



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:40 AM UTC

PDB ID : 4RKM / pdb\_00004rkm  
Title : Wolinella succinogenes octaheme sulfite reductase MccA, form I  
Authors : Hermann, B.; Kern, M.; La Pietra, L.; Simon, J.; Einsle, O.  
Deposited on : 2014-10-13  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

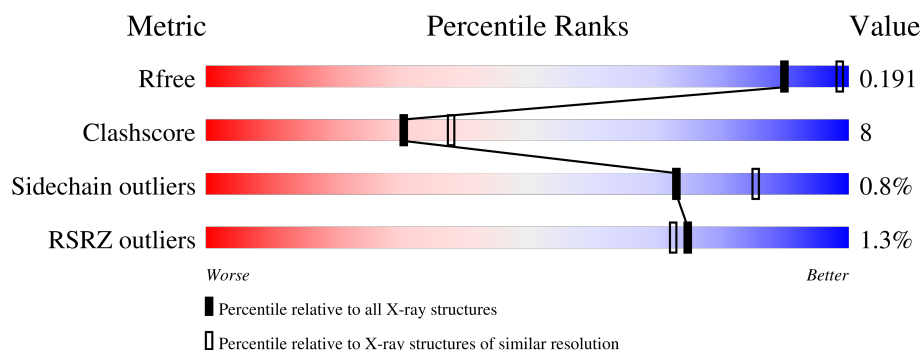
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



| Metric             | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|--------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$         | 180053                      | 6164 (2.20-2.20)                                      |
| Clashscore         | 190562                      | 6851 (2.20-2.20)                                      |
| Sidechain outliers | 187428                      | 6769 (2.20-2.20)                                      |
| RSRZ outliers      | 180081                      | 6166 (2.20-2.20)                                      |

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     | 732    | <div> <div>%</div> <div>86% 10%</div> </div>     |
| 1   | B     | 732    | <div> <div>85% 5% 10%</div> </div>               |
| 1   | C     | 732    | <div> <div>%</div> <div>85% 5% 10%</div> </div>  |
| 1   | D     | 732    | <div> <div>2%</div> <div>85% 5% 10%</div> </div> |
| 1   | E     | 732    | <div> <div>2%</div> <div>84% 6% 10%</div> </div> |
| 1   | F     | 732    | <div> <div>%</div> <div>84% 5% 10%</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 1   | G     | 732    | <div><div><div>%</div><div><div></div><div>84%</div><div>5%</div><div>10%</div></div></div></div>  |
| 1   | H     | 732    | <div><div><div>%</div><div><div></div><div>86%</div><div></div><div>10%</div></div></div></div>    |
| 1   | I     | 732    | <div><div><div></div><div><div></div><div>85%</div><div></div><div>10%</div></div></div></div>     |
| 1   | J     | 732    | <div><div><div>2%</div><div><div></div><div>84%</div><div>5%</div><div>10%</div></div></div></div> |
| 1   | K     | 732    | <div><div><div>%</div><div><div></div><div>85%</div><div>5%</div><div>10%</div></div></div></div>  |
| 1   | L     | 732    | <div><div><div>2%</div><div><div></div><div>85%</div><div>5%</div><div>10%</div></div></div></div> |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 70014 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 MccA.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | B     | 660      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5232  | 3289 | 920 | 988 | 35 |         |         |       |
| 1   | C     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | D     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | E     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | F     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | H     | 660      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5232  | 3289 | 920 | 988 | 35 |         |         |       |
| 1   | I     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | J     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | K     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | L     | 659      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5224  | 3283 | 919 | 987 | 35 |         |         |       |
| 1   | G     | 658      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5218  | 3280 | 918 | 985 | 35 |         |         |       |

There are 360 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| A     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| A     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| A     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| A     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| A     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| A     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| A     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| A     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| A     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| A     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| A     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| A     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| A     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| A     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| A     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| A     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| A     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| A     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| A     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| A     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| A     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| B     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| B     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| B     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| B     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| B     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| B     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| B     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| B     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| B     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| B     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| B     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| B     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| B     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| B     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| B     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| B     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| B     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| B     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| B     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| B     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| B     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| B     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| B     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| B     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| B     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| B     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| B     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| B     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| B     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| C     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| C     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| C     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| C     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| C     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| C     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| C     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| C     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| C     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| C     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| C     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| C     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| C     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| C     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| C     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| C     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| C     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| C     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| C     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| C     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| C     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| C     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| D     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| D     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| D     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| D     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| D     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| D     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| D     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| D     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| D     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| D     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| D     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| D     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| D     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| D     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| D     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| D     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| D     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| D     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| D     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| D     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| D     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| D     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| D     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| E     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| E     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| E     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| E     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| E     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| E     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| E     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| E     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| E     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| E     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| E     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| E     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| E     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| E     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| E     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| E     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| E     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| E     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| E     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| E     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| E     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| E     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| E     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| E     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| E     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| E     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| E     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| E     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| E     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| F     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| F     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| F     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| F     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| F     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| F     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| F     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| F     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| F     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| F     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| F     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| F     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| F     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| F     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| F     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| F     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| F     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| F     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| F     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| F     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| F     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| F     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| H     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| H     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| H     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| H     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| H     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| H     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| H     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| H     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| H     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| H     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| H     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| H     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| H     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| H     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| H     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| H     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| H     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| H     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| H     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| H     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| H     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| H     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| H     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| I     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| I     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| I     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| I     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| I     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| I     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| I     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| I     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| I     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| I     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| I     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| I     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| I     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| I     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| I     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| I     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| I     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| I     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| I     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| I     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| I     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| I     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| J     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| J     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| J     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| J     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| J     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| J     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| J     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| J     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| J     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| J     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| J     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| J     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| J     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| J     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| J     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| J     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| J     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| J     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| J     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| J     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| J     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| J     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| J     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| J     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| J     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| J     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| J     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| J     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| J     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| J     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| K     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| K     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| K     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| K     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| K     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| K     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| K     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| K     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| K     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| K     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| K     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| K     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| K     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| K     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| K     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| K     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| K     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| K     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| K     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| K     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| K     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| K     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| L     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| L     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| L     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| L     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| L     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| L     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| L     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| L     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| L     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| L     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| L     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| L     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| L     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| L     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| L     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| L     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| L     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| L     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| L     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| L     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| L     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| L     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| L     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| G     | 691     | SER      | -      | expression tag | UNP Q7MSJ8 |
| G     | 692     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| G     | 693     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| G     | 694     | SER      | -      | expression tag | UNP Q7MSJ8 |
| G     | 695     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| G     | 696     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| G     | 697     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| G     | 698     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| G     | 699     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| G     | 700     | LYS      | -      | expression tag | UNP Q7MSJ8 |
| G     | 701     | GLY      | -      | expression tag | UNP Q7MSJ8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 702     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| G     | 703     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| G     | 704     | SER      | -      | expression tag | UNP Q7MSJ8 |
| G     | 705     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| G     | 706     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| G     | 707     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| G     | 708     | SER      | -      | expression tag | UNP Q7MSJ8 |
| G     | 709     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| G     | 710     | GLY      | -      | expression tag | UNP Q7MSJ8 |
| G     | 711     | SER      | -      | expression tag | UNP Q7MSJ8 |
| G     | 712     | ALA      | -      | expression tag | UNP Q7MSJ8 |
| G     | 713     | TRP      | -      | expression tag | UNP Q7MSJ8 |
| G     | 714     | SER      | -      | expression tag | UNP Q7MSJ8 |
| G     | 715     | HIS      | -      | expression tag | UNP Q7MSJ8 |
| G     | 716     | PRO      | -      | expression tag | UNP Q7MSJ8 |
| G     | 717     | GLN      | -      | expression tag | UNP Q7MSJ8 |
| G     | 718     | PHE      | -      | expression tag | UNP Q7MSJ8 |
| G     | 719     | GLU      | -      | expression tag | UNP Q7MSJ8 |
| G     | 720     | LYS      | -      | expression tag | UNP Q7MSJ8 |

- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

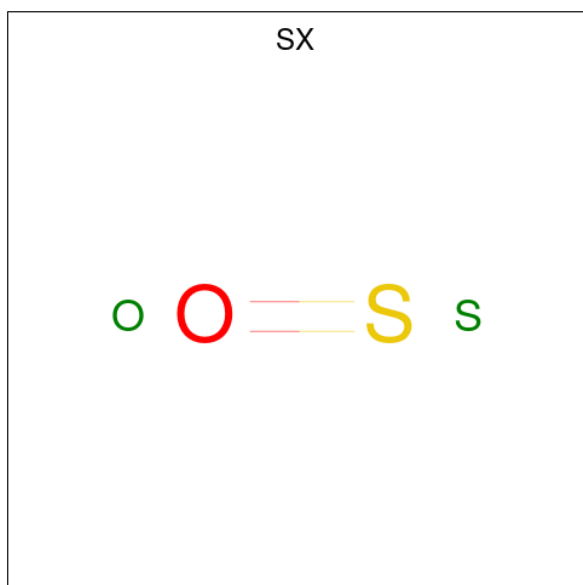
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | A     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | C     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | D     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | E     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | F     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | H     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | I     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | J     | 1        | Total Cu<br>1 1 | 0       | 0       |
| 2   | K     | 1        | Total Cu<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | L     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | G     | 1        | Total | Cu | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is SULFUR OXIDE (CCD ID: SX) (formula: OS).



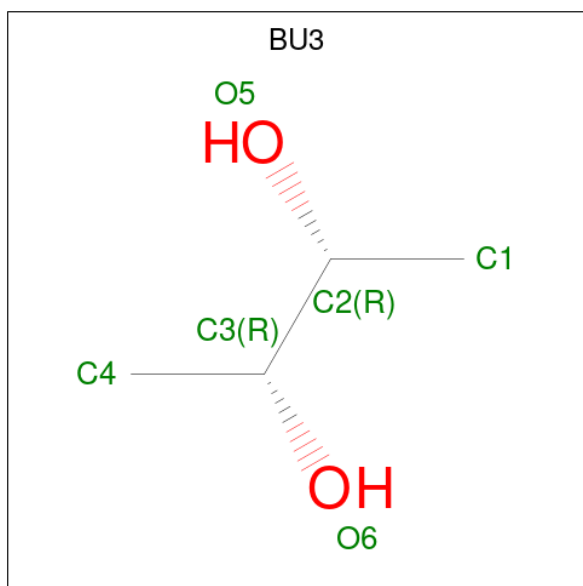
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>).



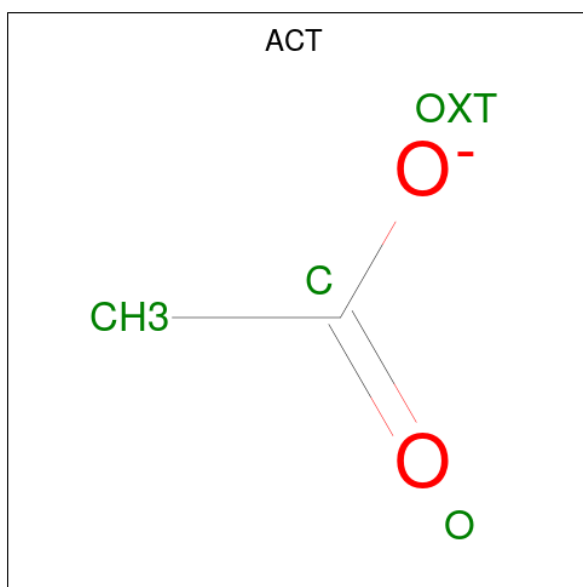
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 4 | 2 |         |         |

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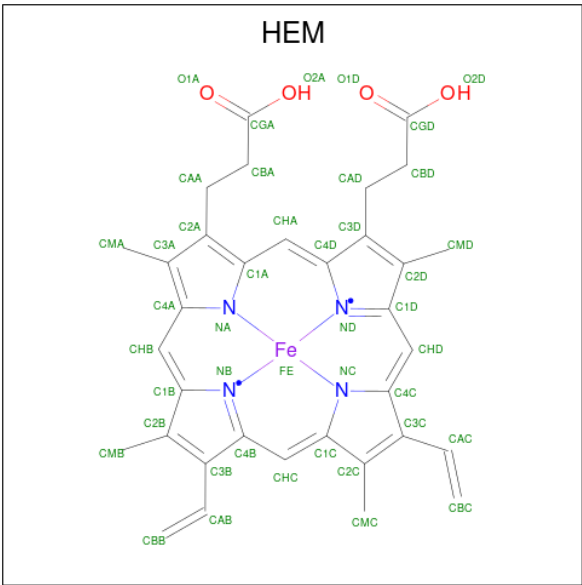
| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | E     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | H     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | I     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | I     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | J     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | J     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | K     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | K     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | L     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | L     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>6 4 2 | 0       | 0       |
| 4   | G     | 1        | Total C O<br>6 4 2 | 0       | 0       |

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 4     | 2 | 2 |         |         |

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



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

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 6   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

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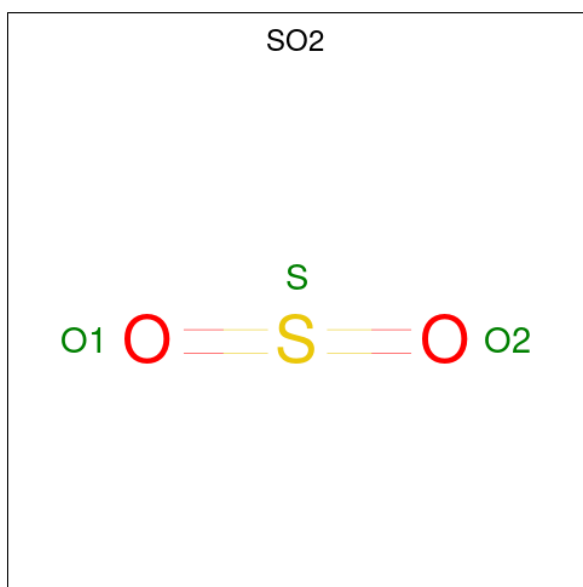
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 6   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 7 is SULFUR DIOXIDE (CCD ID: SO2) (formula: O<sub>2</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |
| 7   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |
| 7   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |
| 7   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 3     | 2 | 1 |         |         |

- Molecule 8 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 8   | A     | 416      | Total | O   | 0       | 0       |
|     |       |          | 416   | 416 |         |         |
| 8   | B     | 298      | Total | O   | 0       | 0       |
|     |       |          | 298   | 298 |         |         |
| 8   | C     | 285      | Total | O   | 0       | 0       |
|     |       |          | 285   | 285 |         |         |
| 8   | D     | 307      | Total | O   | 0       | 0       |
|     |       |          | 307   | 307 |         |         |
| 8   | E     | 219      | Total | O   | 0       | 0       |
|     |       |          | 219   | 219 |         |         |
| 8   | F     | 245      | Total | O   | 0       | 0       |
|     |       |          | 245   | 245 |         |         |
| 8   | H     | 250      | Total | O   | 0       | 0       |
|     |       |          | 250   | 250 |         |         |
| 8   | I     | 218      | Total | O   | 0       | 0       |
|     |       |          | 218   | 218 |         |         |

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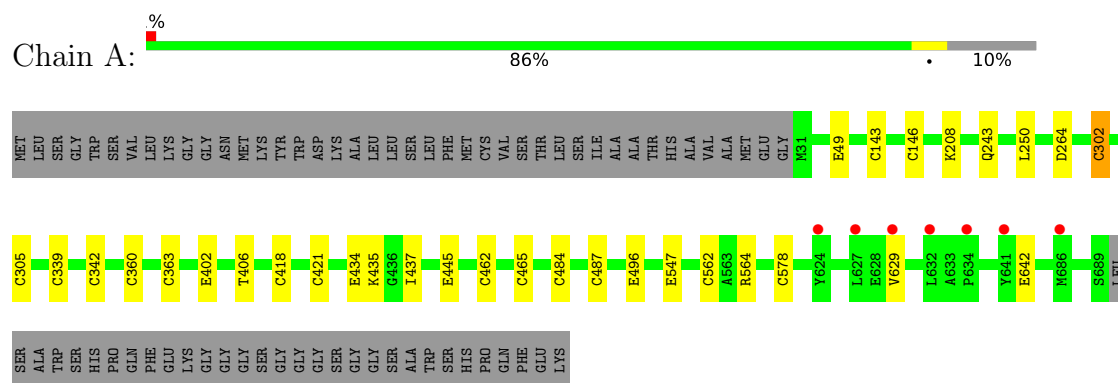
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 8   | J     | 180      | Total<br>180 | O<br>180 | 0       | 0       |
| 8   | K     | 158      | Total<br>158 | O<br>158 | 0       | 0       |
| 8   | L     | 126      | Total<br>126 | O<br>126 | 0       | 0       |
| 8   | G     | 232      | Total<br>232 | O<br>232 | 0       | 0       |

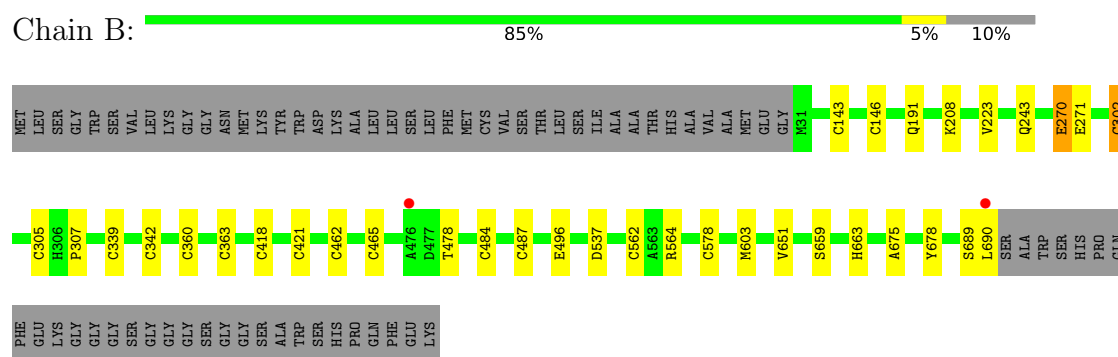
### 3 Residue-property plots [i](#)

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

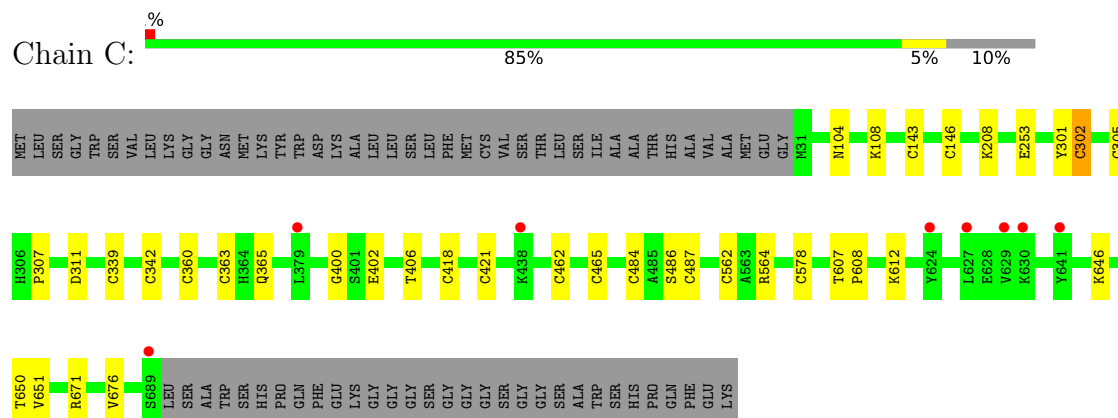
#### • Molecule 1: MccA



#### • Molecule 1: MccA

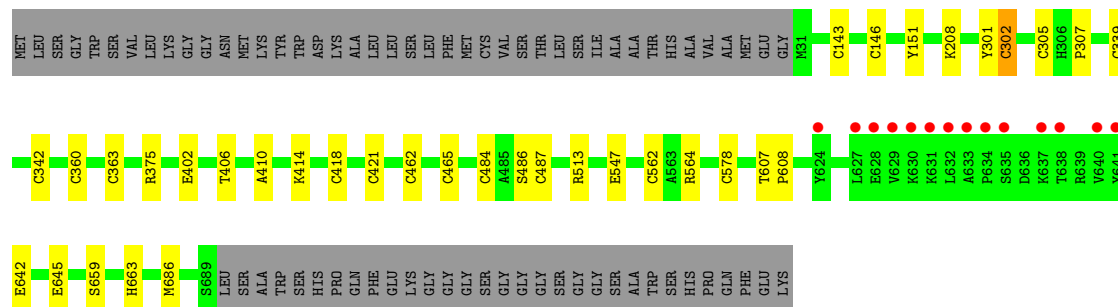


#### • Molecule 1: MccA



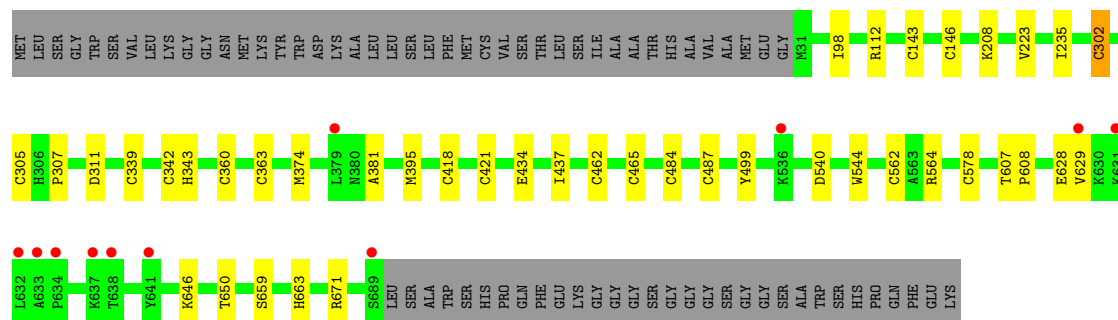
## ● Molecule 1: MccA

Chain D: 



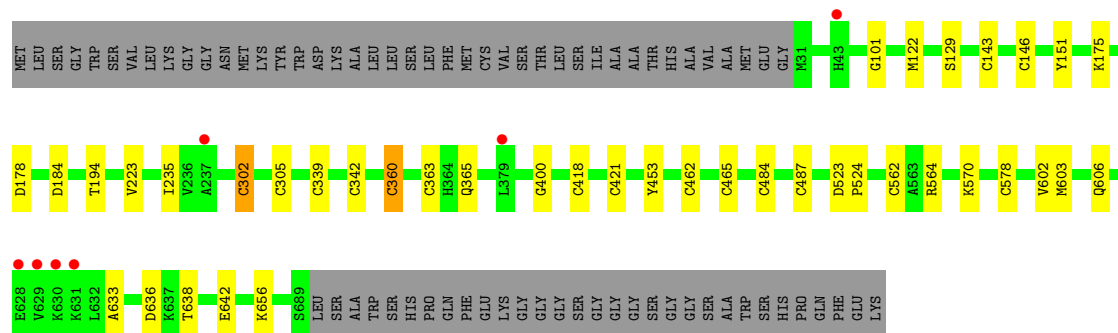
## ● Molecule 1: MccA

Chain E: 



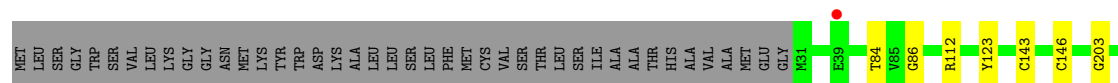
## ● Molecule 1: MccA

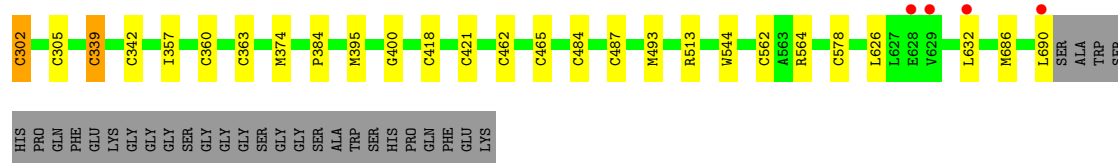
Chain F: 



## ● Molecule 1: MccA

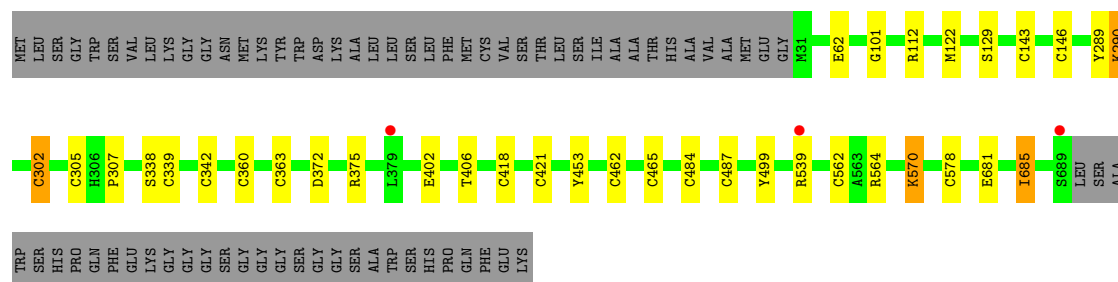
Chain H: 





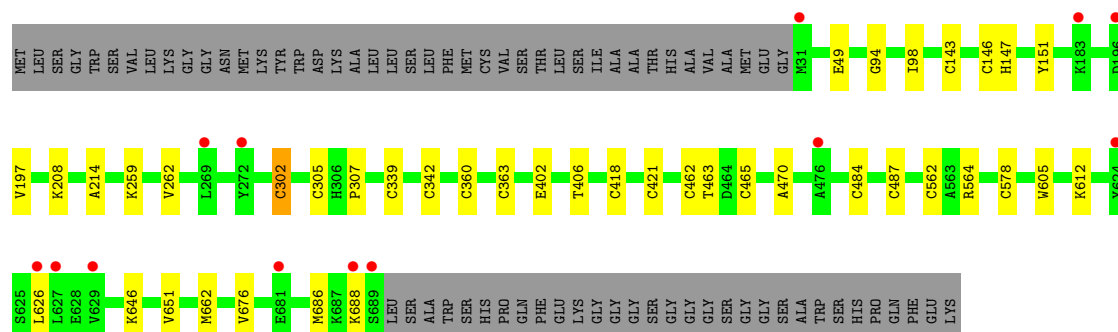
• Molecule 1: MccA

Chain I: 85% 10%



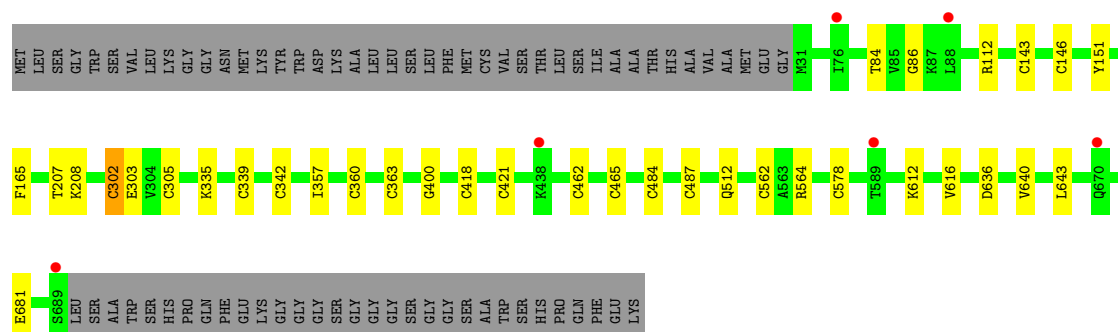
• Molecule 1: MccA

Chain J: 84% 5% 10%



• Molecule 1: MccA

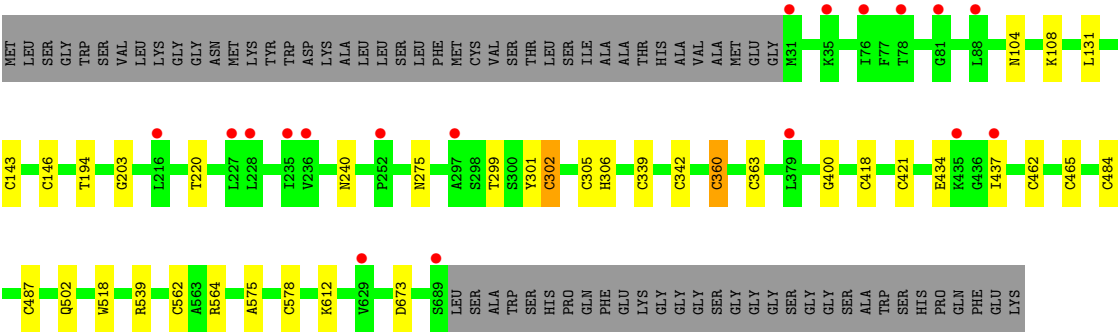
Chain K: 85% 5% 10%



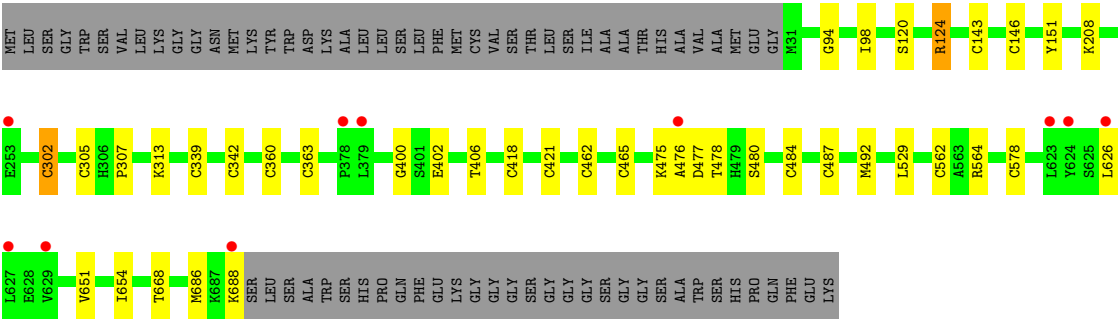
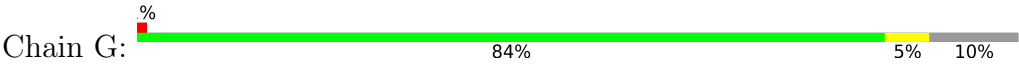
• Molecule 1: MccA

Chain L: 85% 5% 10%





● Molecule 1: MccA



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.12Å 103.04Å 233.07Å<br>90.00° 98.46° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.37 – 2.20<br>49.37 – 2.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (49.37-2.20)<br>99.8 (49.37-2.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.20                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.54 (at 2.20Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0049                                             | Depositor        |
| R, $R_{free}$                                                           | 0.184 , 0.220<br>(Not available) , 0.191                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 24857 reflections (4.96%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.014                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 35.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 70014                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 39.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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: CU1, SX, BU3, HEM, ACT, SO2

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     | 0.48         | 0/5354  | 0.72        | 0/7212         |
| 1   | B     | 0.44         | 0/5362  | 0.72        | 0/7223         |
| 1   | C     | 0.45         | 0/5354  | 0.72        | 0/7212         |
| 1   | D     | 0.43         | 0/5354  | 0.72        | 0/7212         |
| 1   | E     | 0.43         | 0/5354  | 0.71        | 1/7212 (0.0%)  |
| 1   | F     | 0.44         | 0/5354  | 0.72        | 0/7212         |
| 1   | G     | 0.44         | 0/5348  | 0.72        | 0/7204         |
| 1   | H     | 0.43         | 0/5362  | 0.72        | 0/7223         |
| 1   | I     | 0.44         | 0/5354  | 0.71        | 0/7212         |
| 1   | J     | 0.42         | 0/5354  | 0.71        | 0/7212         |
| 1   | K     | 0.42         | 0/5354  | 0.72        | 0/7212         |
| 1   | L     | 0.43         | 0/5354  | 0.72        | 0/7212         |
| All | All   | 0.44         | 0/64258 | 0.72        | 1/86558 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 98  | ILE  | CB-CA-C | -5.41 | 106.24      | 111.05   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5224  | 0        | 5051     | 72      | 0            |
| 1   | B     | 5232  | 0        | 5063     | 68      | 0            |
| 1   | C     | 5224  | 0        | 5052     | 74      | 0            |
| 1   | D     | 5224  | 0        | 5054     | 72      | 0            |
| 1   | E     | 5224  | 0        | 5052     | 77      | 0            |
| 1   | F     | 5224  | 0        | 5052     | 72      | 0            |
| 1   | G     | 5218  | 0        | 5048     | 73      | 0            |
| 1   | H     | 5232  | 0        | 5064     | 70      | 0            |
| 1   | I     | 5224  | 0        | 5053     | 68      | 0            |
| 1   | J     | 5224  | 0        | 5054     | 71      | 0            |
| 1   | K     | 5224  | 0        | 5053     | 68      | 0            |
| 1   | L     | 5224  | 0        | 5054     | 72      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 1     | 0        | 0        | 0       | 0            |
| 2   | J     | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 2     | 0        | 0        | 0       | 0            |
| 3   | B     | 2     | 0        | 0        | 0       | 0            |
| 3   | C     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 2     | 0        | 0        | 0       | 0            |
| 3   | F     | 2     | 0        | 0        | 0       | 0            |
| 3   | G     | 2     | 0        | 0        | 0       | 0            |
| 3   | H     | 2     | 0        | 0        | 0       | 0            |
| 3   | J     | 2     | 0        | 0        | 0       | 0            |
| 3   | K     | 2     | 0        | 0        | 0       | 0            |
| 3   | L     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 12    | 0        | 20       | 0       | 0            |
| 4   | B     | 18    | 0        | 30       | 0       | 0            |
| 4   | C     | 12    | 0        | 20       | 0       | 0            |
| 4   | D     | 12    | 0        | 20       | 0       | 0            |
| 4   | E     | 12    | 0        | 20       | 2       | 0            |
| 4   | F     | 18    | 0        | 30       | 0       | 0            |
| 4   | G     | 12    | 0        | 20       | 0       | 0            |
| 4   | H     | 18    | 0        | 30       | 1       | 0            |
| 4   | I     | 12    | 0        | 20       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | J     | 12    | 0        | 20       | 0       | 0            |
| 4   | K     | 12    | 0        | 20       | 1       | 0            |
| 4   | L     | 12    | 0        | 20       | 0       | 0            |
| 5   | A     | 4     | 0        | 3        | 0       | 0            |
| 5   | B     | 4     | 0        | 3        | 0       | 0            |
| 5   | C     | 4     | 0        | 3        | 1       | 0            |
| 5   | D     | 4     | 0        | 3        | 0       | 0            |
| 5   | E     | 4     | 0        | 3        | 0       | 0            |
| 5   | F     | 4     | 0        | 3        | 1       | 0            |
| 5   | G     | 4     | 0        | 3        | 0       | 0            |
| 5   | H     | 4     | 0        | 3        | 0       | 0            |
| 5   | I     | 4     | 0        | 3        | 0       | 0            |
| 5   | J     | 4     | 0        | 3        | 0       | 0            |
| 5   | K     | 4     | 0        | 3        | 0       | 0            |
| 5   | L     | 4     | 0        | 3        | 0       | 0            |
| 6   | A     | 344   | 0        | 240      | 64      | 0            |
| 6   | B     | 344   | 0        | 240      | 65      | 0            |
| 6   | C     | 344   | 0        | 240      | 70      | 0            |
| 6   | D     | 344   | 0        | 240      | 67      | 0            |
| 6   | E     | 344   | 0        | 240      | 65      | 0            |
| 6   | F     | 344   | 0        | 240      | 61      | 0            |
| 6   | G     | 344   | 0        | 240      | 65      | 0            |
| 6   | H     | 344   | 0        | 240      | 67      | 0            |
| 6   | I     | 344   | 0        | 240      | 58      | 0            |
| 6   | J     | 344   | 0        | 240      | 64      | 0            |
| 6   | K     | 344   | 0        | 240      | 63      | 0            |
| 6   | L     | 344   | 0        | 240      | 75      | 0            |
| 7   | A     | 3     | 0        | 0        | 0       | 0            |
| 7   | D     | 3     | 0        | 0        | 0       | 0            |
| 7   | G     | 3     | 0        | 0        | 0       | 0            |
| 7   | I     | 3     | 0        | 0        | 0       | 0            |
| 8   | A     | 416   | 0        | 0        | 2       | 0            |
| 8   | B     | 298   | 0        | 0        | 0       | 0            |
| 8   | C     | 285   | 0        | 0        | 0       | 0            |
| 8   | D     | 307   | 0        | 0        | 1       | 0            |
| 8   | E     | 219   | 0        | 0        | 1       | 0            |
| 8   | F     | 245   | 0        | 0        | 0       | 0            |
| 8   | G     | 232   | 0        | 0        | 0       | 0            |
| 8   | H     | 250   | 0        | 0        | 0       | 0            |
| 8   | I     | 218   | 0        | 0        | 0       | 0            |
| 8   | J     | 180   | 0        | 0        | 0       | 0            |
| 8   | K     | 158   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | L     | 126   | 0        | 0        | 0       | 0            |
| All | All   | 70014 | 0        | 63836    | 897     | 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 8.

