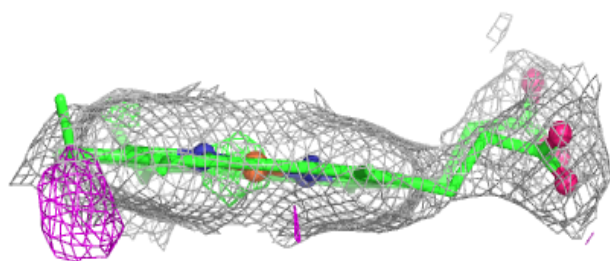
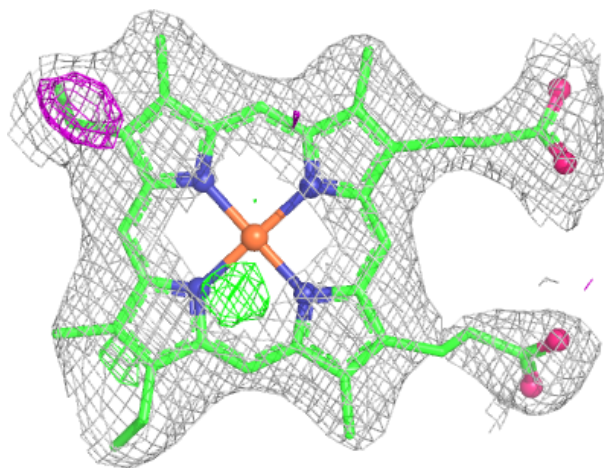
**Electron density around HEM M 501:**

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



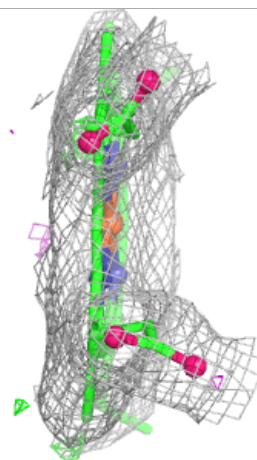
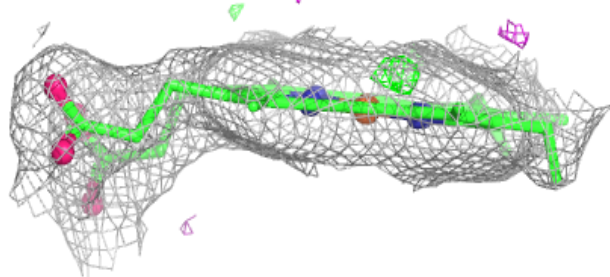
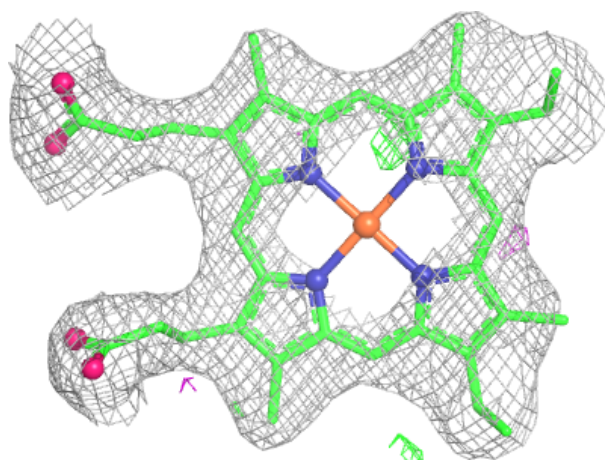
**Electron density around HEM E 301:**