All (897) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:A:462:CYS:SG | 6:A:811:HEM:HAB | 1.41                     | 1.55              |
| 1:A:339:CYS:SG | 6:A:808:HEM:CAB | 2.04                     | 1.46              |
| 1:A:462:CYS:SG | 6:A:811:HEM:CAB | 2.02                     | 1.46              |
| 1:F:462:CYS:SG | 6:F:812:HEM:CAB | 2.03                     | 1.46              |
| 1:A:484:CYS:SG | 6:A:812:HEM:CAB | 2.05                     | 1.45              |
| 1:C:462:CYS:SG | 6:C:811:HEM:CAB | 2.03                     | 1.45              |
| 1:B:339:CYS:SG | 6:B:809:HEM:CAB | 2.05                     | 1.44              |
| 1:I:462:CYS:SG | 6:I:811:HEM:CAB | 2.06                     | 1.44              |
| 1:C:418:CYS:SG | 6:C:810:HEM:CAB | 2.03                     | 1.44              |
| 1:H:484:CYS:SG | 6:H:813:HEM:CAB | 2.04                     | 1.44              |
| 1:E:339:CYS:SG | 6:E:808:HEM:CAB | 2.06                     | 1.43              |
| 1:E:462:CYS:SG | 6:E:811:HEM:CAB | 2.05                     | 1.43              |
| 1:D:484:CYS:SG | 6:D:812:HEM:CAB | 2.07                     | 1.43              |
| 1:F:562:CYS:SG | 6:F:814:HEM:CAB | 2.07                     | 1.43              |
| 1:K:143:CYS:SG | 6:K:806:HEM:HAB | 1.57                     | 1.43              |
| 1:D:418:CYS:SG | 6:D:810:HEM:CAB | 2.07                     | 1.42              |
| 1:I:339:CYS:SG | 6:I:808:HEM:CAB | 2.07                     | 1.42              |
| 1:C:562:CYS:SG | 6:C:813:HEM:CAB | 2.08                     | 1.42              |
| 1:E:484:CYS:SG | 6:E:812:HEM:CAB | 2.08                     | 1.41              |
| 1:C:339:CYS:SG | 6:C:808:HEM:CAB | 2.08                     | 1.41              |
| 1:K:462:CYS:SG | 6:K:811:HEM:CAB | 2.09                     | 1.41              |
| 1:G:418:CYS:SG | 6:G:810:HEM:CAB | 2.06                     | 1.41              |
| 1:D:562:CYS:SG | 6:D:813:HEM:CAB | 2.08                     | 1.41              |
| 1:A:418:CYS:SG | 6:A:810:HEM:CAB | 2.07                     | 1.41              |
| 1:C:360:CYS:SG | 6:C:809:HEM:CAB | 2.09                     | 1.40              |
| 1:A:562:CYS:SG | 6:A:813:HEM:CAB | 2.08                     | 1.40              |
| 1:C:484:CYS:SG | 6:C:812:HEM:CAB | 2.09                     | 1.40              |
| 1:D:462:CYS:SG | 6:D:811:HEM:CAB | 2.09                     | 1.40              |
| 1:E:418:CYS:SG | 6:E:810:HEM:CAB | 2.09                     | 1.40              |
| 1:B:562:CYS:SG | 6:B:814:HEM:CAB | 2.08                     | 1.40              |
| 1:I:484:CYS:SG | 6:I:812:HEM:CAB | 2.10                     | 1.40              |
| 1:L:339:CYS:SG | 6:L:808:HEM:CAB | 2.10                     | 1.40              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:B:418:CYS:SG | 6:B:811:HEM:CAB | 2.08                     | 1.39              |
| 1:B:143:CYS:SG | 6:B:807:HEM:CAB | 2.10                     | 1.39              |
| 1:G:484:CYS:SG | 6:G:812:HEM:CAB | 2.11                     | 1.39              |
| 1:G:562:CYS:SG | 6:G:813:HEM:CAB | 2.11                     | 1.39              |
| 1:D:339:CYS:SG | 6:D:808:HEM:CAB | 2.09                     | 1.39              |
| 1:J:462:CYS:SG | 6:J:811:HEM:CAB | 2.10                     | 1.39              |
| 1:I:363:CYS:SG | 6:I:809:HEM:CAC | 2.11                     | 1.39              |
| 1:I:418:CYS:SG | 6:I:810:HEM:CAB | 2.09                     | 1.39              |
| 1:J:339:CYS:SG | 6:J:808:HEM:CAB | 2.11                     | 1.39              |
| 1:J:562:CYS:SG | 6:J:813:HEM:CAB | 2.11                     | 1.39              |
| 1:E:562:CYS:SG | 6:E:813:HEM:CAB | 2.09                     | 1.38              |
| 1:L:562:CYS:SG | 6:L:813:HEM:CAB | 2.11                     | 1.38              |
| 1:K:339:CYS:SG | 6:K:808:HEM:CAB | 2.10                     | 1.38              |
| 1:G:143:CYS:SG | 6:G:806:HEM:CAB | 2.10                     | 1.38              |
| 1:D:143:CYS:SG | 6:D:806:HEM:CAB | 2.11                     | 1.38              |
| 1:F:418:CYS:SG | 6:F:811:HEM:CAB | 2.12                     | 1.38              |
| 1:H:462:CYS:SG | 6:H:812:HEM:CAB | 2.09                     | 1.38              |
| 1:J:484:CYS:SG | 6:J:812:HEM:CAB | 2.12                     | 1.37              |
| 1:I:562:CYS:SG | 6:I:813:HEM:CAB | 2.12                     | 1.37              |
| 1:H:418:CYS:SG | 6:H:811:HEM:CAB | 2.11                     | 1.37              |
| 1:J:418:CYS:SG | 6:J:810:HEM:CAB | 2.10                     | 1.37              |
| 1:K:143:CYS:SG | 6:K:806:HEM:CAB | 2.10                     | 1.37              |
| 1:C:143:CYS:SG | 6:C:806:HEM:CAB | 2.13                     | 1.36              |
| 1:C:363:CYS:SG | 6:C:809:HEM:CAC | 2.14                     | 1.36              |
| 1:A:363:CYS:SG | 6:A:809:HEM:CAC | 2.13                     | 1.36              |
| 1:J:143:CYS:SG | 6:J:806:HEM:CAB | 2.12                     | 1.35              |
| 1:K:562:CYS:SG | 6:K:813:HEM:CAB | 2.12                     | 1.35              |
| 1:D:363:CYS:SG | 6:D:809:HEM:CAC | 2.14                     | 1.35              |
| 1:L:484:CYS:SG | 6:L:812:HEM:CAB | 2.14                     | 1.35              |
| 1:B:360:CYS:SG | 6:B:810:HEM:CAB | 2.15                     | 1.35              |
| 1:E:360:CYS:SG | 6:E:809:HEM:CAB | 2.13                     | 1.35              |
| 1:D:360:CYS:SG | 6:D:809:HEM:CAB | 2.15                     | 1.34              |
| 1:L:418:CYS:SG | 6:L:810:HEM:CAB | 2.15                     | 1.34              |
| 1:F:363:CYS:SG | 6:F:810:HEM:CAC | 2.14                     | 1.34              |
| 1:H:418:CYS:HG | 6:H:811:HEM:CAB | 1.41                     | 1.34              |
| 1:L:143:CYS:SG | 6:L:806:HEM:CAB | 2.15                     | 1.34              |
| 1:E:363:CYS:SG | 6:E:809:HEM:CAC | 2.16                     | 1.34              |
| 1:H:143:CYS:SG | 6:H:807:HEM:CAB | 2.15                     | 1.33              |
| 1:C:305:CYS:SG | 6:C:807:HEM:CAC | 2.16                     | 1.33              |
| 1:K:363:CYS:SG | 6:K:809:HEM:CAC | 2.16                     | 1.33              |
| 1:L:360:CYS:SG | 6:L:809:HEM:CAB | 2.17                     | 1.33              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:B:363:CYS:SG | 6:B:810:HEM:CAC | 2.16                     | 1.33              |
| 1:A:418:CYS:HG | 6:A:810:HEM:CAB | 1.36                     | 1.32              |
| 1:E:143:CYS:SG | 6:E:806:HEM:CAB | 2.17                     | 1.32              |
| 1:E:418:CYS:HG | 6:E:810:HEM:CAB | 1.40                     | 1.32              |
| 1:E:305:CYS:SG | 6:E:807:HEM:CAC | 2.17                     | 1.32              |
| 1:H:487:CYS:SG | 6:H:813:HEM:CAC | 2.18                     | 1.31              |
| 1:K:360:CYS:SG | 6:K:809:HEM:CAB | 2.18                     | 1.31              |
| 1:A:487:CYS:SG | 6:A:812:HEM:CAC | 2.18                     | 1.31              |
| 1:F:360:CYS:SG | 6:F:810:HEM:CAB | 2.18                     | 1.31              |
| 1:H:360:CYS:SG | 6:H:810:HEM:CAB | 2.18                     | 1.31              |
| 1:I:143:CYS:SG | 6:I:806:HEM:CAB | 2.18                     | 1.31              |
| 1:J:305:CYS:SG | 6:J:807:HEM:CAC | 2.19                     | 1.31              |
| 1:L:462:CYS:SG | 6:L:811:HEM:CAB | 2.19                     | 1.31              |
| 1:A:360:CYS:SG | 6:A:809:HEM:CAB | 2.18                     | 1.31              |
| 1:G:360:CYS:SG | 6:G:809:HEM:CAB | 2.19                     | 1.31              |
| 1:H:305:CYS:SG | 6:H:808:HEM:CAC | 2.19                     | 1.30              |
| 1:I:305:CYS:SG | 6:I:807:HEM:CAC | 2.19                     | 1.30              |
| 1:I:360:CYS:SG | 6:I:809:HEM:CAB | 2.19                     | 1.30              |
| 1:J:363:CYS:SG | 6:J:809:HEM:CAC | 2.19                     | 1.30              |
| 1:D:305:CYS:SG | 6:D:807:HEM:CAC | 2.19                     | 1.30              |
| 1:F:578:CYS:SG | 6:F:814:HEM:CAC | 2.19                     | 1.30              |
| 1:K:305:CYS:SG | 6:K:807:HEM:CAC | 2.20                     | 1.30              |
| 1:C:342:CYS:SG | 6:C:808:HEM:CAC | 2.19                     | 1.30              |
| 1:D:487:CYS:SG | 6:D:812:HEM:CAC | 2.20                     | 1.30              |
| 1:C:339:CYS:HG | 6:C:808:HEM:CAB | 1.40                     | 1.29              |
| 1:E:578:CYS:SG | 6:E:813:HEM:CAC | 2.19                     | 1.29              |
| 1:I:342:CYS:SG | 6:I:808:HEM:CAC | 2.20                     | 1.29              |
| 1:B:305:CYS:SG | 6:B:808:HEM:CAC | 2.18                     | 1.29              |
| 1:C:146:CYS:SG | 6:C:806:HEM:CAC | 2.20                     | 1.29              |
| 1:F:146:CYS:SG | 6:F:807:HEM:CAC | 2.20                     | 1.29              |
| 1:G:487:CYS:SG | 6:G:812:HEM:CAC | 2.21                     | 1.29              |
| 1:E:487:CYS:SG | 6:E:812:HEM:CAC | 2.20                     | 1.29              |
| 1:B:487:CYS:SG | 6:B:813:HEM:CAC | 2.21                     | 1.29              |
| 1:K:487:CYS:SG | 6:K:812:HEM:CAC | 2.21                     | 1.29              |
| 1:F:487:CYS:SG | 6:F:813:HEM:CAC | 2.22                     | 1.28              |
| 1:H:465:CYS:SG | 6:H:812:HEM:CAC | 2.21                     | 1.28              |
| 1:A:146:CYS:SG | 6:A:806:HEM:CAC | 2.22                     | 1.28              |
| 1:C:487:CYS:SG | 6:C:812:HEM:CAC | 2.20                     | 1.28              |
| 1:H:578:CYS:HG | 6:H:814:HEM:CAC | 1.46                     | 1.28              |
| 1:D:342:CYS:SG | 6:D:808:HEM:CAC | 2.22                     | 1.28              |
| 1:E:146:CYS:SG | 6:E:806:HEM:CAC | 2.22                     | 1.28              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:H:578:CYS:SG | 6:H:814:HEM:CAC | 2.20                     | 1.28              |
| 1:J:578:CYS:SG | 6:J:813:HEM:CAC | 2.22                     | 1.28              |
| 1:G:465:CYS:SG | 6:G:811:HEM:CAC | 2.22                     | 1.28              |
| 1:B:465:CYS:SG | 6:B:812:HEM:CAC | 2.22                     | 1.28              |
| 1:B:342:CYS:SG | 6:B:809:HEM:CAC | 2.22                     | 1.27              |
| 1:J:487:CYS:SG | 6:J:812:HEM:CAC | 2.22                     | 1.27              |
| 1:K:578:CYS:SG | 6:K:813:HEM:CAC | 2.21                     | 1.27              |
| 1:L:487:CYS:SG | 6:L:812:HEM:CAC | 2.22                     | 1.27              |
| 1:C:465:CYS:SG | 6:C:811:HEM:CAC | 2.23                     | 1.27              |
| 1:K:146:CYS:SG | 6:K:806:HEM:CAC | 2.22                     | 1.27              |
| 1:K:465:CYS:SG | 6:K:811:HEM:CAC | 2.21                     | 1.27              |
| 1:A:421:CYS:SG | 6:A:810:HEM:CAC | 2.22                     | 1.27              |
| 1:I:487:CYS:SG | 6:I:812:HEM:CAC | 2.22                     | 1.27              |
| 1:D:578:CYS:SG | 6:D:813:HEM:CAC | 2.21                     | 1.27              |
| 1:H:421:CYS:HG | 6:H:811:HEM:CAC | 1.45                     | 1.27              |
| 1:J:146:CYS:SG | 6:J:806:HEM:CAC | 2.22                     | 1.27              |
| 1:L:578:CYS:SG | 6:L:813:HEM:HAC | 1.73                     | 1.26              |
| 1:F:305:CYS:SG | 6:F:808:HEM:CAC | 2.23                     | 1.26              |
| 1:L:342:CYS:SG | 6:L:808:HEM:CAC | 2.23                     | 1.26              |
| 1:J:342:CYS:SG | 6:J:808:HEM:CAC | 2.22                     | 1.26              |
| 1:B:578:CYS:SG | 6:B:814:HEM:CAC | 2.24                     | 1.26              |
| 1:L:578:CYS:SG | 6:L:813:HEM:CAC | 2.22                     | 1.26              |
| 1:B:146:CYS:SG | 6:B:807:HEM:CAC | 2.22                     | 1.25              |
| 1:G:342:CYS:SG | 6:G:808:HEM:CAC | 2.23                     | 1.25              |
| 1:I:578:CYS:SG | 6:I:813:HEM:CAC | 2.23                     | 1.25              |
| 1:L:465:CYS:SG | 6:L:811:HEM:CAC | 2.24                     | 1.25              |
| 1:F:465:CYS:SG | 6:F:812:HEM:CAC | 2.24                     | 1.25              |
| 1:H:342:CYS:SG | 6:H:809:HEM:CAC | 2.24                     | 1.25              |
| 1:H:421:CYS:SG | 6:H:811:HEM:CAC | 2.25                     | 1.25              |
| 1:F:421:CYS:SG | 6:F:811:HEM:CAC | 2.25                     | 1.24              |
| 1:J:465:CYS:SG | 6:J:811:HEM:CAC | 2.24                     | 1.24              |
| 1:D:418:CYS:HG | 6:D:810:HEM:CAB | 1.45                     | 1.24              |
| 1:L:421:CYS:SG | 6:L:810:HEM:CAC | 2.25                     | 1.23              |
| 1:E:342:CYS:SG | 6:E:808:HEM:CAC | 2.26                     | 1.23              |
| 1:H:146:CYS:SG | 6:H:807:HEM:CAC | 2.26                     | 1.23              |
| 1:J:421:CYS:SG | 6:J:810:HEM:CAC | 2.27                     | 1.23              |
| 1:A:465:CYS:SG | 6:A:811:HEM:CAC | 2.26                     | 1.23              |
| 1:C:578:CYS:SG | 6:C:813:HEM:CAC | 2.25                     | 1.23              |
| 1:E:421:CYS:SG | 6:E:810:HEM:CAC | 2.27                     | 1.22              |
| 1:G:578:CYS:SG | 6:G:813:HEM:CAC | 2.27                     | 1.22              |
| 1:C:421:CYS:SG | 6:C:810:HEM:CAC | 2.27                     | 1.22              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:G:421:CYS:SG | 6:G:810:HEM:CAC | 2.27                     | 1.22              |
| 1:B:421:CYS:SG | 6:B:811:HEM:CAC | 2.27                     | 1.22              |
| 1:K:421:CYS:SG | 6:K:810:HEM:CAC | 2.29                     | 1.21              |
| 1:H:302:CYS:SG | 6:H:808:HEM:CAB | 2.30                     | 1.19              |
| 1:J:487:CYS:SG | 6:J:812:HEM:CBC | 2.31                     | 1.19              |
| 1:K:302:CYS:SG | 6:K:807:HEM:C3B | 2.37                     | 1.18              |
| 1:L:302:CYS:SG | 6:L:807:HEM:CAB | 2.31                     | 1.18              |
| 1:D:339:CYS:SG | 6:D:808:HEM:HAB | 1.73                     | 1.18              |
| 1:J:360:CYS:HG | 6:J:809:HEM:CAB | 1.55                     | 1.18              |
| 1:J:302:CYS:SG | 6:J:807:HEM:CAB | 2.33                     | 1.17              |
| 1:G:360:CYS:HG | 6:G:809:HEM:CAB | 1.54                     | 1.17              |
| 1:F:302:CYS:SG | 6:F:808:HEM:CAB | 2.34                     | 1.16              |
| 1:C:302:CYS:SG | 6:C:807:HEM:CAB | 2.33                     | 1.16              |
| 1:A:302:CYS:SG | 6:A:807:HEM:CAB | 2.34                     | 1.15              |
| 1:B:302:CYS:SG | 6:B:808:HEM:CAB | 2.35                     | 1.15              |
| 1:F:418:CYS:HG | 6:F:811:HEM:CAB | 1.55                     | 1.15              |
| 1:E:302:CYS:SG | 6:E:807:HEM:CAB | 2.36                     | 1.13              |
| 1:K:418:CYS:SG | 6:K:810:HEM:CBB | 2.36                     | 1.12              |
| 1:L:360:CYS:HG | 6:L:809:HEM:CAB | 1.58                     | 1.12              |
| 1:F:143:CYS:SG | 6:F:807:HEM:CBB | 2.36                     | 1.12              |
| 1:H:578:CYS:SG | 6:H:814:HEM:CBC | 2.39                     | 1.11              |
| 1:C:339:CYS:SG | 6:C:808:HEM:HAB | 1.83                     | 1.11              |
| 1:I:418:CYS:HG | 6:I:810:HEM:CAB | 1.50                     | 1.11              |
| 1:G:302:CYS:SG | 6:G:807:HEM:CAB | 2.39                     | 1.11              |
| 1:B:360:CYS:HG | 6:B:810:HEM:CAB | 1.54                     | 1.11              |
| 1:H:462:CYS:SG | 6:H:812:HEM:CBB | 2.41                     | 1.08              |
| 1:J:363:CYS:HG | 6:J:809:HEM:CAC | 1.61                     | 1.08              |
| 1:K:578:CYS:SG | 6:K:813:HEM:CBC | 2.42                     | 1.07              |
| 1:L:487:CYS:SG | 6:L:812:HEM:CBC | 2.43                     | 1.06              |
| 1:L:462:CYS:SG | 6:L:811:HEM:HAB | 1.94                     | 1.06              |
| 1:E:360:CYS:HG | 6:E:809:HEM:CAB | 1.57                     | 1.06              |
| 1:F:484:CYS:SG | 6:F:813:HEM:HAB | 1.92                     | 1.05              |
| 1:B:578:CYS:SG | 6:B:814:HEM:CBC | 2.44                     | 1.05              |
| 1:J:302:CYS:SG | 6:J:807:HEM:C3B | 2.50                     | 1.05              |
| 1:C:562:CYS:SG | 6:C:813:HEM:CBB | 2.45                     | 1.04              |
| 1:B:305:CYS:SG | 6:B:808:HEM:CBC | 2.46                     | 1.04              |
| 1:D:360:CYS:HG | 6:D:809:HEM:CAB | 1.61                     | 1.04              |
| 1:J:305:CYS:SG | 6:J:807:HEM:CBC | 2.45                     | 1.04              |
| 1:J:462:CYS:SG | 6:J:811:HEM:CBB | 2.46                     | 1.04              |
| 1:L:146:CYS:SG | 6:L:806:HEM:CBC | 2.44                     | 1.04              |
| 1:I:462:CYS:SG | 6:I:811:HEM:CBB | 2.44                     | 1.04              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:L:562:CYS:SG | 6:L:813:HEM:CBB | 2.45                     | 1.03              |
| 1:K:484:CYS:SG | 6:K:812:HEM:CBB | 2.46                     | 1.03              |
| 1:K:562:CYS:SG | 6:K:813:HEM:CBB | 2.46                     | 1.03              |
| 1:I:562:CYS:SG | 6:I:813:HEM:CBB | 2.47                     | 1.02              |
| 1:J:146:CYS:SG | 6:J:806:HEM:CBC | 2.47                     | 1.02              |
| 1:A:143:CYS:SG | 6:A:806:HEM:HAB | 1.93                     | 1.02              |
| 1:L:302:CYS:SG | 6:L:807:HEM:C3B | 2.52                     | 1.02              |
| 1:L:305:CYS:SG | 6:L:807:HEM:CBC | 2.47                     | 1.02              |
| 1:D:487:CYS:SG | 6:D:812:HEM:CBC | 2.48                     | 1.01              |
| 1:E:484:CYS:SG | 6:E:812:HEM:CBB | 2.47                     | 1.01              |
| 1:E:418:CYS:SG | 6:E:810:HEM:CBB | 2.49                     | 1.01              |
| 1:B:462:CYS:SG | 6:B:812:HEM:CBB | 2.48                     | 1.01              |
| 1:C:302:CYS:SG | 6:C:807:HEM:C3B | 2.53                     | 1.01              |
| 1:A:418:CYS:SG | 6:A:810:HEM:HAB | 1.95                     | 1.00              |
| 1:I:418:CYS:SG | 6:I:810:HEM:CBB | 2.48                     | 1.00              |
| 1:D:562:CYS:SG | 6:D:813:HEM:CBB | 2.49                     | 1.00              |
| 1:B:562:CYS:SG | 6:B:814:HEM:CBB | 2.50                     | 1.00              |
| 1:G:462:CYS:SG | 6:G:811:HEM:CBB | 2.50                     | 1.00              |
| 1:G:487:CYS:SG | 6:G:812:HEM:CBC | 2.49                     | 1.00              |
| 1:E:462:CYS:SG | 6:E:811:HEM:CBB | 2.48                     | 1.00              |
| 1:F:360:CYS:HG | 6:F:810:HEM:CAB | 1.64                     | 0.99              |
| 1:L:418:CYS:SG | 6:L:810:HEM:CBB | 2.49                     | 0.99              |
| 1:C:143:CYS:SG | 6:C:806:HEM:HAB | 1.99                     | 0.99              |
| 1:E:305:CYS:SG | 6:E:807:HEM:CBC | 2.50                     | 0.99              |
| 1:F:418:CYS:SG | 6:F:811:HEM:HAB | 2.01                     | 0.99              |
| 1:B:302:CYS:SG | 6:B:808:HEM:C3B | 2.55                     | 0.99              |
| 1:C:305:CYS:SG | 6:C:807:HEM:CBC | 2.51                     | 0.99              |
| 1:D:418:CYS:SG | 6:D:810:HEM:HAB | 2.01                     | 0.99              |
| 1:L:339:CYS:SG | 6:L:808:HEM:CBB | 2.51                     | 0.99              |
| 1:H:487:CYS:SG | 6:H:813:HEM:CBC | 2.51                     | 0.99              |
| 1:A:484:CYS:SG | 6:A:812:HEM:CBB | 2.51                     | 0.99              |
| 1:A:578:CYS:SG | 6:A:813:HEM:CBC | 2.51                     | 0.99              |
| 1:B:484:CYS:SG | 6:B:813:HEM:CBB | 2.49                     | 0.99              |
| 1:E:302:CYS:SG | 6:E:807:HEM:C3B | 2.56                     | 0.99              |
| 1:G:562:CYS:SG | 6:G:813:HEM:CBB | 2.51                     | 0.99              |
| 1:A:339:CYS:SG | 6:A:808:HEM:HAB | 1.99                     | 0.98              |
| 1:B:339:CYS:SG | 6:B:809:HEM:HAB | 2.02                     | 0.98              |
| 1:K:342:CYS:SG | 6:K:808:HEM:CBC | 2.51                     | 0.98              |
| 1:E:487:CYS:SG | 6:E:812:HEM:CBC | 2.51                     | 0.97              |
| 1:G:146:CYS:SG | 6:G:806:HEM:CBC | 2.51                     | 0.97              |
| 1:I:360:CYS:HG | 6:I:809:HEM:CAB | 1.69                     | 0.97              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:B:418:CYS:SG | 6:B:811:HEM:HAB | 2.02                     | 0.97              |
| 1:D:484:CYS:SG | 6:D:812:HEM:CBB | 2.53                     | 0.97              |
| 1:E:339:CYS:SG | 6:E:808:HEM:CBB | 2.53                     | 0.97              |
| 1:H:339:CYS:SG | 6:H:809:HEM:HAB | 2.05                     | 0.97              |
| 1:K:339:CYS:SG | 6:K:808:HEM:HAB | 2.05                     | 0.97              |
| 1:F:562:CYS:SG | 6:F:814:HEM:CBB | 2.51                     | 0.96              |
| 1:G:339:CYS:SG | 6:G:808:HEM:CBB | 2.53                     | 0.96              |
| 1:B:487:CYS:SG | 6:B:813:HEM:CBC | 2.53                     | 0.96              |
| 1:F:578:CYS:SG | 6:F:814:HEM:CBC | 2.53                     | 0.96              |
| 1:A:484:CYS:SG | 6:A:812:HEM:HAB | 2.03                     | 0.96              |
| 1:D:462:CYS:SG | 6:D:811:HEM:CBB | 2.54                     | 0.95              |
| 1:F:302:CYS:SG | 6:F:808:HEM:C3B | 2.59                     | 0.95              |
| 1:H:484:CYS:SG | 6:H:813:HEM:HAB | 2.06                     | 0.95              |
| 1:L:421:CYS:SG | 6:L:810:HEM:CBC | 2.53                     | 0.95              |
| 1:G:143:CYS:SG | 6:G:806:HEM:HAB | 2.06                     | 0.95              |
| 1:D:146:CYS:SG | 6:D:806:HEM:CBC | 2.54                     | 0.95              |
| 1:I:484:CYS:SG | 6:I:812:HEM:HAB | 2.04                     | 0.95              |
| 1:G:418:CYS:SG | 6:G:810:HEM:CBB | 2.53                     | 0.95              |
| 1:G:484:CYS:SG | 6:G:812:HEM:CBB | 2.54                     | 0.95              |
| 1:J:339:CYS:SG | 6:J:808:HEM:HAB | 2.07                     | 0.95              |
| 1:L:484:CYS:SG | 6:L:812:HEM:CBB | 2.54                     | 0.95              |
| 1:B:465:CYS:SG | 6:B:812:HEM:CBC | 2.54                     | 0.95              |
| 1:E:578:CYS:SG | 6:E:813:HEM:CBC | 2.54                     | 0.95              |
| 1:A:302:CYS:SG | 6:A:807:HEM:C3B | 2.59                     | 0.95              |
| 1:C:462:CYS:SG | 6:C:811:HEM:HAB | 2.06                     | 0.95              |
| 1:J:484:CYS:SG | 6:J:812:HEM:CBB | 2.54                     | 0.95              |
| 1:A:339:CYS:SG | 6:A:808:HEM:CBB | 2.55                     | 0.95              |
| 1:C:465:CYS:SG | 6:C:811:HEM:CBC | 2.54                     | 0.95              |
| 1:D:484:CYS:SG | 6:D:812:HEM:HAB | 2.03                     | 0.94              |
| 1:G:339:CYS:SG | 6:G:808:HEM:HAB | 2.05                     | 0.94              |
| 1:C:484:CYS:SG | 6:C:812:HEM:HAB | 2.05                     | 0.94              |
| 1:D:578:CYS:SG | 6:D:813:HEM:CBC | 2.54                     | 0.94              |
| 1:B:363:CYS:SG | 6:B:810:HEM:CBC | 2.55                     | 0.94              |
| 1:D:143:CYS:SG | 6:D:806:HEM:HAB | 2.05                     | 0.94              |
| 1:H:418:CYS:SG | 6:H:811:HEM:CBB | 2.55                     | 0.94              |
| 1:J:562:CYS:SG | 6:J:813:HEM:CBB | 2.54                     | 0.94              |
| 1:K:487:CYS:SG | 6:K:812:HEM:CBC | 2.56                     | 0.94              |
| 1:L:339:CYS:SG | 6:L:808:HEM:HAB | 2.06                     | 0.93              |
| 1:C:418:CYS:SG | 6:C:810:HEM:HAB | 2.06                     | 0.93              |
| 1:F:462:CYS:SG | 6:F:812:HEM:HAB | 2.05                     | 0.93              |
| 1:G:305:CYS:SG | 6:G:807:HEM:CBC | 2.56                     | 0.93              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:E:339:CYS:SG | 6:E:808:HEM:HAB | 2.06                     | 0.93              |
| 1:F:562:CYS:SG | 6:F:814:HEM:HAB | 2.07                     | 0.92              |
| 1:H:421:CYS:HG | 6:H:811:HEM:CBC | 1.80                     | 0.92              |
| 1:I:578:CYS:SG | 6:I:813:HEM:CBC | 2.57                     | 0.92              |
| 1:H:143:CYS:SG | 6:H:807:HEM:HAB | 2.06                     | 0.92              |
| 1:I:146:CYS:SG | 6:I:806:HEM:CBC | 2.57                     | 0.92              |
| 1:H:146:CYS:SG | 6:H:807:HEM:CBC | 2.58                     | 0.92              |
| 1:J:484:CYS:SG | 6:J:812:HEM:HAB | 2.09                     | 0.92              |
| 1:H:360:CYS:SG | 6:H:810:HEM:CBB | 2.58                     | 0.92              |
| 1:H:418:CYS:SG | 6:H:811:HEM:HAB | 2.10                     | 0.92              |
| 1:B:421:CYS:SG | 6:B:811:HEM:CBC | 2.58                     | 0.92              |
| 1:A:305:CYS:SG | 6:A:807:HEM:CBC | 2.57                     | 0.91              |
| 1:B:143:CYS:SG | 6:B:807:HEM:CBB | 2.58                     | 0.91              |
| 1:C:578:CYS:SG | 6:C:813:HEM:CBC | 2.57                     | 0.91              |
| 1:H:363:CYS:SG | 6:H:810:HEM:CBC | 2.58                     | 0.91              |
| 1:I:339:CYS:SG | 6:I:808:HEM:CBB | 2.57                     | 0.91              |
| 1:F:465:CYS:SG | 6:F:812:HEM:CBC | 2.57                     | 0.91              |
| 1:G:143:CYS:SG | 6:G:806:HEM:CBB | 2.58                     | 0.91              |
| 1:I:484:CYS:SG | 6:I:812:HEM:CBB | 2.57                     | 0.91              |
| 1:H:465:CYS:SG | 6:H:812:HEM:CBC | 2.59                     | 0.91              |
| 1:F:305:CYS:SG | 6:F:808:HEM:CBC | 2.59                     | 0.91              |
| 1:E:562:CYS:SG | 6:E:813:HEM:CBB | 2.58                     | 0.91              |
| 1:I:487:CYS:SG | 6:I:812:HEM:CBC | 2.59                     | 0.91              |
| 1:B:418:CYS:SG | 6:B:811:HEM:CBB | 2.60                     | 0.90              |
| 1:D:418:CYS:SG | 6:D:810:HEM:CBB | 2.59                     | 0.90              |
| 1:J:339:CYS:SG | 6:J:808:HEM:CBB | 2.58                     | 0.90              |
| 1:C:342:CYS:SG | 6:C:808:HEM:CBC | 2.59                     | 0.90              |
| 1:K:360:CYS:HG | 6:K:809:HEM:CAB | 1.74                     | 0.90              |
| 1:C:487:CYS:SG | 6:C:812:HEM:CBC | 2.59                     | 0.90              |
| 1:E:462:CYS:SG | 6:E:811:HEM:HAB | 2.10                     | 0.90              |
| 1:E:562:CYS:SG | 6:E:813:HEM:HAB | 2.11                     | 0.90              |
| 1:I:143:CYS:SG | 6:I:806:HEM:CBB | 2.60                     | 0.90              |
| 1:G:478:THR:O  | 6:G:813:HEM:O2D | 1.88                     | 0.90              |
| 1:K:339:CYS:SG | 6:K:808:HEM:CBB | 2.58                     | 0.89              |
| 1:H:562:CYS:SG | 6:H:814:HEM:CBB | 2.60                     | 0.89              |
| 1:K:143:CYS:HG | 6:K:806:HEM:HAB | 1.12                     | 0.89              |
| 1:K:465:CYS:SG | 6:K:811:HEM:CBC | 2.60                     | 0.89              |
| 1:A:562:CYS:SG | 6:A:813:HEM:CBB | 2.60                     | 0.89              |
| 1:A:465:CYS:SG | 6:A:811:HEM:CBC | 2.59                     | 0.89              |
| 1:D:143:CYS:SG | 6:D:806:HEM:CBB | 2.59                     | 0.89              |
| 1:I:363:CYS:SG | 6:I:809:HEM:C3C | 2.65                     | 0.89              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:C:363:CYS:SG | 6:C:809:HEM:HAC | 2.12                     | 0.89              |
| 1:E:146:CYS:SG | 6:E:806:HEM:CBC | 2.61                     | 0.89              |
| 1:I:462:CYS:SG | 6:I:811:HEM:HAB | 2.11                     | 0.89              |
| 1:J:418:CYS:SG | 6:J:810:HEM:HAB | 2.09                     | 0.89              |
| 1:L:143:CYS:SG | 6:L:806:HEM:CBB | 2.61                     | 0.89              |
| 1:E:421:CYS:SG | 6:E:810:HEM:CBC | 2.61                     | 0.88              |
| 1:G:302:CYS:SG | 6:G:807:HEM:C3B | 2.66                     | 0.88              |
| 1:D:360:CYS:SG | 6:D:809:HEM:CBB | 2.61                     | 0.88              |
| 1:F:418:CYS:SG | 6:F:811:HEM:CBB | 2.62                     | 0.88              |
| 1:E:484:CYS:SG | 6:E:812:HEM:HAB | 2.09                     | 0.88              |
| 1:D:462:CYS:SG | 6:D:811:HEM:HAB | 2.11                     | 0.88              |
| 1:D:363:CYS:SG | 6:D:809:HEM:CBC | 2.60                     | 0.88              |
| 1:E:418:CYS:SG | 6:E:810:HEM:HAB | 2.10                     | 0.88              |
| 1:I:363:CYS:SG | 6:I:809:HEM:HAC | 2.14                     | 0.88              |
| 1:B:146:CYS:SG | 6:B:807:HEM:CBC | 2.62                     | 0.87              |
| 1:H:462:CYS:SG | 6:H:812:HEM:HAB | 2.13                     | 0.87              |
| 1:K:146:CYS:SG | 6:K:806:HEM:CBC | 2.61                     | 0.87              |
| 1:G:421:CYS:SG | 6:G:810:HEM:CBC | 2.61                     | 0.87              |
| 1:F:146:CYS:SG | 6:F:807:HEM:CBC | 2.62                     | 0.87              |
| 1:G:562:CYS:SG | 6:G:813:HEM:HAB | 2.14                     | 0.87              |
| 1:D:305:CYS:SG | 6:D:807:HEM:C3C | 2.68                     | 0.87              |
| 1:L:143:CYS:SG | 6:L:806:HEM:HAB | 2.11                     | 0.87              |
| 1:B:305:CYS:SG | 6:B:808:HEM:C3C | 2.68                     | 0.87              |
| 1:A:143:CYS:SG | 6:A:806:HEM:CBB | 2.62                     | 0.87              |
| 1:A:562:CYS:SG | 6:A:813:HEM:HAB | 2.11                     | 0.87              |
| 1:D:363:CYS:SG | 6:D:809:HEM:C3C | 2.68                     | 0.86              |
| 1:E:305:CYS:SG | 6:E:807:HEM:C3C | 2.68                     | 0.86              |
| 1:H:363:CYS:SG | 6:H:810:HEM:C3C | 2.68                     | 0.86              |
| 1:J:305:CYS:SG | 6:J:807:HEM:C3C | 2.67                     | 0.86              |
| 1:A:363:CYS:SG | 6:A:809:HEM:CBC | 2.62                     | 0.86              |
| 1:H:143:CYS:SG | 6:H:807:HEM:CBB | 2.62                     | 0.86              |
| 1:J:421:CYS:SG | 6:J:810:HEM:CBC | 2.64                     | 0.86              |
| 1:F:484:CYS:SG | 6:F:813:HEM:CBB | 2.63                     | 0.86              |
| 1:I:305:CYS:SG | 6:I:807:HEM:C3C | 2.68                     | 0.86              |
| 1:A:342:CYS:SG | 6:A:808:HEM:CBC | 2.62                     | 0.86              |
| 1:G:342:CYS:SG | 6:G:808:HEM:CBC | 2.63                     | 0.86              |
| 1:E:418:CYS:HG | 6:E:810:HEM:CBB | 1.85                     | 0.86              |
| 1:K:484:CYS:SG | 6:K:812:HEM:HAB | 2.15                     | 0.86              |
| 1:G:465:CYS:SG | 6:G:811:HEM:C3C | 2.69                     | 0.86              |
| 1:F:363:CYS:SG | 6:F:810:HEM:CBC | 2.64                     | 0.85              |
| 1:F:305:CYS:SG | 6:F:808:HEM:C3C | 2.70                     | 0.85              |

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| Atom-1         | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 1:B:342:CYS:SG | 6:B:809:HEM:CBC | 2.64                     | 0.85              |
| 1:C:360:CYS:SG | 6:C:809:HEM:HAB | 2.17                     | 0.85              |
| 1:K:363:CYS:SG | 6:K:809:HEM:C3C | 2.69                     | 0.85              |
| 1:B:562:CYS:SG | 6:B:814:HEM:HAB | 2.16                     | 0.85              |
| 1:D:342:CYS:SG | 6:D:808:HEM:CBC | 2.63                     | 0.85              |
| 1:L:360:CYS:SG | 6:L:809:HEM:CBB | 2.64                     | 0.85              |
| 1:A:418:CYS:SG | 6:A:810:HEM:CBB | 2.65                     | 0.84              |
| 1:C:360:CYS:SG | 6:C:809:HEM:CBB | 2.65                     | 0.84              |
| 1:F:363:CYS:SG | 6:F:810:HEM:HAC | 2.16                     | 0.84              |
| 1:C:562:CYS:SG | 6:C:813:HEM:HAB | 2.15                     | 0.84              |
| 1:B:302:CYS:HG | 6:B:808:HEM:CAB | 1.84                     | 0.84              |
| 1:F:360:CYS:SG | 6:F:810:HEM:CBB | 2.64                     | 0.84              |
| 1:L:465:CYS:SG | 6:L:811:HEM:CBC | 2.65                     | 0.84              |
| 1:L:484:CYS:SG | 6:L:812:HEM:HAB | 2.18                     | 0.84              |
| 1:C:484:CYS:SG | 6:C:812:HEM:CBB | 2.64                     | 0.84              |
| 1:E:363:CYS:SG | 6:E:809:HEM:CBC | 2.66                     | 0.83              |
| 1:C:363:CYS:SG | 6:C:809:HEM:C3C | 2.70                     | 0.83              |
| 1:G:363:CYS:SG | 6:G:809:HEM:C3C | 2.70                     | 0.83              |
| 1:A:421:CYS:SG | 6:A:810:HEM:CBC | 2.66                     | 0.83              |
| 1:G:302:CYS:HG | 6:G:807:HEM:CAB | 1.88                     | 0.83              |
| 1:B:462:CYS:SG | 6:B:812:HEM:HAB | 2.14                     | 0.83              |
| 1:F:421:CYS:SG | 6:F:811:HEM:CBC | 2.68                     | 0.82              |
| 1:A:360:CYS:SG | 6:A:809:HEM:CBB | 2.67                     | 0.82              |
| 1:H:342:CYS:SG | 6:H:809:HEM:CBC | 2.67                     | 0.82              |
| 1:B:360:CYS:SG | 6:B:810:HEM:CBB | 2.66                     | 0.82              |
| 1:F:143:CYS:SG | 6:F:807:HEM:HAB | 2.17                     | 0.82              |
| 1:H:339:CYS:SG | 6:H:809:HEM:CBB | 2.67                     | 0.82              |
| 1:D:421:CYS:SG | 6:D:810:HEM:CBC | 2.68                     | 0.82              |
| 1:I:421:CYS:SG | 6:I:810:HEM:C3C | 2.72                     | 0.82              |
| 1:B:478:THR:O  | 6:B:814:HEM:O2D | 1.97                     | 0.82              |
| 1:I:143:CYS:SG | 6:I:806:HEM:HAB | 2.18                     | 0.82              |
| 1:J:363:CYS:SG | 6:J:809:HEM:CBC | 2.68                     | 0.82              |
| 1:A:363:CYS:SG | 6:A:809:HEM:HAC | 2.19                     | 0.81              |
| 1:I:421:CYS:SG | 6:I:810:HEM:CBC | 2.68                     | 0.81              |
| 1:I:342:CYS:SG | 6:I:808:HEM:CBC | 2.68                     | 0.81              |
| 1:F:146:CYS:SG | 6:F:807:HEM:C3C | 2.73                     | 0.81              |
| 1:L:305:CYS:SG | 6:L:807:HEM:C3C | 2.72                     | 0.81              |
| 1:C:421:CYS:SG | 6:C:810:HEM:CBC | 2.68                     | 0.81              |
| 1:J:360:CYS:SG | 6:J:809:HEM:CBB | 2.69                     | 0.81              |
| 1:H:465:CYS:SG | 6:H:812:HEM:C3C | 2.73                     | 0.81              |
| 1:L:421:CYS:SG | 6:L:810:HEM:C3C | 2.74                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:342:CYS:SG   | 6:E:808:HEM:CBC  | 2.69                     | 0.80              |
| 1:A:363:CYS:SG   | 6:A:809:HEM:C3C  | 2.74                     | 0.80              |
| 1:J:562:CYS:SG   | 6:J:813:HEM:C3B  | 2.74                     | 0.80              |
| 1:K:418:CYS:SG   | 6:K:810:HEM:HAB  | 2.16                     | 0.80              |
| 1:G:305:CYS:SG   | 6:G:807:HEM:C3C  | 2.74                     | 0.80              |
| 1:J:465:CYS:SG   | 6:J:811:HEM:C3C  | 2.75                     | 0.80              |
| 1:K:465:CYS:SG   | 6:K:811:HEM:C3C  | 2.74                     | 0.80              |
| 1:A:146:CYS:SG   | 6:A:806:HEM:C3C  | 2.75                     | 0.80              |
| 1:B:360:CYS:SG   | 6:B:810:HEM:HAB  | 2.21                     | 0.80              |
| 1:I:465:CYS:SG   | 6:I:811:HEM:C3C  | 2.74                     | 0.80              |
| 1:L:562:CYS:SG   | 6:L:813:HEM:HAB  | 2.20                     | 0.80              |
| 1:G:360:CYS:SG   | 6:G:809:HEM:CBB  | 2.69                     | 0.80              |
| 1:F:339:CYS:SG   | 6:F:809:HEM:CBB  | 2.71                     | 0.79              |
| 1:A:418:CYS:HG   | 6:A:810:HEM:CBB  | 1.96                     | 0.79              |
| 1:K:363:CYS:SG   | 6:K:809:HEM:CBC  | 2.71                     | 0.79              |
| 1:H:302:CYS:HG   | 6:H:808:HEM:CAB  | 1.91                     | 0.79              |
| 1:A:562:CYS:SG   | 6:A:813:HEM:C3B  | 2.75                     | 0.79              |
| 1:A:360:CYS:SG   | 6:A:809:HEM:HAB  | 2.22                     | 0.79              |
| 6:L:807:HEM:HMD1 | 6:L:807:HEM:CGD  | 2.12                     | 0.79              |
| 1:K:462:CYS:SG   | 6:K:811:HEM:HAB  | 2.20                     | 0.79              |
| 1:B:146:CYS:SG   | 6:B:807:HEM:C3C  | 2.77                     | 0.78              |
| 1:G:363:CYS:SG   | 6:G:809:HEM:CBC  | 2.72                     | 0.78              |
| 1:D:146:CYS:SG   | 6:D:806:HEM:C3C  | 2.77                     | 0.78              |
| 1:K:363:CYS:SG   | 6:K:809:HEM:HAC  | 2.24                     | 0.78              |
| 6:C:807:HEM:CGD  | 6:C:807:HEM:HMD1 | 2.14                     | 0.78              |
| 1:I:418:CYS:HG   | 6:I:810:HEM:CBB  | 1.94                     | 0.78              |
| 1:I:146:CYS:SG   | 6:I:806:HEM:C3C  | 2.77                     | 0.78              |
| 1:E:462:CYS:SG   | 6:E:811:HEM:C3B  | 2.77                     | 0.78              |
| 1:E:465:CYS:SG   | 6:E:811:HEM:C3C  | 2.77                     | 0.78              |
| 1:B:339:CYS:SG   | 6:B:809:HEM:C3B  | 2.78                     | 0.77              |
| 1:L:363:CYS:SG   | 6:L:809:HEM:HAC  | 2.24                     | 0.77              |
| 1:K:487:CYS:SG   | 6:K:812:HEM:C3C  | 2.76                     | 0.77              |
| 1:G:465:CYS:SG   | 6:G:811:HEM:CBC  | 2.72                     | 0.77              |
| 1:D:418:CYS:HG   | 6:D:810:HEM:CBB  | 1.98                     | 0.77              |
| 1:C:484:CYS:SG   | 6:C:812:HEM:C3B  | 2.78                     | 0.77              |
| 1:F:418:CYS:HG   | 6:F:811:HEM:CBB  | 1.95                     | 0.77              |
| 1:I:363:CYS:SG   | 6:I:809:HEM:CBC  | 2.73                     | 0.77              |
| 1:F:342:CYS:SG   | 6:F:809:HEM:C3C  | 2.78                     | 0.77              |
| 1:D:421:CYS:SG   | 6:D:810:HEM:C3C  | 2.79                     | 0.76              |
| 1:C:146:CYS:SG   | 6:C:806:HEM:C3C  | 2.78                     | 0.76              |
| 6:I:807:HEM:HMD1 | 6:I:807:HEM:CGD  | 2.14                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:K:807:HEM:HMD1 | 6:K:807:HEM:CGD  | 2.15                     | 0.76              |
| 1:A:578:CYS:SG   | 6:A:813:HEM:C3C  | 2.78                     | 0.76              |
| 1:L:363:CYS:SG   | 6:L:809:HEM:CBC  | 2.73                     | 0.76              |
| 1:G:146:CYS:SG   | 6:G:806:HEM:C3C  | 2.77                     | 0.76              |
| 1:G:208:LYS:HG3  | 6:G:807:HEM:HMA2 | 1.68                     | 0.76              |
| 6:D:807:HEM:HMD1 | 6:D:807:HEM:CGD  | 2.14                     | 0.76              |
| 1:J:562:CYS:SG   | 6:J:813:HEM:HAB  | 2.22                     | 0.76              |
| 1:J:360:CYS:SG   | 6:J:809:HEM:C3B  | 2.71                     | 0.76              |
| 1:L:146:CYS:SG   | 6:L:806:HEM:C3C  | 2.78                     | 0.76              |
| 1:K:421:CYS:SG   | 6:K:810:HEM:CBC  | 2.73                     | 0.76              |
| 1:H:146:CYS:SG   | 6:H:807:HEM:C3C  | 2.78                     | 0.76              |
| 1:H:421:CYS:SG   | 6:H:811:HEM:C3C  | 2.76                     | 0.76              |
| 1:J:421:CYS:SG   | 6:J:810:HEM:C3C  | 2.79                     | 0.76              |
| 1:F:302:CYS:HG   | 6:F:808:HEM:CAB  | 1.99                     | 0.76              |
| 1:E:562:CYS:SG   | 6:E:813:HEM:C3B  | 2.78                     | 0.76              |
| 1:B:465:CYS:SG   | 6:B:812:HEM:C3C  | 2.79                     | 0.75              |
| 1:B:562:CYS:SG   | 6:B:814:HEM:C3B  | 2.79                     | 0.75              |
| 1:H:487:CYS:SG   | 6:H:813:HEM:C3C  | 2.79                     | 0.75              |
| 1:E:421:CYS:SG   | 6:E:810:HEM:C3C  | 2.79                     | 0.75              |
| 1:L:465:CYS:SG   | 6:L:811:HEM:C3C  | 2.79                     | 0.75              |
| 1:F:421:CYS:SG   | 6:F:811:HEM:C3C  | 2.78                     | 0.75              |
| 1:G:360:CYS:SG   | 6:G:809:HEM:HAB  | 2.25                     | 0.75              |
| 1:E:302:CYS:HG   | 6:E:807:HEM:CAB  | 1.89                     | 0.75              |
| 1:A:421:CYS:SG   | 6:A:810:HEM:C3C  | 2.79                     | 0.75              |
| 1:C:143:CYS:SG   | 6:C:806:HEM:CBB  | 2.73                     | 0.75              |
| 1:D:465:CYS:SG   | 6:D:811:HEM:C3C  | 2.80                     | 0.75              |
| 6:E:810:HEM:HMC1 | 6:E:810:HEM:HBC2 | 1.69                     | 0.75              |
| 1:L:342:CYS:SG   | 6:L:808:HEM:C3C  | 2.80                     | 0.75              |
| 1:B:421:CYS:SG   | 6:B:811:HEM:C3C  | 2.79                     | 0.74              |
| 1:A:487:CYS:SG   | 6:A:812:HEM:C3C  | 2.81                     | 0.74              |
| 1:F:342:CYS:SG   | 6:F:809:HEM:HAC  | 2.25                     | 0.74              |
| 1:K:421:CYS:SG   | 6:K:810:HEM:C3C  | 2.80                     | 0.74              |
| 1:C:462:CYS:SG   | 6:C:811:HEM:C3B  | 2.80                     | 0.74              |
| 1:D:360:CYS:SG   | 6:D:809:HEM:HAB  | 2.26                     | 0.74              |
| 1:E:360:CYS:SG   | 6:E:809:HEM:C3B  | 2.73                     | 0.74              |
| 1:F:462:CYS:SG   | 6:F:812:HEM:C3B  | 2.79                     | 0.74              |
| 1:C:421:CYS:SG   | 6:C:810:HEM:C3C  | 2.81                     | 0.74              |
| 1:A:339:CYS:SG   | 6:A:808:HEM:C3B  | 2.81                     | 0.74              |
| 1:G:462:CYS:SG   | 6:G:811:HEM:C3B  | 2.81                     | 0.73              |
| 1:K:462:CYS:SG   | 6:K:811:HEM:C3B  | 2.80                     | 0.73              |
| 1:F:465:CYS:SG   | 6:F:812:HEM:C3C  | 2.81                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:465:CYS:SG   | 6:C:811:HEM:C3C  | 2.81                     | 0.73              |
| 6:L:810:HEM:HBC2 | 6:L:810:HEM:HMC1 | 1.71                     | 0.73              |
| 1:F:484:CYS:SG   | 6:F:813:HEM:C3B  | 2.82                     | 0.73              |
| 1:H:562:CYS:SG   | 6:H:814:HEM:C3B  | 2.80                     | 0.72              |
| 1:I:360:CYS:SG   | 6:I:809:HEM:HAB  | 2.25                     | 0.72              |
| 1:I:360:CYS:SG   | 6:I:809:HEM:CBB  | 2.78                     | 0.72              |
| 1:J:302:CYS:HG   | 6:J:807:HEM:CAB  | 1.93                     | 0.72              |
| 1:G:487:CYS:SG   | 6:G:812:HEM:C3C  | 2.82                     | 0.72              |
| 1:C:562:CYS:SG   | 6:C:813:HEM:C3B  | 2.82                     | 0.72              |
| 1:K:562:CYS:SG   | 6:K:813:HEM:C3B  | 2.82                     | 0.72              |
| 1:D:462:CYS:SG   | 6:D:811:HEM:C3B  | 2.81                     | 0.72              |
| 1:K:562:CYS:SG   | 6:K:813:HEM:HAB  | 2.24                     | 0.72              |
| 1:C:339:CYS:HG   | 6:C:808:HEM:CBB  | 2.02                     | 0.72              |
| 1:C:418:CYS:SG   | 6:C:810:HEM:C3B  | 2.81                     | 0.72              |
| 1:F:578:CYS:SG   | 6:F:814:HEM:C3C  | 2.83                     | 0.72              |
| 1:H:342:CYS:SG   | 6:H:809:HEM:C3C  | 2.82                     | 0.72              |
| 1:K:418:CYS:SG   | 6:K:810:HEM:C3B  | 2.82                     | 0.72              |
| 1:D:342:CYS:SG   | 6:D:808:HEM:HAC  | 2.30                     | 0.71              |
| 1:I:462:CYS:SG   | 6:I:811:HEM:C3B  | 2.81                     | 0.71              |
| 1:I:342:CYS:SG   | 6:I:808:HEM:HAC  | 2.27                     | 0.71              |
| 1:D:339:CYS:SG   | 6:D:808:HEM:C3B  | 2.84                     | 0.71              |
| 1:A:484:CYS:SG   | 6:A:812:HEM:C3B  | 2.83                     | 0.71              |
| 1:L:360:CYS:SG   | 6:L:809:HEM:C3B  | 2.73                     | 0.71              |
| 1:D:562:CYS:SG   | 6:D:813:HEM:C3B  | 2.82                     | 0.71              |
| 1:K:146:CYS:SG   | 6:K:806:HEM:C3C  | 2.82                     | 0.71              |
| 1:C:342:CYS:SG   | 6:C:808:HEM:HAC  | 2.28                     | 0.71              |
| 1:K:360:CYS:SG   | 6:K:809:HEM:HAB  | 2.27                     | 0.71              |
| 1:C:487:CYS:SG   | 6:C:812:HEM:C3C  | 2.84                     | 0.70              |
| 1:C:487:CYS:SG   | 6:C:812:HEM:HAC  | 2.30                     | 0.70              |
| 1:D:487:CYS:SG   | 6:D:812:HEM:C3C  | 2.83                     | 0.70              |
| 1:J:146:CYS:SG   | 6:J:806:HEM:C3C  | 2.83                     | 0.70              |
| 1:J:578:CYS:SG   | 6:J:813:HEM:C3C  | 2.83                     | 0.70              |
| 1:L:462:CYS:SG   | 6:L:811:HEM:C3B  | 2.79                     | 0.70              |
| 1:G:342:CYS:SG   | 6:G:808:HEM:HAC  | 2.30                     | 0.70              |
| 1:C:342:CYS:SG   | 6:C:808:HEM:C3C  | 2.83                     | 0.70              |
| 1:C:578:CYS:SG   | 6:C:813:HEM:C3C  | 2.84                     | 0.70              |
| 1:I:302:CYS:HG   | 6:I:807:HEM:CAB  | 1.91                     | 0.70              |
| 1:B:487:CYS:SG   | 6:B:813:HEM:C3C  | 2.83                     | 0.70              |
| 1:F:360:CYS:SG   | 6:F:810:HEM:C3B  | 2.78                     | 0.70              |
| 1:G:562:CYS:SG   | 6:G:813:HEM:C3B  | 2.85                     | 0.70              |
| 1:H:484:CYS:SG   | 6:H:813:HEM:C3B  | 2.84                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:421:CYS:SG   | 6:G:810:HEM:C3C  | 2.84                     | 0.70              |
| 1:J:363:CYS:HG   | 6:J:809:HEM:CBC  | 2.05                     | 0.70              |
| 1:E:578:CYS:SG   | 6:E:813:HEM:C3C  | 2.85                     | 0.69              |
| 1:L:562:CYS:SG   | 6:L:813:HEM:C3B  | 2.84                     | 0.69              |
| 1:I:487:CYS:SG   | 6:I:812:HEM:C3C  | 2.85                     | 0.69              |
| 1:K:360:CYS:SG   | 6:K:809:HEM:C3B  | 2.77                     | 0.69              |
| 1:B:484:CYS:SG   | 6:B:813:HEM:C3B  | 2.84                     | 0.69              |
| 1:E:578:CYS:SG   | 6:E:813:HEM:HAC  | 2.31                     | 0.69              |
| 1:A:208:LYS:HG3  | 6:A:807:HEM:HMA2 | 1.73                     | 0.69              |
| 1:B:360:CYS:SG   | 6:B:810:HEM:C3B  | 2.74                     | 0.69              |
| 1:F:143:CYS:SG   | 6:F:807:HEM:C3B  | 2.85                     | 0.69              |
| 6:F:808:HEM:HMD1 | 6:F:808:HEM:CGD  | 2.23                     | 0.69              |
| 1:I:578:CYS:SG   | 6:I:813:HEM:C3C  | 2.86                     | 0.69              |
| 1:C:339:CYS:SG   | 6:C:808:HEM:C3B  | 2.83                     | 0.68              |
| 1:D:578:CYS:SG   | 6:D:813:HEM:C3C  | 2.85                     | 0.68              |
| 1:A:487:CYS:SG   | 6:A:812:HEM:HAC  | 2.29                     | 0.68              |
| 1:J:363:CYS:SG   | 6:J:809:HEM:HAC  | 2.28                     | 0.68              |
| 1:L:487:CYS:SG   | 6:L:812:HEM:C3C  | 2.86                     | 0.68              |
| 1:F:339:CYS:SG   | 6:F:809:HEM:C3B  | 2.85                     | 0.68              |
| 6:G:807:HEM:HMD1 | 6:G:807:HEM:CGD  | 2.22                     | 0.68              |
| 1:A:342:CYS:SG   | 6:A:808:HEM:HAC  | 2.32                     | 0.68              |
| 1:K:342:CYS:SG   | 6:K:808:HEM:C3C  | 2.86                     | 0.68              |
| 1:B:418:CYS:SG   | 6:B:811:HEM:C3B  | 2.85                     | 0.68              |
| 1:J:339:CYS:SG   | 6:J:808:HEM:C3B  | 2.87                     | 0.68              |
| 1:E:363:CYS:SG   | 6:E:809:HEM:HAC  | 2.26                     | 0.68              |
| 6:H:808:HEM:HMD1 | 6:H:808:HEM:CGD  | 2.24                     | 0.68              |
| 1:L:302:CYS:HG   | 6:L:807:HEM:CAB  | 2.06                     | 0.68              |
| 1:E:342:CYS:SG   | 6:E:808:HEM:C3C  | 2.86                     | 0.68              |
| 1:J:342:CYS:SG   | 6:J:808:HEM:C3C  | 2.85                     | 0.68              |
| 6:L:807:HEM:HMC1 | 6:L:807:HEM:HBC2 | 1.76                     | 0.67              |
| 1:A:302:CYS:HG   | 6:A:807:HEM:CAB  | 1.97                     | 0.67              |
| 1:G:143:CYS:SG   | 6:G:806:HEM:C3B  | 2.87                     | 0.67              |
| 1:F:487:CYS:SG   | 6:F:813:HEM:C3C  | 2.88                     | 0.67              |
| 1:K:339:CYS:SG   | 6:K:808:HEM:C3B  | 2.88                     | 0.67              |
| 1:H:360:CYS:SG   | 6:H:810:HEM:HAB  | 2.31                     | 0.67              |
| 1:L:562:CYS:HG   | 6:L:813:HEM:CAB  | 2.06                     | 0.67              |
| 6:B:808:HEM:CGD  | 6:B:808:HEM:HMD1 | 2.25                     | 0.67              |
| 1:D:363:CYS:SG   | 6:D:809:HEM:HAC  | 2.27                     | 0.67              |
| 1:E:143:CYS:HG   | 6:E:806:HEM:CAB  | 2.03                     | 0.67              |
| 1:E:143:CYS:HG   | 6:E:806:HEM:HAB  | 1.58                     | 0.67              |
| 1:E:342:CYS:SG   | 6:E:808:HEM:HAC  | 2.34                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:342:CYS:SG   | 6:J:808:HEM:HAC  | 2.29                     | 0.66              |
| 1:D:418:CYS:SG   | 6:D:810:HEM:C3B  | 2.84                     | 0.66              |
| 1:L:360:CYS:SG   | 6:L:809:HEM:HAB  | 2.28                     | 0.66              |
| 1:G:578:CYS:SG   | 6:G:813:HEM:C3C  | 2.88                     | 0.66              |
| 1:G:626:LEU:HB3  | 1:G:686:MET:HE2  | 1.76                     | 0.66              |
| 6:B:808:HEM:HMC1 | 6:B:808:HEM:HBC2 | 1.78                     | 0.66              |
| 1:H:339:CYS:SG   | 6:H:809:HEM:C3B  | 2.89                     | 0.65              |
| 6:C:807:HEM:HMC1 | 6:C:807:HEM:HBC2 | 1.78                     | 0.65              |
| 1:I:562:CYS:SG   | 6:I:813:HEM:C3B  | 2.90                     | 0.65              |
| 1:H:626:LEU:HD13 | 1:H:686:MET:HE2  | 1.79                     | 0.65              |
| 1:I:484:CYS:SG   | 6:I:812:HEM:C3B  | 2.88                     | 0.65              |
| 1:C:339:CYS:SG   | 6:C:808:HEM:CBB  | 2.84                     | 0.65              |
| 1:J:462:CYS:SG   | 6:J:811:HEM:C3B  | 2.88                     | 0.65              |
| 1:A:342:CYS:SG   | 6:A:808:HEM:C3C  | 2.89                     | 0.65              |
| 1:A:360:CYS:HG   | 6:A:809:HEM:CBB  | 2.06                     | 0.65              |
| 1:K:146:CYS:SG   | 6:K:806:HEM:HAC  | 2.35                     | 0.65              |
| 1:G:120:SER:OG   | 1:G:124:ARG:HG3  | 1.97                     | 0.65              |
| 6:E:807:HEM:HMC1 | 6:E:807:HEM:HBC2 | 1.79                     | 0.64              |
| 1:H:360:CYS:HG   | 6:H:810:HEM:CBB  | 2.06                     | 0.64              |
| 1:B:363:CYS:SG   | 6:B:810:HEM:HAC  | 2.31                     | 0.64              |
| 1:I:487:CYS:SG   | 6:I:812:HEM:HAC  | 2.35                     | 0.64              |
| 1:A:421:CYS:SG   | 6:A:810:HEM:HAC  | 2.33                     | 0.64              |
| 1:B:208:LYS:HG3  | 6:B:808:HEM:HMA2 | 1.79                     | 0.64              |
| 1:D:484:CYS:SG   | 6:D:812:HEM:C3B  | 2.87                     | 0.64              |
| 1:E:484:CYS:SG   | 6:E:812:HEM:C3B  | 2.88                     | 0.64              |
| 1:L:484:CYS:SG   | 6:L:812:HEM:C3B  | 2.88                     | 0.64              |
| 1:B:462:CYS:SG   | 6:B:812:HEM:C3B  | 2.89                     | 0.64              |
| 1:C:143:CYS:SG   | 6:C:806:HEM:C3B  | 2.91                     | 0.64              |
| 6:B:811:HEM:HMC1 | 6:B:811:HEM:HBC2 | 1.80                     | 0.63              |
| 1:H:342:CYS:SG   | 6:H:809:HEM:HAC  | 2.33                     | 0.63              |
| 1:C:146:CYS:SG   | 6:C:806:HEM:HAC  | 2.30                     | 0.63              |
| 1:C:302:CYS:HG   | 6:C:807:HEM:CAB  | 2.08                     | 0.63              |
| 1:K:484:CYS:SG   | 6:K:812:HEM:C3B  | 2.90                     | 0.63              |
| 1:G:339:CYS:SG   | 6:G:808:HEM:C3B  | 2.89                     | 0.63              |
| 1:C:208:LYS:HG3  | 6:C:807:HEM:HMA2 | 1.80                     | 0.63              |
| 1:I:465:CYS:SG   | 6:I:811:HEM:HAC  | 2.35                     | 0.63              |
| 1:D:360:CYS:SG   | 6:D:809:HEM:C3B  | 2.74                     | 0.63              |
| 1:D:143:CYS:SG   | 6:D:806:HEM:C3B  | 2.89                     | 0.63              |
| 6:J:807:HEM:HMC1 | 6:J:807:HEM:HBC2 | 1.81                     | 0.63              |
| 1:L:143:CYS:SG   | 6:L:806:HEM:C3B  | 2.91                     | 0.63              |
| 1:A:305:CYS:SG   | 6:A:807:HEM:HAC  | 2.31                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:487:CYS:SG   | 6:F:813:HEM:HAC  | 2.33                     | 0.62              |
| 1:L:578:CYS:SG   | 6:L:813:HEM:C3C  | 2.93                     | 0.62              |
| 1:E:143:CYS:SG   | 6:E:806:HEM:C3B  | 2.91                     | 0.62              |
| 1:G:475:LYS:O    | 1:G:476:ALA:O    | 2.17                     | 0.62              |
| 1:D:375:ARG:NH1  | 8:D:1036:HOH:O   | 2.31                     | 0.62              |
| 1:J:484:CYS:SG   | 6:J:812:HEM:C3B  | 2.91                     | 0.62              |
| 1:H:462:CYS:SG   | 6:H:812:HEM:C3B  | 2.91                     | 0.61              |
| 1:B:689:SER:O    | 1:B:690:LEU:HB2  | 2.01                     | 0.61              |
| 1:B:487:CYS:SG   | 6:B:813:HEM:HAC  | 2.36                     | 0.61              |
| 6:F:808:HEM:HMC1 | 6:F:808:HEM:HBC2 | 1.82                     | 0.61              |
| 1:D:421:CYS:SG   | 6:D:810:HEM:HAC  | 2.37                     | 0.61              |
| 1:J:418:CYS:SG   | 6:J:810:HEM:C3B  | 2.92                     | 0.61              |
| 1:B:342:CYS:SG   | 6:B:809:HEM:HAC  | 2.34                     | 0.60              |
| 1:I:418:CYS:SG   | 6:I:810:HEM:C3B  | 2.86                     | 0.60              |
| 1:L:502:GLN:O    | 1:L:539:ARG:NH2  | 2.35                     | 0.60              |
| 1:G:360:CYS:SG   | 6:G:809:HEM:C3B  | 2.78                     | 0.60              |
| 6:A:813:HEM:HMC1 | 6:A:813:HEM:HBC2 | 1.84                     | 0.60              |
| 1:G:143:CYS:HG   | 6:G:806:HEM:CAB  | 2.13                     | 0.60              |
| 1:A:143:CYS:SG   | 6:A:806:HEM:C3B  | 2.91                     | 0.59              |
| 6:K:813:HEM:HBB2 | 6:K:813:HEM:HMB1 | 1.84                     | 0.59              |
| 1:C:302:CYS:SG   | 6:C:807:HEM:CBB  | 2.89                     | 0.59              |
| 6:H:808:HEM:HMC1 | 6:H:808:HEM:HBC2 | 1.84                     | 0.59              |
| 1:I:143:CYS:SG   | 6:I:806:HEM:C3B  | 2.93                     | 0.59              |
| 1:J:626:LEU:HB3  | 1:J:686:MET:HE2  | 1.85                     | 0.59              |
| 1:L:339:CYS:SG   | 6:L:808:HEM:C3B  | 2.93                     | 0.59              |
| 1:E:418:CYS:SG   | 6:E:810:HEM:C3B  | 2.87                     | 0.59              |
| 1:K:302:CYS:SG   | 6:K:807:HEM:C2B  | 2.95                     | 0.58              |
| 1:J:305:CYS:CB   | 6:J:807:HEM:C3C  | 2.86                     | 0.58              |
| 1:H:360:CYS:SG   | 6:H:810:HEM:C3B  | 2.77                     | 0.58              |
| 1:F:578:CYS:SG   | 6:F:814:HEM:HAC  | 2.34                     | 0.58              |
| 1:G:465:CYS:SG   | 6:G:811:HEM:HAC  | 2.36                     | 0.57              |
| 1:A:418:CYS:SG   | 6:A:810:HEM:C3B  | 2.85                     | 0.57              |
| 1:I:578:CYS:SG   | 6:I:813:HEM:HAC  | 2.37                     | 0.57              |
| 1:B:146:CYS:SG   | 6:B:807:HEM:HAC  | 2.38                     | 0.56              |
| 1:K:465:CYS:SG   | 6:K:811:HEM:HAC  | 2.40                     | 0.56              |
| 1:F:146:CYS:SG   | 6:F:807:HEM:HAC  | 2.37                     | 0.56              |
| 1:A:434:GLU:HB2  | 1:A:437:ILE:HD12 | 1.86                     | 0.56              |
| 1:H:578:CYS:SG   | 6:H:814:HEM:C3C  | 2.86                     | 0.56              |
| 6:L:812:HEM:HMC2 | 6:L:812:HEM:HBC2 | 1.88                     | 0.56              |
| 6:G:807:HEM:HMC1 | 6:G:807:HEM:HBC2 | 1.86                     | 0.56              |
| 1:H:143:CYS:SG   | 6:H:807:HEM:C3B  | 2.96                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:208:LYS:HG3  | 6:K:807:HEM:HMA2 | 1.86                     | 0.56              |
| 1:B:418:CYS:HG   | 6:B:811:HEM:CAB  | 2.16                     | 0.55              |
| 1:A:302:CYS:SG   | 6:A:807:HEM:CBB  | 2.93                     | 0.55              |
| 1:K:143:CYS:SG   | 6:K:806:HEM:CBB  | 2.90                     | 0.55              |
| 1:L:575:ALA:HB3  | 6:L:813:HEM:HBC1 | 1.88                     | 0.55              |
| 1:A:146:CYS:SG   | 6:A:806:HEM:HAC  | 2.36                     | 0.55              |
| 1:D:302:CYS:SG   | 6:D:807:HEM:CBB  | 2.93                     | 0.55              |
| 1:J:612:LYS:HE3  | 1:J:676:VAL:HG21 | 1.88                     | 0.55              |
| 1:I:421:CYS:SG   | 6:I:810:HEM:HAC  | 2.38                     | 0.54              |
| 1:K:305:CYS:CB   | 6:K:807:HEM:C3C  | 2.90                     | 0.54              |
| 1:D:208:LYS:HG3  | 6:D:807:HEM:HMA2 | 1.88                     | 0.54              |
| 1:A:402:GLU:O    | 1:A:406:THR:HG23 | 2.08                     | 0.54              |
| 1:D:402:GLU:O    | 1:D:406:THR:HG23 | 2.07                     | 0.54              |
| 1:G:578:CYS:SG   | 6:G:813:HEM:HAC  | 2.40                     | 0.54              |
| 1:E:302:CYS:SG   | 6:E:807:HEM:CBB  | 2.95                     | 0.54              |
| 1:G:476:ALA:O    | 1:G:480:SER:HB3  | 2.06                     | 0.54              |
| 1:A:305:CYS:CB   | 6:A:807:HEM:C3C  | 2.90                     | 0.53              |
| 1:D:487:CYS:SG   | 6:D:812:HEM:HAC  | 2.39                     | 0.53              |
| 1:D:578:CYS:SG   | 6:D:813:HEM:HAC  | 2.36                     | 0.53              |
| 1:C:578:CYS:SG   | 6:C:813:HEM:HAC  | 2.42                     | 0.53              |
| 1:A:462:CYS:SG   | 6:A:811:HEM:C3B  | 2.91                     | 0.53              |
| 6:K:810:HEM:HMB1 | 6:K:810:HEM:HBB2 | 1.90                     | 0.53              |
| 6:G:810:HEM:HBB2 | 6:G:810:HEM:HMB1 | 1.91                     | 0.53              |
| 1:H:400:GLY:HA3  | 6:H:808:HEM:HMD2 | 1.89                     | 0.53              |
| 1:C:612:LYS:HE3  | 1:C:676:VAL:HG21 | 1.91                     | 0.53              |
| 1:B:305:CYS:CB   | 6:B:808:HEM:C3C  | 2.92                     | 0.53              |
| 1:H:487:CYS:SG   | 6:H:813:HEM:HAC  | 2.36                     | 0.53              |
| 1:B:302:CYS:SG   | 6:B:808:HEM:CBB  | 2.95                     | 0.52              |
| 1:E:208:LYS:HG3  | 6:E:807:HEM:HMA2 | 1.92                     | 0.52              |
| 1:E:484:CYS:CB   | 6:E:812:HEM:CAB  | 2.87                     | 0.52              |
| 1:E:540:ASP:O    | 4:E:804:BU3:H3   | 2.10                     | 0.52              |
| 1:F:146:CYS:CB   | 6:F:807:HEM:C3C  | 2.93                     | 0.52              |
| 1:G:302:CYS:SG   | 6:G:807:HEM:CBB  | 2.98                     | 0.52              |
| 1:F:302:CYS:SG   | 6:F:808:HEM:CBB  | 2.98                     | 0.52              |
| 1:H:302:CYS:SG   | 6:H:808:HEM:CBB  | 2.96                     | 0.52              |
| 1:G:305:CYS:C    | 1:G:307:PRO:HD3  | 2.35                     | 0.51              |
| 1:L:305:CYS:CB   | 6:L:807:HEM:C3C  | 2.94                     | 0.51              |
| 1:L:400:GLY:HA3  | 6:L:807:HEM:HMD2 | 1.92                     | 0.51              |
| 1:L:146:CYS:CB   | 6:L:806:HEM:C3C  | 2.94                     | 0.51              |
| 1:L:575:ALA:CB   | 6:L:813:HEM:CBC  | 2.89                     | 0.51              |
| 1:G:146:CYS:CB   | 6:G:806:HEM:C3C  | 2.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:578:CYS:SG   | 6:J:813:HEM:HAC  | 2.37                     | 0.51              |
| 1:A:435:LYS:NZ   | 1:A:445:GLU:OE1  | 2.43                     | 0.51              |
| 1:C:146:CYS:CB   | 6:C:806:HEM:C3C  | 2.94                     | 0.51              |
| 1:D:146:CYS:CB   | 6:D:806:HEM:C3C  | 2.94                     | 0.51              |
| 1:F:305:CYS:CB   | 6:F:808:HEM:C3C  | 2.94                     | 0.51              |
| 1:G:484:CYS:CB   | 6:G:812:HEM:CAB  | 2.89                     | 0.51              |
| 1:A:360:CYS:SG   | 6:A:809:HEM:C3B  | 2.80                     | 0.51              |
| 1:A:49:GLU:HG2   | 8:A:1274:HOH:O   | 2.11                     | 0.50              |
| 1:A:629:VAL:HG12 | 1:A:629:VAL:O    | 2.11                     | 0.50              |
| 1:B:603:MET:HE2  | 1:B:603:MET:HA   | 1.93                     | 0.50              |
| 1:F:363:CYS:CB   | 6:F:810:HEM:C3C  | 2.95                     | 0.50              |
| 1:L:465:CYS:SG   | 6:L:811:HEM:HAC  | 2.39                     | 0.50              |
| 1:L:518:TRP:HE1  | 6:L:811:HEM:HBB2 | 1.76                     | 0.50              |
| 1:D:339:CYS:SG   | 6:D:808:HEM:CBB  | 2.95                     | 0.49              |
| 1:I:484:CYS:HB3  | 6:I:812:HEM:C3B  | 2.48                     | 0.49              |
| 1:L:104:ASN:O    | 1:L:108:LYS:HG2  | 2.12                     | 0.49              |
| 1:L:342:CYS:SG   | 6:L:808:HEM:HAC  | 2.40                     | 0.49              |
| 6:B:809:HEM:HBC1 | 6:B:810:HEM:CHC  | 2.42                     | 0.49              |
| 1:C:421:CYS:SG   | 6:C:810:HEM:HAC  | 2.41                     | 0.49              |
| 1:F:603:MET:HE1  | 1:F:606:GLN:OE1  | 2.12                     | 0.49              |
| 1:H:84:THR:OG1   | 1:H:86:GLY:O     | 2.25                     | 0.49              |
| 1:B:465:CYS:SG   | 6:B:812:HEM:HAC  | 2.43                     | 0.49              |
| 6:J:812:HEM:HBC2 | 6:J:812:HEM:HMC2 | 1.95                     | 0.48              |
| 1:K:421:CYS:SG   | 6:K:810:HEM:HAC  | 2.43                     | 0.48              |
| 1:B:305:CYS:C    | 1:B:307:PRO:HD3  | 2.37                     | 0.48              |
| 1:J:360:CYS:HG   | 6:J:809:HEM:CBB  | 2.21                     | 0.48              |
| 1:A:146:CYS:CB   | 6:A:806:HEM:C3C  | 2.96                     | 0.48              |
| 1:C:486:SER:HB2  | 6:C:813:HEM:HBC2 | 1.96                     | 0.48              |
| 1:F:223:VAL:CG2  | 1:F:235:ILE:HD13 | 2.43                     | 0.48              |
| 1:I:146:CYS:CB   | 6:I:806:HEM:C3C  | 2.96                     | 0.48              |
| 1:I:484:CYS:CB   | 6:I:812:HEM:CAB  | 2.89                     | 0.48              |
| 1:L:562:CYS:HG   | 6:L:813:HEM:HAB  | 1.76                     | 0.48              |
| 6:L:806:HEM:HBC2 | 6:L:806:HEM:HMC2 | 1.96                     | 0.48              |
| 1:G:487:CYS:SG   | 6:G:812:HEM:HAC  | 2.40                     | 0.48              |
| 1:I:146:CYS:SG   | 6:I:806:HEM:HAC  | 2.44                     | 0.48              |
| 1:A:462:CYS:SG   | 6:A:811:HEM:CBB  | 2.94                     | 0.47              |
| 1:D:360:CYS:HG   | 6:D:809:HEM:CBB  | 2.20                     | 0.47              |
| 1:E:146:CYS:SG   | 6:E:806:HEM:HAC  | 2.40                     | 0.47              |
| 1:F:101:GLY:CA   | 1:F:122:MET:HE3  | 2.44                     | 0.47              |
| 1:J:463:THR:HG22 | 1:J:470:ALA:HB2  | 1.96                     | 0.47              |
| 1:G:484:CYS:HB3  | 6:G:812:HEM:C3B  | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:681:GLU:O    | 1:I:685:ILE:HD12 | 2.14                     | 0.47              |
| 1:J:421:CYS:SG   | 6:J:810:HEM:HAC  | 2.45                     | 0.47              |
| 1:J:465:CYS:SG   | 6:J:811:HEM:HAC  | 2.41                     | 0.47              |
| 1:K:165:PHE:CZ   | 1:K:335:LYS:HD3  | 2.49                     | 0.47              |
| 1:C:465:CYS:SG   | 6:C:811:HEM:HAC  | 2.43                     | 0.47              |
| 1:E:305:CYS:CB   | 6:E:807:HEM:C3C  | 2.97                     | 0.47              |
| 1:K:487:CYS:SG   | 6:K:812:HEM:HAC  | 2.41                     | 0.47              |
| 1:E:607:THR:HB   | 1:E:608:PRO:HD3  | 1.96                     | 0.47              |
| 1:A:547:GLU:HG3  | 8:A:1296:HOH:O   | 2.15                     | 0.47              |
| 1:G:305:CYS:CB   | 6:G:807:HEM:C3C  | 2.98                     | 0.47              |
| 1:C:400:GLY:HA3  | 6:C:807:HEM:HMD2 | 1.98                     | 0.47              |
| 1:F:421:CYS:SG   | 6:F:811:HEM:HAC  | 2.40                     | 0.46              |
| 1:E:374:MET:HE1  | 1:E:381:ALA:HA   | 1.97                     | 0.46              |
| 1:C:305:CYS:CB   | 6:C:807:HEM:C3C  | 2.99                     | 0.46              |
| 1:H:418:CYS:SG   | 6:H:811:HEM:C3B  | 2.89                     | 0.46              |
| 1:K:305:CYS:HB2  | 6:K:807:HEM:C3C  | 2.50                     | 0.46              |
| 1:B:243:GLN:HB3  | 1:B:496:GLU:OE2  | 2.14                     | 0.46              |
| 1:C:305:CYS:C    | 1:C:307:PRO:HD3  | 2.40                     | 0.46              |
| 1:E:646:LYS:NZ   | 8:E:1118:HOH:O   | 2.49                     | 0.46              |
| 1:H:146:CYS:CB   | 6:H:807:HEM:C3C  | 2.99                     | 0.46              |
| 1:I:372:ASP:OD1  | 1:I:375:ARG:NH2  | 2.48                     | 0.46              |
| 1:A:363:CYS:CB   | 6:A:809:HEM:C3C  | 2.99                     | 0.46              |
| 1:I:305:CYS:C    | 1:I:307:PRO:HD3  | 2.40                     | 0.46              |
| 6:L:808:HEM:HBC1 | 6:L:809:HEM:CHC  | 2.46                     | 0.46              |
| 1:C:301:TYR:CD2  | 6:C:807:HEM:HAB  | 2.51                     | 0.46              |
| 1:I:289:TYR:CE2  | 1:I:290:LYS:HE2  | 2.51                     | 0.46              |
| 1:J:146:CYS:SG   | 6:J:806:HEM:HAC  | 2.45                     | 0.46              |
| 1:D:484:CYS:CB   | 6:D:812:HEM:CAB  | 2.91                     | 0.45              |
| 1:E:112:ARG:HB2  | 1:K:151:TYR:CE1  | 2.51                     | 0.45              |
| 1:F:365:GLN:NE2  | 5:F:806:ACT:O    | 2.48                     | 0.45              |
| 1:I:305:CYS:SG   | 6:I:807:HEM:HAC  | 2.39                     | 0.45              |
| 1:G:654:ILE:HD12 | 1:G:668:THR:HG23 | 1.98                     | 0.45              |
| 1:A:484:CYS:CB   | 6:A:812:HEM:CAB  | 2.93                     | 0.45              |
| 1:B:675:ALA:HA   | 1:B:678:TYR:CD2  | 2.52                     | 0.45              |
| 1:E:311:ASP:OD1  | 1:E:311:ASP:C    | 2.59                     | 0.45              |
| 6:E:810:HEM:HMB1 | 6:E:810:HEM:HBB2 | 1.97                     | 0.45              |
| 1:K:302:CYS:HG   | 6:K:807:HEM:CAB  | 2.10                     | 0.45              |
| 1:G:475:LYS:O    | 1:G:476:ALA:C    | 2.60                     | 0.45              |
| 1:C:650:THR:HG23 | 1:C:671:ARG:HG2  | 1.98                     | 0.45              |
| 1:C:365:GLN:OE1  | 5:C:805:ACT:H1   | 2.17                     | 0.45              |
| 1:G:402:GLU:O    | 1:G:406:THR:HG23 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:305:CYS:HB2  | 6:A:807:HEM:C3C  | 2.51                     | 0.45              |
| 1:E:305:CYS:SG   | 6:E:807:HEM:HAC  | 2.43                     | 0.45              |
| 1:E:659:SER:HB3  | 1:E:663:HIS:CE1  | 2.52                     | 0.45              |
| 1:G:360:CYS:HG   | 6:G:809:HEM:CBB  | 2.16                     | 0.45              |
| 1:I:499:TYR:O    | 1:I:539:ARG:NH2  | 2.50                     | 0.45              |
| 1:K:146:CYS:CB   | 6:K:806:HEM:C3C  | 3.00                     | 0.44              |
| 1:J:305:CYS:C    | 1:J:307:PRO:HD3  | 2.42                     | 0.44              |
| 1:K:357:ILE:HB   | 4:K:803:BU3:H11  | 1.99                     | 0.44              |
| 1:F:363:CYS:HB2  | 6:F:810:HEM:C3C  | 2.51                     | 0.44              |
| 1:L:220:THR:HA   | 1:L:240:ASN:ND2  | 2.33                     | 0.44              |
| 1:G:94:GLY:O     | 1:G:98:ILE:HB    | 2.16                     | 0.44              |
| 1:D:146:CYS:SG   | 6:D:806:HEM:HAC  | 2.44                     | 0.44              |
| 1:D:486:SER:HB2  | 6:D:813:HEM:HBC2 | 1.99                     | 0.44              |
| 6:J:813:HEM:HBD1 | 6:J:813:HEM:HMD2 | 1.98                     | 0.44              |
| 1:G:688:LYS:HD3  | 1:G:688:LYS:N    | 2.33                     | 0.44              |
| 1:F:223:VAL:HG22 | 1:F:235:ILE:HD13 | 1.99                     | 0.44              |
| 1:A:243:GLN:HB3  | 1:A:496:GLU:OE2  | 2.18                     | 0.44              |
| 1:G:421:CYS:SG   | 6:G:810:HEM:HAC  | 2.45                     | 0.44              |
| 1:J:208:LYS:HG3  | 6:J:807:HEM:HMA3 | 1.99                     | 0.44              |
| 6:C:807:HEM:HBB2 | 6:C:807:HEM:HMB2 | 2.00                     | 0.44              |
| 6:D:811:HEM:HMC2 | 6:D:811:HEM:HBC2 | 1.99                     | 0.44              |
| 1:F:633:ALA:O    | 1:F:636:ASP:N    | 2.44                     | 0.44              |
| 1:B:578:CYS:SG   | 6:B:814:HEM:HAC  | 2.43                     | 0.43              |
| 1:C:104:ASN:O    | 1:C:108:LYS:HG2  | 2.17                     | 0.43              |
| 6:C:810:HEM:HMB1 | 6:C:810:HEM:HBB2 | 2.00                     | 0.43              |
| 1:D:305:CYS:C    | 1:D:307:PRO:HD3  | 2.43                     | 0.43              |
| 1:H:123:TYR:CE1  | 6:H:808:HEM:HBC2 | 2.54                     | 0.43              |
| 1:J:305:CYS:HB2  | 6:J:807:HEM:C3C  | 2.53                     | 0.43              |
| 1:J:402:GLU:O    | 1:J:406:THR:HG23 | 2.19                     | 0.43              |
| 1:K:400:GLY:HA3  | 6:K:807:HEM:HMD2 | 2.00                     | 0.43              |
| 1:F:453:TYR:CD2  | 1:F:570:LYS:HG2  | 2.54                     | 0.43              |
| 1:H:203:GLY:HA3  | 6:H:808:HEM:HMA1 | 2.01                     | 0.43              |
| 1:H:305:CYS:SG   | 6:H:808:HEM:HAC  | 2.39                     | 0.43              |
| 1:D:410:ALA:O    | 1:D:414:LYS:HG2  | 2.19                     | 0.43              |
| 1:E:343:HIS:CE1  | 6:E:808:HEM:ND   | 2.86                     | 0.43              |
| 1:K:207:THR:HG23 | 1:K:512:GLN:HG3  | 2.00                     | 0.43              |
| 1:J:302:CYS:SG   | 6:J:807:HEM:CBB  | 3.04                     | 0.43              |
| 1:D:305:CYS:HB2  | 6:D:807:HEM:C3C  | 2.53                     | 0.43              |
| 1:D:659:SER:HB3  | 1:D:663:HIS:CE1  | 2.54                     | 0.43              |
| 6:H:814:HEM:HMC2 | 6:H:814:HEM:HBC2 | 1.99                     | 0.43              |
| 1:B:270:GLU:HG2  | 1:B:271:GLU:N    | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:151:TYR:CE1  | 1:K:112:ARG:HB2  | 2.54                     | 0.43              |
| 1:D:305:CYS:SG   | 6:D:807:HEM:HAC  | 2.43                     | 0.43              |
| 1:F:151:TYR:CE1  | 1:I:112:ARG:HB2  | 2.53                     | 0.43              |
| 1:L:131:LEU:HD21 | 1:L:299:THR:HG21 | 2.01                     | 0.43              |
| 1:L:434:GLU:HB2  | 1:L:437:ILE:HD12 | 2.01                     | 0.43              |
| 1:G:400:GLY:HA3  | 6:G:807:HEM:HMD2 | 2.00                     | 0.43              |
| 6:D:808:HEM:HBC1 | 6:D:809:HEM:CHC  | 2.48                     | 0.43              |
| 1:F:602:VAL:HG12 | 1:F:603:MET:HE2  | 2.00                     | 0.43              |
| 1:H:493:MET:HB2  | 1:H:513:ARG:HB2  | 2.01                     | 0.43              |
| 1:I:402:GLU:O    | 1:I:406:THR:HG23 | 2.18                     | 0.43              |
| 1:I:453:TYR:CD2  | 1:I:570:LYS:HD2  | 2.54                     | 0.43              |
| 1:H:302:CYS:SG   | 6:H:808:HEM:HAB  | 2.48                     | 0.43              |
| 1:L:360:CYS:HG   | 6:L:809:HEM:CBB  | 2.18                     | 0.43              |
| 1:E:223:VAL:HG22 | 1:E:235:ILE:HD13 | 2.01                     | 0.43              |
| 1:K:143:CYS:SG   | 6:K:806:HEM:C3B  | 3.00                     | 0.43              |
| 1:H:395:MET:HG2  | 1:H:544:TRP:CE2  | 2.54                     | 0.42              |
| 1:K:84:THR:OG1   | 1:K:86:GLY:O     | 2.37                     | 0.42              |
| 1:L:339:CYS:HA   | 6:L:808:HEM:CHC  | 2.49                     | 0.42              |
| 6:L:807:HEM:HBB2 | 6:L:807:HEM:HMB2 | 2.00                     | 0.42              |
| 6:G:806:HEM:HMC2 | 6:G:806:HEM:HBC2 | 2.01                     | 0.42              |
| 1:H:484:CYS:CB   | 6:H:813:HEM:CAB  | 2.95                     | 0.42              |
| 1:K:612:LYS:O    | 1:K:616:VAL:HG23 | 2.18                     | 0.42              |
| 6:K:808:HEM:HBC2 | 6:K:808:HEM:HMC2 | 2.01                     | 0.42              |
| 1:L:305:CYS:HB2  | 6:L:807:HEM:C3C  | 2.55                     | 0.42              |
| 1:E:499:TYR:CD1  | 4:E:804:BU3:H43  | 2.54                     | 0.42              |
| 1:F:642:GLU:OE2  | 1:J:646:LYS:NZ   | 2.42                     | 0.42              |
| 1:H:374:MET:HE1  | 1:H:384:PRO:HA   | 2.01                     | 0.42              |
| 1:E:360:CYS:HG   | 6:E:809:HEM:CBB  | 2.19                     | 0.42              |
| 6:J:813:HEM:HBD1 | 6:J:813:HEM:CMD  | 2.50                     | 0.42              |
| 1:G:363:CYS:CB   | 6:G:809:HEM:C3C  | 3.03                     | 0.42              |
| 1:B:191:GLN:HG2  | 1:B:223:VAL:O    | 2.19                     | 0.42              |
| 6:B:808:HEM:HBB2 | 6:B:808:HEM:HMB2 | 2.00                     | 0.42              |
| 6:C:807:HEM:HMD1 | 6:C:807:HEM:CBD  | 2.50                     | 0.42              |
| 1:D:607:THR:HB   | 1:D:608:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:264:ASP:OD1  | 1:A:264:ASP:N    | 2.51                     | 0.42              |
| 1:F:302:CYS:SG   | 6:F:808:HEM:HAB  | 2.50                     | 0.42              |
| 6:H:807:HEM:HBC2 | 6:H:807:HEM:CMC  | 2.50                     | 0.42              |
| 1:J:197:VAL:O    | 1:J:214:ALA:N    | 2.53                     | 0.42              |
| 1:L:301:TYR:CD2  | 6:L:807:HEM:HAB  | 2.55                     | 0.42              |
| 1:H:374:MET:CE   | 1:H:384:PRO:HA   | 2.50                     | 0.42              |
| 1:I:101:GLY:CA   | 1:I:122:MET:HE3  | 2.49                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:L:812:HEM:HBC2 | 6:L:812:HEM:CMC  | 2.50                     | 0.42              |
| 1:G:492:MET:CE   | 1:G:529:LEU:HD21 | 2.49                     | 0.42              |
| 1:J:259:LYS:HA   | 1:J:262:VAL:O    | 2.20                     | 0.41              |
| 1:L:302:CYS:SG   | 6:L:807:HEM:HAB  | 2.47                     | 0.41              |
| 1:C:607:THR:HB   | 1:C:608:PRO:HD3  | 2.02                     | 0.41              |
| 1:E:395:MET:HG2  | 1:E:544:TRP:CE2  | 2.55                     | 0.41              |
| 1:L:612:LYS:NZ   | 1:L:673:ASP:OD1  | 2.43                     | 0.41              |
| 1:G:476:ALA:O    | 1:G:477:ASP:CB   | 2.68                     | 0.41              |
| 6:H:809:HEM:HBC1 | 6:H:810:HEM:CHC  | 2.50                     | 0.41              |
| 1:I:62:GLU:OE1   | 1:I:129:SER:OG   | 2.25                     | 0.41              |
| 1:I:302:CYS:SG   | 6:I:807:HEM:C2B  | 3.12                     | 0.41              |
| 1:L:203:GLY:HA2  | 6:L:807:HEM:HBA2 | 2.02                     | 0.41              |
| 1:E:628:GLU:O    | 1:E:629:VAL:HG22 | 2.19                     | 0.41              |
| 1:A:642:GLU:OE2  | 1:C:646:LYS:HE3  | 2.21                     | 0.41              |
| 1:D:642:GLU:HG3  | 1:E:646:LYS:HE3  | 2.03                     | 0.41              |
| 1:F:400:GLY:HA3  | 6:F:808:HEM:HMD2 | 2.03                     | 0.41              |
| 1:L:306:HIS:CE1  | 6:L:809:HEM:HMD2 | 2.56                     | 0.41              |
| 1:C:311:ASP:OD1  | 1:C:311:ASP:C    | 2.63                     | 0.41              |
| 1:C:402:GLU:O    | 1:C:406:THR:HG23 | 2.21                     | 0.41              |
| 1:F:184:ASP:OD1  | 1:F:184:ASP:N    | 2.52                     | 0.41              |
| 1:H:112:ARG:HB2  | 1:G:151:TYR:CE1  | 2.56                     | 0.41              |
| 1:K:636:ASP:O    | 1:K:640:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:360:CYS:HG   | 6:B:810:HEM:CBB  | 2.16                     | 0.41              |
| 1:D:301:TYR:CD2  | 6:D:807:HEM:HAB  | 2.56                     | 0.41              |
| 1:J:151:TYR:CD1  | 1:J:151:TYR:C    | 2.98                     | 0.41              |
| 1:J:302:CYS:SG   | 6:J:807:HEM:C2B  | 3.10                     | 0.41              |
| 1:K:643:LEU:HD11 | 1:K:681:GLU:HG2  | 2.02                     | 0.41              |
| 1:F:523:ASP:CG   | 1:F:524:PRO:HD2  | 2.46                     | 0.41              |
| 1:I:338:SER:O    | 1:I:339:CYS:C    | 2.64                     | 0.41              |
| 1:J:94:GLY:O     | 1:J:98:ILE:HB    | 2.21                     | 0.41              |
| 1:J:143:CYS:SG   | 6:J:806:HEM:C3B  | 3.03                     | 0.41              |
| 1:B:305:CYS:HB2  | 6:B:808:HEM:C3C  | 2.55                     | 0.41              |
| 1:E:434:GLU:HB2  | 1:E:437:ILE:HD12 | 2.03                     | 0.41              |
| 1:F:175:LYS:HE3  | 1:F:178:ASP:OD2  | 2.21                     | 0.41              |
| 1:B:659:SER:HB3  | 1:B:663:HIS:CE1  | 2.56                     | 0.40              |
| 1:H:357:ILE:HB   | 4:H:803:BU3:H11  | 2.02                     | 0.40              |
| 6:G:812:HEM:HMC2 | 6:G:812:HEM:HBC2 | 2.03                     | 0.40              |
| 1:E:305:CYS:C    | 1:E:307:PRO:HD3  | 2.46                     | 0.40              |
| 1:H:421:CYS:SG   | 6:H:811:HEM:HAC  | 2.45                     | 0.40              |
| 1:J:147:HIS:CE1  | 6:J:806:HEM:ND   | 2.89                     | 0.40              |
| 1:J:605:TRP:HE3  | 1:J:662:MET:SD   | 2.44                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:513:ARG:NH1  | 6:D:810:HEM:O1A  | 2.55                     | 0.40              |
| 1:E:484:CYS:CB   | 6:E:812:HEM:C3B  | 3.05                     | 0.40              |
| 1:E:650:THR:HG23 | 1:E:671:ARG:HB3  | 2.04                     | 0.40              |
| 6:L:809:HEM:HMB2 | 6:L:809:HEM:HBB2 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 559/613 (91%)   | 556 (100%) | 3 (0%)   | 81          | 90 |
| 1   | B     | 560/613 (91%)   | 555 (99%)  | 5 (1%)   | 70          | 84 |
| 1   | C     | 559/613 (91%)   | 555 (99%)  | 4 (1%)   | 76          | 87 |
| 1   | D     | 559/613 (91%)   | 554 (99%)  | 5 (1%)   | 70          | 84 |
| 1   | E     | 559/613 (91%)   | 557 (100%) | 2 (0%)   | 84          | 92 |
| 1   | F     | 559/613 (91%)   | 552 (99%)  | 7 (1%)   | 61          | 76 |
| 1   | G     | 558/613 (91%)   | 553 (99%)  | 5 (1%)   | 70          | 84 |
| 1   | H     | 560/613 (91%)   | 555 (99%)  | 5 (1%)   | 70          | 84 |
| 1   | I     | 559/613 (91%)   | 554 (99%)  | 5 (1%)   | 70          | 84 |
| 1   | J     | 559/613 (91%)   | 554 (99%)  | 5 (1%)   | 70          | 84 |
| 1   | K     | 559/613 (91%)   | 556 (100%) | 3 (0%)   | 81          | 90 |
| 1   | L     | 559/613 (91%)   | 554 (99%)  | 5 (1%)   | 70          | 84 |
| All | All   | 6709/7356 (91%) | 6655 (99%) | 54 (1%)  | 73          | 85 |