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



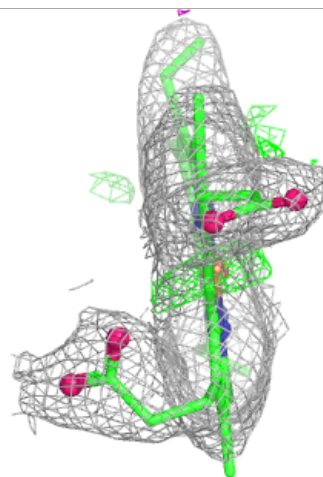
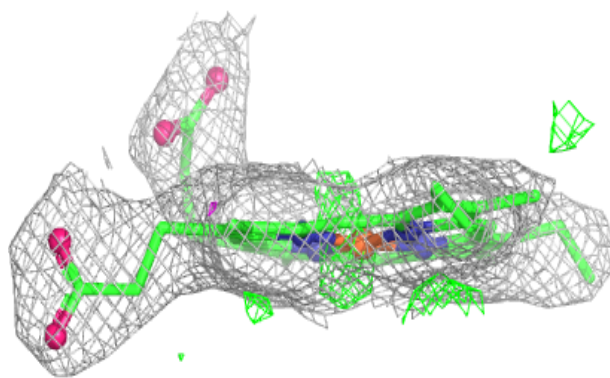
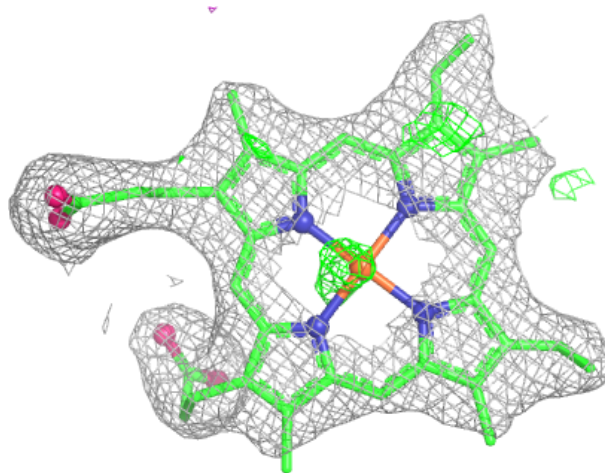
**Electron density around HEM Q 301:**

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



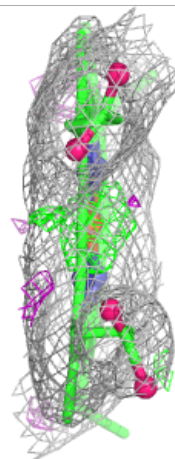
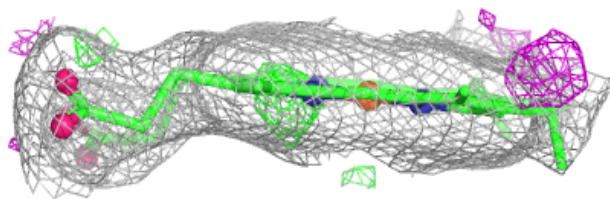
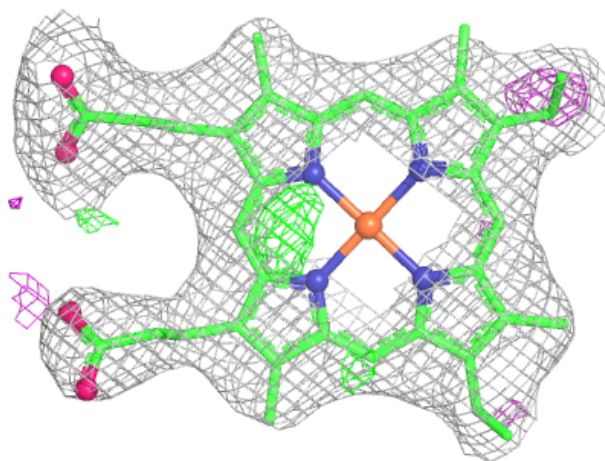
**Electron density around HEM G 501:**