All (54) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 250 | LEU  |
| 1   | A     | 302 | CYS  |
| 1   | A     | 564 | ARG  |
| 1   | B     | 270 | GLU  |
| 1   | B     | 302 | CYS  |
| 1   | B     | 537 | ASP  |
| 1   | B     | 564 | ARG  |
| 1   | B     | 651 | VAL  |
| 1   | C     | 253 | GLU  |
| 1   | C     | 302 | CYS  |
| 1   | C     | 564 | ARG  |
| 1   | C     | 651 | VAL  |
| 1   | D     | 302 | CYS  |
| 1   | D     | 547 | GLU  |
| 1   | D     | 564 | ARG  |
| 1   | D     | 645 | GLU  |
| 1   | D     | 686 | MET  |
| 1   | E     | 302 | CYS  |
| 1   | E     | 564 | ARG  |
| 1   | F     | 129 | SER  |
| 1   | F     | 194 | THR  |
| 1   | F     | 302 | CYS  |
| 1   | F     | 360 | CYS  |
| 1   | F     | 564 | ARG  |
| 1   | F     | 638 | THR  |
| 1   | F     | 656 | LYS  |
| 1   | H     | 302 | CYS  |
| 1   | H     | 339 | CYS  |
| 1   | H     | 564 | ARG  |
| 1   | H     | 632 | LEU  |
| 1   | H     | 690 | LEU  |
| 1   | I     | 290 | LYS  |
| 1   | I     | 302 | CYS  |
| 1   | I     | 564 | ARG  |
| 1   | I     | 570 | LYS  |
| 1   | I     | 685 | ILE  |
| 1   | J     | 49  | GLU  |
| 1   | J     | 302 | CYS  |
| 1   | J     | 564 | ARG  |
| 1   | J     | 651 | VAL  |
| 1   | J     | 688 | LYS  |
| 1   | K     | 302 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 303 | GLU  |
| 1   | K     | 564 | ARG  |
| 1   | L     | 194 | THR  |
| 1   | L     | 275 | ASN  |
| 1   | L     | 302 | CYS  |
| 1   | L     | 360 | CYS  |
| 1   | L     | 564 | ARG  |
| 1   | G     | 124 | ARG  |
| 1   | G     | 302 | CYS  |
| 1   | G     | 313 | LYS  |
| 1   | G     | 564 | ARG  |
| 1   | G     | 651 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 365 | GLN  |
| 1   | A     | 446 | GLN  |
| 1   | A     | 497 | ASN  |
| 1   | A     | 648 | GLN  |
| 1   | B     | 497 | ASN  |
| 1   | B     | 621 | GLN  |
| 1   | B     | 670 | GLN  |
| 1   | C     | 446 | GLN  |
| 1   | D     | 497 | ASN  |
| 1   | D     | 648 | GLN  |
| 1   | E     | 43  | HIS  |
| 1   | E     | 64  | GLN  |
| 1   | E     | 380 | ASN  |
| 1   | E     | 446 | GLN  |
| 1   | E     | 497 | ASN  |
| 1   | E     | 606 | GLN  |
| 1   | F     | 43  | HIS  |
| 1   | H     | 64  | GLN  |
| 1   | H     | 73  | ASN  |
| 1   | H     | 377 | ASN  |
| 1   | H     | 497 | ASN  |
| 1   | H     | 648 | GLN  |
| 1   | I     | 497 | ASN  |
| 1   | J     | 64  | GLN  |
| 1   | J     | 380 | ASN  |
| 1   | J     | 512 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 43  | HIS  |
| 1   | K     | 241 | GLN  |
| 1   | K     | 621 | GLN  |
| 1   | L     | 104 | ASN  |
| 1   | L     | 377 | ASN  |
| 1   | L     | 600 | ASN  |
| 1   | L     | 670 | GLN  |
| 1   | G     | 446 | GLN  |
| 1   | G     | 497 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 161 ligands modelled in this entry, 12 are monoatomic - leaving 149 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 | $\# Z  > 2$ |
| 5   | ACT  | D     | 805 | -    | 3,3,3        | 0.88 | 0           | 3,3,3       | 0.52 | 0           |
| 6   | HEM  | K     | 806 | 1    | 50,50,50     | 2.46 | 12 (24%)    | 67,82,82    | 2.55 | 21 (31%)    |
| 6   | HEM  | G     | 809 | 1    | 50,50,50     | 2.44 | 11 (22%)    | 67,82,82    | 2.12 | 17 (25%)    |
| 6   | HEM  | F     | 813 | 1    | 50,50,50     | 2.40 | 9 (18%)     | 67,82,82    | 2.39 | 15 (22%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | HEM  | F     | 814 | 1    | 50,50,50     | 2.44 | 11 (22%) | 67,82,82    | 2.28 | 15 (22%) |
| 4   | BU3  | E     | 804 | -    | 4,5,5        | 0.31 | 0        | 6,6,6       | 0.29 | 0        |
| 6   | HEM  | K     | 808 | 1    | 50,50,50     | 2.41 | 9 (18%)  | 67,82,82    | 2.19 | 14 (20%) |
| 4   | BU3  | K     | 804 | -    | 4,5,5        | 0.50 | 0        | 6,6,6       | 0.27 | 0        |
| 4   | BU3  | L     | 804 | -    | 4,5,5        | 0.43 | 0        | 6,6,6       | 0.35 | 0        |
| 4   | BU3  | G     | 803 | -    | 4,5,5        | 0.45 | 0        | 6,6,6       | 0.27 | 0        |
| 6   | HEM  | A     | 812 | 1    | 50,50,50     | 2.39 | 10 (20%) | 67,82,82    | 2.44 | 20 (29%) |
| 6   | HEM  | J     | 809 | 1    | 50,50,50     | 2.49 | 10 (20%) | 67,82,82    | 2.16 | 17 (25%) |
| 6   | HEM  | I     | 808 | 1    | 50,50,50     | 2.40 | 10 (20%) | 67,82,82    | 2.22 | 14 (20%) |
| 7   | SO2  | G     | 814 | 6    | 2,2,2        | 1.72 | 0        | 1,1,1       | 1.58 | 0        |
| 4   | BU3  | H     | 803 | -    | 4,5,5        | 0.32 | 0        | 6,6,6       | 0.24 | 0        |
| 5   | ACT  | B     | 806 | -    | 3,3,3        | 0.78 | 0        | 3,3,3       | 0.97 | 0        |
| 6   | HEM  | B     | 814 | 1    | 50,50,50     | 2.46 | 10 (20%) | 67,82,82    | 2.21 | 15 (22%) |
| 6   | HEM  | I     | 806 | 1    | 50,50,50     | 2.46 | 9 (18%)  | 67,82,82    | 2.21 | 16 (23%) |
| 6   | HEM  | G     | 811 | 1    | 50,50,50     | 2.45 | 12 (24%) | 67,82,82    | 2.36 | 16 (23%) |
| 6   | HEM  | F     | 808 | 1,3  | 50,50,50     | 2.48 | 10 (20%) | 67,82,82    | 2.17 | 16 (23%) |
| 6   | HEM  | G     | 808 | 1    | 50,50,50     | 2.44 | 10 (20%) | 67,82,82    | 2.20 | 13 (19%) |
| 6   | HEM  | C     | 813 | 1    | 50,50,50     | 2.42 | 10 (20%) | 67,82,82    | 2.27 | 14 (20%) |
| 6   | HEM  | E     | 808 | 1    | 50,50,50     | 2.39 | 12 (24%) | 67,82,82    | 2.31 | 14 (20%) |
| 4   | BU3  | B     | 804 | -    | 4,5,5        | 0.40 | 0        | 6,6,6       | 0.32 | 0        |
| 4   | BU3  | B     | 803 | -    | 4,5,5        | 0.41 | 0        | 6,6,6       | 0.20 | 0        |
| 5   | ACT  | K     | 805 | -    | 3,3,3        | 0.84 | 0        | 3,3,3       | 0.62 | 0        |
| 6   | HEM  | L     | 808 | 1    | 50,50,50     | 2.47 | 9 (18%)  | 67,82,82    | 2.19 | 14 (20%) |
| 7   | SO2  | A     | 814 | 6    | 2,2,2        | 1.74 | 0        | 1,1,1       | 1.43 | 0        |
| 6   | HEM  | D     | 813 | 1    | 50,50,50     | 2.43 | 10 (20%) | 67,82,82    | 2.27 | 14 (20%) |
| 6   | HEM  | H     | 809 | 1    | 50,50,50     | 2.46 | 11 (22%) | 67,82,82    | 2.16 | 14 (20%) |
| 6   | HEM  | F     | 811 | 1    | 50,50,50     | 2.42 | 10 (20%) | 67,82,82    | 2.32 | 18 (26%) |
| 6   | HEM  | F     | 812 | 1    | 50,50,50     | 2.38 | 7 (14%)  | 67,82,82    | 2.40 | 13 (19%) |
| 6   | HEM  | D     | 806 | 1    | 50,50,50     | 2.40 | 7 (14%)  | 67,82,82    | 2.31 | 16 (23%) |
| 5   | ACT  | J     | 805 | -    | 3,3,3        | 0.77 | 0        | 3,3,3       | 0.94 | 0        |
| 6   | HEM  | L     | 813 | 1    | 50,50,50     | 2.44 | 8 (16%)  | 67,82,82    | 2.26 | 19 (28%) |
| 6   | HEM  | C     | 809 | 1    | 50,50,50     | 2.43 | 9 (18%)  | 67,82,82    | 2.22 | 15 (22%) |
| 6   | HEM  | B     | 807 | 1    | 50,50,50     | 2.37 | 9 (18%)  | 67,82,82    | 2.27 | 16 (23%) |
| 5   | ACT  | H     | 806 | -    | 3,3,3        | 0.78 | 0        | 3,3,3       | 0.81 | 0        |
| 6   | HEM  | E     | 812 | 1    | 50,50,50     | 2.43 | 9 (18%)  | 67,82,82    | 2.25 | 17 (25%) |
| 4   | BU3  | D     | 804 | -    | 4,5,5        | 0.48 | 0        | 6,6,6       | 0.36 | 0        |
| 5   | ACT  | E     | 805 | -    | 3,3,3        | 0.75 | 0        | 3,3,3       | 0.92 | 0        |
| 6   | HEM  | H     | 812 | 1    | 50,50,50     | 2.41 | 9 (18%)  | 67,82,82    | 2.24 | 15 (22%) |



| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | HEM  | G     | 807 | 1,3,7 | 50,50,50     | 2.46 | 12 (24%) | 67,82,82    | 2.22 | 14 (20%) |
| 6   | HEM  | K     | 811 | 1     | 50,50,50     | 2.45 | 10 (20%) | 67,82,82    | 2.24 | 13 (19%) |
| 6   | HEM  | B     | 809 | 1     | 50,50,50     | 2.42 | 12 (24%) | 67,82,82    | 2.38 | 15 (22%) |
| 5   | ACT  | G     | 805 | -     | 3,3,3        | 0.83 | 0        | 3,3,3       | 0.64 | 0        |
| 6   | HEM  | L     | 812 | 1     | 50,50,50     | 2.45 | 9 (18%)  | 67,82,82    | 2.15 | 15 (22%) |
| 6   | HEM  | J     | 811 | 1     | 50,50,50     | 2.44 | 12 (24%) | 67,82,82    | 2.36 | 15 (22%) |
| 4   | BU3  | A     | 803 | -     | 4,5,5        | 0.37 | 0        | 6,6,6       | 0.32 | 0        |
| 5   | ACT  | L     | 805 | -     | 3,3,3        | 0.84 | 0        | 3,3,3       | 0.56 | 0        |
| 6   | HEM  | G     | 813 | 1     | 50,50,50     | 2.46 | 9 (18%)  | 67,82,82    | 2.20 | 18 (26%) |
| 3   | SX   | J     | 802 | 6     | 0,1,1        | -    | -        | -           | -    | -        |
| 6   | HEM  | E     | 806 | 1     | 50,50,50     | 2.43 | 11 (22%) | 67,82,82    | 2.27 | 14 (20%) |
| 6   | HEM  | A     | 811 | 1     | 50,50,50     | 2.42 | 12 (24%) | 67,82,82    | 2.51 | 21 (31%) |
| 6   | HEM  | C     | 811 | 1     | 50,50,50     | 2.40 | 9 (18%)  | 67,82,82    | 2.36 | 15 (22%) |
| 6   | HEM  | I     | 811 | 1     | 50,50,50     | 2.39 | 8 (16%)  | 67,82,82    | 2.39 | 14 (20%) |
| 6   | HEM  | K     | 807 | 1,3   | 50,50,50     | 2.47 | 11 (22%) | 67,82,82    | 2.20 | 13 (19%) |
| 6   | HEM  | H     | 810 | 1     | 50,50,50     | 2.48 | 9 (18%)  | 67,82,82    | 2.16 | 17 (25%) |
| 6   | HEM  | C     | 806 | 1     | 50,50,50     | 2.36 | 11 (22%) | 67,82,82    | 2.31 | 14 (20%) |
| 4   | BU3  | L     | 803 | -     | 4,5,5        | 0.46 | 0        | 6,6,6       | 0.18 | 0        |
| 6   | HEM  | B     | 811 | 1     | 50,50,50     | 2.43 | 9 (18%)  | 67,82,82    | 2.29 | 19 (28%) |
| 6   | HEM  | B     | 812 | 1     | 50,50,50     | 2.42 | 9 (18%)  | 67,82,82    | 2.26 | 15 (22%) |
| 6   | HEM  | H     | 807 | 1     | 50,50,50     | 2.44 | 8 (16%)  | 67,82,82    | 2.28 | 15 (22%) |
| 3   | SX   | B     | 802 | 6     | 0,1,1        | -    | -        | -           | -    | -        |
| 6   | HEM  | J     | 810 | 1     | 50,50,50     | 2.44 | 10 (20%) | 67,82,82    | 2.21 | 17 (25%) |
| 4   | BU3  | B     | 805 | -     | 4,5,5        | 0.33 | 0        | 6,6,6       | 0.26 | 0        |
| 6   | HEM  | A     | 813 | 1     | 50,50,50     | 2.49 | 12 (24%) | 67,82,82    | 2.29 | 15 (22%) |
| 6   | HEM  | L     | 807 | 1,3   | 50,50,50     | 2.48 | 10 (20%) | 67,82,82    | 2.20 | 13 (19%) |
| 6   | HEM  | K     | 812 | 1     | 50,50,50     | 2.45 | 11 (22%) | 67,82,82    | 2.20 | 14 (20%) |
| 4   | BU3  | I     | 804 | -     | 4,5,5        | 0.52 | 0        | 6,6,6       | 0.31 | 0        |
| 6   | HEM  | C     | 810 | 1     | 50,50,50     | 2.45 | 11 (22%) | 67,82,82    | 2.38 | 19 (28%) |
| 3   | SX   | H     | 802 | 6     | 0,1,1        | -    | -        | -           | -    | -        |
| 4   | BU3  | H     | 805 | -     | 4,5,5        | 0.28 | 0        | 6,6,6       | 0.58 | 0        |
| 6   | HEM  | K     | 809 | 1     | 50,50,50     | 2.51 | 9 (18%)  | 67,82,82    | 2.04 | 14 (20%) |
| 3   | SX   | A     | 802 | 6     | 0,1,1        | -    | -        | -           | -    | -        |
| 3   | SX   | C     | 802 | 6     | 0,1,1        | -    | -        | -           | -    | -        |
| 6   | HEM  | D     | 807 | 1,7   | 50,50,50     | 2.46 | 10 (20%) | 67,82,82    | 2.16 | 13 (19%) |
| 3   | SX   | G     | 802 | 6     | 0,1,1        | -    | -        | -           | -    | -        |
| 6   | HEM  | D     | 811 | 1     | 50,50,50     | 2.40 | 8 (16%)  | 67,82,82    | 2.31 | 16 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | HEM  | D     | 812 | 1    | 50,50,50     | 2.40 | 10 (20%) | 67,82,82    | 2.27 | 16 (23%) |
| 6   | HEM  | E     | 810 | 1    | 50,50,50     | 2.42 | 10 (20%) | 67,82,82    | 2.29 | 16 (23%) |
| 6   | HEM  | I     | 810 | 1    | 50,50,50     | 2.38 | 10 (20%) | 67,82,82    | 2.28 | 17 (25%) |
| 6   | HEM  | L     | 809 | 1    | 50,50,50     | 2.51 | 11 (22%) | 67,82,82    | 2.15 | 15 (22%) |
| 6   | HEM  | D     | 809 | 1    | 50,50,50     | 2.44 | 11 (22%) | 67,82,82    | 2.14 | 15 (22%) |
| 6   | HEM  | H     | 811 | 1    | 50,50,50     | 2.38 | 9 (18%)  | 67,82,82    | 2.30 | 18 (26%) |
| 4   | BU3  | C     | 804 | -    | 4,5,5        | 0.33 | 0        | 6,6,6       | 0.29 | 0        |
| 6   | HEM  | H     | 808 | 1,3  | 50,50,50     | 2.49 | 10 (20%) | 67,82,82    | 2.22 | 14 (20%) |
| 6   | HEM  | L     | 811 | 1    | 50,50,50     | 2.45 | 8 (16%)  | 67,82,82    | 2.27 | 20 (29%) |
| 6   | HEM  | A     | 810 | 1    | 50,50,50     | 2.37 | 10 (20%) | 67,82,82    | 2.34 | 17 (25%) |
| 6   | HEM  | I     | 809 | 1    | 50,50,50     | 2.43 | 9 (18%)  | 67,82,82    | 2.07 | 15 (22%) |
| 4   | BU3  | F     | 804 | -    | 4,5,5        | 0.45 | 0        | 6,6,6       | 0.31 | 0        |
| 4   | BU3  | E     | 803 | -    | 4,5,5        | 0.32 | 0        | 6,6,6       | 0.27 | 0        |
| 4   | BU3  | G     | 804 | -    | 4,5,5        | 0.41 | 0        | 6,6,6       | 0.26 | 0        |
| 6   | HEM  | J     | 806 | 1    | 50,50,50     | 2.45 | 11 (22%) | 67,82,82    | 2.48 | 19 (28%) |
| 6   | HEM  | B     | 808 | 1,3  | 50,50,50     | 2.45 | 10 (20%) | 67,82,82    | 2.20 | 12 (17%) |
| 3   | SX   | F     | 802 | 6    | 0,1,1        | -    | -        | -           | -    | -        |
| 4   | BU3  | F     | 805 | -    | 4,5,5        | 0.42 | 0        | 6,6,6       | 0.23 | 0        |
| 4   | BU3  | J     | 804 | -    | 4,5,5        | 0.47 | 0        | 6,6,6       | 0.23 | 0        |
| 6   | HEM  | J     | 808 | 1    | 50,50,50     | 2.46 | 11 (22%) | 67,82,82    | 2.21 | 15 (22%) |
| 6   | HEM  | F     | 807 | 1    | 50,50,50     | 2.45 | 12 (24%) | 67,82,82    | 2.35 | 14 (20%) |
| 6   | HEM  | D     | 808 | 1    | 50,50,50     | 2.45 | 12 (24%) | 67,82,82    | 2.36 | 16 (23%) |
| 6   | HEM  | G     | 810 | 1    | 50,50,50     | 2.38 | 8 (16%)  | 67,82,82    | 2.28 | 16 (23%) |
| 6   | HEM  | C     | 808 | 1    | 50,50,50     | 2.38 | 12 (24%) | 67,82,82    | 2.32 | 17 (25%) |
| 6   | HEM  | J     | 807 | 1,3  | 50,50,50     | 2.50 | 11 (22%) | 67,82,82    | 2.19 | 13 (19%) |
| 6   | HEM  | E     | 809 | 1    | 50,50,50     | 2.48 | 11 (22%) | 67,82,82    | 2.15 | 17 (25%) |
| 6   | HEM  | J     | 813 | 1    | 50,50,50     | 2.49 | 10 (20%) | 67,82,82    | 2.11 | 14 (20%) |
| 7   | SO2  | D     | 802 | 6    | 2,2,2        | 1.81 | 0        | 1,1,1       | 1.52 | 0        |
| 5   | ACT  | F     | 806 | -    | 3,3,3        | 0.80 | 0        | 3,3,3       | 0.87 | 0        |
| 3   | SX   | K     | 802 | 6    | 0,1,1        | -    | -        | -           | -    | -        |
| 6   | HEM  | H     | 814 | 1    | 50,50,50     | 2.43 | 11 (22%) | 67,82,82    | 2.21 | 15 (22%) |
| 6   | HEM  | E     | 813 | 1    | 50,50,50     | 2.44 | 11 (22%) | 67,82,82    | 2.25 | 15 (22%) |
| 6   | HEM  | I     | 813 | 1    | 50,50,50     | 2.47 | 12 (24%) | 67,82,82    | 2.27 | 16 (23%) |
| 6   | HEM  | I     | 807 | 1,7  | 50,50,50     | 2.45 | 11 (22%) | 67,82,82    | 2.22 | 14 (20%) |
| 6   | HEM  | A     | 808 | 1    | 50,50,50     | 2.38 | 11 (22%) | 67,82,82    | 2.25 | 14 (20%) |
| 3   | SX   | L     | 802 | 6    | 0,1,1        | -    | -        | -           | -    | -        |
| 6   | HEM  | A     | 806 | 1    | 50,50,50     | 2.39 | 11 (22%) | 67,82,82    | 2.31 | 16 (23%) |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | HEM  | J     | 812 | 1     | 50,50,50     | 2.44 | 10 (20%) | 67,82,82    | 2.26 | 13 (19%) |
| 6   | HEM  | F     | 809 | 1     | 50,50,50     | 2.46 | 10 (20%) | 67,82,82    | 2.24 | 16 (23%) |
| 6   | HEM  | K     | 813 | 1     | 50,50,50     | 2.48 | 11 (22%) | 67,82,82    | 2.26 | 16 (23%) |
| 4   | BU3  | F     | 803 | -     | 4,5,5        | 0.39 | 0        | 6,6,6       | 0.41 | 0        |
| 7   | SO2  | I     | 802 | 6     | 2,2,2        | 1.83 | 0        | 1,1,1       | 1.49 | 0        |
| 6   | HEM  | B     | 813 | 1     | 50,50,50     | 2.43 | 11 (22%) | 67,82,82    | 2.30 | 16 (23%) |
| 4   | BU3  | H     | 804 | -     | 4,5,5        | 0.40 | 0        | 6,6,6       | 0.30 | 0        |
| 6   | HEM  | C     | 812 | 1     | 50,50,50     | 2.46 | 10 (20%) | 67,82,82    | 2.31 | 17 (25%) |
| 6   | HEM  | I     | 812 | 1     | 50,50,50     | 2.39 | 10 (20%) | 67,82,82    | 2.30 | 15 (22%) |
| 5   | ACT  | A     | 805 | -     | 3,3,3        | 0.72 | 0        | 3,3,3       | 0.98 | 0        |
| 5   | ACT  | C     | 805 | -     | 3,3,3        | 0.79 | 0        | 3,3,3       | 0.89 | 0        |
| 6   | HEM  | E     | 811 | 1     | 50,50,50     | 2.40 | 9 (18%)  | 67,82,82    | 2.37 | 15 (22%) |
| 6   | HEM  | K     | 810 | 1     | 50,50,50     | 2.42 | 8 (16%)  | 67,82,82    | 2.27 | 17 (25%) |
| 5   | ACT  | I     | 805 | -     | 3,3,3        | 0.82 | 0        | 3,3,3       | 0.71 | 0        |
| 4   | BU3  | A     | 804 | -     | 4,5,5        | 0.38 | 0        | 6,6,6       | 0.38 | 0        |
| 6   | HEM  | G     | 812 | 1     | 50,50,50     | 2.42 | 8 (16%)  | 67,82,82    | 2.30 | 18 (26%) |
| 4   | BU3  | C     | 803 | -     | 4,5,5        | 0.35 | 0        | 6,6,6       | 0.33 | 0        |
| 6   | HEM  | B     | 810 | 1     | 50,50,50     | 2.41 | 11 (22%) | 67,82,82    | 2.17 | 14 (20%) |
| 4   | BU3  | J     | 803 | -     | 4,5,5        | 0.34 | 0        | 6,6,6       | 0.30 | 0        |
| 4   | BU3  | D     | 803 | -     | 4,5,5        | 0.38 | 0        | 6,6,6       | 0.16 | 0        |
| 6   | HEM  | D     | 810 | 1     | 50,50,50     | 2.38 | 9 (18%)  | 67,82,82    | 2.38 | 17 (25%) |
| 6   | HEM  | G     | 806 | 1     | 50,50,50     | 2.42 | 9 (18%)  | 67,82,82    | 2.24 | 13 (19%) |
| 6   | HEM  | E     | 807 | 1,3   | 50,50,50     | 2.43 | 8 (16%)  | 67,82,82    | 2.19 | 12 (17%) |
| 4   | BU3  | K     | 803 | -     | 4,5,5        | 0.36 | 0        | 6,6,6       | 0.39 | 0        |
| 6   | HEM  | L     | 806 | 1     | 50,50,50     | 2.47 | 10 (20%) | 67,82,82    | 2.18 | 14 (20%) |
| 6   | HEM  | A     | 809 | 1     | 50,50,50     | 2.39 | 9 (18%)  | 67,82,82    | 2.01 | 15 (22%) |
| 4   | BU3  | I     | 803 | -     | 4,5,5        | 0.40 | 0        | 6,6,6       | 0.18 | 0        |
| 6   | HEM  | A     | 807 | 1,3,7 | 50,50,50     | 2.43 | 9 (18%)  | 67,82,82    | 2.12 | 13 (19%) |
| 6   | HEM  | C     | 807 | 1,3   | 50,50,50     | 2.44 | 8 (16%)  | 67,82,82    | 2.13 | 13 (19%) |
| 6   | HEM  | H     | 813 | 1     | 50,50,50     | 2.40 | 11 (22%) | 67,82,82    | 2.30 | 15 (22%) |
| 6   | HEM  | L     | 810 | 1     | 50,50,50     | 2.43 | 10 (20%) | 67,82,82    | 2.28 | 15 (22%) |
| 6   | HEM  | F     | 810 | 1     | 50,50,50     | 2.48 | 11 (22%) | 67,82,82    | 2.12 | 17 (25%) |
| 3   | SX   | E     | 802 | 6     | 0,1,1        | -    | -        | -           | -    | -        |