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



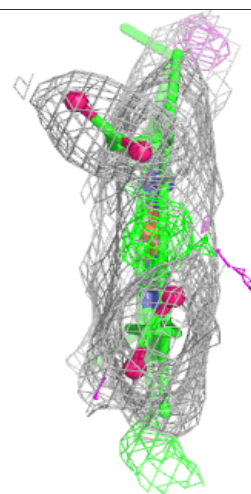
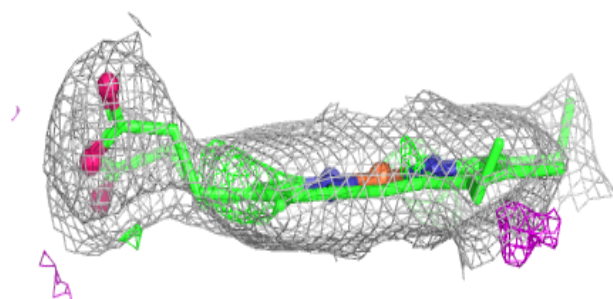
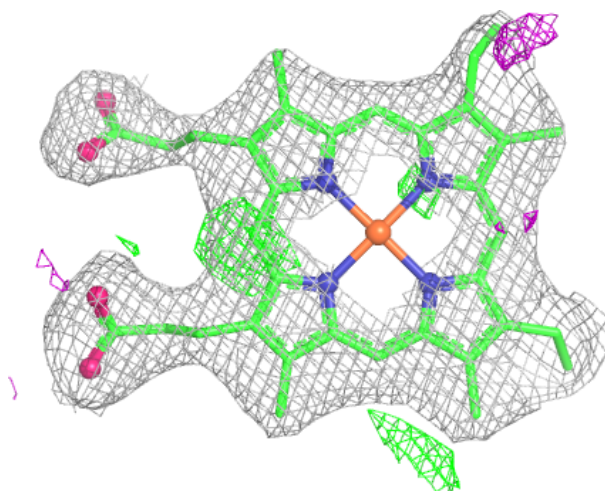
**Electron density around HEM B 301:**

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



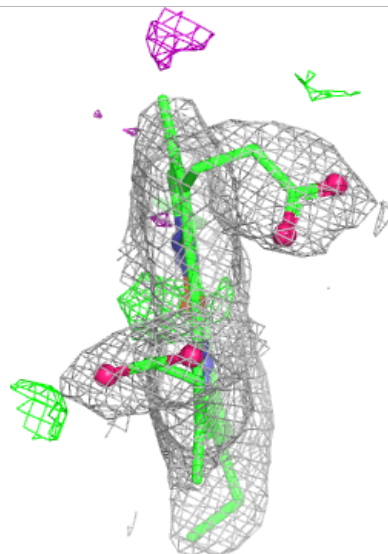
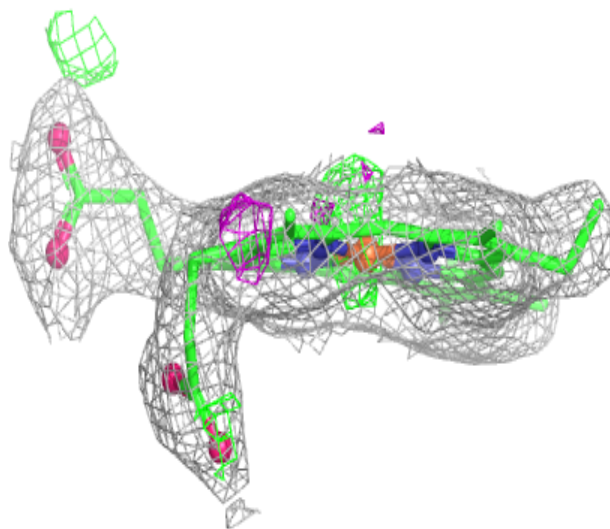
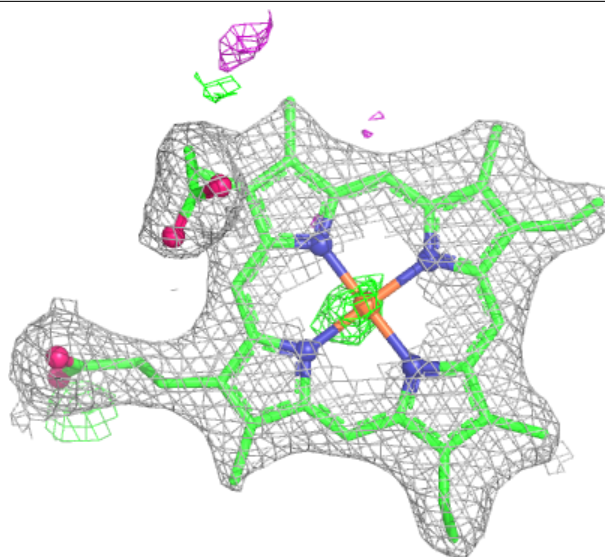
**Electron density around HEM K 301:**