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

| Mol | Type | Chain | Res | Link  | Chirals | Torsions   | Rings |
|-----|------|-------|-----|-------|---------|------------|-------|
| 6   | HEM  | K     | 806 | 1     | -       | 3/14/54/54 | -     |
| 6   | HEM  | G     | 809 | 1     | -       | 0/14/54/54 | -     |
| 6   | HEM  | F     | 813 | 1     | -       | 2/14/54/54 | -     |
| 6   | HEM  | F     | 814 | 1     | -       | 4/14/54/54 | -     |
| 4   | BU3  | E     | 804 | -     | -       | 0/4/4/4    | -     |
| 6   | HEM  | K     | 808 | 1     | -       | 3/14/54/54 | -     |
| 4   | BU3  | K     | 804 | -     | -       | 4/4/4/4    | -     |
| 4   | BU3  | L     | 804 | -     | -       | 4/4/4/4    | -     |
| 4   | BU3  | G     | 803 | -     | -       | 4/4/4/4    | -     |
| 6   | HEM  | A     | 812 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | J     | 809 | 1     | -       | 2/14/54/54 | -     |
| 6   | HEM  | I     | 808 | 1     | -       | 3/14/54/54 | -     |
| 4   | BU3  | H     | 803 | -     | -       | 0/4/4/4    | -     |
| 6   | HEM  | B     | 814 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | I     | 806 | 1     | -       | 1/14/54/54 | -     |
| 6   | HEM  | G     | 811 | 1     | -       | 2/14/54/54 | -     |
| 6   | HEM  | F     | 808 | 1,3   | -       | 2/14/54/54 | -     |
| 6   | HEM  | G     | 808 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | C     | 813 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | E     | 808 | 1     | -       | 5/14/54/54 | -     |
| 4   | BU3  | B     | 804 | -     | -       | 4/4/4/4    | -     |
| 4   | BU3  | B     | 803 | -     | -       | 4/4/4/4    | -     |
| 6   | HEM  | L     | 808 | 1     | -       | 3/14/54/54 | -     |
| 6   | HEM  | D     | 813 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | H     | 809 | 1     | -       | 3/14/54/54 | -     |
| 6   | HEM  | F     | 811 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | F     | 812 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | D     | 806 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | L     | 813 | 1     | -       | 5/14/54/54 | -     |
| 6   | HEM  | C     | 809 | 1     | -       | 2/14/54/54 | -     |
| 6   | HEM  | B     | 807 | 1     | -       | 1/14/54/54 | -     |
| 6   | HEM  | E     | 812 | 1     | -       | 4/14/54/54 | -     |
| 4   | BU3  | D     | 804 | -     | -       | 4/4/4/4    | -     |
| 6   | HEM  | H     | 812 | 1     | -       | 2/14/54/54 | -     |
| 6   | HEM  | G     | 807 | 1,3,7 | -       | 3/14/54/54 | -     |
| 6   | HEM  | K     | 811 | 1     | -       | 4/14/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 6   | HEM  | B     | 809 | 1    | -       | 3/14/54/54 | -     |
| 6   | HEM  | L     | 812 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | J     | 811 | 1    | -       | 2/14/54/54 | -     |
| 4   | BU3  | A     | 803 | -    | -       | 4/4/4/4    | -     |
| 6   | HEM  | G     | 813 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | E     | 806 | 1    | -       | 1/14/54/54 | -     |
| 6   | HEM  | A     | 811 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | C     | 811 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | I     | 811 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | K     | 807 | 1,3  | -       | 4/14/54/54 | -     |
| 6   | HEM  | H     | 810 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | C     | 806 | 1    | -       | 2/14/54/54 | -     |
| 4   | BU3  | L     | 803 | -    | -       | 4/4/4/4    | -     |
| 6   | HEM  | B     | 811 | 1    | -       | 5/14/54/54 | -     |
| 6   | HEM  | B     | 812 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | H     | 807 | 1    | -       | 1/14/54/54 | -     |
| 6   | HEM  | J     | 810 | 1    | -       | 4/14/54/54 | -     |
| 4   | BU3  | B     | 805 | -    | -       | 0/4/4/4    | -     |
| 6   | HEM  | A     | 813 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | L     | 807 | 1,3  | -       | 3/14/54/54 | -     |
| 6   | HEM  | K     | 812 | 1    | -       | 4/14/54/54 | -     |
| 4   | BU3  | I     | 804 | -    | -       | 4/4/4/4    | -     |
| 6   | HEM  | C     | 810 | 1    | -       | 2/14/54/54 | -     |
| 4   | BU3  | H     | 805 | -    | -       | 0/4/4/4    | -     |
| 6   | HEM  | K     | 809 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | D     | 807 | 1,7  | -       | 2/14/54/54 | -     |
| 6   | HEM  | D     | 811 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | D     | 812 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | I     | 810 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | E     | 810 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | L     | 809 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | D     | 809 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | H     | 811 | 1    | -       | 4/14/54/54 | -     |
| 4   | BU3  | C     | 804 | -    | -       | 4/4/4/4    | -     |
| 6   | HEM  | H     | 808 | 1,3  | -       | 4/14/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 6   | HEM  | L     | 811 | 1    | -       | 6/14/54/54 | -     |
| 6   | HEM  | A     | 810 | 1    | -       | 5/14/54/54 | -     |
| 6   | HEM  | I     | 809 | 1    | -       | 2/14/54/54 | -     |
| 4   | BU3  | F     | 804 | -    | -       | 4/4/4/4    | -     |
| 4   | BU3  | E     | 803 | -    | -       | 1/4/4/4    | -     |
| 4   | BU3  | G     | 804 | -    | -       | 0/4/4/4    | -     |
| 6   | HEM  | J     | 806 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | B     | 808 | 1,3  | -       | 4/14/54/54 | -     |
| 4   | BU3  | F     | 805 | -    | -       | 4/4/4/4    | -     |
| 4   | BU3  | J     | 804 | -    | -       | 4/4/4/4    | -     |
| 6   | HEM  | J     | 808 | 1    | -       | 3/14/54/54 | -     |
| 6   | HEM  | F     | 807 | 1    | -       | 1/14/54/54 | -     |
| 6   | HEM  | D     | 808 | 1    | -       | 3/14/54/54 | -     |
| 6   | HEM  | G     | 810 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | C     | 808 | 1    | -       | 5/14/54/54 | -     |
| 6   | HEM  | J     | 807 | 1,3  | -       | 3/14/54/54 | -     |
| 6   | HEM  | E     | 809 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | J     | 813 | 1    | -       | 6/14/54/54 | -     |
| 6   | HEM  | H     | 814 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | E     | 813 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | I     | 813 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | I     | 807 | 1,7  | -       | 3/14/54/54 | -     |
| 6   | HEM  | A     | 808 | 1    | -       | 3/14/54/54 | -     |
| 6   | HEM  | K     | 813 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | A     | 806 | 1    | -       | 2/14/54/54 | -     |
| 6   | HEM  | J     | 812 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | F     | 809 | 1    | -       | 3/14/54/54 | -     |
| 4   | BU3  | F     | 803 | -    | -       | 4/4/4/4    | -     |
| 6   | HEM  | B     | 813 | 1    | -       | 4/14/54/54 | -     |
| 4   | BU3  | H     | 804 | -    | -       | 4/4/4/4    | -     |
| 6   | HEM  | C     | 812 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | I     | 812 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | E     | 811 | 1    | -       | 4/14/54/54 | -     |
| 6   | HEM  | K     | 810 | 1    | -       | 2/14/54/54 | -     |
| 4   | BU3  | A     | 804 | -    | -       | 4/4/4/4    | -     |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions   | Rings |
|-----|------|-------|-----|-------|---------|------------|-------|
| 6   | HEM  | G     | 812 | 1     | -       | 4/14/54/54 | -     |
| 4   | BU3  | C     | 803 | -     | -       | 4/4/4/4    | -     |
| 6   | HEM  | B     | 810 | 1     | -       | 2/14/54/54 | -     |
| 4   | BU3  | J     | 803 | -     | -       | 4/4/4/4    | -     |
| 4   | BU3  | D     | 803 | -     | -       | 0/4/4/4    | -     |
| 6   | HEM  | D     | 810 | 1     | -       | 5/14/54/54 | -     |
| 6   | HEM  | G     | 806 | 1     | -       | 1/14/54/54 | -     |
| 6   | HEM  | E     | 807 | 1,3   | -       | 2/14/54/54 | -     |
| 4   | BU3  | K     | 803 | -     | -       | 0/4/4/4    | -     |
| 6   | HEM  | L     | 806 | 1     | -       | 1/14/54/54 | -     |
| 6   | HEM  | A     | 809 | 1     | -       | 2/14/54/54 | -     |
| 4   | BU3  | I     | 803 | -     | -       | 4/4/4/4    | -     |
| 6   | HEM  | A     | 807 | 1,3,7 | -       | 2/14/54/54 | -     |
| 6   | HEM  | C     | 807 | 1,3   | -       | 2/14/54/54 | -     |
| 6   | HEM  | H     | 813 | 1     | -       | 3/14/54/54 | -     |
| 6   | HEM  | L     | 810 | 1     | -       | 4/14/54/54 | -     |
| 6   | HEM  | F     | 810 | 1     | -       | 2/14/54/54 | -     |