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



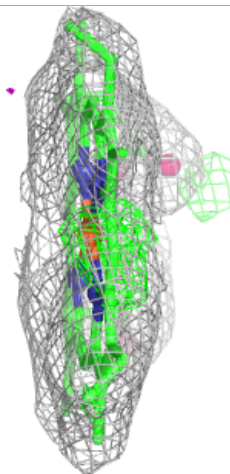
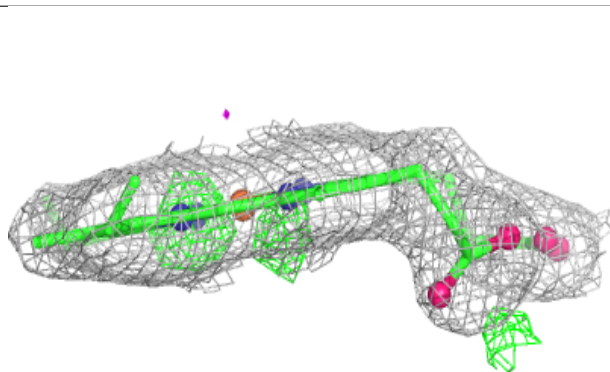
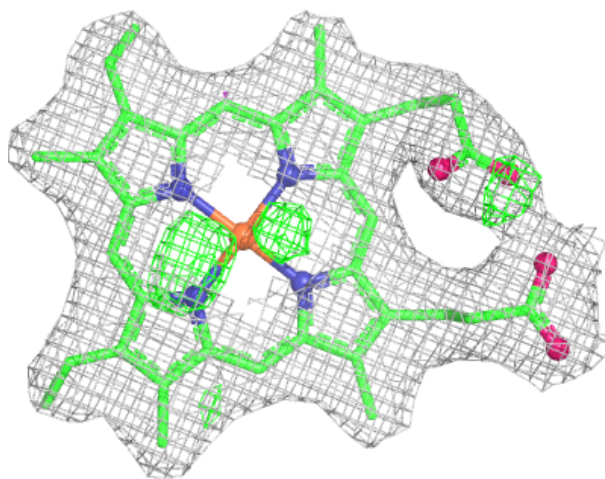
**Electron density around HEM P 501:**

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



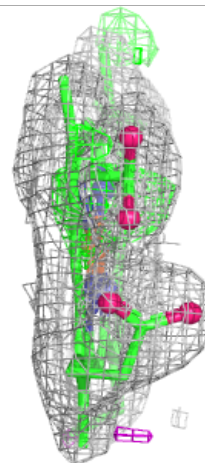
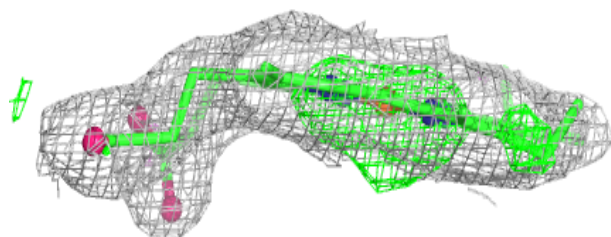
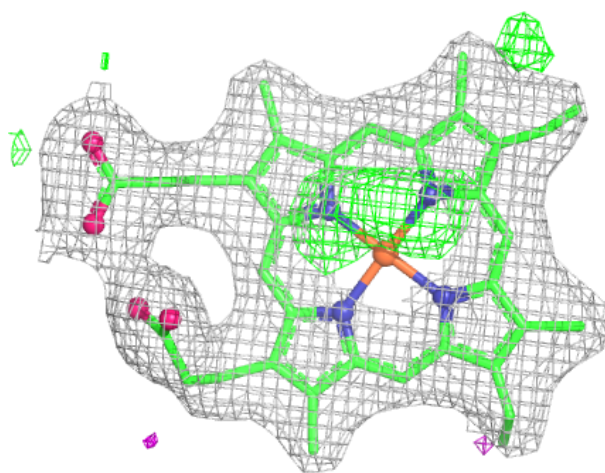
**Electron density around HEM P 502:**

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



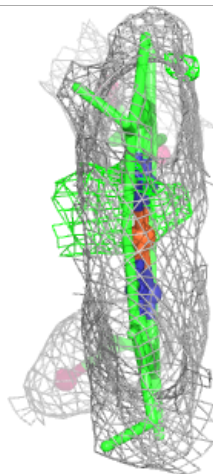
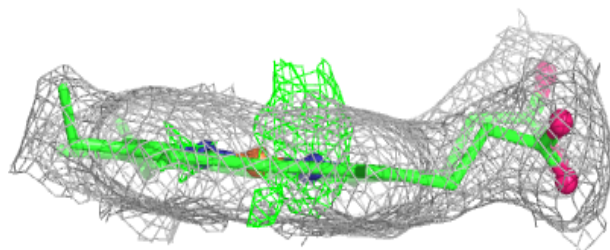
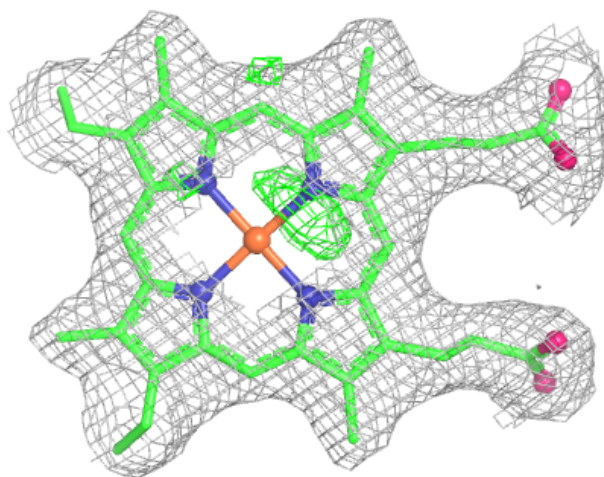
**Electron density around HEM G 502:**

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



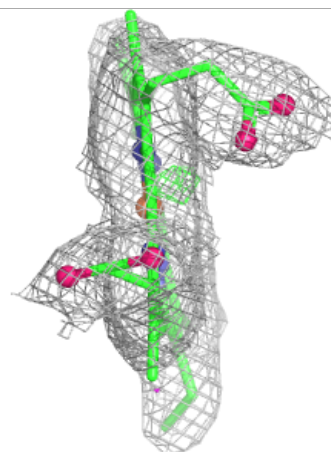
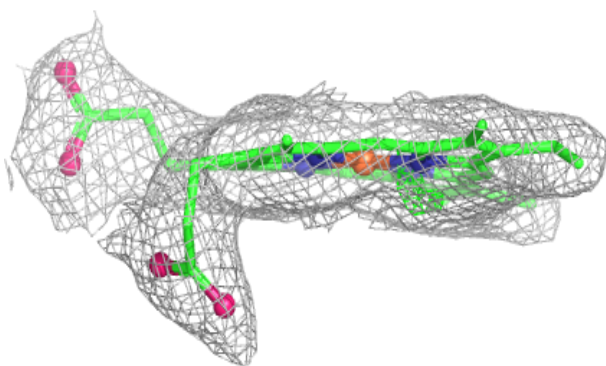
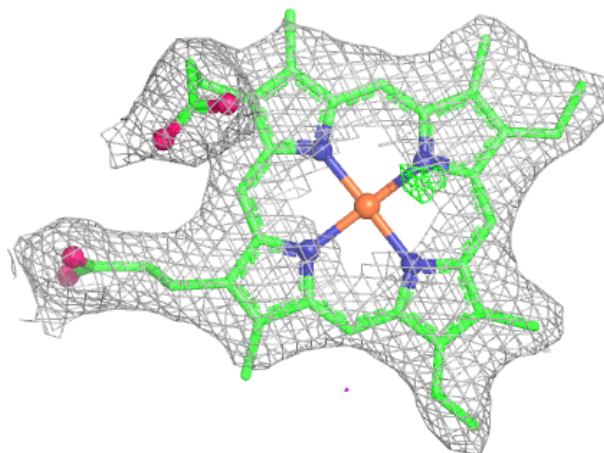
**Electron density around HEM H 301:**