All (960) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | K     | 809 | HEM  | FE-NB | 12.67 | 2.33        | 1.94     |
| 6   | L     | 813 | HEM  | FE-NB | 12.66 | 2.33        | 1.94     |
| 6   | L     | 809 | HEM  | FE-NB | 12.58 | 2.33        | 1.94     |
| 6   | H     | 810 | HEM  | FE-NB | 12.55 | 2.33        | 1.94     |
| 6   | J     | 807 | HEM  | FE-NB | 12.48 | 2.33        | 1.94     |
| 6   | L     | 811 | HEM  | FE-NB | 12.45 | 2.33        | 1.94     |
| 6   | H     | 808 | HEM  | FE-NB | 12.45 | 2.33        | 1.94     |
| 6   | J     | 809 | HEM  | FE-NB | 12.43 | 2.33        | 1.94     |
| 6   | L     | 807 | HEM  | FE-NB | 12.42 | 2.33        | 1.94     |
| 6   | F     | 808 | HEM  | FE-NB | 12.41 | 2.33        | 1.94     |
| 6   | K     | 807 | HEM  | FE-NB | 12.40 | 2.33        | 1.94     |
| 6   | K     | 813 | HEM  | FE-NB | 12.36 | 2.33        | 1.94     |
| 6   | F     | 810 | HEM  | FE-NB | 12.36 | 2.32        | 1.94     |
| 6   | L     | 812 | HEM  | FE-NB | 12.35 | 2.32        | 1.94     |
| 6   | I     | 809 | HEM  | FE-NB | 12.35 | 2.32        | 1.94     |
| 6   | L     | 808 | HEM  | FE-NB | 12.31 | 2.32        | 1.94     |
| 6   | J     | 812 | HEM  | FE-NB | 12.31 | 2.32        | 1.94     |
| 6   | B     | 808 | HEM  | FE-NB | 12.30 | 2.32        | 1.94     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | J     | 813 | HEM  | FE-NB | 12.29 | 2.32        | 1.94     |
| 6   | K     | 812 | HEM  | FE-NB | 12.27 | 2.32        | 1.94     |
| 6   | D     | 807 | HEM  | FE-NB | 12.26 | 2.32        | 1.94     |
| 6   | B     | 814 | HEM  | FE-NB | 12.25 | 2.32        | 1.94     |
| 6   | I     | 806 | HEM  | FE-NB | 12.24 | 2.32        | 1.94     |
| 6   | I     | 807 | HEM  | FE-NB | 12.24 | 2.32        | 1.94     |
| 6   | E     | 809 | HEM  | FE-NB | 12.22 | 2.32        | 1.94     |
| 6   | L     | 806 | HEM  | FE-NB | 12.20 | 2.32        | 1.94     |
| 6   | F     | 809 | HEM  | FE-NB | 12.17 | 2.32        | 1.94     |
| 6   | G     | 807 | HEM  | FE-NB | 12.17 | 2.32        | 1.94     |
| 6   | G     | 809 | HEM  | FE-NB | 12.15 | 2.32        | 1.94     |
| 6   | K     | 811 | HEM  | FE-NB | 12.12 | 2.32        | 1.94     |
| 6   | D     | 809 | HEM  | FE-NB | 12.11 | 2.32        | 1.94     |
| 6   | J     | 808 | HEM  | FE-NB | 12.10 | 2.32        | 1.94     |
| 6   | K     | 806 | HEM  | FE-NB | 12.10 | 2.32        | 1.94     |
| 6   | J     | 806 | HEM  | FE-NB | 12.10 | 2.32        | 1.94     |
| 6   | G     | 812 | HEM  | FE-NB | 12.06 | 2.32        | 1.94     |
| 6   | E     | 807 | HEM  | FE-NB | 12.05 | 2.32        | 1.94     |
| 6   | J     | 810 | HEM  | FE-NB | 12.02 | 2.31        | 1.94     |
| 6   | G     | 813 | HEM  | FE-NB | 12.02 | 2.31        | 1.94     |
| 6   | H     | 809 | HEM  | FE-NB | 12.01 | 2.31        | 1.94     |
| 6   | C     | 807 | HEM  | FE-NB | 11.99 | 2.31        | 1.94     |
| 6   | D     | 813 | HEM  | FE-NB | 11.98 | 2.31        | 1.94     |
| 6   | C     | 809 | HEM  | FE-NB | 11.98 | 2.31        | 1.94     |
| 6   | B     | 810 | HEM  | FE-NB | 11.97 | 2.31        | 1.94     |
| 6   | I     | 813 | HEM  | FE-NB | 11.97 | 2.31        | 1.94     |
| 6   | K     | 810 | HEM  | FE-NB | 11.96 | 2.31        | 1.94     |
| 6   | E     | 812 | HEM  | FE-NB | 11.95 | 2.31        | 1.94     |
| 6   | E     | 813 | HEM  | FE-NB | 11.93 | 2.31        | 1.94     |
| 6   | I     | 811 | HEM  | FE-NB | 11.93 | 2.31        | 1.94     |
| 6   | G     | 806 | HEM  | FE-NB | 11.93 | 2.31        | 1.94     |
| 6   | C     | 812 | HEM  | FE-NB | 11.93 | 2.31        | 1.94     |
| 6   | A     | 807 | HEM  | FE-NB | 11.93 | 2.31        | 1.94     |
| 6   | K     | 808 | HEM  | FE-NB | 11.93 | 2.31        | 1.94     |
| 6   | F     | 807 | HEM  | FE-NB | 11.91 | 2.31        | 1.94     |
| 6   | H     | 807 | HEM  | FE-NB | 11.90 | 2.31        | 1.94     |
| 6   | A     | 813 | HEM  | FE-NB | 11.89 | 2.31        | 1.94     |
| 6   | H     | 814 | HEM  | FE-NB | 11.88 | 2.31        | 1.94     |
| 6   | G     | 811 | HEM  | FE-NB | 11.88 | 2.31        | 1.94     |
| 6   | H     | 812 | HEM  | FE-NB | 11.87 | 2.31        | 1.94     |
| 6   | F     | 814 | HEM  | FE-NB | 11.87 | 2.31        | 1.94     |
| 6   | D     | 806 | HEM  | FE-NB | 11.85 | 2.31        | 1.94     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | D     | 808 | HEM  | FE-NB  | 11.85 | 2.31        | 1.94     |
| 6   | E     | 806 | HEM  | FE-NB  | 11.85 | 2.31        | 1.94     |
| 6   | B     | 813 | HEM  | FE-NB  | 11.82 | 2.31        | 1.94     |
| 6   | I     | 808 | HEM  | FE-NB  | 11.82 | 2.31        | 1.94     |
| 6   | H     | 813 | HEM  | FE-NB  | 11.82 | 2.31        | 1.94     |
| 6   | E     | 810 | HEM  | FE-NB  | 11.76 | 2.31        | 1.94     |
| 6   | B     | 812 | HEM  | FE-NB  | 11.76 | 2.31        | 1.94     |
| 6   | G     | 808 | HEM  | FE-NB  | 11.75 | 2.31        | 1.94     |
| 6   | B     | 811 | HEM  | FE-NB  | 11.75 | 2.31        | 1.94     |
| 6   | C     | 811 | HEM  | FE-NB  | 11.75 | 2.31        | 1.94     |
| 6   | A     | 809 | HEM  | FE-NB  | 11.73 | 2.31        | 1.94     |
| 6   | E     | 808 | HEM  | FE-NB  | 11.72 | 2.31        | 1.94     |
| 6   | J     | 811 | HEM  | FE-NB  | 11.72 | 2.31        | 1.94     |
| 6   | L     | 810 | HEM  | FE-NB  | 11.70 | 2.30        | 1.94     |
| 6   | D     | 811 | HEM  | FE-NB  | 11.67 | 2.30        | 1.94     |
| 6   | D     | 812 | HEM  | FE-NB  | 11.67 | 2.30        | 1.94     |
| 6   | C     | 810 | HEM  | FE-NB  | 11.67 | 2.30        | 1.94     |
| 6   | I     | 810 | HEM  | FE-NB  | 11.66 | 2.30        | 1.94     |
| 6   | C     | 813 | HEM  | FE-NB  | 11.64 | 2.30        | 1.94     |
| 6   | B     | 809 | HEM  | FE-NB  | 11.63 | 2.30        | 1.94     |
| 6   | B     | 807 | HEM  | FE-NB  | 11.63 | 2.30        | 1.94     |
| 6   | H     | 811 | HEM  | FE-NB  | 11.62 | 2.30        | 1.94     |
| 6   | E     | 811 | HEM  | FE-NB  | 11.60 | 2.30        | 1.94     |
| 6   | G     | 810 | HEM  | FE-NB  | 11.57 | 2.30        | 1.94     |
| 6   | A     | 811 | HEM  | FE-NB  | 11.54 | 2.30        | 1.94     |
| 6   | F     | 811 | HEM  | FE-NB  | 11.54 | 2.30        | 1.94     |
| 6   | F     | 813 | HEM  | FE-NB  | 11.48 | 2.30        | 1.94     |
| 6   | I     | 812 | HEM  | FE-NB  | 11.46 | 2.30        | 1.94     |
| 6   | A     | 806 | HEM  | FE-NB  | 11.42 | 2.30        | 1.94     |
| 6   | C     | 806 | HEM  | FE-NB  | 11.40 | 2.30        | 1.94     |
| 6   | A     | 808 | HEM  | FE-NB  | 11.39 | 2.30        | 1.94     |
| 6   | D     | 810 | HEM  | FE-NB  | 11.37 | 2.29        | 1.94     |
| 6   | C     | 808 | HEM  | FE-NB  | 11.30 | 2.29        | 1.94     |
| 6   | F     | 812 | HEM  | FE-NB  | 11.30 | 2.29        | 1.94     |
| 6   | A     | 810 | HEM  | FE-NB  | 11.25 | 2.29        | 1.94     |
| 6   | A     | 812 | HEM  | FE-NB  | 11.15 | 2.29        | 1.94     |
| 6   | A     | 810 | HEM  | C1B-NB | -6.04 | 1.29        | 1.40     |
| 6   | H     | 809 | HEM  | C1B-NB | -5.79 | 1.30        | 1.40     |
| 6   | A     | 812 | HEM  | C1B-NB | -5.76 | 1.30        | 1.40     |
| 6   | D     | 811 | HEM  | C1B-NB | -5.73 | 1.30        | 1.40     |
| 6   | G     | 812 | HEM  | C1B-NB | -5.73 | 1.30        | 1.40     |
| 6   | A     | 808 | HEM  | C1B-NB | -5.67 | 1.30        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | C     | 810 | HEM  | C1B-NB | -5.63 | 1.30        | 1.40     |
| 6   | G     | 810 | HEM  | C1B-NB | -5.61 | 1.30        | 1.40     |
| 6   | E     | 809 | HEM  | C1B-NB | -5.60 | 1.30        | 1.40     |
| 6   | B     | 811 | HEM  | C1B-NB | -5.58 | 1.30        | 1.40     |
| 6   | J     | 809 | HEM  | C1B-NB | -5.54 | 1.30        | 1.40     |
| 6   | L     | 810 | HEM  | C1B-NB | -5.53 | 1.30        | 1.40     |
| 6   | F     | 808 | HEM  | C1B-NB | -5.53 | 1.30        | 1.40     |
| 6   | A     | 813 | HEM  | C1B-NB | -5.53 | 1.30        | 1.40     |
| 6   | E     | 806 | HEM  | C1B-NB | -5.50 | 1.30        | 1.40     |
| 6   | E     | 812 | HEM  | C1B-NB | -5.49 | 1.30        | 1.40     |
| 6   | F     | 810 | HEM  | C1B-NB | -5.48 | 1.30        | 1.40     |
| 6   | I     | 813 | HEM  | C1B-NB | -5.48 | 1.30        | 1.40     |
| 6   | A     | 811 | HEM  | C1B-NB | -5.48 | 1.30        | 1.40     |
| 6   | D     | 810 | HEM  | C1B-NB | -5.45 | 1.30        | 1.40     |
| 6   | B     | 810 | HEM  | C1B-NB | -5.44 | 1.30        | 1.40     |
| 6   | B     | 812 | HEM  | C1B-NB | -5.44 | 1.30        | 1.40     |
| 6   | A     | 807 | HEM  | C1B-NB | -5.43 | 1.30        | 1.40     |
| 6   | C     | 809 | HEM  | C1B-NB | -5.43 | 1.30        | 1.40     |
| 6   | L     | 808 | HEM  | C1B-NB | -5.43 | 1.30        | 1.40     |
| 6   | E     | 811 | HEM  | C1B-NB | -5.43 | 1.30        | 1.40     |
| 6   | C     | 813 | HEM  | C1B-NB | -5.42 | 1.30        | 1.40     |
| 6   | L     | 809 | HEM  | C1B-NB | -5.42 | 1.30        | 1.40     |
| 6   | L     | 806 | HEM  | C1B-NB | -5.41 | 1.30        | 1.40     |
| 6   | G     | 811 | HEM  | C1B-NB | -5.38 | 1.30        | 1.40     |
| 6   | F     | 811 | HEM  | C1B-NB | -5.37 | 1.31        | 1.40     |
| 6   | D     | 812 | HEM  | C1B-NB | -5.37 | 1.31        | 1.40     |
| 6   | K     | 810 | HEM  | C1B-NB | -5.37 | 1.31        | 1.40     |
| 6   | E     | 810 | HEM  | C1B-NB | -5.36 | 1.31        | 1.40     |
| 6   | D     | 808 | HEM  | C1B-NB | -5.36 | 1.31        | 1.40     |
| 6   | F     | 807 | HEM  | C1B-NB | -5.36 | 1.31        | 1.40     |
| 6   | H     | 808 | HEM  | C1B-NB | -5.35 | 1.31        | 1.40     |
| 6   | I     | 810 | HEM  | C1B-NB | -5.35 | 1.31        | 1.40     |
| 6   | I     | 808 | HEM  | C1B-NB | -5.34 | 1.31        | 1.40     |
| 6   | C     | 807 | HEM  | C1B-NB | -5.32 | 1.31        | 1.40     |
| 6   | L     | 807 | HEM  | C1B-NB | -5.32 | 1.31        | 1.40     |
| 6   | B     | 809 | HEM  | C1B-NB | -5.32 | 1.31        | 1.40     |
| 6   | B     | 813 | HEM  | C1B-NB | -5.32 | 1.31        | 1.40     |
| 6   | C     | 812 | HEM  | C1B-NB | -5.32 | 1.31        | 1.40     |
| 6   | F     | 813 | HEM  | C1B-NB | -5.31 | 1.31        | 1.40     |
| 6   | J     | 810 | HEM  | C1B-NB | -5.30 | 1.31        | 1.40     |
| 6   | K     | 809 | HEM  | C1B-NB | -5.29 | 1.31        | 1.40     |
| 6   | H     | 814 | HEM  | C1B-NB | -5.29 | 1.31        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | F     | 812 | HEM  | C1B-NB | -5.28 | 1.31        | 1.40     |
| 6   | D     | 807 | HEM  | C1B-NB | -5.28 | 1.31        | 1.40     |
| 6   | D     | 813 | HEM  | C1B-NB | -5.26 | 1.31        | 1.40     |
| 6   | J     | 811 | HEM  | C1B-NB | -5.25 | 1.31        | 1.40     |
| 6   | F     | 814 | HEM  | C1B-NB | -5.24 | 1.31        | 1.40     |
| 6   | I     | 809 | HEM  | C1B-NB | -5.24 | 1.31        | 1.40     |
| 6   | K     | 807 | HEM  | C1B-NB | -5.24 | 1.31        | 1.40     |
| 6   | H     | 810 | HEM  | C1B-NB | -5.23 | 1.31        | 1.40     |
| 6   | J     | 807 | HEM  | C1B-NB | -5.22 | 1.31        | 1.40     |
| 6   | B     | 814 | HEM  | C1B-NB | -5.22 | 1.31        | 1.40     |
| 6   | D     | 809 | HEM  | C1B-NB | -5.21 | 1.31        | 1.40     |
| 6   | K     | 813 | HEM  | C1B-NB | -5.20 | 1.31        | 1.40     |
| 6   | H     | 812 | HEM  | C1B-NB | -5.20 | 1.31        | 1.40     |
| 6   | G     | 809 | HEM  | C1B-NB | -5.20 | 1.31        | 1.40     |
| 6   | G     | 808 | HEM  | C1B-NB | -5.19 | 1.31        | 1.40     |
| 6   | G     | 813 | HEM  | C1B-NB | -5.19 | 1.31        | 1.40     |
| 6   | K     | 811 | HEM  | C1B-NB | -5.19 | 1.31        | 1.40     |
| 6   | K     | 812 | HEM  | C1B-NB | -5.19 | 1.31        | 1.40     |
| 6   | I     | 811 | HEM  | C1B-NB | -5.18 | 1.31        | 1.40     |
| 6   | K     | 806 | HEM  | C1B-NB | -5.18 | 1.31        | 1.40     |
| 6   | I     | 806 | HEM  | C1B-NB | -5.14 | 1.31        | 1.40     |
| 6   | I     | 807 | HEM  | C1B-NB | -5.13 | 1.31        | 1.40     |
| 6   | K     | 808 | HEM  | C1B-NB | -5.13 | 1.31        | 1.40     |
| 6   | H     | 811 | HEM  | C1B-NB | -5.13 | 1.31        | 1.40     |
| 6   | J     | 813 | HEM  | C1B-NB | -5.11 | 1.31        | 1.40     |
| 6   | L     | 812 | HEM  | C1B-NB | -5.10 | 1.31        | 1.40     |
| 6   | E     | 807 | HEM  | C1B-NB | -5.10 | 1.31        | 1.40     |
| 6   | L     | 813 | HEM  | C1B-NB | -5.10 | 1.31        | 1.40     |
| 6   | J     | 808 | HEM  | C1B-NB | -5.09 | 1.31        | 1.40     |
| 6   | B     | 807 | HEM  | C1B-NB | -5.06 | 1.31        | 1.40     |
| 6   | F     | 809 | HEM  | C1B-NB | -5.05 | 1.31        | 1.40     |
| 6   | C     | 806 | HEM  | C1B-NB | -5.04 | 1.31        | 1.40     |
| 6   | B     | 808 | HEM  | C1B-NB | -5.03 | 1.31        | 1.40     |
| 6   | E     | 813 | HEM  | C1B-NB | -5.03 | 1.31        | 1.40     |
| 6   | C     | 811 | HEM  | C1B-NB | -5.02 | 1.31        | 1.40     |
| 6   | I     | 812 | HEM  | C1B-NB | -5.01 | 1.31        | 1.40     |
| 6   | G     | 807 | HEM  | C1B-NB | -5.00 | 1.31        | 1.40     |
| 6   | A     | 806 | HEM  | C1B-NB | -4.98 | 1.31        | 1.40     |
| 6   | L     | 811 | HEM  | C1B-NB | -4.97 | 1.31        | 1.40     |
| 6   | J     | 812 | HEM  | C1B-NB | -4.96 | 1.31        | 1.40     |
| 6   | G     | 806 | HEM  | C1B-NB | -4.96 | 1.31        | 1.40     |
| 6   | D     | 806 | HEM  | C1B-NB | -4.95 | 1.31        | 1.40     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | H     | 807 | HEM  | C1B-NB | -4.91 | 1.31        | 1.40     |
| 6   | C     | 808 | HEM  | C1B-NB | -4.86 | 1.31        | 1.40     |
| 6   | A     | 809 | HEM  | C1B-NB | -4.86 | 1.31        | 1.40     |
| 6   | H     | 813 | HEM  | C1B-NB | -4.83 | 1.31        | 1.40     |
| 6   | J     | 806 | HEM  | C1B-NB | -4.81 | 1.31        | 1.40     |
| 6   | E     | 808 | HEM  | C1B-NB | -4.77 | 1.32        | 1.40     |
| 6   | F     | 812 | HEM  | C4B-NB | -4.71 | 1.29        | 1.38     |
| 6   | D     | 812 | HEM  | C4B-NB | -4.66 | 1.29        | 1.38     |
| 6   | E     | 812 | HEM  | C4B-NB | -4.55 | 1.29        | 1.38     |
| 6   | H     | 814 | HEM  | C4B-NB | -4.42 | 1.30        | 1.38     |
| 6   | D     | 808 | HEM  | C4B-NB | -4.40 | 1.30        | 1.38     |
| 6   | D     | 806 | HEM  | FE-NC  | 4.40  | 2.09        | 1.95     |
| 6   | H     | 812 | HEM  | C4B-NB | -4.37 | 1.30        | 1.38     |
| 6   | E     | 811 | HEM  | C4B-NB | -4.37 | 1.30        | 1.38     |
| 6   | C     | 813 | HEM  | FE-NC  | 4.36  | 2.09        | 1.95     |
| 6   | F     | 807 | HEM  | C4B-NB | -4.34 | 1.30        | 1.38     |
| 6   | L     | 810 | HEM  | FE-NC  | 4.33  | 2.09        | 1.95     |
| 6   | C     | 813 | HEM  | C4B-NB | -4.32 | 1.30        | 1.38     |
| 6   | A     | 812 | HEM  | C4B-NB | -4.32 | 1.30        | 1.38     |
| 6   | I     | 810 | HEM  | FE-NC  | 4.32  | 2.09        | 1.95     |
| 6   | H     | 809 | HEM  | C4B-NB | -4.31 | 1.30        | 1.38     |
| 6   | C     | 811 | HEM  | C4B-NB | -4.31 | 1.30        | 1.38     |
| 6   | J     | 808 | HEM  | C4B-NB | -4.30 | 1.30        | 1.38     |
| 6   | B     | 807 | HEM  | C4B-NB | -4.30 | 1.30        | 1.38     |
| 6   | I     | 811 | HEM  | C4B-NB | -4.30 | 1.30        | 1.38     |
| 6   | A     | 808 | HEM  | C4B-NB | -4.29 | 1.30        | 1.38     |
| 6   | C     | 810 | HEM  | C4B-NB | -4.29 | 1.30        | 1.38     |
| 6   | C     | 812 | HEM  | C4B-NB | -4.29 | 1.30        | 1.38     |
| 6   | F     | 813 | HEM  | C4B-NB | -4.29 | 1.30        | 1.38     |
| 6   | A     | 806 | HEM  | C4B-NB | -4.28 | 1.30        | 1.38     |
| 6   | C     | 806 | HEM  | C4B-NB | -4.28 | 1.30        | 1.38     |
| 6   | A     | 813 | HEM  | C4B-NB | -4.26 | 1.30        | 1.38     |
| 6   | H     | 810 | HEM  | FE-NC  | 4.26  | 2.09        | 1.95     |
| 6   | B     | 811 | HEM  | FE-NC  | 4.26  | 2.09        | 1.95     |
| 6   | C     | 808 | HEM  | C4B-NB | -4.26 | 1.30        | 1.38     |
| 6   | B     | 813 | HEM  | C4B-NB | -4.26 | 1.30        | 1.38     |
| 6   | G     | 811 | HEM  | FE-NC  | 4.26  | 2.09        | 1.95     |
| 6   | L     | 811 | HEM  | FE-NC  | 4.25  | 2.09        | 1.95     |
| 6   | B     | 811 | HEM  | C4B-NB | -4.24 | 1.30        | 1.38     |
| 6   | D     | 811 | HEM  | C4B-NB | -4.24 | 1.30        | 1.38     |
| 6   | K     | 811 | HEM  | C4B-NB | -4.24 | 1.30        | 1.38     |
| 6   | F     | 811 | HEM  | FE-NC  | 4.24  | 2.09        | 1.95     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | J     | 811 | HEM  | C4B-NB | -4.22 | 1.30        | 1.38     |
| 6   | L     | 806 | HEM  | FE-NC  | 4.22  | 2.09        | 1.95     |
| 6   | H     | 813 | HEM  | C4B-NB | -4.22 | 1.30        | 1.38     |
| 6   | A     | 809 | HEM  | C4B-NB | -4.22 | 1.30        | 1.38     |
| 6   | A     | 810 | HEM  | C4B-NB | -4.21 | 1.30        | 1.38     |
| 6   | G     | 808 | HEM  | C4B-NB | -4.21 | 1.30        | 1.38     |
| 6   | B     | 808 | HEM  | FE-NC  | 4.20  | 2.09        | 1.95     |
| 6   | G     | 811 | HEM  | C4B-NB | -4.19 | 1.30        | 1.38     |
| 6   | H     | 808 | HEM  | FE-NC  | 4.19  | 2.09        | 1.95     |
| 6   | F     | 812 | HEM  | FE-NC  | 4.19  | 2.09        | 1.95     |
| 6   | I     | 812 | HEM  | C4B-NB | -4.18 | 1.30        | 1.38     |
| 6   | A     | 807 | HEM  | C4B-NB | -4.17 | 1.30        | 1.38     |
| 6   | I     | 808 | HEM  | C4B-NB | -4.17 | 1.30        | 1.38     |
| 6   | L     | 813 | HEM  | FE-NC  | 4.17  | 2.08        | 1.95     |
| 6   | G     | 810 | HEM  | FE-NC  | 4.16  | 2.08        | 1.95     |
| 6   | H     | 807 | HEM  | FE-NC  | 4.16  | 2.08        | 1.95     |
| 6   | F     | 809 | HEM  | C4B-NB | -4.15 | 1.30        | 1.38     |
| 6   | I     | 813 | HEM  | FE-NC  | 4.15  | 2.08        | 1.95     |
| 6   | G     | 812 | HEM  | C4B-NB | -4.15 | 1.30        | 1.38     |
| 6   | I     | 806 | HEM  | FE-NC  | 4.14  | 2.08        | 1.95     |
| 6   | F     | 807 | HEM  | FE-NC  | 4.14  | 2.08        | 1.95     |
| 6   | E     | 808 | HEM  | C4B-NB | -4.14 | 1.30        | 1.38     |
| 6   | B     | 814 | HEM  | C4B-NB | -4.13 | 1.30        | 1.38     |
| 6   | K     | 806 | HEM  | FE-NC  | 4.12  | 2.08        | 1.95     |
| 6   | D     | 810 | HEM  | FE-NC  | 4.11  | 2.08        | 1.95     |
| 6   | D     | 810 | HEM  | C4B-NB | -4.11 | 1.30        | 1.38     |
| 6   | G     | 810 | HEM  | C4B-NB | -4.11 | 1.30        | 1.38     |
| 6   | J     | 811 | HEM  | FE-NC  | 4.10  | 2.08        | 1.95     |
| 6   | G     | 813 | HEM  | FE-NC  | 4.10  | 2.08        | 1.95     |
| 6   | D     | 806 | HEM  | C4B-NB | -4.09 | 1.30        | 1.38     |
| 6   | J     | 813 | HEM  | C4B-NB | -4.09 | 1.30        | 1.38     |
| 6   | H     | 811 | HEM  | FE-NC  | 4.09  | 2.08        | 1.95     |
| 6   | E     | 806 | HEM  | C4B-NB | -4.09 | 1.30        | 1.38     |
| 6   | F     | 811 | HEM  | C4B-NB | -4.09 | 1.30        | 1.38     |
| 6   | K     | 810 | HEM  | C4B-NB | -4.08 | 1.30        | 1.38     |
| 6   | L     | 806 | HEM  | C4B-NB | -4.08 | 1.30        | 1.38     |
| 6   | J     | 810 | HEM  | C4B-NB | -4.07 | 1.30        | 1.38     |
| 6   | J     | 810 | HEM  | FE-NC  | 4.07  | 2.08        | 1.95     |
| 6   | E     | 813 | HEM  | C4B-NB | -4.07 | 1.30        | 1.38     |
| 6   | D     | 807 | HEM  | FE-NC  | 4.07  | 2.08        | 1.95     |
| 6   | L     | 808 | HEM  | C4B-NB | -4.07 | 1.30        | 1.38     |
| 6   | B     | 814 | HEM  | FE-NC  | 4.07  | 2.08        | 1.95     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 6   | K     | 813 | HEM  | FE-NC  | 4.06  | 2.08        | 1.95     |
| 6   | C     | 807 | HEM  | FE-NC  | 4.06  | 2.08        | 1.95     |
| 6   | C     | 810 | HEM  | FE-NC  | 4.06  | 2.08        | 1.95     |
| 6   | E     | 810 | HEM  | C4B-NB | -4.05 | 1.30        | 1.38     |
| 6   | K     | 810 | HEM  | FE-NC  | 4.05  | 2.08        | 1.95     |
| 6   | H     | 807 | HEM  | C4B-NB | -4.05 | 1.30        | 1.38     |
| 6   | E     | 807 | HEM  | FE-NC  | 4.04  | 2.08        | 1.95     |
| 6   | B     | 812 | HEM  | FE-NC  | 4.04  | 2.08        | 1.95     |
| 6   | E     | 810 | HEM  | FE-NC  | 4.04  | 2.08        | 1.95     |
| 6   | G     | 808 | HEM  | FE-NC  | 4.04  | 2.08        | 1.95     |
| 6   | F     | 814 | HEM  | C4B-NB | -4.03 | 1.30        | 1.38     |
| 6   | L     | 812 | HEM  | FE-NC  | 4.03  | 2.08        | 1.95     |
| 6   | C     | 807 | HEM  | C4B-NB | -4.03 | 1.30        | 1.38     |
| 6   | F     | 813 | HEM  | FE-NC  | 4.03  | 2.08        | 1.95     |
| 6   | D     | 813 | HEM  | C4B-NB | -4.03 | 1.30        | 1.38     |
| 6   | K     | 807 | HEM  | C4B-NB | -4.03 | 1.30        | 1.38     |
| 6   | E     | 807 | HEM  | C4B-NB | -4.02 | 1.30        | 1.38     |
| 6   | G     | 806 | HEM  | FE-NC  | 4.02  | 2.08        | 1.95     |
| 6   | K     | 811 | HEM  | FE-NC  | 4.01  | 2.08        | 1.95     |
| 6   | G     | 807 | HEM  | C4B-NB | -4.01 | 1.31        | 1.38     |
| 6   | F     | 814 | HEM  | FE-NC  | 4.00  | 2.08        | 1.95     |
| 6   | J     | 812 | HEM  | C4B-NB | -3.99 | 1.31        | 1.38     |
| 6   | D     | 807 | HEM  | C4B-NB | -3.99 | 1.31        | 1.38     |
| 6   | B     | 809 | HEM  | C4B-NB | -3.98 | 1.31        | 1.38     |
| 6   | J     | 806 | HEM  | FE-NC  | 3.98  | 2.08        | 1.95     |
| 6   | H     | 813 | HEM  | FE-NC  | 3.98  | 2.08        | 1.95     |
| 6   | G     | 809 | HEM  | FE-NC  | 3.97  | 2.08        | 1.95     |
| 6   | G     | 806 | HEM  | C4B-NB | -3.97 | 1.31        | 1.38     |
| 6   | E     | 813 | HEM  | FE-NC  | 3.95  | 2.08        | 1.95     |
| 6   | K     | 808 | HEM  | FE-NC  | 3.95  | 2.08        | 1.95     |
| 6   | K     | 807 | HEM  | FE-NC  | 3.95  | 2.08        | 1.95     |
| 6   | D     | 813 | HEM  | FE-NC  | 3.95  | 2.08        | 1.95     |
| 6   | C     | 811 | HEM  | FE-NC  | 3.94  | 2.08        | 1.95     |
| 6   | L     | 813 | HEM  | C4B-NB | -3.93 | 1.31        | 1.38     |
| 6   | K     | 808 | HEM  | C4B-NB | -3.93 | 1.31        | 1.38     |
| 6   | K     | 809 | HEM  | C4B-NB | -3.93 | 1.31        | 1.38     |
| 6   | I     | 809 | HEM  | FE-NC  | 3.92  | 2.08        | 1.95     |
| 6   | G     | 812 | HEM  | FE-NC  | 3.91  | 2.08        | 1.95     |
| 6   | I     | 807 | HEM  | C4B-NB | -3.91 | 1.31        | 1.38     |
| 6   | L     | 812 | HEM  | C4B-NB | -3.91 | 1.31        | 1.38     |
| 6   | A     | 810 | HEM  | FE-NC  | 3.91  | 2.08        | 1.95     |
| 6   | E     | 809 | HEM  | C4B-NB | -3.91 | 1.31        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | K     | 809 | HEM  | FE-NC   | 3.91  | 2.08        | 1.95     |
| 6   | D     | 809 | HEM  | C4B-NB  | -3.90 | 1.31        | 1.38     |
| 6   | G     | 810 | HEM  | CBB-CAB | 3.90  | 1.49        | 1.30     |
| 6   | G     | 813 | HEM  | C4B-NB  | -3.90 | 1.31        | 1.38     |
| 6   | L     | 811 | HEM  | C4B-NB  | -3.90 | 1.31        | 1.38     |
| 6   | B     | 813 | HEM  | FE-NC   | 3.90  | 2.08        | 1.95     |
| 6   | I     | 812 | HEM  | FE-NC   | 3.89  | 2.08        | 1.95     |
| 6   | A     | 806 | HEM  | FE-NC   | 3.89  | 2.08        | 1.95     |
| 6   | E     | 811 | HEM  | FE-NC   | 3.89  | 2.08        | 1.95     |
| 6   | J     | 809 | HEM  | FE-NC   | 3.88  | 2.08        | 1.95     |
| 6   | E     | 808 | HEM  | FE-NC   | 3.87  | 2.07        | 1.95     |
| 6   | H     | 811 | HEM  | C4B-NB  | -3.87 | 1.31        | 1.38     |
| 6   | H     | 810 | HEM  | CBC-CAC | 3.87  | 1.49        | 1.30     |
| 6   | L     | 807 | HEM  | C4B-NB  | -3.86 | 1.31        | 1.38     |
| 6   | J     | 808 | HEM  | FE-NC   | 3.86  | 2.07        | 1.95     |
| 6   | B     | 812 | HEM  | C4B-NB  | -3.86 | 1.31        | 1.38     |
| 6   | L     | 812 | HEM  | CBB-CAB | 3.86  | 1.48        | 1.30     |
| 6   | I     | 809 | HEM  | C4B-NB  | -3.85 | 1.31        | 1.38     |
| 6   | I     | 813 | HEM  | C4B-NB  | -3.85 | 1.31        | 1.38     |
| 6   | B     | 808 | HEM  | C4B-NB  | -3.85 | 1.31        | 1.38     |
| 6   | J     | 810 | HEM  | CBB-CAB | 3.85  | 1.48        | 1.30     |
| 6   | E     | 806 | HEM  | FE-NC   | 3.85  | 2.07        | 1.95     |
| 6   | J     | 807 | HEM  | FE-NC   | 3.85  | 2.07        | 1.95     |
| 6   | G     | 806 | HEM  | CBC-CAC | 3.84  | 1.48        | 1.30     |
| 6   | A     | 813 | HEM  | FE-NC   | 3.84  | 2.07        | 1.95     |
| 6   | B     | 809 | HEM  | FE-NC   | 3.84  | 2.07        | 1.95     |
| 6   | I     | 810 | HEM  | C4B-NB  | -3.83 | 1.31        | 1.38     |
| 6   | G     | 811 | HEM  | CBC-CAC | 3.83  | 1.48        | 1.30     |
| 6   | L     | 806 | HEM  | CBC-CAC | 3.83  | 1.48        | 1.30     |
| 6   | C     | 809 | HEM  | FE-NC   | 3.83  | 2.07        | 1.95     |
| 6   | L     | 807 | HEM  | FE-NC   | 3.83  | 2.07        | 1.95     |
| 6   | I     | 806 | HEM  | C4B-NB  | -3.83 | 1.31        | 1.38     |
| 6   | C     | 813 | HEM  | CBB-CAB | 3.83  | 1.48        | 1.30     |
| 6   | C     | 809 | HEM  | CBB-CAB | 3.83  | 1.48        | 1.30     |
| 6   | J     | 813 | HEM  | FE-NC   | 3.82  | 2.07        | 1.95     |
| 6   | F     | 813 | HEM  | CBB-CAB | 3.82  | 1.48        | 1.30     |
| 6   | K     | 806 | HEM  | CBC-CAC | 3.82  | 1.48        | 1.30     |
| 6   | G     | 809 | HEM  | CBB-CAB | 3.82  | 1.48        | 1.30     |
| 6   | C     | 809 | HEM  | C4B-NB  | -3.81 | 1.31        | 1.38     |
| 6   | K     | 812 | HEM  | FE-NC   | 3.81  | 2.07        | 1.95     |
| 6   | F     | 810 | HEM  | C4B-NB  | -3.81 | 1.31        | 1.38     |
| 6   | A     | 811 | HEM  | FE-NC   | 3.81  | 2.07        | 1.95     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | E     | 812 | HEM  | FE-NC   | 3.81  | 2.07        | 1.95     |
| 6   | F     | 809 | HEM  | CBB-CAB | 3.81  | 1.48        | 1.30     |
| 6   | L     | 809 | HEM  | CBC-CAC | 3.80  | 1.48        | 1.30     |
| 6   | C     | 811 | HEM  | CBC-CAC | 3.80  | 1.48        | 1.30     |
| 6   | H     | 807 | HEM  | CBC-CAC | 3.80  | 1.48        | 1.30     |
| 6   | B     | 813 | HEM  | CBB-CAB | 3.80  | 1.48        | 1.30     |
| 6   | A     | 809 | HEM  | CBC-CAC | 3.80  | 1.48        | 1.30     |
| 6   | C     | 810 | HEM  | CBB-CAB | 3.80  | 1.48        | 1.30     |
| 6   | I     | 811 | HEM  | CBC-CAC | 3.80  | 1.48        | 1.30     |
| 6   | L     | 810 | HEM  | C4B-NB  | -3.79 | 1.31        | 1.38     |
| 6   | J     | 807 | HEM  | C4B-NB  | -3.79 | 1.31        | 1.38     |
| 6   | E     | 813 | HEM  | CBC-CAC | 3.79  | 1.48        | 1.30     |
| 6   | I     | 806 | HEM  | CBC-CAC | 3.79  | 1.48        | 1.30     |
| 6   | F     | 807 | HEM  | CBC-CAC | 3.79  | 1.48        | 1.30     |
| 6   | F     | 814 | HEM  | CBB-CAB | 3.79  | 1.48        | 1.30     |
| 6   | G     | 811 | HEM  | CBB-CAB | 3.79  | 1.48        | 1.30     |
| 6   | E     | 812 | HEM  | CBC-CAC | 3.78  | 1.48        | 1.30     |
| 6   | H     | 814 | HEM  | FE-NC   | 3.78  | 2.07        | 1.95     |
| 6   | C     | 806 | HEM  | FE-NC   | 3.78  | 2.07        | 1.95     |
| 6   | J     | 812 | HEM  | FE-NC   | 3.78  | 2.07        | 1.95     |
| 6   | L     | 811 | HEM  | CBC-CAC | 3.78  | 1.48        | 1.30     |
| 6   | H     | 812 | HEM  | CBC-CAC | 3.78  | 1.48        | 1.30     |
| 6   | K     | 810 | HEM  | CBB-CAB | 3.78  | 1.48        | 1.30     |
| 6   | H     | 808 | HEM  | C4B-NB  | -3.78 | 1.31        | 1.38     |
| 6   | L     | 809 | HEM  | CBB-CAB | 3.78  | 1.48        | 1.30     |
| 6   | F     | 809 | HEM  | FE-NC   | 3.78  | 2.07        | 1.95     |
| 6   | D     | 811 | HEM  | CBC-CAC | 3.78  | 1.48        | 1.30     |
| 6   | C     | 806 | HEM  | CBB-CAB | 3.78  | 1.48        | 1.30     |
| 6   | J     | 813 | HEM  | CBC-CAC | 3.78  | 1.48        | 1.30     |
| 6   | B     | 812 | HEM  | CBC-CAC | 3.78  | 1.48        | 1.30     |
| 6   | J     | 813 | HEM  | CBB-CAB | 3.77  | 1.48        | 1.30     |
| 6   | E     | 811 | HEM  | CBB-CAB | 3.77  | 1.48        | 1.30     |
| 6   | E     | 811 | HEM  | CBC-CAC | 3.77  | 1.48        | 1.30     |
| 6   | H     | 814 | HEM  | CBB-CAB | 3.77  | 1.48        | 1.30     |
| 6   | B     | 812 | HEM  | CBB-CAB | 3.77  | 1.48        | 1.30     |
| 6   | J     | 809 | HEM  | CBB-CAB | 3.77  | 1.48        | 1.30     |
| 6   | H     | 807 | HEM  | CBB-CAB | 3.77  | 1.48        | 1.30     |
| 6   | J     | 806 | HEM  | CBC-CAC | 3.77  | 1.48        | 1.30     |
| 6   | L     | 810 | HEM  | CBB-CAB | 3.76  | 1.48        | 1.30     |
| 6   | B     | 814 | HEM  | CBB-CAB | 3.76  | 1.48        | 1.30     |
| 6   | J     | 812 | HEM  | CBB-CAB | 3.76  | 1.48        | 1.30     |
| 6   | A     | 812 | HEM  | CBB-CAB | 3.76  | 1.48        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | K     | 813 | HEM  | CBB-CAB | 3.75  | 1.48        | 1.30     |
| 6   | K     | 811 | HEM  | CBB-CAB | 3.75  | 1.48        | 1.30     |
| 6   | L     | 813 | HEM  | CBB-CAB | 3.75  | 1.48        | 1.30     |
| 6   | E     | 809 | HEM  | FE-NC   | 3.75  | 2.07        | 1.95     |
| 6   | G     | 806 | HEM  | CBB-CAB | 3.75  | 1.48        | 1.30     |
| 6   | I     | 813 | HEM  | CBB-CAB | 3.75  | 1.48        | 1.30     |
| 6   | E     | 806 | HEM  | CBB-CAB | 3.75  | 1.48        | 1.30     |
| 6   | F     | 808 | HEM  | CBB-CAB | 3.74  | 1.48        | 1.30     |
| 6   | G     | 808 | HEM  | CBB-CAB | 3.74  | 1.48        | 1.30     |
| 6   | G     | 813 | HEM  | CBB-CAB | 3.74  | 1.48        | 1.30     |
| 6   | C     | 807 | HEM  | CBC-CAC | 3.74  | 1.48        | 1.30     |
| 6   | B     | 810 | HEM  | CBC-CAC | 3.74  | 1.48        | 1.30     |
| 6   | J     | 811 | HEM  | CBB-CAB | 3.74  | 1.48        | 1.30     |
| 6   | C     | 808 | HEM  | CBB-CAB | 3.74  | 1.48        | 1.30     |
| 6   | K     | 813 | HEM  | CBC-CAC | 3.74  | 1.48        | 1.30     |
| 6   | J     | 812 | HEM  | CBC-CAC | 3.73  | 1.48        | 1.30     |
| 6   | L     | 808 | HEM  | FE-NC   | 3.73  | 2.07        | 1.95     |
| 6   | J     | 809 | HEM  | CBC-CAC | 3.73  | 1.48        | 1.30     |
| 6   | J     | 807 | HEM  | CBC-CAC | 3.73  | 1.48        | 1.30     |
| 6   | E     | 810 | HEM  | CBB-CAB | 3.73  | 1.48        | 1.30     |
| 6   | E     | 809 | HEM  | CBC-CAC | 3.73  | 1.48        | 1.30     |
| 6   | D     | 806 | HEM  | CBC-CAC | 3.73  | 1.48        | 1.30     |
| 6   | I     | 806 | HEM  | CBB-CAB | 3.73  | 1.48        | 1.30     |
| 6   | A     | 807 | HEM  | CBC-CAC | 3.73  | 1.48        | 1.30     |
| 6   | E     | 807 | HEM  | CBC-CAC | 3.73  | 1.48        | 1.30     |
| 6   | G     | 812 | HEM  | CBB-CAB | 3.72  | 1.48        | 1.30     |
| 6   | H     | 812 | HEM  | FE-NC   | 3.72  | 2.07        | 1.95     |
| 6   | J     | 811 | HEM  | CBC-CAC | 3.72  | 1.48        | 1.30     |
| 6   | G     | 807 | HEM  | CBB-CAB | 3.72  | 1.48        | 1.30     |
| 6   | B     | 810 | HEM  | C4B-NB  | -3.72 | 1.31        | 1.38     |
| 6   | L     | 809 | HEM  | FE-NC   | 3.72  | 2.07        | 1.95     |
| 6   | E     | 806 | HEM  | CBC-CAC | 3.72  | 1.48        | 1.30     |
| 6   | K     | 809 | HEM  | CBC-CAC | 3.72  | 1.48        | 1.30     |
| 6   | A     | 813 | HEM  | CBC-CAC | 3.72  | 1.48        | 1.30     |
| 6   | D     | 811 | HEM  | FE-NC   | 3.71  | 2.07        | 1.95     |
| 6   | I     | 807 | HEM  | FE-NC   | 3.71  | 2.07        | 1.95     |
| 6   | G     | 809 | HEM  | CBC-CAC | 3.71  | 1.48        | 1.30     |
| 6   | D     | 813 | HEM  | CBC-CAC | 3.71  | 1.48        | 1.30     |
| 6   | I     | 813 | HEM  | CBC-CAC | 3.71  | 1.48        | 1.30     |
| 6   | G     | 812 | HEM  | CBC-CAC | 3.71  | 1.48        | 1.30     |
| 6   | K     | 812 | HEM  | CBB-CAB | 3.71  | 1.48        | 1.30     |
| 6   | J     | 807 | HEM  | CBB-CAB | 3.70  | 1.48        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | F     | 808 | HEM  | C4B-NB  | -3.70 | 1.31        | 1.38     |
| 6   | G     | 813 | HEM  | CBC-CAC | 3.70  | 1.48        | 1.30     |
| 6   | D     | 809 | HEM  | FE-NC   | 3.70  | 2.07        | 1.95     |
| 6   | B     | 810 | HEM  | CBB-CAB | 3.70  | 1.48        | 1.30     |
| 6   | L     | 812 | HEM  | CBC-CAC | 3.70  | 1.48        | 1.30     |
| 6   | H     | 814 | HEM  | CBC-CAC | 3.70  | 1.48        | 1.30     |
| 6   | H     | 810 | HEM  | C4B-NB  | -3.70 | 1.31        | 1.38     |
| 6   | D     | 813 | HEM  | CBB-CAB | 3.70  | 1.48        | 1.30     |
| 6   | F     | 810 | HEM  | CBC-CAC | 3.70  | 1.48        | 1.30     |
| 6   | B     | 810 | HEM  | FE-NC   | 3.70  | 2.07        | 1.95     |
| 6   | K     | 813 | HEM  | C4B-NB  | -3.70 | 1.31        | 1.38     |
| 6   | K     | 808 | HEM  | CBC-CAC | 3.70  | 1.48        | 1.30     |
| 6   | J     | 809 | HEM  | C4B-NB  | -3.70 | 1.31        | 1.38     |
| 6   | I     | 811 | HEM  | FE-NC   | 3.70  | 2.07        | 1.95     |
| 6   | D     | 811 | HEM  | CBB-CAB | 3.69  | 1.48        | 1.30     |
| 6   | A     | 810 | HEM  | CBB-CAB | 3.69  | 1.48        | 1.30     |
| 6   | D     | 812 | HEM  | CBC-CAC | 3.69  | 1.48        | 1.30     |
| 6   | A     | 812 | HEM  | CBC-CAC | 3.69  | 1.48        | 1.30     |
| 6   | B     | 814 | HEM  | CBC-CAC | 3.69  | 1.48        | 1.30     |
| 6   | K     | 811 | HEM  | CBC-CAC | 3.69  | 1.48        | 1.30     |
| 6   | I     | 809 | HEM  | CBC-CAC | 3.69  | 1.48        | 1.30     |
| 6   | B     | 807 | HEM  | FE-NC   | 3.69  | 2.07        | 1.95     |
| 6   | A     | 811 | HEM  | C4B-NB  | -3.69 | 1.31        | 1.38     |
| 6   | L     | 806 | HEM  | CBB-CAB | 3.68  | 1.48        | 1.30     |
| 6   | C     | 813 | HEM  | CBC-CAC | 3.68  | 1.48        | 1.30     |
| 6   | I     | 807 | HEM  | CBC-CAC | 3.68  | 1.48        | 1.30     |
| 6   | E     | 809 | HEM  | CBB-CAB | 3.68  | 1.48        | 1.30     |
| 6   | A     | 813 | HEM  | CBB-CAB | 3.68  | 1.48        | 1.30     |
| 6   | F     | 808 | HEM  | CBC-CAC | 3.68  | 1.48        | 1.30     |
| 6   | H     | 809 | HEM  | CBB-CAB | 3.68  | 1.48        | 1.30     |
| 6   | L     | 807 | HEM  | CBC-CAC | 3.68  | 1.48        | 1.30     |
| 6   | F     | 814 | HEM  | CBC-CAC | 3.68  | 1.48        | 1.30     |
| 6   | E     | 813 | HEM  | CBB-CAB | 3.67  | 1.48        | 1.30     |
| 6   | J     | 810 | HEM  | CBC-CAC | 3.67  | 1.48        | 1.30     |
| 6   | L     | 807 | HEM  | CBB-CAB | 3.67  | 1.48        | 1.30     |
| 6   | H     | 811 | HEM  | CBB-CAB | 3.67  | 1.48        | 1.30     |
| 6   | A     | 806 | HEM  | CBC-CAC | 3.67  | 1.48        | 1.30     |
| 6   | D     | 809 | HEM  | CBC-CAC | 3.67  | 1.48        | 1.30     |
| 6   | H     | 813 | HEM  | CBC-CAC | 3.67  | 1.48        | 1.30     |
| 6   | A     | 811 | HEM  | CBC-CAC | 3.67  | 1.48        | 1.30     |
| 6   | D     | 810 | HEM  | CBB-CAB | 3.66  | 1.48        | 1.30     |
| 6   | C     | 809 | HEM  | CBC-CAC | 3.66  | 1.48        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | H     | 812 | HEM  | CBB-CAB | 3.66  | 1.48        | 1.30     |
| 6   | K     | 812 | HEM  | C4B-NB  | -3.66 | 1.31        | 1.38     |
| 6   | D     | 810 | HEM  | CBC-CAC | 3.65  | 1.47        | 1.30     |
| 6   | C     | 811 | HEM  | CBB-CAB | 3.65  | 1.47        | 1.30     |
| 6   | A     | 807 | HEM  | FE-NC   | 3.65  | 2.07        | 1.95     |
| 6   | B     | 809 | HEM  | CBB-CAB | 3.65  | 1.47        | 1.30     |
| 6   | I     | 812 | HEM  | CBB-CAB | 3.65  | 1.47        | 1.30     |
| 6   | G     | 807 | HEM  | CBC-CAC | 3.65  | 1.47        | 1.30     |
| 6   | L     | 808 | HEM  | CBC-CAC | 3.65  | 1.47        | 1.30     |
| 6   | L     | 811 | HEM  | CBB-CAB | 3.64  | 1.47        | 1.30     |
| 6   | I     | 812 | HEM  | CBC-CAC | 3.64  | 1.47        | 1.30     |
| 6   | B     | 811 | HEM  | CBB-CAB | 3.64  | 1.47        | 1.30     |
| 6   | C     | 812 | HEM  | CBC-CAC | 3.64  | 1.47        | 1.30     |
| 6   | D     | 809 | HEM  | CBB-CAB | 3.64  | 1.47        | 1.30     |
| 6   | I     | 810 | HEM  | CBB-CAB | 3.64  | 1.47        | 1.30     |
| 6   | H     | 813 | HEM  | CBB-CAB | 3.64  | 1.47        | 1.30     |
| 6   | K     | 808 | HEM  | CBB-CAB | 3.64  | 1.47        | 1.30     |
| 6   | F     | 811 | HEM  | CBC-CAC | 3.64  | 1.47        | 1.30     |
| 6   | B     | 807 | HEM  | CBC-CAC | 3.63  | 1.47        | 1.30     |
| 6   | C     | 806 | HEM  | CBC-CAC | 3.63  | 1.47        | 1.30     |
| 6   | H     | 809 | HEM  | CBC-CAC | 3.63  | 1.47        | 1.30     |
| 6   | F     | 810 | HEM  | CBB-CAB | 3.63  | 1.47        | 1.30     |
| 6   | B     | 808 | HEM  | CBC-CAC | 3.62  | 1.47        | 1.30     |
| 6   | I     | 808 | HEM  | CBB-CAB | 3.62  | 1.47        | 1.30     |
| 6   | D     | 808 | HEM  | FE-NC   | 3.62  | 2.07        | 1.95     |
| 6   | A     | 809 | HEM  | FE-NC   | 3.62  | 2.07        | 1.95     |
| 6   | C     | 812 | HEM  | CBB-CAB | 3.62  | 1.47        | 1.30     |
| 6   | F     | 813 | HEM  | CBC-CAC | 3.62  | 1.47        | 1.30     |
| 6   | H     | 808 | HEM  | CBB-CAB | 3.62  | 1.47        | 1.30     |
| 6   | A     | 806 | HEM  | CBB-CAB | 3.62  | 1.47        | 1.30     |
| 6   | G     | 808 | HEM  | CBC-CAC | 3.62  | 1.47        | 1.30     |
| 6   | C     | 808 | HEM  | CBC-CAC | 3.62  | 1.47        | 1.30     |
| 6   | K     | 809 | HEM  | CBB-CAB | 3.61  | 1.47        | 1.30     |
| 6   | A     | 809 | HEM  | CBB-CAB | 3.61  | 1.47        | 1.30     |
| 6   | E     | 812 | HEM  | CBB-CAB | 3.61  | 1.47        | 1.30     |
| 6   | D     | 808 | HEM  | CBB-CAB | 3.61  | 1.47        | 1.30     |
| 6   | J     | 808 | HEM  | CBB-CAB | 3.61  | 1.47        | 1.30     |
| 6   | I     | 810 | HEM  | CBC-CAC | 3.61  | 1.47        | 1.30     |
| 6   | E     | 807 | HEM  | CBB-CAB | 3.61  | 1.47        | 1.30     |
| 6   | F     | 810 | HEM  | FE-NC   | 3.60  | 2.07        | 1.95     |
| 6   | F     | 812 | HEM  | CBC-CAC | 3.60  | 1.47        | 1.30     |
| 6   | I     | 811 | HEM  | CBB-CAB | 3.60  | 1.47        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | I     | 808 | HEM  | FE-NC   | 3.60  | 2.07        | 1.95     |
| 6   | D     | 807 | HEM  | CBC-CAC | 3.59  | 1.47        | 1.30     |
| 6   | A     | 808 | HEM  | CBB-CAB | 3.59  | 1.47        | 1.30     |
| 6   | F     | 811 | HEM  | CBB-CAB | 3.59  | 1.47        | 1.30     |
| 6   | D     | 812 | HEM  | FE-NC   | 3.59  | 2.07        | 1.95     |
| 6   | K     | 807 | HEM  | CBC-CAC | 3.59  | 1.47        | 1.30     |
| 6   | L     | 808 | HEM  | CBB-CAB | 3.59  | 1.47        | 1.30     |
| 6   | G     | 810 | HEM  | CBC-CAC | 3.59  | 1.47        | 1.30     |
| 6   | K     | 812 | HEM  | CBC-CAC | 3.58  | 1.47        | 1.30     |
| 6   | L     | 810 | HEM  | CBC-CAC | 3.58  | 1.47        | 1.30     |
| 6   | D     | 807 | HEM  | CBB-CAB | 3.58  | 1.47        | 1.30     |
| 6   | H     | 810 | HEM  | CBB-CAB | 3.58  | 1.47        | 1.30     |
| 6   | E     | 808 | HEM  | CBB-CAB | 3.58  | 1.47        | 1.30     |
| 6   | G     | 809 | HEM  | C4B-NB  | -3.57 | 1.31        | 1.38     |
| 6   | E     | 808 | HEM  | CBC-CAC | 3.57  | 1.47        | 1.30     |
| 6   | H     | 811 | HEM  | CBC-CAC | 3.57  | 1.47        | 1.30     |
| 6   | C     | 808 | HEM  | FE-NC   | 3.57  | 2.07        | 1.95     |
| 6   | B     | 807 | HEM  | CBB-CAB | 3.57  | 1.47        | 1.30     |
| 6   | H     | 808 | HEM  | CBC-CAC | 3.57  | 1.47        | 1.30     |
| 6   | A     | 807 | HEM  | CBB-CAB | 3.57  | 1.47        | 1.30     |
| 6   | I     | 809 | HEM  | CBB-CAB | 3.57  | 1.47        | 1.30     |
| 6   | G     | 807 | HEM  | FE-NC   | 3.56  | 2.06        | 1.95     |
| 6   | C     | 812 | HEM  | FE-NC   | 3.56  | 2.06        | 1.95     |
| 6   | B     | 813 | HEM  | CBC-CAC | 3.56  | 1.47        | 1.30     |
| 6   | D     | 812 | HEM  | CBB-CAB | 3.56  | 1.47        | 1.30     |
| 6   | I     | 807 | HEM  | CBB-CAB | 3.56  | 1.47        | 1.30     |
| 6   | C     | 807 | HEM  | CBB-CAB | 3.55  | 1.47        | 1.30     |
| 6   | F     | 808 | HEM  | FE-NC   | 3.54  | 2.06        | 1.95     |
| 6   | J     | 806 | HEM  | CBB-CAB | 3.54  | 1.47        | 1.30     |
| 6   | E     | 810 | HEM  | CBC-CAC | 3.54  | 1.47        | 1.30     |
| 6   | B     | 808 | HEM  | CBB-CAB | 3.53  | 1.47        | 1.30     |
| 6   | K     | 810 | HEM  | CBC-CAC | 3.52  | 1.47        | 1.30     |
| 6   | F     | 809 | HEM  | CBC-CAC | 3.52  | 1.47        | 1.30     |
| 6   | F     | 807 | HEM  | CBB-CAB | 3.52  | 1.47        | 1.30     |
| 6   | A     | 808 | HEM  | CBC-CAC | 3.51  | 1.47        | 1.30     |
| 6   | B     | 811 | HEM  | CBC-CAC | 3.51  | 1.47        | 1.30     |
| 6   | C     | 810 | HEM  | CBC-CAC | 3.51  | 1.47        | 1.30     |
| 6   | A     | 811 | HEM  | CBB-CAB | 3.51  | 1.47        | 1.30     |
| 6   | K     | 806 | HEM  | CBB-CAB | 3.51  | 1.47        | 1.30     |
| 6   | I     | 808 | HEM  | CBC-CAC | 3.51  | 1.47        | 1.30     |
| 6   | H     | 809 | HEM  | FE-NC   | 3.50  | 2.06        | 1.95     |
| 6   | K     | 807 | HEM  | CBB-CAB | 3.50  | 1.47        | 1.30     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | J     | 808 | HEM  | CBC-CAC | 3.50  | 1.47        | 1.30     |
| 6   | L     | 809 | HEM  | C4B-NB  | -3.49 | 1.32        | 1.38     |
| 6   | A     | 810 | HEM  | CBC-CAC | 3.48  | 1.47        | 1.30     |
| 6   | D     | 808 | HEM  | CBC-CAC | 3.48  | 1.47        | 1.30     |
| 6   | B     | 809 | HEM  | CBC-CAC | 3.46  | 1.47        | 1.30     |
| 6   | A     | 812 | HEM  | FE-NC   | 3.45  | 2.06        | 1.95     |
| 6   | J     | 806 | HEM  | C4B-NB  | -3.45 | 1.32        | 1.38     |
| 6   | F     | 812 | HEM  | CBB-CAB | 3.45  | 1.46        | 1.30     |
| 6   | J     | 809 | HEM  | C4D-ND  | -3.41 | 1.34        | 1.40     |
| 6   | H     | 807 | HEM  | C4D-ND  | -3.39 | 1.34        | 1.40     |
| 6   | K     | 806 | HEM  | C4B-NB  | -3.38 | 1.32        | 1.38     |
| 6   | F     | 812 | HEM  | C4D-ND  | -3.37 | 1.34        | 1.40     |
| 6   | D     | 806 | HEM  | CBB-CAB | 3.36  | 1.46        | 1.30     |
| 6   | C     | 810 | HEM  | C4D-ND  | -3.31 | 1.34        | 1.40     |
| 6   | A     | 812 | HEM  | C4D-ND  | -3.31 | 1.34        | 1.40     |
| 6   | G     | 806 | HEM  | C4D-ND  | -3.30 | 1.34        | 1.40     |
| 6   | A     | 808 | HEM  | FE-NC   | 3.28  | 2.06        | 1.95     |
| 6   | A     | 813 | HEM  | C4D-ND  | -3.28 | 1.34        | 1.40     |
| 6   | E     | 809 | HEM  | C4D-ND  | -3.27 | 1.34        | 1.40     |
| 6   | C     | 808 | HEM  | C4D-ND  | -3.26 | 1.34        | 1.40     |
| 6   | K     | 809 | HEM  | C4D-ND  | -3.23 | 1.34        | 1.40     |
| 6   | E     | 808 | HEM  | C4D-ND  | -3.22 | 1.34        | 1.40     |
| 6   | F     | 810 | HEM  | C4D-ND  | -3.21 | 1.34        | 1.40     |
| 6   | L     | 813 | HEM  | CBC-CAC | 3.21  | 1.45        | 1.30     |
| 6   | J     | 808 | HEM  | C4D-ND  | -3.19 | 1.34        | 1.40     |
| 6   | E     | 813 | HEM  | C4D-ND  | -3.19 | 1.34        | 1.40     |
| 6   | J     | 811 | HEM  | C4D-ND  | -3.19 | 1.34        | 1.40     |
| 6   | I     | 813 | HEM  | C4D-ND  | -3.18 | 1.34        | 1.40     |
| 6   | B     | 809 | HEM  | C4D-ND  | -3.17 | 1.34        | 1.40     |
| 6   | H     | 809 | HEM  | C4D-ND  | -3.17 | 1.34        | 1.40     |
| 6   | G     | 807 | HEM  | C4D-ND  | -3.16 | 1.34        | 1.40     |
| 6   | G     | 813 | HEM  | C4D-ND  | -3.16 | 1.34        | 1.40     |
| 6   | K     | 811 | HEM  | C4D-ND  | -3.15 | 1.34        | 1.40     |
| 6   | J     | 813 | HEM  | C4D-ND  | -3.14 | 1.34        | 1.40     |
| 6   | K     | 813 | HEM  | C4D-ND  | -3.13 | 1.34        | 1.40     |
| 6   | F     | 811 | HEM  | C4D-ND  | -3.12 | 1.34        | 1.40     |
| 6   | D     | 813 | HEM  | C4D-ND  | -3.12 | 1.34        | 1.40     |
| 6   | B     | 812 | HEM  | C4D-ND  | -3.07 | 1.34        | 1.40     |
| 6   | J     | 806 | HEM  | C4D-ND  | -3.06 | 1.35        | 1.40     |
| 6   | A     | 813 | HEM  | C3C-C4C | -3.05 | 1.40        | 1.46     |
| 6   | D     | 812 | HEM  | C4D-ND  | -3.05 | 1.35        | 1.40     |
| 6   | D     | 808 | HEM  | C4D-ND  | -3.04 | 1.35        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | D     | 806 | HEM  | C4D-ND  | -3.03 | 1.35        | 1.40     |
| 6   | L     | 806 | HEM  | C4D-ND  | -3.03 | 1.35        | 1.40     |
| 6   | A     | 811 | HEM  | C4D-ND  | -3.02 | 1.35        | 1.40     |
| 6   | H     | 812 | HEM  | C4D-ND  | -3.01 | 1.35        | 1.40     |
| 6   | G     | 811 | HEM  | C4D-ND  | -3.01 | 1.35        | 1.40     |
| 6   | I     | 806 | HEM  | C4D-ND  | -2.99 | 1.35        | 1.40     |
| 6   | L     | 808 | HEM  | C4D-ND  | -2.98 | 1.35        | 1.40     |
| 6   | F     | 809 | HEM  | C4D-ND  | -2.98 | 1.35        | 1.40     |
| 6   | H     | 808 | HEM  | C4D-ND  | -2.97 | 1.35        | 1.40     |
| 6   | J     | 810 | HEM  | C4D-ND  | -2.97 | 1.35        | 1.40     |
| 6   | F     | 807 | HEM  | C4D-ND  | -2.97 | 1.35        | 1.40     |
| 6   | I     | 807 | HEM  | C4D-ND  | -2.96 | 1.35        | 1.40     |
| 6   | L     | 809 | HEM  | C4D-ND  | -2.96 | 1.35        | 1.40     |
| 6   | H     | 810 | HEM  | C4D-ND  | -2.95 | 1.35        | 1.40     |
| 6   | C     | 811 | HEM  | C4D-ND  | -2.95 | 1.35        | 1.40     |
| 6   | L     | 810 | HEM  | C4D-ND  | -2.95 | 1.35        | 1.40     |
| 6   | E     | 806 | HEM  | C4D-ND  | -2.95 | 1.35        | 1.40     |
| 6   | H     | 814 | HEM  | C4D-ND  | -2.95 | 1.35        | 1.40     |
| 6   | G     | 808 | HEM  | C4D-ND  | -2.94 | 1.35        | 1.40     |
| 6   | B     | 810 | HEM  | C4D-ND  | -2.94 | 1.35        | 1.40     |
| 6   | C     | 813 | HEM  | C4D-ND  | -2.94 | 1.35        | 1.40     |
| 6   | E     | 812 | HEM  | C4D-ND  | -2.93 | 1.35        | 1.40     |
| 6   | C     | 812 | HEM  | C3C-C4C | -2.93 | 1.40        | 1.46     |
| 6   | D     | 811 | HEM  | C4D-ND  | -2.93 | 1.35        | 1.40     |
| 6   | I     | 810 | HEM  | C4D-ND  | -2.92 | 1.35        | 1.40     |
| 6   | C     | 806 | HEM  | C4D-ND  | -2.92 | 1.35        | 1.40     |
| 6   | K     | 808 | HEM  | C4D-ND  | -2.91 | 1.35        | 1.40     |
| 6   | B     | 808 | HEM  | C4D-ND  | -2.91 | 1.35        | 1.40     |
| 6   | E     | 811 | HEM  | C4D-ND  | -2.91 | 1.35        | 1.40     |
| 6   | C     | 807 | HEM  | C4D-ND  | -2.90 | 1.35        | 1.40     |
| 6   | B     | 814 | HEM  | C4D-ND  | -2.89 | 1.35        | 1.40     |
| 6   | K     | 806 | HEM  | C4D-ND  | -2.89 | 1.35        | 1.40     |
| 6   | C     | 812 | HEM  | C4D-ND  | -2.89 | 1.35        | 1.40     |
| 6   | B     | 807 | HEM  | C4D-ND  | -2.88 | 1.35        | 1.40     |
| 6   | F     | 813 | HEM  | C4D-ND  | -2.86 | 1.35        | 1.40     |
| 6   | K     | 810 | HEM  | C4D-ND  | -2.85 | 1.35        | 1.40     |
| 6   | E     | 810 | HEM  | C4D-ND  | -2.85 | 1.35        | 1.40     |
| 6   | L     | 807 | HEM  | C4D-ND  | -2.85 | 1.35        | 1.40     |
| 6   | A     | 806 | HEM  | C4D-ND  | -2.84 | 1.35        | 1.40     |
| 6   | A     | 808 | HEM  | C4D-ND  | -2.83 | 1.35        | 1.40     |
| 6   | H     | 811 | HEM  | C4D-ND  | -2.83 | 1.35        | 1.40     |
| 6   | F     | 814 | HEM  | C4D-ND  | -2.83 | 1.35        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | I     | 812 | HEM  | C4D-ND  | -2.82 | 1.35        | 1.40     |
| 6   | A     | 809 | HEM  | C4D-ND  | -2.81 | 1.35        | 1.40     |
| 6   | F     | 808 | HEM  | C4D-ND  | -2.79 | 1.35        | 1.40     |
| 6   | B     | 811 | HEM  | C4D-ND  | -2.78 | 1.35        | 1.40     |
| 6   | G     | 809 | HEM  | C4D-ND  | -2.78 | 1.35        | 1.40     |
| 6   | K     | 812 | HEM  | C4D-ND  | -2.76 | 1.35        | 1.40     |
| 6   | H     | 813 | HEM  | C4D-ND  | -2.75 | 1.35        | 1.40     |
| 6   | B     | 813 | HEM  | C4D-ND  | -2.74 | 1.35        | 1.40     |
| 6   | A     | 807 | HEM  | C4D-ND  | -2.73 | 1.35        | 1.40     |
| 6   | D     | 809 | HEM  | C4C-NC  | -2.73 | 1.34        | 1.39     |
| 6   | C     | 809 | HEM  | C4D-ND  | -2.73 | 1.35        | 1.40     |
| 6   | D     | 809 | HEM  | C4D-ND  | -2.73 | 1.35        | 1.40     |
| 6   | G     | 807 | HEM  | C3C-C4C | -2.72 | 1.41        | 1.46     |
| 6   | D     | 807 | HEM  | C4D-ND  | -2.72 | 1.35        | 1.40     |
| 6   | L     | 813 | HEM  | C4D-ND  | -2.70 | 1.35        | 1.40     |
| 6   | E     | 807 | HEM  | C4D-ND  | -2.70 | 1.35        | 1.40     |
| 6   | J     | 807 | HEM  | C4D-ND  | -2.70 | 1.35        | 1.40     |
| 6   | G     | 810 | HEM  | C4D-ND  | -2.70 | 1.35        | 1.40     |
| 6   | K     | 807 | HEM  | C4D-ND  | -2.69 | 1.35        | 1.40     |
| 6   | B     | 809 | HEM  | C4C-NC  | -2.68 | 1.34        | 1.39     |
| 6   | D     | 810 | HEM  | C4D-ND  | -2.68 | 1.35        | 1.40     |
| 6   | J     | 812 | HEM  | C4D-ND  | -2.68 | 1.35        | 1.40     |
| 6   | I     | 808 | HEM  | C4D-ND  | -2.66 | 1.35        | 1.40     |
| 6   | A     | 811 | HEM  | C4C-NC  | -2.62 | 1.34        | 1.39     |
| 6   | L     | 812 | HEM  | C4D-ND  | -2.62 | 1.35        | 1.40     |
| 6   | E     | 809 | HEM  | C3C-C4C | -2.62 | 1.41        | 1.46     |
| 6   | I     | 811 | HEM  | C4D-ND  | -2.62 | 1.35        | 1.40     |
| 6   | F     | 814 | HEM  | C3C-C4C | -2.59 | 1.41        | 1.46     |
| 6   | C     | 812 | HEM  | C1D-ND  | -2.58 | 1.33        | 1.38     |
| 6   | C     | 808 | HEM  | C4C-NC  | -2.58 | 1.34        | 1.39     |
| 6   | L     | 809 | HEM  | C3C-C4C | -2.57 | 1.41        | 1.46     |
| 6   | F     | 811 | HEM  | C3C-C4C | -2.55 | 1.41        | 1.46     |
| 6   | K     | 813 | HEM  | C3C-C4C | -2.55 | 1.41        | 1.46     |
| 6   | F     | 808 | HEM  | C1D-ND  | -2.55 | 1.33        | 1.38     |
| 6   | I     | 813 | HEM  | C4C-NC  | -2.54 | 1.34        | 1.39     |
| 6   | A     | 810 | HEM  | C4D-ND  | -2.54 | 1.35        | 1.40     |
| 6   | L     | 811 | HEM  | C4D-ND  | -2.53 | 1.35        | 1.40     |
| 6   | D     | 809 | HEM  | C1C-C2C | -2.53 | 1.40        | 1.45     |
| 6   | J     | 813 | HEM  | C4C-NC  | -2.53 | 1.34        | 1.39     |
| 6   | F     | 810 | HEM  | C4C-NC  | -2.53 | 1.34        | 1.39     |
| 6   | J     | 808 | HEM  | C3C-C4C | -2.51 | 1.41        | 1.46     |
| 6   | K     | 807 | HEM  | C3C-C4C | -2.51 | 1.41        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | J     | 813 | HEM  | C3C-C4C | -2.50 | 1.41        | 1.46     |
| 6   | F     | 810 | HEM  | C3C-C4C | -2.50 | 1.41        | 1.46     |
| 6   | A     | 810 | HEM  | C3C-C4C | -2.50 | 1.41        | 1.46     |
| 6   | F     | 813 | HEM  | C3C-C4C | -2.49 | 1.41        | 1.46     |
| 6   | J     | 808 | HEM  | C4C-NC  | -2.49 | 1.34        | 1.39     |
| 6   | L     | 809 | HEM  | C1D-ND  | -2.49 | 1.34        | 1.38     |
| 6   | K     | 812 | HEM  | C3C-C4C | -2.48 | 1.41        | 1.46     |
| 6   | F     | 814 | HEM  | C4C-NC  | -2.48 | 1.34        | 1.39     |
| 6   | F     | 809 | HEM  | C3C-C4C | -2.48 | 1.41        | 1.46     |
| 6   | G     | 813 | HEM  | C3C-C4C | -2.48 | 1.41        | 1.46     |
| 6   | J     | 806 | HEM  | CHC-C1C | 2.47  | 1.43        | 1.38     |
| 6   | A     | 811 | HEM  | C1D-ND  | -2.47 | 1.34        | 1.38     |
| 6   | L     | 813 | HEM  | C1C-C2C | -2.47 | 1.40        | 1.45     |
| 6   | K     | 806 | HEM  | CHC-C1C | 2.46  | 1.43        | 1.38     |
| 6   | E     | 809 | HEM  | C4C-NC  | -2.45 | 1.35        | 1.39     |
| 6   | B     | 808 | HEM  | C3C-C4C | -2.44 | 1.41        | 1.46     |
| 6   | I     | 813 | HEM  | C3C-C4C | -2.44 | 1.41        | 1.46     |
| 6   | F     | 811 | HEM  | C4C-NC  | -2.44 | 1.35        | 1.39     |
| 6   | D     | 808 | HEM  | C4C-NC  | -2.43 | 1.35        | 1.39     |
| 6   | E     | 806 | HEM  | C1D-ND  | -2.43 | 1.34        | 1.38     |
| 6   | J     | 807 | HEM  | C3C-C4C | -2.43 | 1.41        | 1.46     |
| 6   | J     | 807 | HEM  | C1D-ND  | -2.43 | 1.34        | 1.38     |
| 6   | G     | 807 | HEM  | C1D-ND  | -2.43 | 1.34        | 1.38     |
| 6   | I     | 812 | HEM  | C3C-C4C | -2.42 | 1.41        | 1.46     |
| 6   | J     | 808 | HEM  | C1C-C2C | -2.42 | 1.40        | 1.45     |
| 6   | C     | 809 | HEM  | C3C-C4C | -2.41 | 1.41        | 1.46     |
| 6   | G     | 813 | HEM  | C4C-NC  | -2.41 | 1.35        | 1.39     |
| 6   | B     | 809 | HEM  | C1D-ND  | -2.40 | 1.34        | 1.38     |
| 6   | L     | 807 | HEM  | C1D-ND  | -2.40 | 1.34        | 1.38     |
| 6   | A     | 808 | HEM  | C1C-C2C | -2.40 | 1.40        | 1.45     |
| 6   | C     | 810 | HEM  | C4C-NC  | -2.39 | 1.35        | 1.39     |
| 6   | I     | 809 | HEM  | C4D-ND  | -2.38 | 1.36        | 1.40     |
| 6   | D     | 810 | HEM  | C3C-C4C | -2.38 | 1.41        | 1.46     |
| 6   | G     | 809 | HEM  | C3C-C4C | -2.38 | 1.41        | 1.46     |
| 6   | K     | 807 | HEM  | C1D-ND  | -2.38 | 1.34        | 1.38     |
| 6   | G     | 809 | HEM  | C4C-NC  | -2.38 | 1.35        | 1.39     |
| 6   | A     | 811 | HEM  | C3C-C4C | -2.37 | 1.41        | 1.46     |
| 6   | A     | 808 | HEM  | C1D-ND  | -2.37 | 1.34        | 1.38     |
| 6   | C     | 807 | HEM  | C1D-ND  | -2.36 | 1.34        | 1.38     |
| 6   | E     | 813 | HEM  | C3C-C4C | -2.36 | 1.41        | 1.46     |
| 6   | D     | 808 | HEM  | C3C-C4C | -2.36 | 1.41        | 1.46     |
| 6   | K     | 806 | HEM  | C1D-ND  | -2.36 | 1.34        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | C     | 812 | HEM  | C4C-NC  | -2.35 | 1.35        | 1.39     |
| 6   | H     | 814 | HEM  | C4C-NC  | -2.35 | 1.35        | 1.39     |
| 6   | J     | 806 | HEM  | C1D-ND  | -2.35 | 1.34        | 1.38     |
| 6   | J     | 806 | HEM  | C3B-C4B | 2.35  | 1.49        | 1.44     |
| 6   | L     | 806 | HEM  | C4C-NC  | -2.35 | 1.35        | 1.39     |
| 6   | K     | 806 | HEM  | C3B-C4B | 2.35  | 1.49        | 1.44     |
| 6   | E     | 810 | HEM  | C3C-C4C | -2.35 | 1.41        | 1.46     |
| 6   | F     | 808 | HEM  | C3C-C4C | -2.34 | 1.41        | 1.46     |
| 6   | A     | 813 | HEM  | C1D-ND  | -2.34 | 1.34        | 1.38     |
| 6   | I     | 808 | HEM  | C4C-NC  | -2.34 | 1.35        | 1.39     |
| 6   | G     | 812 | HEM  | C4D-ND  | -2.34 | 1.36        | 1.40     |
| 6   | H     | 808 | HEM  | C3C-C4C | -2.34 | 1.41        | 1.46     |
| 6   | E     | 811 | HEM  | C1D-ND  | -2.33 | 1.34        | 1.38     |
| 6   | D     | 809 | HEM  | C3C-C4C | -2.33 | 1.42        | 1.46     |
| 6   | H     | 813 | HEM  | C4C-NC  | -2.32 | 1.35        | 1.39     |
| 6   | H     | 809 | HEM  | C4C-NC  | -2.32 | 1.35        | 1.39     |
| 6   | B     | 807 | HEM  | C1D-ND  | -2.32 | 1.34        | 1.38     |
| 6   | I     | 808 | HEM  | C3C-C4C | -2.32 | 1.42        | 1.46     |
| 6   | L     | 810 | HEM  | C3C-C4C | -2.31 | 1.42        | 1.46     |
| 6   | A     | 808 | HEM  | C3C-C4C | -2.31 | 1.42        | 1.46     |
| 6   | D     | 808 | HEM  | C1D-ND  | -2.31 | 1.34        | 1.38     |
| 6   | B     | 814 | HEM  | C4C-NC  | -2.31 | 1.35        | 1.39     |
| 6   | E     | 813 | HEM  | C4C-NC  | -2.31 | 1.35        | 1.39     |
| 6   | D     | 809 | HEM  | C1D-ND  | -2.31 | 1.34        | 1.38     |
| 6   | J     | 813 | HEM  | C1D-ND  | -2.31 | 1.34        | 1.38     |
| 6   | A     | 812 | HEM  | C3C-C4C | -2.31 | 1.42        | 1.46     |
| 6   | I     | 807 | HEM  | C3C-C4C | -2.30 | 1.42        | 1.46     |
| 6   | H     | 814 | HEM  | C3C-C4C | -2.29 | 1.42        | 1.46     |
| 6   | K     | 807 | HEM  | C4C-NC  | -2.29 | 1.35        | 1.39     |
| 6   | C     | 811 | HEM  | C1D-ND  | -2.29 | 1.34        | 1.38     |
| 6   | C     | 809 | HEM  | C1D-ND  | -2.29 | 1.34        | 1.38     |
| 6   | B     | 810 | HEM  | C3C-C4C | -2.29 | 1.42        | 1.46     |
| 6   | L     | 808 | HEM  | C1D-ND  | -2.29 | 1.34        | 1.38     |
| 6   | J     | 811 | HEM  | CHB-C1B | 2.28  | 1.43        | 1.38     |
| 6   | F     | 811 | HEM  | C1C-C2C | -2.28 | 1.40        | 1.45     |
| 6   | I     | 807 | HEM  | C1D-ND  | -2.28 | 1.34        | 1.38     |
| 6   | B     | 808 | HEM  | C4C-NC  | -2.28 | 1.35        | 1.39     |
| 6   | K     | 811 | HEM  | C1D-ND  | -2.28 | 1.34        | 1.38     |
| 6   | E     | 808 | HEM  | C3C-C4C | -2.28 | 1.42        | 1.46     |
| 6   | K     | 813 | HEM  | C4C-NC  | -2.28 | 1.35        | 1.39     |
| 6   | F     | 809 | HEM  | C1C-C2C | -2.28 | 1.40        | 1.45     |
| 6   | E     | 811 | HEM  | C4C-NC  | -2.27 | 1.35        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | C     | 808 | HEM  | C3C-C4C | -2.27 | 1.42        | 1.46     |
| 6   | D     | 807 | HEM  | C4C-NC  | -2.27 | 1.35        | 1.39     |
| 6   | A     | 807 | HEM  | C1D-ND  | -2.26 | 1.34        | 1.38     |
| 6   | D     | 813 | HEM  | C4C-NC  | -2.26 | 1.35        | 1.39     |
| 6   | A     | 813 | HEM  | C4C-NC  | -2.26 | 1.35        | 1.39     |
| 6   | L     | 806 | HEM  | C1D-ND  | -2.26 | 1.34        | 1.38     |
| 6   | C     | 808 | HEM  | C1D-ND  | -2.25 | 1.34        | 1.38     |
| 6   | E     | 808 | HEM  | CHB-C1B | 2.25  | 1.43        | 1.38     |
| 6   | E     | 808 | HEM  | C4C-NC  | -2.25 | 1.35        | 1.39     |
| 6   | B     | 811 | HEM  | C3C-C4C | -2.25 | 1.42        | 1.46     |
| 6   | B     | 813 | HEM  | C3C-C4C | -2.24 | 1.42        | 1.46     |
| 6   | G     | 808 | HEM  | C4C-NC  | -2.24 | 1.35        | 1.39     |
| 6   | J     | 809 | HEM  | C3C-C4C | -2.24 | 1.42        | 1.46     |
| 6   | J     | 811 | HEM  | C3C-C4C | -2.23 | 1.42        | 1.46     |
| 6   | B     | 812 | HEM  | C3C-C4C | -2.23 | 1.42        | 1.46     |
| 6   | H     | 812 | HEM  | CHB-C1B | 2.23  | 1.42        | 1.38     |
| 6   | H     | 808 | HEM  | C1D-ND  | -2.23 | 1.34        | 1.38     |
| 6   | F     | 807 | HEM  | C3C-C4C | -2.22 | 1.42        | 1.46     |
| 6   | F     | 810 | HEM  | C1D-ND  | -2.22 | 1.34        | 1.38     |
| 6   | C     | 810 | HEM  | C1C-C2C | -2.22 | 1.40        | 1.45     |
| 6   | J     | 808 | HEM  | C1D-ND  | -2.22 | 1.34        | 1.38     |
| 6   | A     | 810 | HEM  | C1C-C2C | -2.22 | 1.40        | 1.45     |
| 6   | A     | 806 | HEM  | CHB-C1B | 2.22  | 1.42        | 1.38     |
| 6   | E     | 812 | HEM  | C3C-C4C | -2.22 | 1.42        | 1.46     |
| 6   | E     | 813 | HEM  | C1D-ND  | -2.22 | 1.34        | 1.38     |
| 6   | C     | 806 | HEM  | CHB-C1B | 2.21  | 1.42        | 1.38     |
| 6   | I     | 810 | HEM  | C3C-C4C | -2.21 | 1.42        | 1.46     |
| 6   | H     | 814 | HEM  | C1D-ND  | -2.21 | 1.34        | 1.38     |
| 6   | J     | 809 | HEM  | C1D-ND  | -2.21 | 1.34        | 1.38     |
| 6   | C     | 806 | HEM  | C1C-C2C | -2.20 | 1.41        | 1.45     |
| 6   | E     | 806 | HEM  | CHB-C1B | 2.20  | 1.42        | 1.38     |
| 6   | A     | 812 | HEM  | C1D-ND  | -2.20 | 1.34        | 1.38     |
| 6   | H     | 812 | HEM  | C1D-ND  | -2.20 | 1.34        | 1.38     |
| 6   | B     | 811 | HEM  | C4C-NC  | -2.20 | 1.35        | 1.39     |
| 6   | G     | 809 | HEM  | C1C-C2C | -2.19 | 1.41        | 1.45     |
| 6   | L     | 809 | HEM  | C4C-NC  | -2.19 | 1.35        | 1.39     |
| 6   | E     | 809 | HEM  | C1D-ND  | -2.19 | 1.34        | 1.38     |
| 6   | A     | 813 | HEM  | CHB-C1B | 2.19  | 1.42        | 1.38     |
| 6   | B     | 808 | HEM  | C1D-ND  | -2.19 | 1.34        | 1.38     |
| 6   | L     | 810 | HEM  | C4C-NC  | -2.18 | 1.35        | 1.39     |
| 6   | K     | 812 | HEM  | C1D-ND  | -2.18 | 1.34        | 1.38     |
| 6   | I     | 806 | HEM  | CHB-C1B | 2.18  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | H     | 809 | HEM  | C1C-C2C | -2.18 | 1.41        | 1.45     |
| 6   | A     | 812 | HEM  | C4C-NC  | -2.17 | 1.35        | 1.39     |
| 6   | G     | 808 | HEM  | C1D-ND  | -2.17 | 1.34        | 1.38     |
| 6   | A     | 810 | HEM  | C1D-ND  | -2.17 | 1.34        | 1.38     |
| 6   | B     | 809 | HEM  | C3C-C4C | -2.17 | 1.42        | 1.46     |
| 6   | B     | 814 | HEM  | C3C-C4C | -2.17 | 1.42        | 1.46     |
| 6   | G     | 811 | HEM  | FE-ND   | -2.17 | 1.88        | 1.94     |
| 6   | H     | 811 | HEM  | C3C-C4C | -2.17 | 1.42        | 1.46     |
| 6   | G     | 806 | HEM  | C1D-ND  | -2.17 | 1.34        | 1.38     |
| 6   | B     | 814 | HEM  | CHB-C1B | 2.16  | 1.42        | 1.38     |
| 6   | I     | 808 | HEM  | C1C-C2C | -2.16 | 1.41        | 1.45     |
| 6   | K     | 811 | HEM  | C4C-NC  | -2.16 | 1.35        | 1.39     |
| 6   | A     | 808 | HEM  | C4C-NC  | -2.16 | 1.35        | 1.39     |
| 6   | H     | 807 | HEM  | C3C-C4C | -2.16 | 1.42        | 1.46     |
| 6   | F     | 809 | HEM  | C4C-NC  | -2.16 | 1.35        | 1.39     |
| 6   | H     | 809 | HEM  | C1D-ND  | -2.16 | 1.34        | 1.38     |
| 6   | D     | 811 | HEM  | C1D-ND  | -2.16 | 1.34        | 1.38     |
| 6   | B     | 812 | HEM  | C1D-ND  | -2.15 | 1.34        | 1.38     |
| 6   | E     | 810 | HEM  | C4C-NC  | -2.15 | 1.35        | 1.39     |
| 6   | F     | 808 | HEM  | C4C-NC  | -2.15 | 1.35        | 1.39     |
| 6   | B     | 810 | HEM  | C1D-ND  | -2.15 | 1.34        | 1.38     |
| 6   | F     | 807 | HEM  | C1D-ND  | -2.14 | 1.34        | 1.38     |
| 6   | H     | 814 | HEM  | C1C-C2C | -2.14 | 1.41        | 1.45     |
| 6   | K     | 812 | HEM  | C4C-NC  | -2.14 | 1.35        | 1.39     |
| 6   | K     | 808 | HEM  | C4C-NC  | -2.14 | 1.35        | 1.39     |
| 6   | J     | 807 | HEM  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 6   | A     | 806 | HEM  | C1D-ND  | -2.14 | 1.34        | 1.38     |
| 6   | L     | 811 | HEM  | CHB-C1B | 2.13  | 1.42        | 1.38     |
| 6   | B     | 809 | HEM  | C1C-C2C | -2.13 | 1.41        | 1.45     |
| 6   | J     | 810 | HEM  | C4C-NC  | -2.13 | 1.35        | 1.39     |
| 6   | E     | 810 | HEM  | C1D-ND  | -2.13 | 1.34        | 1.38     |
| 6   | C     | 806 | HEM  | C1D-ND  | -2.13 | 1.34        | 1.38     |
| 6   | D     | 812 | HEM  | C4C-NC  | -2.13 | 1.35        | 1.39     |
| 6   | F     | 810 | HEM  | C1C-C2C | -2.13 | 1.41        | 1.45     |
| 6   | D     | 813 | HEM  | C3C-C4C | -2.13 | 1.42        | 1.46     |
| 6   | H     | 809 | HEM  | C3C-C4C | -2.13 | 1.42        | 1.46     |
| 6   | G     | 811 | HEM  | C1C-C2C | -2.13 | 1.41        | 1.45     |
| 6   | H     | 813 | HEM  | C1D-ND  | -2.12 | 1.34        | 1.38     |
| 6   | J     | 809 | HEM  | C4C-NC  | -2.12 | 1.35        | 1.39     |
| 6   | G     | 810 | HEM  | C1C-C2C | -2.12 | 1.41        | 1.45     |
| 6   | C     | 810 | HEM  | C3C-C4C | -2.12 | 1.42        | 1.46     |
| 6   | J     | 812 | HEM  | C3C-C4C | -2.12 | 1.42        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | G     | 807 | HEM  | C4C-NC  | -2.12 | 1.35        | 1.39     |
| 6   | K     | 808 | HEM  | CHB-C1B | 2.12  | 1.42        | 1.38     |
| 6   | H     | 810 | HEM  | C1D-ND  | -2.12 | 1.34        | 1.38     |
| 6   | K     | 813 | HEM  | C1D-ND  | -2.12 | 1.34        | 1.38     |
| 6   | G     | 811 | HEM  | C3C-C4C | -2.11 | 1.42        | 1.46     |
| 6   | H     | 810 | HEM  | C4C-NC  | -2.11 | 1.35        | 1.39     |
| 6   | F     | 814 | HEM  | C1D-ND  | -2.11 | 1.34        | 1.38     |
| 6   | J     | 812 | HEM  | C4C-NC  | -2.11 | 1.35        | 1.39     |
| 6   | C     | 808 | HEM  | C1A-C2A | -2.11 | 1.40        | 1.44     |
| 6   | I     | 812 | HEM  | CHB-C1B | 2.11  | 1.42        | 1.38     |
| 6   | L     | 807 | HEM  | C3C-C4C | -2.11 | 1.42        | 1.46     |
| 6   | J     | 811 | HEM  | C1C-C2C | -2.11 | 1.41        | 1.45     |
| 6   | G     | 809 | HEM  | C1D-ND  | -2.11 | 1.34        | 1.38     |
| 6   | A     | 806 | HEM  | C3C-C4C | -2.11 | 1.42        | 1.46     |
| 6   | L     | 808 | HEM  | C3C-C4C | -2.11 | 1.42        | 1.46     |
| 6   | I     | 811 | HEM  | C4C-NC  | -2.10 | 1.35        | 1.39     |
| 6   | D     | 807 | HEM  | C1D-ND  | -2.10 | 1.34        | 1.38     |
| 6   | J     | 812 | HEM  | C1D-ND  | -2.10 | 1.34        | 1.38     |
| 6   | B     | 810 | HEM  | C4C-NC  | -2.10 | 1.35        | 1.39     |
| 6   | E     | 812 | HEM  | C1C-C2C | -2.10 | 1.41        | 1.45     |
| 6   | E     | 806 | HEM  | C3C-C4C | -2.09 | 1.42        | 1.46     |
| 6   | L     | 809 | HEM  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 6   | K     | 810 | HEM  | C3C-C4C | -2.09 | 1.42        | 1.46     |
| 6   | A     | 809 | HEM  | C4C-NC  | -2.09 | 1.35        | 1.39     |
| 6   | E     | 809 | HEM  | C1C-C2C | -2.09 | 1.41        | 1.45     |
| 6   | G     | 807 | HEM  | C3B-C4B | 2.08  | 1.49        | 1.44     |
| 6   | J     | 806 | HEM  | C3C-C4C | -2.08 | 1.42        | 1.46     |
| 6   | K     | 809 | HEM  | C3C-C4C | -2.08 | 1.42        | 1.46     |
| 6   | C     | 813 | HEM  | C1D-ND  | -2.08 | 1.34        | 1.38     |
| 6   | A     | 807 | HEM  | C4C-NC  | -2.08 | 1.35        | 1.39     |
| 6   | I     | 807 | HEM  | C4C-NC  | -2.08 | 1.35        | 1.39     |
| 6   | D     | 808 | HEM  | C1C-C2C | -2.08 | 1.41        | 1.45     |
| 6   | B     | 813 | HEM  | C1C-C2C | -2.08 | 1.41        | 1.45     |
| 6   | D     | 812 | HEM  | C3C-C4C | -2.08 | 1.42        | 1.46     |
| 6   | L     | 812 | HEM  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 6   | D     | 813 | HEM  | C1D-ND  | -2.07 | 1.34        | 1.38     |
| 6   | E     | 808 | HEM  | C1D-ND  | -2.07 | 1.34        | 1.38     |
| 6   | L     | 806 | HEM  | CHB-C1B | 2.07  | 1.42        | 1.38     |
| 6   | H     | 813 | HEM  | C3C-C4C | -2.07 | 1.42        | 1.46     |
| 6   | I     | 810 | HEM  | C1C-C2C | -2.07 | 1.41        | 1.45     |
| 6   | G     | 812 | HEM  | C3C-C4C | -2.07 | 1.42        | 1.46     |
| 6   | I     | 809 | HEM  | C4C-NC  | -2.07 | 1.35        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | E     | 808 | HEM  | C1C-C2C | -2.07 | 1.41        | 1.45     |
| 6   | K     | 806 | HEM  | C3C-C4C | -2.07 | 1.42        | 1.46     |
| 6   | D     | 810 | HEM  | C1D-ND  | -2.06 | 1.34        | 1.38     |
| 6   | I     | 813 | HEM  | CHB-C1B | 2.06  | 1.42        | 1.38     |
| 6   | D     | 808 | HEM  | C1A-C2A | -2.06 | 1.40        | 1.44     |
| 6   | J     | 811 | HEM  | C4C-NC  | -2.06 | 1.35        | 1.39     |
| 6   | I     | 810 | HEM  | C4C-NC  | -2.06 | 1.35        | 1.39     |
| 6   | C     | 810 | HEM  | C1A-C2A | -2.06 | 1.40        | 1.44     |
| 6   | D     | 807 | HEM  | C3C-C4C | -2.06 | 1.42        | 1.46     |
| 6   | G     | 811 | HEM  | C1D-ND  | -2.06 | 1.34        | 1.38     |
| 6   | I     | 807 | HEM  | CHC-C1C | 2.05  | 1.42        | 1.38     |
| 6   | I     | 809 | HEM  | C1D-ND  | -2.04 | 1.34        | 1.38     |
| 6   | G     | 807 | HEM  | CHC-C1C | 2.04  | 1.42        | 1.38     |
| 6   | J     | 810 | HEM  | C1D-ND  | -2.04 | 1.34        | 1.38     |
| 6   | K     | 806 | HEM  | C4C-NC  | -2.04 | 1.35        | 1.39     |
| 6   | E     | 806 | HEM  | C4C-NC  | -2.04 | 1.35        | 1.39     |
| 6   | B     | 810 | HEM  | C1C-C2C | -2.04 | 1.41        | 1.45     |
| 6   | F     | 814 | HEM  | CHB-C1B | 2.04  | 1.42        | 1.38     |
| 6   | I     | 812 | HEM  | C1D-ND  | -2.03 | 1.34        | 1.38     |
| 6   | L     | 807 | HEM  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 6   | A     | 813 | HEM  | C1C-C2C | -2.03 | 1.41        | 1.45     |
| 6   | F     | 813 | HEM  | C1D-ND  | -2.03 | 1.34        | 1.38     |
| 6   | G     | 806 | HEM  | C3C-C4C | -2.03 | 1.42        | 1.46     |
| 6   | J     | 807 | HEM  | C3B-C4B | 2.03  | 1.48        | 1.44     |
| 6   | C     | 811 | HEM  | C4C-NC  | -2.03 | 1.35        | 1.39     |
| 6   | A     | 811 | HEM  | C1B-C2B | -2.03 | 1.40        | 1.44     |
| 6   | A     | 811 | HEM  | FE-ND   | -2.03 | 1.88        | 1.94     |
| 6   | I     | 806 | HEM  | C3C-C4C | -2.03 | 1.42        | 1.46     |
| 6   | J     | 811 | HEM  | C1D-ND  | -2.02 | 1.34        | 1.38     |
| 6   | L     | 810 | HEM  | C1C-C2C | -2.02 | 1.41        | 1.45     |
| 6   | K     | 807 | HEM  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 6   | H     | 808 | HEM  | C4C-NC  | -2.02 | 1.35        | 1.39     |
| 6   | G     | 811 | HEM  | C4C-NC  | -2.02 | 1.35        | 1.39     |
| 6   | E     | 813 | HEM  | FE-ND   | -2.02 | 1.88        | 1.94     |
| 6   | B     | 813 | HEM  | C4C-NC  | -2.02 | 1.35        | 1.39     |
| 6   | A     | 806 | HEM  | C4C-NC  | -2.02 | 1.35        | 1.39     |
| 6   | H     | 813 | HEM  | CHB-C1B | 2.02  | 1.42        | 1.38     |
| 6   | F     | 807 | HEM  | C1A-C2A | -2.02 | 1.40        | 1.44     |
| 6   | J     | 810 | HEM  | C3C-C4C | -2.02 | 1.42        | 1.46     |
| 6   | B     | 813 | HEM  | C1D-ND  | -2.02 | 1.34        | 1.38     |
| 6   | F     | 807 | HEM  | CHB-C1B | 2.02  | 1.42        | 1.38     |
| 6   | K     | 813 | HEM  | CHB-C1B | 2.02  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 6   | E     | 807 | HEM  | C1D-ND  | -2.01 | 1.34        | 1.38     |
| 6   | I     | 813 | HEM  | C1D-ND  | -2.01 | 1.34        | 1.38     |
| 6   | G     | 808 | HEM  | FE-ND   | -2.01 | 1.88        | 1.94     |
| 6   | C     | 806 | HEM  | C3C-C4C | -2.01 | 1.42        | 1.46     |
| 6   | K     | 811 | HEM  | C3C-C4C | -2.01 | 1.42        | 1.46     |
| 6   | F     | 807 | HEM  | C4C-NC  | -2.01 | 1.35        | 1.39     |
| 6   | H     | 811 | HEM  | C1D-ND  | -2.01 | 1.34        | 1.38     |
| 6   | I     | 813 | HEM  | CHC-C1C | 2.01  | 1.42        | 1.38     |
| 6   | C     | 813 | HEM  | C3C-C4C | -2.01 | 1.42        | 1.46     |
| 6   | B     | 807 | HEM  | C3C-C4C | -2.01 | 1.42        | 1.46     |
| 6   | D     | 812 | HEM  | C1D-ND  | -2.01 | 1.34        | 1.38     |
| 6   | C     | 813 | HEM  | FE-ND   | -2.00 | 1.88        | 1.94     |
| 6   | L     | 812 | HEM  | C3C-C4C | -2.00 | 1.42        | 1.46     |
| 6   | K     | 809 | HEM  | C4C-NC  | -2.00 | 1.35        | 1.39     |
| 6   | A     | 809 | HEM  | C3C-C4C | -2.00 | 1.42        | 1.46     |
| 6   | K     | 812 | HEM  | CHC-C1C | 2.00  | 1.42        | 1.38     |
| 6   | B     | 809 | HEM  | FE-ND   | -2.00 | 1.88        | 1.94     |
| 6   | C     | 808 | HEM  | FE-ND   | -2.00 | 1.88        | 1.94     |