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



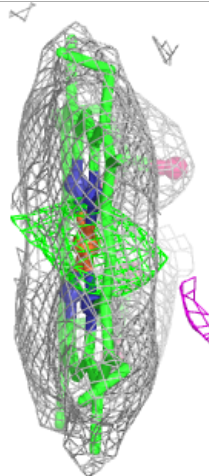
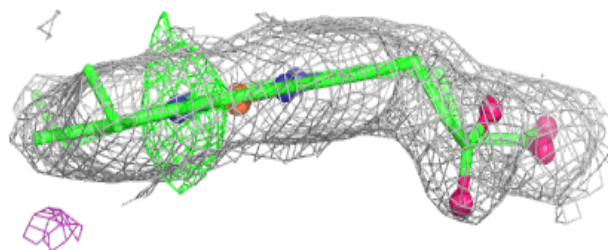
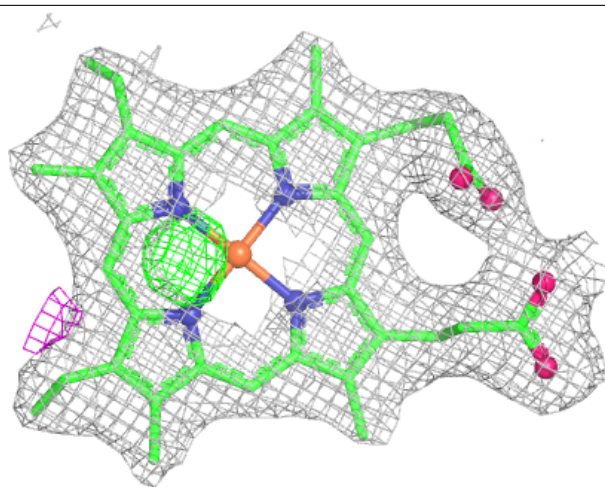
**Electron density around HEM D 501:**

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



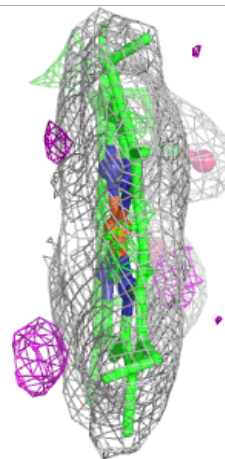
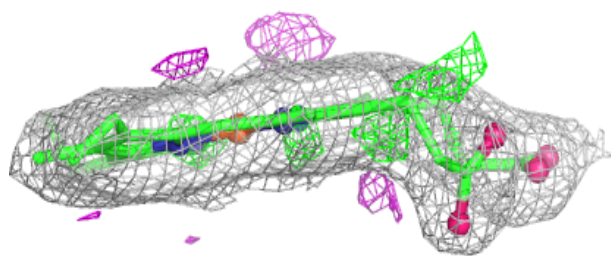
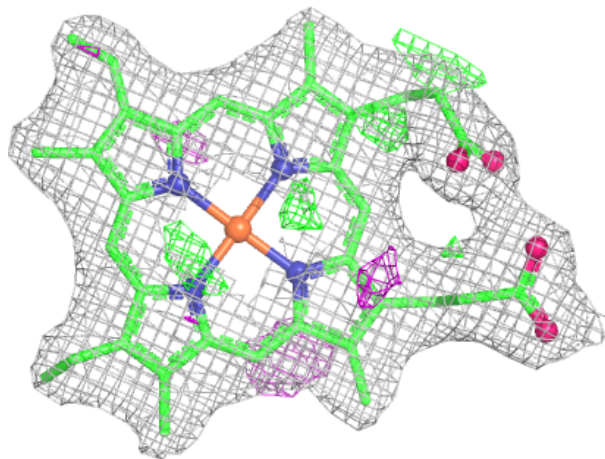
**Electron density around HEM J 502:**