All (1483) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 6   | K     | 806 | HEM  | C3B-C4B-NB | -10.94 | 101.61      | 109.47   |
| 6   | A     | 811 | HEM  | C3B-C4B-NB | -10.71 | 101.77      | 109.47   |
| 6   | J     | 806 | HEM  | C3B-C4B-NB | -10.70 | 101.79      | 109.47   |
| 6   | F     | 812 | HEM  | C1B-NB-C4B | 10.66  | 117.83      | 105.21   |
| 6   | A     | 812 | HEM  | C1B-NB-C4B | 10.66  | 117.83      | 105.21   |
| 6   | C     | 811 | HEM  | C1B-NB-C4B | 10.62  | 117.79      | 105.21   |
| 6   | J     | 811 | HEM  | C1B-NB-C4B | 10.52  | 117.67      | 105.21   |
| 6   | F     | 807 | HEM  | C1B-NB-C4B | 10.52  | 117.66      | 105.21   |
| 6   | B     | 809 | HEM  | C1B-NB-C4B | 10.47  | 117.61      | 105.21   |
| 6   | E     | 811 | HEM  | C1B-NB-C4B | 10.46  | 117.59      | 105.21   |
| 6   | D     | 810 | HEM  | C1B-NB-C4B | 10.44  | 117.57      | 105.21   |
| 6   | C     | 810 | HEM  | C1B-NB-C4B | 10.40  | 117.53      | 105.21   |
| 6   | C     | 806 | HEM  | C1B-NB-C4B | 10.36  | 117.48      | 105.21   |
| 6   | A     | 811 | HEM  | C1B-NB-C4B | 10.34  | 117.45      | 105.21   |
| 6   | I     | 811 | HEM  | C1B-NB-C4B | 10.33  | 117.44      | 105.21   |
| 6   | F     | 813 | HEM  | C1B-NB-C4B | 10.29  | 117.40      | 105.21   |
| 6   | D     | 811 | HEM  | C1B-NB-C4B | 10.28  | 117.38      | 105.21   |
| 6   | E     | 806 | HEM  | C1B-NB-C4B | 10.26  | 117.36      | 105.21   |
| 6   | A     | 808 | HEM  | C1B-NB-C4B | 10.25  | 117.34      | 105.21   |
| 6   | A     | 813 | HEM  | C1B-NB-C4B | 10.18  | 117.26      | 105.21   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 6   | C     | 812 | HEM  | C1B-NB-C4B | 10.17 | 117.25      | 105.21   |
| 6   | K     | 806 | HEM  | C1B-NB-C4B | 10.17 | 117.25      | 105.21   |
| 6   | J     | 806 | HEM  | C1B-NB-C4B | 10.10 | 117.17      | 105.21   |
| 6   | D     | 813 | HEM  | C1B-NB-C4B | 10.10 | 117.16      | 105.21   |
| 6   | I     | 812 | HEM  | C1B-NB-C4B | 10.09 | 117.16      | 105.21   |
| 6   | G     | 811 | HEM  | C1B-NB-C4B | 10.09 | 117.15      | 105.21   |
| 6   | H     | 812 | HEM  | C1B-NB-C4B | 10.08 | 117.14      | 105.21   |
| 6   | B     | 807 | HEM  | C1B-NB-C4B | 10.08 | 117.14      | 105.21   |
| 6   | B     | 813 | HEM  | C1B-NB-C4B | 10.08 | 117.14      | 105.21   |
| 6   | D     | 808 | HEM  | C1B-NB-C4B | 10.07 | 117.13      | 105.21   |
| 6   | H     | 813 | HEM  | C1B-NB-C4B | 10.07 | 117.13      | 105.21   |
| 6   | B     | 812 | HEM  | C1B-NB-C4B | 10.06 | 117.12      | 105.21   |
| 6   | A     | 810 | HEM  | C1B-NB-C4B | 10.05 | 117.11      | 105.21   |
| 6   | E     | 808 | HEM  | C1B-NB-C4B | 10.03 | 117.08      | 105.21   |
| 6   | D     | 806 | HEM  | C1B-NB-C4B | 10.02 | 117.07      | 105.21   |
| 6   | G     | 806 | HEM  | C1B-NB-C4B | 10.02 | 117.07      | 105.21   |
| 6   | A     | 806 | HEM  | C1B-NB-C4B | 10.00 | 117.05      | 105.21   |
| 6   | H     | 807 | HEM  | C1B-NB-C4B | 10.00 | 117.05      | 105.21   |
| 6   | F     | 814 | HEM  | C1B-NB-C4B | 9.99  | 117.03      | 105.21   |
| 6   | G     | 810 | HEM  | C1B-NB-C4B | 9.97  | 117.01      | 105.21   |
| 6   | C     | 813 | HEM  | C1B-NB-C4B | 9.96  | 117.01      | 105.21   |
| 6   | G     | 812 | HEM  | C1B-NB-C4B | 9.92  | 116.96      | 105.21   |
| 6   | I     | 813 | HEM  | C1B-NB-C4B | 9.88  | 116.91      | 105.21   |
| 6   | G     | 808 | HEM  | C1B-NB-C4B | 9.88  | 116.91      | 105.21   |
| 6   | E     | 810 | HEM  | C1B-NB-C4B | 9.88  | 116.90      | 105.21   |
| 6   | J     | 812 | HEM  | C1B-NB-C4B | 9.87  | 116.89      | 105.21   |
| 6   | K     | 808 | HEM  | C1B-NB-C4B | 9.86  | 116.89      | 105.21   |
| 6   | D     | 812 | HEM  | C1B-NB-C4B | 9.85  | 116.87      | 105.21   |
| 6   | E     | 812 | HEM  | C1B-NB-C4B | 9.84  | 116.86      | 105.21   |
| 6   | F     | 811 | HEM  | C1B-NB-C4B | 9.82  | 116.84      | 105.21   |
| 6   | K     | 811 | HEM  | C1B-NB-C4B | 9.82  | 116.83      | 105.21   |
| 6   | L     | 810 | HEM  | C1B-NB-C4B | 9.81  | 116.83      | 105.21   |
| 6   | C     | 809 | HEM  | C1B-NB-C4B | 9.81  | 116.83      | 105.21   |
| 6   | C     | 808 | HEM  | C1B-NB-C4B | 9.80  | 116.82      | 105.21   |
| 6   | K     | 813 | HEM  | C1B-NB-C4B | 9.80  | 116.81      | 105.21   |
| 6   | H     | 808 | HEM  | C1B-NB-C4B | 9.80  | 116.81      | 105.21   |
| 6   | L     | 808 | HEM  | C1B-NB-C4B | 9.77  | 116.78      | 105.21   |
| 6   | I     | 808 | HEM  | C1B-NB-C4B | 9.77  | 116.78      | 105.21   |
| 6   | E     | 807 | HEM  | C1B-NB-C4B | 9.76  | 116.77      | 105.21   |
| 6   | H     | 811 | HEM  | C1B-NB-C4B | 9.75  | 116.76      | 105.21   |
| 6   | I     | 806 | HEM  | C1B-NB-C4B | 9.75  | 116.75      | 105.21   |
| 6   | K     | 812 | HEM  | C1B-NB-C4B | 9.73  | 116.73      | 105.21   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 6   | E     | 813 | HEM  | C1B-NB-C4B | 9.71  | 116.71      | 105.21   |
| 6   | I     | 810 | HEM  | C1B-NB-C4B | 9.70  | 116.69      | 105.21   |
| 6   | L     | 806 | HEM  | C1B-NB-C4B | 9.68  | 116.68      | 105.21   |
| 6   | L     | 811 | HEM  | C1B-NB-C4B | 9.68  | 116.67      | 105.21   |
| 6   | H     | 814 | HEM  | C1B-NB-C4B | 9.64  | 116.62      | 105.21   |
| 6   | K     | 810 | HEM  | C1B-NB-C4B | 9.63  | 116.61      | 105.21   |
| 6   | B     | 814 | HEM  | C1B-NB-C4B | 9.63  | 116.61      | 105.21   |
| 6   | J     | 810 | HEM  | C1B-NB-C4B | 9.57  | 116.54      | 105.21   |
| 6   | B     | 811 | HEM  | C1B-NB-C4B | 9.56  | 116.53      | 105.21   |
| 6   | B     | 810 | HEM  | C1B-NB-C4B | 9.55  | 116.52      | 105.21   |
| 6   | D     | 807 | HEM  | C1B-NB-C4B | 9.52  | 116.49      | 105.21   |
| 6   | H     | 809 | HEM  | C1B-NB-C4B | 9.52  | 116.48      | 105.21   |
| 6   | G     | 807 | HEM  | C1B-NB-C4B | 9.51  | 116.47      | 105.21   |
| 6   | J     | 808 | HEM  | C1B-NB-C4B | 9.50  | 116.45      | 105.21   |
| 6   | F     | 809 | HEM  | C1B-NB-C4B | 9.48  | 116.44      | 105.21   |
| 6   | I     | 807 | HEM  | C1B-NB-C4B | 9.47  | 116.42      | 105.21   |
| 6   | F     | 813 | HEM  | C3B-C4B-NB | -9.46 | 102.68      | 109.47   |
| 6   | C     | 807 | HEM  | C1B-NB-C4B | 9.45  | 116.40      | 105.21   |
| 6   | B     | 808 | HEM  | C1B-NB-C4B | 9.43  | 116.37      | 105.21   |
| 6   | K     | 807 | HEM  | C1B-NB-C4B | 9.39  | 116.33      | 105.21   |
| 6   | H     | 810 | HEM  | C1B-NB-C4B | 9.36  | 116.29      | 105.21   |
| 6   | J     | 807 | HEM  | C1B-NB-C4B | 9.36  | 116.29      | 105.21   |
| 6   | F     | 808 | HEM  | C1B-NB-C4B | 9.35  | 116.27      | 105.21   |
| 6   | G     | 813 | HEM  | C1B-NB-C4B | 9.35  | 116.27      | 105.21   |
| 6   | J     | 813 | HEM  | C1B-NB-C4B | 9.34  | 116.27      | 105.21   |
| 6   | L     | 807 | HEM  | C1B-NB-C4B | 9.29  | 116.21      | 105.21   |
| 6   | L     | 812 | HEM  | C1B-NB-C4B | 9.28  | 116.19      | 105.21   |
| 6   | I     | 811 | HEM  | C3B-C4B-NB | -9.26 | 102.81      | 109.47   |
| 6   | A     | 807 | HEM  | C1B-NB-C4B | 9.23  | 116.13      | 105.21   |
| 6   | E     | 809 | HEM  | C1B-NB-C4B | 9.23  | 116.13      | 105.21   |
| 6   | J     | 809 | HEM  | C1B-NB-C4B | 9.22  | 116.13      | 105.21   |
| 6   | G     | 809 | HEM  | C1B-NB-C4B | 9.21  | 116.11      | 105.21   |
| 6   | B     | 809 | HEM  | C3B-C4B-NB | -9.19 | 102.86      | 109.47   |
| 6   | F     | 812 | HEM  | C3B-C4B-NB | -9.18 | 102.88      | 109.47   |
| 6   | C     | 811 | HEM  | C3B-C4B-NB | -9.15 | 102.90      | 109.47   |
| 6   | E     | 811 | HEM  | C3B-C4B-NB | -9.15 | 102.90      | 109.47   |
| 6   | I     | 809 | HEM  | C1B-NB-C4B | 9.14  | 116.03      | 105.21   |
| 6   | L     | 809 | HEM  | C1B-NB-C4B | 9.12  | 116.01      | 105.21   |
| 6   | D     | 808 | HEM  | C3B-C4B-NB | -9.09 | 102.94      | 109.47   |
| 6   | D     | 809 | HEM  | C1B-NB-C4B | 9.04  | 115.91      | 105.21   |
| 6   | F     | 810 | HEM  | C1B-NB-C4B | 8.93  | 115.78      | 105.21   |
| 6   | A     | 812 | HEM  | C3B-C4B-NB | -8.92 | 103.06      | 109.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 6   | J     | 811 | HEM  | C3B-C4B-NB | -8.90 | 103.08      | 109.47   |
| 6   | A     | 806 | HEM  | C3B-C4B-NB | -8.72 | 103.21      | 109.47   |
| 6   | C     | 808 | HEM  | C3B-C4B-NB | -8.65 | 103.26      | 109.47   |
| 6   | J     | 812 | HEM  | C3B-C4B-NB | -8.64 | 103.26      | 109.47   |
| 6   | L     | 813 | HEM  | C1B-NB-C4B | 8.61  | 115.41      | 105.21   |
| 6   | G     | 811 | HEM  | C3B-C4B-NB | -8.61 | 103.28      | 109.47   |
| 6   | D     | 810 | HEM  | C3B-C4B-NB | -8.61 | 103.28      | 109.47   |
| 6   | C     | 812 | HEM  | C3B-C4B-NB | -8.61 | 103.29      | 109.47   |
| 6   | D     | 811 | HEM  | C3B-C4B-NB | -8.58 | 103.31      | 109.47   |
| 6   | K     | 809 | HEM  | C1B-NB-C4B | 8.58  | 115.36      | 105.21   |
| 6   | G     | 806 | HEM  | C3B-C4B-NB | -8.57 | 103.31      | 109.47   |
| 6   | H     | 807 | HEM  | C3B-C4B-NB | -8.53 | 103.34      | 109.47   |
| 6   | D     | 807 | HEM  | C3B-C4B-NB | -8.53 | 103.34      | 109.47   |
| 6   | F     | 807 | HEM  | C3B-C4B-NB | -8.53 | 103.34      | 109.47   |
| 6   | A     | 810 | HEM  | C3B-C4B-NB | -8.52 | 103.35      | 109.47   |
| 6   | A     | 809 | HEM  | C1B-NB-C4B | 8.51  | 115.28      | 105.21   |
| 6   | D     | 812 | HEM  | C3B-C4B-NB | -8.49 | 103.37      | 109.47   |
| 6   | F     | 809 | HEM  | C3B-C4B-NB | -8.46 | 103.39      | 109.47   |
| 6   | L     | 807 | HEM  | C3B-C4B-NB | -8.46 | 103.39      | 109.47   |
| 6   | E     | 808 | HEM  | C3B-C4B-NB | -8.46 | 103.39      | 109.47   |
| 6   | H     | 811 | HEM  | C3B-C4B-NB | -8.44 | 103.41      | 109.47   |
| 6   | I     | 807 | HEM  | C3B-C4B-NB | -8.43 | 103.41      | 109.47   |
| 6   | I     | 812 | HEM  | C3B-C4B-NB | -8.43 | 103.42      | 109.47   |
| 6   | H     | 813 | HEM  | C3B-C4B-NB | -8.42 | 103.42      | 109.47   |
| 6   | F     | 811 | HEM  | C3B-C4B-NB | -8.41 | 103.43      | 109.47   |
| 6   | G     | 807 | HEM  | C3B-C4B-NB | -8.41 | 103.43      | 109.47   |
| 6   | K     | 807 | HEM  | C3B-C4B-NB | -8.39 | 103.44      | 109.47   |
| 6   | C     | 806 | HEM  | C3B-C4B-NB | -8.34 | 103.48      | 109.47   |
| 6   | H     | 808 | HEM  | C3B-C4B-NB | -8.34 | 103.48      | 109.47   |
| 6   | F     | 814 | HEM  | C3B-C4B-NB | -8.31 | 103.50      | 109.47   |
| 6   | E     | 810 | HEM  | C3B-C4B-NB | -8.31 | 103.50      | 109.47   |
| 6   | G     | 810 | HEM  | C3B-C4B-NB | -8.31 | 103.50      | 109.47   |
| 6   | J     | 807 | HEM  | C3B-C4B-NB | -8.29 | 103.52      | 109.47   |
| 6   | B     | 813 | HEM  | C3B-C4B-NB | -8.28 | 103.52      | 109.47   |
| 6   | E     | 807 | HEM  | C3B-C4B-NB | -8.28 | 103.52      | 109.47   |
| 6   | C     | 810 | HEM  | C3B-C4B-NB | -8.27 | 103.53      | 109.47   |
| 6   | B     | 807 | HEM  | C3B-C4B-NB | -8.27 | 103.53      | 109.47   |
| 6   | K     | 811 | HEM  | C3B-C4B-NB | -8.23 | 103.56      | 109.47   |
| 6   | B     | 812 | HEM  | C3B-C4B-NB | -8.18 | 103.59      | 109.47   |
| 6   | B     | 808 | HEM  | C3B-C4B-NB | -8.13 | 103.63      | 109.47   |
| 6   | A     | 807 | HEM  | C3B-C4B-NB | -8.13 | 103.63      | 109.47   |
| 6   | E     | 812 | HEM  | C3B-C4B-NB | -8.09 | 103.66      | 109.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 6   | D     | 813 | HEM  | C3B-C4B-NB | -8.07 | 103.67      | 109.47   |
| 6   | J     | 810 | HEM  | C3B-C4B-NB | -8.07 | 103.67      | 109.47   |
| 6   | A     | 808 | HEM  | C3B-C4B-NB | -8.05 | 103.68      | 109.47   |
| 6   | I     | 813 | HEM  | C3B-C4B-NB | -8.05 | 103.69      | 109.47   |
| 6   | K     | 812 | HEM  | C3B-C4B-NB | -8.03 | 103.70      | 109.47   |
| 6   | G     | 812 | HEM  | C3B-C4B-NB | -8.02 | 103.71      | 109.47   |
| 6   | E     | 806 | HEM  | C3B-C4B-NB | -8.02 | 103.71      | 109.47   |
| 6   | C     | 813 | HEM  | C3B-C4B-NB | -8.01 | 103.71      | 109.47   |
| 6   | L     | 808 | HEM  | C3B-C4B-NB | -7.98 | 103.74      | 109.47   |
| 6   | K     | 810 | HEM  | C3B-C4B-NB | -7.96 | 103.75      | 109.47   |
| 6   | E     | 813 | HEM  | C3B-C4B-NB | -7.96 | 103.75      | 109.47   |
| 6   | D     | 806 | HEM  | C3B-C4B-NB | -7.92 | 103.78      | 109.47   |
| 6   | F     | 808 | HEM  | C3B-C4B-NB | -7.89 | 103.80      | 109.47   |
| 6   | I     | 810 | HEM  | C3B-C4B-NB | -7.89 | 103.80      | 109.47   |
| 6   | H     | 812 | HEM  | C3B-C4B-NB | -7.89 | 103.80      | 109.47   |
| 6   | K     | 808 | HEM  | C3B-C4B-NB | -7.85 | 103.83      | 109.47   |
| 6   | B     | 811 | HEM  | C3B-C4B-NB | -7.84 | 103.84      | 109.47   |
| 6   | I     | 808 | HEM  | C3B-C4B-NB | -7.81 | 103.86      | 109.47   |
| 6   | K     | 813 | HEM  | C3B-C4B-NB | -7.80 | 103.87      | 109.47   |
| 6   | G     | 808 | HEM  | C3B-C4B-NB | -7.76 | 103.89      | 109.47   |
| 6   | C     | 807 | HEM  | C3B-C4B-NB | -7.75 | 103.90      | 109.47   |
| 6   | L     | 810 | HEM  | C3B-C4B-NB | -7.70 | 103.94      | 109.47   |
| 6   | L     | 812 | HEM  | C3B-C4B-NB | -7.55 | 104.05      | 109.47   |
| 6   | H     | 810 | HEM  | C3B-C4B-NB | -7.51 | 104.08      | 109.47   |
| 6   | I     | 806 | HEM  | C3B-C4B-NB | -7.49 | 104.09      | 109.47   |
| 6   | H     | 814 | HEM  | C3B-C4B-NB | -7.48 | 104.10      | 109.47   |
| 6   | B     | 810 | HEM  | C3B-C4B-NB | -7.45 | 104.11      | 109.47   |
| 6   | A     | 813 | HEM  | C3B-C4B-NB | -7.45 | 104.12      | 109.47   |
| 6   | H     | 809 | HEM  | C3B-C4B-NB | -7.40 | 104.15      | 109.47   |
| 6   | L     | 806 | HEM  | C3B-C4B-NB | -7.37 | 104.18      | 109.47   |
| 6   | C     | 809 | HEM  | C3B-C4B-NB | -7.35 | 104.19      | 109.47   |
| 6   | L     | 809 | HEM  | C3B-C4B-NB | -7.31 | 104.22      | 109.47   |
| 6   | D     | 809 | HEM  | C3B-C4B-NB | -7.31 | 104.22      | 109.47   |
| 6   | J     | 808 | HEM  | C3B-C4B-NB | -7.31 | 104.22      | 109.47   |
| 6   | G     | 813 | HEM  | C3B-C4B-NB | -7.25 | 104.26      | 109.47   |
| 6   | J     | 813 | HEM  | C3B-C4B-NB | -7.17 | 104.32      | 109.47   |
| 6   | B     | 814 | HEM  | C3B-C4B-NB | -7.15 | 104.33      | 109.47   |
| 6   | L     | 811 | HEM  | C3B-C4B-NB | -7.08 | 104.38      | 109.47   |
| 6   | E     | 809 | HEM  | C3B-C4B-NB | -6.94 | 104.48      | 109.47   |
| 6   | G     | 809 | HEM  | C3B-C4B-NB | -6.85 | 104.55      | 109.47   |
| 6   | I     | 809 | HEM  | C3B-C4B-NB | -6.74 | 104.63      | 109.47   |
| 6   | A     | 809 | HEM  | C3B-C4B-NB | -6.72 | 104.64      | 109.47   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 6   | F     | 810 | HEM  | C3B-C4B-NB | -6.69 | 104.66      | 109.47   |
| 6   | J     | 809 | HEM  | C3B-C4B-NB | -6.66 | 104.69      | 109.47   |
| 6   | K     | 809 | HEM  | C3B-C4B-NB | -6.37 | 104.89      | 109.47   |
| 6   | L     | 813 | HEM  | C3B-C4B-NB | -6.22 | 105.00      | 109.47   |
| 6   | D     | 806 | HEM  | CHC-C4B-NB | 6.17  | 131.06      | 124.42   |
| 6   | F     | 807 | HEM  | CHC-C4B-NB | 6.00  | 130.88      | 124.42   |
| 6   | F     | 812 | HEM  | CHC-C4B-NB | 6.00  | 130.88      | 124.42   |
| 6   | D     | 810 | HEM  | CHC-C4B-NB | 5.98  | 130.86      | 124.42   |
| 6   | A     | 812 | HEM  | CHC-C4B-NB | 5.89  | 130.76      | 124.42   |
| 6   | A     | 810 | HEM  | CHC-C4B-NB | 5.84  | 130.71      | 124.42   |
| 6   | C     | 810 | HEM  | CHC-C4B-NB | 5.83  | 130.69      | 124.42   |
| 6   | F     | 813 | HEM  | CHC-C4B-NB | 5.66  | 130.51      | 124.42   |
| 6   | H     | 813 | HEM  | CHC-C4B-NB | 5.65  | 130.50      | 124.42   |
| 6   | B     | 809 | HEM  | CHC-C4B-NB | 5.62  | 130.47      | 124.42   |
| 6   | B     | 811 | HEM  | CHC-C4B-NB | 5.58  | 130.42      | 124.42   |
| 6   | A     | 806 | HEM  | CHC-C4B-NB | 5.55  | 130.40      | 124.42   |
| 6   | C     | 806 | HEM  | CHC-C4B-NB | 5.54  | 130.38      | 124.42   |
| 6   | G     | 810 | HEM  | CHC-C4B-NB | 5.52  | 130.36      | 124.42   |
| 6   | C     | 811 | HEM  | CHC-C4B-NB | 5.49  | 130.33      | 124.42   |
| 6   | I     | 812 | HEM  | CHC-C4B-NB | 5.46  | 130.30      | 124.42   |
| 6   | E     | 808 | HEM  | CHC-C4B-NB | 5.45  | 130.29      | 124.42   |
| 6   | B     | 807 | HEM  | CHC-C4B-NB | 5.41  | 130.25      | 124.42   |
| 6   | I     | 810 | HEM  | CHC-C4B-NB | 5.40  | 130.24      | 124.42   |
| 6   | B     | 814 | HEM  | CHC-C4B-NB | 5.40  | 130.23      | 124.42   |
| 6   | D     | 808 | HEM  | CHC-C4B-NB | 5.37  | 130.20      | 124.42   |
| 6   | G     | 811 | HEM  | CHC-C4B-NB | 5.35  | 130.18      | 124.42   |
| 6   | G     | 812 | HEM  | CHC-C4B-NB | 5.32  | 130.15      | 124.42   |
| 6   | F     | 811 | HEM  | CHC-C4B-NB | 5.32  | 130.15      | 124.42   |
| 6   | C     | 808 | HEM  | CHC-C4B-NB | 5.32  | 130.15      | 124.42   |
| 6   | J     | 811 | HEM  | CHC-C4B-NB | 5.27  | 130.10      | 124.42   |
| 6   | B     | 813 | HEM  | CHC-C4B-NB | 5.24  | 130.06      | 124.42   |
| 6   | H     | 807 | HEM  | CHC-C4B-NB | 5.22  | 130.04      | 124.42   |
| 6   | I     | 811 | HEM  | CHC-C4B-NB | 5.19  | 130.00      | 124.42   |
| 6   | A     | 813 | HEM  | CHC-C4B-NB | 5.16  | 129.98      | 124.42   |
| 6   | C     | 813 | HEM  | CHC-C4B-NB | 5.16  | 129.98      | 124.42   |
| 6   | E     | 811 | HEM  | CHC-C4B-NB | 5.15  | 129.96      | 124.42   |
| 6   | H     | 811 | HEM  | CHC-C4B-NB | 5.14  | 129.96      | 124.42   |
| 6   | D     | 813 | HEM  | CHC-C4B-NB | 5.14  | 129.95      | 124.42   |
| 6   | G     | 811 | HEM  | CHD-C1D-ND | 5.13  | 129.95      | 124.42   |
| 6   | D     | 811 | HEM  | CHC-C4B-NB | 5.12  | 129.93      | 124.42   |
| 6   | B     | 808 | HEM  | CHD-C1D-ND | 5.10  | 129.91      | 124.42   |
| 6   | E     | 810 | HEM  | CHC-C4B-NB | 5.05  | 129.86      | 124.42   |