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



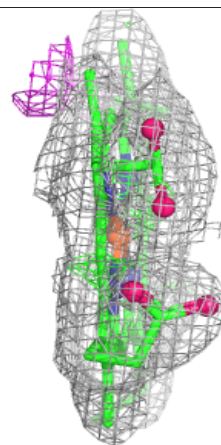
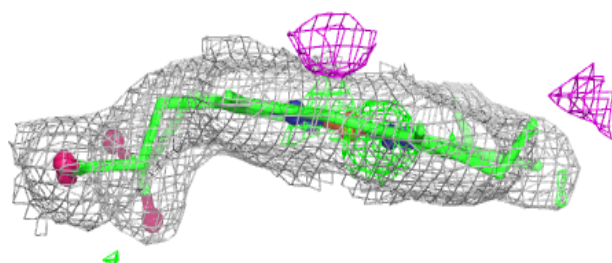
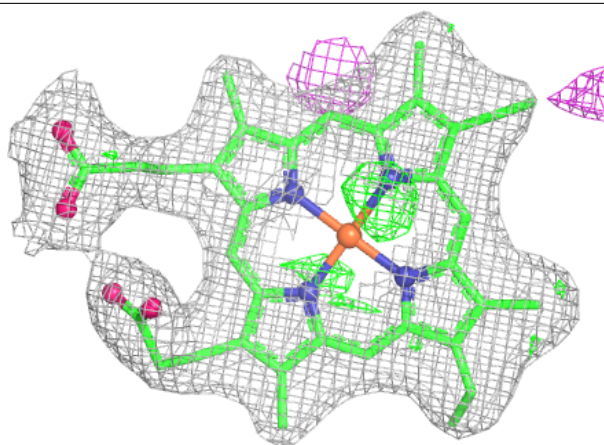
**Electron density around HEM D 502:**

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



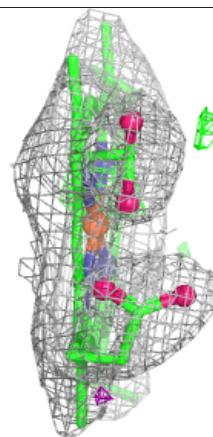
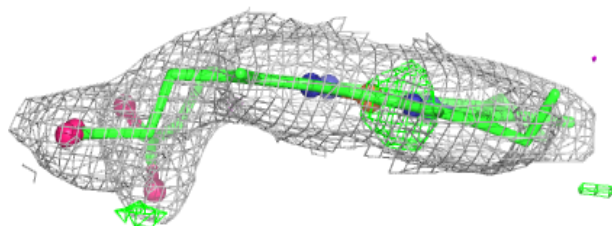
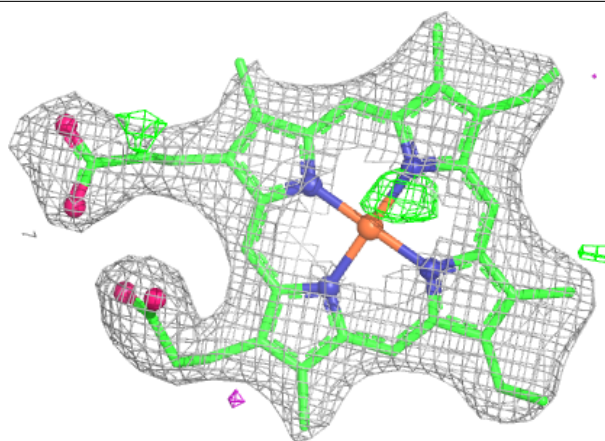
**Electron density around HEM A 502:**

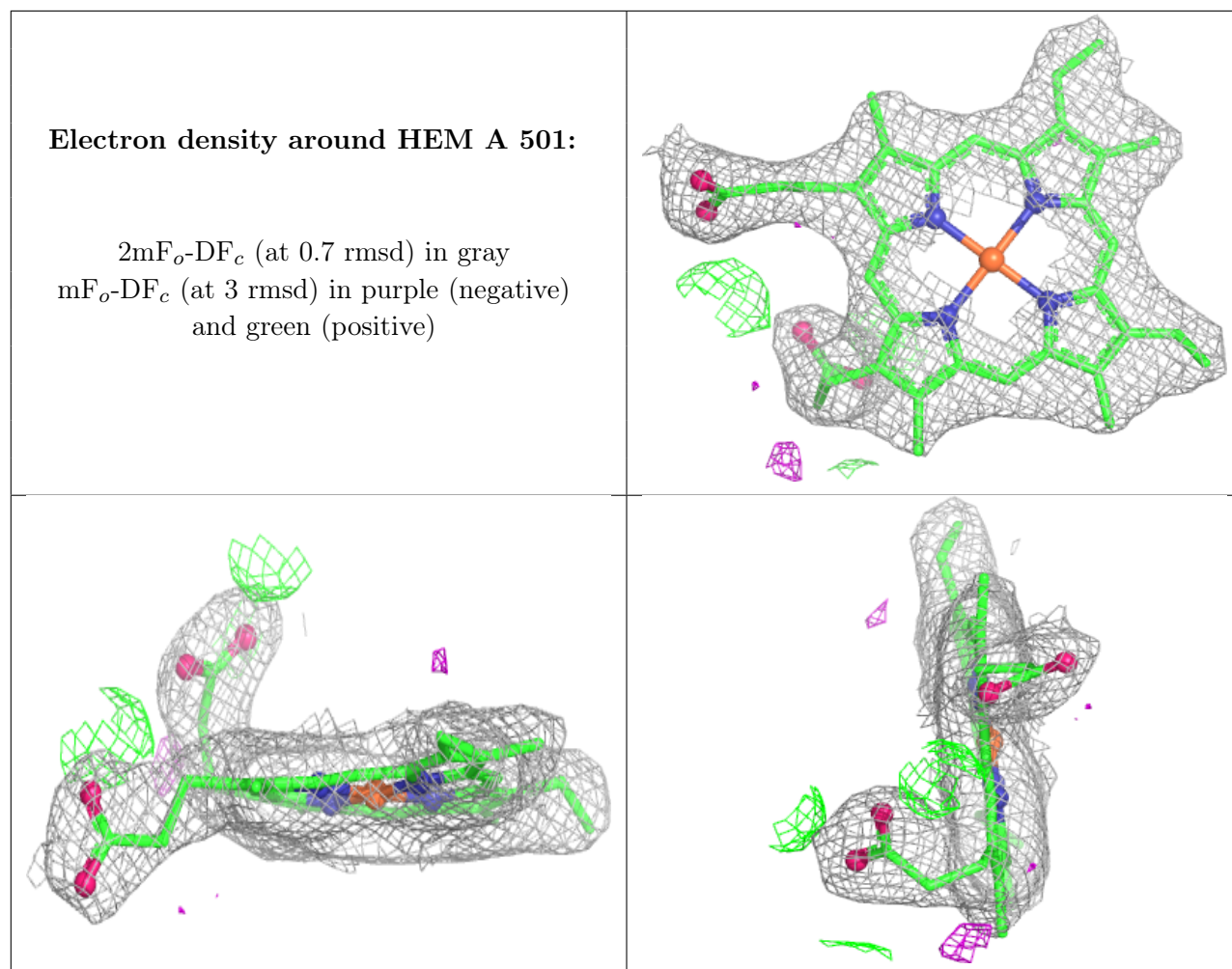
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM M 502:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.