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| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 6   | A     | 808 | HEM  | CHC-C4B-NB | 5.01 | 129.81      | 124.42   |
| 6   | E     | 806 | HEM  | CHC-C4B-NB | 5.00 | 129.80      | 124.42   |
| 6   | C     | 812 | HEM  | CHC-C4B-NB | 4.99 | 129.79      | 124.42   |
| 6   | K     | 810 | HEM  | CHC-C4B-NB | 4.98 | 129.78      | 124.42   |
| 6   | L     | 810 | HEM  | CHC-C4B-NB | 4.98 | 129.78      | 124.42   |
| 6   | L     | 806 | HEM  | CHC-C4B-NB | 4.97 | 129.78      | 124.42   |
| 6   | E     | 812 | HEM  | CHC-C4B-NB | 4.97 | 129.77      | 124.42   |
| 6   | G     | 806 | HEM  | CHC-C4B-NB | 4.95 | 129.75      | 124.42   |
| 6   | F     | 812 | HEM  | CHD-C1D-ND | 4.93 | 129.73      | 124.42   |
| 6   | C     | 813 | HEM  | CHD-C1D-ND | 4.91 | 129.71      | 124.42   |
| 6   | L     | 810 | HEM  | CHD-C1D-ND | 4.90 | 129.70      | 124.42   |
| 6   | F     | 814 | HEM  | CHC-C4B-NB | 4.88 | 129.68      | 124.42   |
| 6   | L     | 811 | HEM  | CHC-C4B-NB | 4.88 | 129.68      | 124.42   |
| 6   | H     | 812 | HEM  | CHC-C4B-NB | 4.86 | 129.65      | 124.42   |
| 6   | J     | 808 | HEM  | CHC-C4B-NB | 4.84 | 129.63      | 124.42   |
| 6   | G     | 813 | HEM  | CHC-C4B-NB | 4.83 | 129.62      | 124.42   |
| 6   | L     | 813 | HEM  | CHC-C1C-NC | 4.83 | 129.71      | 124.45   |
| 6   | E     | 813 | HEM  | CHC-C4B-NB | 4.83 | 129.62      | 124.42   |
| 6   | B     | 812 | HEM  | CHC-C4B-NB | 4.81 | 129.60      | 124.42   |
| 6   | D     | 812 | HEM  | CHC-C4B-NB | 4.79 | 129.58      | 124.42   |
| 6   | I     | 813 | HEM  | CHC-C4B-NB | 4.78 | 129.57      | 124.42   |
| 6   | E     | 813 | HEM  | CHD-C1D-ND | 4.77 | 129.56      | 124.42   |
| 6   | B     | 811 | HEM  | CHD-C1D-ND | 4.74 | 129.52      | 124.42   |
| 6   | L     | 813 | HEM  | CHD-C1D-ND | 4.74 | 129.52      | 124.42   |
| 6   | K     | 808 | HEM  | CHC-C4B-NB | 4.71 | 129.49      | 124.42   |
| 6   | I     | 810 | HEM  | CHD-C1D-ND | 4.70 | 129.48      | 124.42   |
| 6   | D     | 806 | HEM  | CHD-C1D-ND | 4.63 | 129.41      | 124.42   |
| 6   | I     | 808 | HEM  | CHC-C4B-NB | 4.63 | 129.41      | 124.42   |
| 6   | F     | 811 | HEM  | CHD-C1D-ND | 4.62 | 129.40      | 124.42   |
| 6   | E     | 810 | HEM  | CHD-C1D-ND | 4.62 | 129.40      | 124.42   |
| 6   | G     | 810 | HEM  | CHD-C1D-ND | 4.62 | 129.39      | 124.42   |
| 6   | J     | 809 | HEM  | CHD-C1D-ND | 4.61 | 129.38      | 124.42   |
| 6   | L     | 811 | HEM  | CHD-C1D-ND | 4.61 | 129.38      | 124.42   |
| 6   | H     | 808 | HEM  | CHD-C1D-ND | 4.59 | 129.37      | 124.42   |
| 6   | J     | 808 | HEM  | CHD-C1D-ND | 4.56 | 129.34      | 124.42   |
| 6   | I     | 806 | HEM  | CHC-C4B-NB | 4.56 | 129.33      | 124.42   |
| 6   | K     | 810 | HEM  | CHD-C1D-ND | 4.55 | 129.32      | 124.42   |
| 6   | J     | 812 | HEM  | CHC-C4B-NB | 4.55 | 129.32      | 124.42   |
| 6   | K     | 807 | HEM  | CHD-C1D-ND | 4.53 | 129.30      | 124.42   |
| 6   | I     | 811 | HEM  | CHD-C1D-ND | 4.51 | 129.28      | 124.42   |
| 6   | K     | 811 | HEM  | CHD-C1D-ND | 4.50 | 129.27      | 124.42   |
| 6   | F     | 807 | HEM  | CHD-C1D-ND | 4.50 | 129.26      | 124.42   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 6   | C     | 809 | HEM  | CHD-C1D-ND | 4.49  | 129.25      | 124.42   |
| 6   | E     | 808 | HEM  | CHD-C1D-ND | 4.49  | 129.25      | 124.42   |
| 6   | G     | 813 | HEM  | CHD-C1D-ND | 4.47  | 129.24      | 124.42   |
| 6   | A     | 812 | HEM  | CHD-C1D-ND | 4.47  | 129.23      | 124.42   |
| 6   | K     | 813 | HEM  | CHC-C4B-NB | 4.47  | 129.23      | 124.42   |
| 6   | I     | 813 | HEM  | CHD-C1D-ND | 4.46  | 129.22      | 124.42   |
| 6   | H     | 814 | HEM  | CHD-C1D-ND | 4.45  | 129.21      | 124.42   |
| 6   | J     | 810 | HEM  | CHD-C1D-ND | 4.44  | 129.20      | 124.42   |
| 6   | H     | 814 | HEM  | CHC-C4B-NB | 4.42  | 129.18      | 124.42   |
| 6   | B     | 812 | HEM  | CHD-C1D-ND | 4.42  | 129.18      | 124.42   |
| 6   | H     | 807 | HEM  | CHD-C1D-ND | 4.39  | 129.15      | 124.42   |
| 6   | K     | 811 | HEM  | CHC-C4B-NB | 4.38  | 129.13      | 124.42   |
| 6   | L     | 808 | HEM  | CHC-C4B-NB | 4.37  | 129.13      | 124.42   |
| 6   | H     | 810 | HEM  | CHD-C1D-ND | 4.35  | 129.10      | 124.42   |
| 6   | D     | 811 | HEM  | CHD-C1D-ND | 4.35  | 129.10      | 124.42   |
| 6   | J     | 813 | HEM  | CHC-C4B-NB | 4.33  | 129.08      | 124.42   |
| 6   | J     | 810 | HEM  | CHC-C4B-NB | 4.32  | 129.07      | 124.42   |
| 6   | C     | 811 | HEM  | CHD-C1D-ND | 4.31  | 129.06      | 124.42   |
| 6   | H     | 809 | HEM  | CHC-C4B-NB | 4.29  | 129.04      | 124.42   |
| 6   | G     | 808 | HEM  | CHD-C1D-ND | 4.29  | 129.04      | 124.42   |
| 6   | G     | 808 | HEM  | CHC-C4B-NB | 4.29  | 129.04      | 124.42   |
| 6   | C     | 806 | HEM  | C2B-C1B-NB | -4.29 | 104.91      | 109.84   |
| 6   | K     | 809 | HEM  | CHD-C1D-ND | 4.28  | 129.03      | 124.42   |
| 6   | K     | 813 | HEM  | CHD-C1D-ND | 4.28  | 129.03      | 124.42   |
| 6   | E     | 809 | HEM  | CHD-C1D-ND | 4.28  | 129.03      | 124.42   |
| 6   | D     | 813 | HEM  | CHD-C1D-ND | 4.27  | 129.02      | 124.42   |
| 6   | L     | 806 | HEM  | CHD-C1D-ND | 4.25  | 129.00      | 124.42   |
| 6   | L     | 809 | HEM  | CHD-C1D-ND | 4.25  | 128.99      | 124.42   |
| 6   | A     | 811 | HEM  | CHD-C1D-ND | 4.22  | 128.96      | 124.42   |
| 6   | E     | 806 | HEM  | CHD-C1D-ND | 4.22  | 128.96      | 124.42   |
| 6   | E     | 812 | HEM  | CHD-C1D-ND | 4.20  | 128.95      | 124.42   |
| 6   | G     | 812 | HEM  | CHD-C1D-ND | 4.20  | 128.94      | 124.42   |
| 6   | C     | 807 | HEM  | CHD-C1D-ND | 4.19  | 128.93      | 124.42   |
| 6   | E     | 811 | HEM  | CHD-C1D-ND | 4.19  | 128.93      | 124.42   |
| 6   | C     | 809 | HEM  | CHC-C4B-NB | 4.19  | 128.93      | 124.42   |
| 6   | H     | 812 | HEM  | CHD-C1D-ND | 4.18  | 128.92      | 124.42   |
| 6   | L     | 812 | HEM  | CHC-C4B-NB | 4.17  | 128.91      | 124.42   |
| 6   | B     | 814 | HEM  | CHD-C1D-ND | 4.16  | 128.90      | 124.42   |
| 6   | A     | 812 | HEM  | C2B-C1B-NB | -4.16 | 105.06      | 109.84   |
| 6   | C     | 806 | HEM  | CHD-C1D-ND | 4.15  | 128.89      | 124.42   |
| 6   | D     | 810 | HEM  | C2B-C1B-NB | -4.15 | 105.07      | 109.84   |
| 6   | I     | 812 | HEM  | CHD-C1D-ND | 4.14  | 128.88      | 124.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | C     | 811 | HEM  | C2B-C1B-NB  | -4.12 | 105.10      | 109.84   |
| 6   | L     | 807 | HEM  | CHD-C1D-ND  | 4.12  | 128.85      | 124.42   |
| 6   | F     | 807 | HEM  | C2B-C1B-NB  | -4.11 | 105.11      | 109.84   |
| 6   | K     | 812 | HEM  | CHC-C4B-NB  | 4.11  | 128.85      | 124.42   |
| 6   | I     | 807 | HEM  | CHD-C1D-ND  | 4.10  | 128.83      | 124.42   |
| 6   | A     | 813 | HEM  | C2B-C1B-NB  | -4.09 | 105.13      | 109.84   |
| 6   | J     | 813 | HEM  | CHD-C1D-ND  | 4.09  | 128.83      | 124.42   |
| 6   | D     | 810 | HEM  | CHD-C1D-ND  | 4.09  | 128.82      | 124.42   |
| 6   | E     | 806 | HEM  | C2B-C1B-NB  | -4.09 | 105.14      | 109.84   |
| 6   | C     | 810 | HEM  | C2B-C1B-NB  | -4.09 | 105.14      | 109.84   |
| 6   | B     | 808 | HEM  | CHD-C1D-C2D | -4.08 | 118.58      | 125.03   |
| 6   | G     | 807 | HEM  | CHD-C1D-ND  | 4.08  | 128.81      | 124.42   |
| 6   | B     | 809 | HEM  | CHD-C1D-ND  | 4.07  | 128.80      | 124.42   |
| 6   | E     | 808 | HEM  | C2B-C1B-NB  | -4.06 | 105.17      | 109.84   |
| 6   | D     | 809 | HEM  | CHD-C1D-ND  | 4.05  | 128.78      | 124.42   |
| 6   | D     | 812 | HEM  | CHD-C1D-ND  | 4.05  | 128.78      | 124.42   |
| 6   | L     | 812 | HEM  | CHD-C1D-ND  | 4.05  | 128.78      | 124.42   |
| 6   | F     | 810 | HEM  | CHD-C1D-ND  | 4.05  | 128.78      | 124.42   |
| 6   | G     | 809 | HEM  | CHD-C1D-ND  | 4.05  | 128.78      | 124.42   |
| 6   | A     | 813 | HEM  | CHD-C1D-ND  | 4.04  | 128.77      | 124.42   |
| 6   | E     | 807 | HEM  | CHD-C1D-ND  | 4.03  | 128.76      | 124.42   |
| 6   | A     | 807 | HEM  | CHD-C1D-ND  | 4.02  | 128.75      | 124.42   |
| 6   | I     | 806 | HEM  | CHD-C1D-ND  | 4.02  | 128.75      | 124.42   |
| 6   | B     | 813 | HEM  | CHD-C1D-ND  | 4.02  | 128.75      | 124.42   |
| 6   | C     | 810 | HEM  | CHD-C1D-ND  | 4.01  | 128.74      | 124.42   |
| 6   | C     | 813 | HEM  | CHA-C4D-ND  | 4.00  | 129.31      | 124.37   |
| 6   | J     | 812 | HEM  | CHD-C1D-ND  | 4.00  | 128.72      | 124.42   |
| 6   | H     | 810 | HEM  | CHC-C4B-NB  | 3.99  | 128.72      | 124.42   |
| 6   | E     | 807 | HEM  | CHC-C4B-NB  | 3.99  | 128.71      | 124.42   |
| 6   | F     | 809 | HEM  | CHC-C4B-NB  | 3.98  | 128.71      | 124.42   |
| 6   | J     | 811 | HEM  | C2B-C1B-NB  | -3.98 | 105.27      | 109.84   |
| 6   | H     | 813 | HEM  | C2B-C1B-NB  | -3.98 | 105.27      | 109.84   |
| 6   | A     | 810 | HEM  | CHD-C1D-ND  | 3.97  | 128.70      | 124.42   |
| 6   | B     | 809 | HEM  | C2B-C1B-NB  | -3.97 | 105.27      | 109.84   |
| 6   | K     | 806 | HEM  | CHA-C4D-ND  | 3.96  | 129.27      | 124.37   |
| 6   | G     | 811 | HEM  | CHA-C4D-ND  | 3.96  | 129.26      | 124.37   |
| 6   | F     | 813 | HEM  | CHD-C1D-ND  | 3.94  | 128.67      | 124.42   |
| 6   | H     | 812 | HEM  | C2B-C1B-NB  | -3.94 | 105.31      | 109.84   |
| 6   | B     | 810 | HEM  | CHD-C1D-ND  | 3.94  | 128.66      | 124.42   |
| 6   | H     | 813 | HEM  | CHD-C1D-ND  | 3.94  | 128.66      | 124.42   |
| 6   | K     | 809 | HEM  | CHC-C1C-NC  | 3.93  | 128.73      | 124.45   |
| 6   | L     | 813 | HEM  | CHA-C4D-ND  | 3.90  | 129.19      | 124.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | I     | 806 | HEM  | C2B-C1B-NB  | -3.89 | 105.36      | 109.84   |
| 6   | A     | 808 | HEM  | C2B-C1B-NB  | -3.89 | 105.37      | 109.84   |
| 6   | L     | 813 | HEM  | CHC-C4B-NB  | 3.89  | 128.61      | 124.42   |
| 6   | D     | 813 | HEM  | C2B-C1B-NB  | -3.89 | 105.37      | 109.84   |
| 6   | D     | 806 | HEM  | C2B-C1B-NB  | -3.88 | 105.37      | 109.84   |
| 6   | J     | 811 | HEM  | CHD-C1D-ND  | 3.88  | 128.60      | 124.42   |
| 6   | D     | 807 | HEM  | CHD-C1D-ND  | 3.86  | 128.58      | 124.42   |
| 6   | B     | 810 | HEM  | CHC-C4B-NB  | 3.85  | 128.56      | 124.42   |
| 6   | J     | 807 | HEM  | CHD-C1D-ND  | 3.85  | 128.56      | 124.42   |
| 6   | F     | 810 | HEM  | CHC-C1C-NC  | 3.85  | 128.64      | 124.45   |
| 6   | F     | 809 | HEM  | CHA-C4D-ND  | 3.84  | 129.12      | 124.37   |
| 6   | K     | 807 | HEM  | CHC-C4B-NB  | 3.84  | 128.56      | 124.42   |
| 6   | B     | 812 | HEM  | C2B-C1B-NB  | -3.84 | 105.43      | 109.84   |
| 6   | D     | 809 | HEM  | CHC-C4B-NB  | 3.84  | 128.56      | 124.42   |
| 6   | I     | 809 | HEM  | CHD-C1D-ND  | 3.84  | 128.56      | 124.42   |
| 6   | L     | 808 | HEM  | CHD-C1D-ND  | 3.84  | 128.55      | 124.42   |
| 6   | K     | 808 | HEM  | C2B-C1B-NB  | -3.83 | 105.43      | 109.84   |
| 6   | G     | 809 | HEM  | CHC-C4B-NB  | 3.83  | 128.54      | 124.42   |
| 6   | C     | 809 | HEM  | C2B-C1B-NB  | -3.83 | 105.44      | 109.84   |
| 6   | J     | 806 | HEM  | C2B-C1B-NB  | -3.82 | 105.44      | 109.84   |
| 6   | L     | 811 | HEM  | C2B-C1B-NB  | -3.82 | 105.44      | 109.84   |
| 6   | I     | 808 | HEM  | CHD-C1D-ND  | 3.81  | 128.52      | 124.42   |
| 6   | F     | 814 | HEM  | CHD-C1D-ND  | 3.80  | 128.51      | 124.42   |
| 6   | A     | 811 | HEM  | C2B-C1B-NB  | -3.80 | 105.48      | 109.84   |
| 6   | F     | 814 | HEM  | C2B-C1B-NB  | -3.79 | 105.48      | 109.84   |
| 6   | K     | 808 | HEM  | CHD-C1D-ND  | 3.79  | 128.50      | 124.42   |
| 6   | H     | 811 | HEM  | CHD-C1D-ND  | 3.79  | 128.50      | 124.42   |
| 6   | E     | 809 | HEM  | CHC-C1C-NC  | 3.79  | 128.58      | 124.45   |
| 6   | K     | 806 | HEM  | C2B-C1B-NB  | -3.79 | 105.48      | 109.84   |
| 6   | F     | 814 | HEM  | CHA-C4D-ND  | 3.77  | 129.03      | 124.37   |
| 6   | L     | 810 | HEM  | C2B-C1B-NB  | -3.77 | 105.51      | 109.84   |
| 6   | C     | 808 | HEM  | CHD-C1D-ND  | 3.77  | 128.48      | 124.42   |
| 6   | L     | 806 | HEM  | C2B-C1B-NB  | -3.76 | 105.51      | 109.84   |
| 6   | H     | 807 | HEM  | C2B-C1B-NB  | -3.76 | 105.52      | 109.84   |
| 6   | K     | 806 | HEM  | CHD-C1D-ND  | 3.75  | 128.46      | 124.42   |
| 6   | A     | 806 | HEM  | CHD-C1D-ND  | 3.75  | 128.46      | 124.42   |
| 6   | F     | 812 | HEM  | C2B-C1B-NB  | -3.75 | 105.53      | 109.84   |
| 6   | B     | 807 | HEM  | C2B-C1B-NB  | -3.74 | 105.54      | 109.84   |
| 6   | E     | 811 | HEM  | C2B-C1B-NB  | -3.74 | 105.54      | 109.84   |
| 6   | A     | 809 | HEM  | CHD-C1D-ND  | 3.74  | 128.45      | 124.42   |
| 6   | L     | 809 | HEM  | CHC-C1C-NC  | 3.73  | 128.52      | 124.45   |
| 6   | L     | 813 | HEM  | CAC-C3C-C4C | 3.73  | 133.73      | 124.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | D     | 811 | HEM  | C2B-C1B-NB  | -3.73 | 105.55      | 109.84   |
| 6   | C     | 812 | HEM  | CHD-C1D-ND  | 3.73  | 128.43      | 124.42   |
| 6   | G     | 810 | HEM  | C2B-C1B-NB  | -3.73 | 105.56      | 109.84   |
| 6   | H     | 807 | HEM  | CHA-C4D-ND  | 3.73  | 128.97      | 124.37   |
| 6   | B     | 813 | HEM  | CHA-C4D-ND  | 3.72  | 128.96      | 124.37   |
| 6   | B     | 813 | HEM  | C2B-C1B-NB  | -3.71 | 105.57      | 109.84   |
| 6   | J     | 806 | HEM  | CHA-C4D-ND  | 3.71  | 128.96      | 124.37   |
| 6   | G     | 806 | HEM  | CHD-C1D-ND  | 3.71  | 128.41      | 124.42   |
| 6   | I     | 809 | HEM  | CHC-C1C-NC  | 3.71  | 128.49      | 124.45   |
| 6   | K     | 813 | HEM  | CHA-C4D-ND  | 3.71  | 128.95      | 124.37   |
| 6   | G     | 807 | HEM  | CHD-C1D-C2D | -3.70 | 119.19      | 125.03   |
| 6   | G     | 813 | HEM  | CHD-C1D-C2D | -3.69 | 119.20      | 125.03   |
| 6   | G     | 808 | HEM  | C2B-C1B-NB  | -3.69 | 105.60      | 109.84   |
| 6   | D     | 812 | HEM  | CHA-C4D-ND  | 3.69  | 128.93      | 124.37   |
| 6   | B     | 811 | HEM  | CHD-C1D-C2D | -3.68 | 119.21      | 125.03   |
| 6   | J     | 809 | HEM  | CHC-C4B-NB  | 3.68  | 128.39      | 124.42   |
| 6   | I     | 812 | HEM  | C2B-C1B-NB  | -3.68 | 105.61      | 109.84   |
| 6   | L     | 807 | HEM  | CHA-C4D-ND  | 3.66  | 128.90      | 124.37   |
| 6   | B     | 814 | HEM  | C2B-C1B-NB  | -3.66 | 105.63      | 109.84   |
| 6   | H     | 809 | HEM  | CHA-C4D-ND  | 3.66  | 128.89      | 124.37   |
| 6   | K     | 811 | HEM  | CHA-C4D-ND  | 3.65  | 128.88      | 124.37   |
| 6   | F     | 809 | HEM  | CHD-C1D-ND  | 3.65  | 128.35      | 124.42   |
| 6   | B     | 808 | HEM  | CHC-C4B-NB  | 3.64  | 128.34      | 124.42   |
| 6   | G     | 806 | HEM  | C2B-C1B-NB  | -3.62 | 105.68      | 109.84   |
| 6   | J     | 809 | HEM  | CHD-C1D-C2D | -3.62 | 119.32      | 125.03   |
| 6   | G     | 812 | HEM  | C2B-C1B-NB  | -3.60 | 105.70      | 109.84   |
| 6   | L     | 807 | HEM  | CHB-C4A-NA  | 3.60  | 130.39      | 123.86   |
| 6   | D     | 809 | HEM  | CHC-C1C-NC  | 3.60  | 128.37      | 124.45   |
| 6   | F     | 808 | HEM  | CHB-C4A-NA  | 3.60  | 130.38      | 123.86   |
| 6   | I     | 813 | HEM  | C2B-C1B-NB  | -3.60 | 105.71      | 109.84   |
| 6   | H     | 812 | HEM  | CHA-C4D-ND  | 3.59  | 128.81      | 124.37   |
| 6   | K     | 813 | HEM  | C2B-C1B-NB  | -3.59 | 105.71      | 109.84   |
| 6   | B     | 808 | HEM  | CHB-C4A-NA  | 3.59  | 130.37      | 123.86   |
| 6   | K     | 806 | HEM  | CAB-C3B-C2B | -3.58 | 116.78      | 128.43   |
| 6   | F     | 808 | HEM  | CHD-C1D-ND  | 3.58  | 128.28      | 124.42   |
| 6   | K     | 809 | HEM  | CHA-C4D-ND  | 3.58  | 128.79      | 124.37   |
| 6   | H     | 813 | HEM  | CHA-C4D-ND  | 3.58  | 128.79      | 124.37   |
| 6   | K     | 812 | HEM  | C2B-C1B-NB  | -3.58 | 105.73      | 109.84   |
| 6   | A     | 806 | HEM  | C2B-C1B-NB  | -3.58 | 105.73      | 109.84   |
| 6   | F     | 812 | HEM  | CHA-C4D-ND  | 3.58  | 128.79      | 124.37   |
| 6   | H     | 809 | HEM  | CHD-C1D-ND  | 3.57  | 128.27      | 124.42   |
| 6   | G     | 811 | HEM  | C2B-C1B-NB  | -3.57 | 105.73      | 109.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 814 | HEM  | CHB-C4A-NA  | 3.57  | 130.34      | 123.86   |
| 6   | H     | 808 | HEM  | CHC-C4B-NB  | 3.57  | 128.27      | 124.42   |
| 6   | K     | 807 | HEM  | CHB-C4A-NA  | 3.57  | 130.33      | 123.86   |
| 6   | L     | 813 | HEM  | CHB-C4A-NA  | 3.56  | 130.32      | 123.86   |
| 6   | J     | 809 | HEM  | C2B-C1B-NB  | -3.56 | 105.75      | 109.84   |
| 6   | H     | 814 | HEM  | CHA-C4D-ND  | 3.56  | 128.76      | 124.37   |
| 6   | E     | 809 | HEM  | CHC-C4B-NB  | 3.55  | 128.24      | 124.42   |
| 6   | G     | 812 | HEM  | CHB-C4A-NA  | 3.54  | 130.29      | 123.86   |
| 6   | C     | 808 | HEM  | C2B-C1B-NB  | -3.54 | 105.77      | 109.84   |
| 6   | F     | 813 | HEM  | C2B-C1B-NB  | -3.54 | 105.77      | 109.84   |
| 6   | J     | 808 | HEM  | C2B-C1B-NB  | -3.54 | 105.77      | 109.84   |
| 6   | H     | 808 | HEM  | CHD-C1D-C2D | -3.54 | 119.44      | 125.03   |
| 6   | J     | 810 | HEM  | CHA-C4D-ND  | 3.54  | 128.74      | 124.37   |
| 6   | L     | 810 | HEM  | CHD-C1D-C2D | -3.53 | 119.45      | 125.03   |
| 6   | A     | 812 | HEM  | CHD-C1D-C2D | -3.53 | 119.46      | 125.03   |
| 6   | L     | 809 | HEM  | CHD-C1D-C2D | -3.53 | 119.46      | 125.03   |
| 6   | L     | 806 | HEM  | CHA-C4D-ND  | 3.52  | 128.73      | 124.37   |
| 6   | K     | 812 | HEM  | CHD-C1D-ND  | 3.52  | 128.22      | 124.42   |
| 6   | D     | 813 | HEM  | CHD-C1D-C2D | -3.52 | 119.47      | 125.03   |
| 6   | D     | 808 | HEM  | C2B-C1B-NB  | -3.52 | 105.79      | 109.84   |
| 6   | I     | 808 | HEM  | CHA-C4D-ND  | 3.52  | 128.72      | 124.37   |
| 6   | J     | 808 | HEM  | CHB-C4A-NA  | 3.51  | 130.23      | 123.86   |
| 6   | C     | 812 | HEM  | C2B-C1B-NB  | -3.51 | 105.81      | 109.84   |
| 6   | H     | 809 | HEM  | CHC-C1C-NC  | 3.51  | 128.27      | 124.45   |
| 6   | C     | 813 | HEM  | C2B-C1B-NB  | -3.50 | 105.82      | 109.84   |
| 6   | E     | 813 | HEM  | C2B-C1B-NB  | -3.50 | 105.82      | 109.84   |
| 6   | K     | 810 | HEM  | CHD-C1D-C2D | -3.49 | 119.51      | 125.03   |
| 6   | E     | 810 | HEM  | CHA-C4D-ND  | 3.49  | 128.69      | 124.37   |
| 6   | C     | 807 | HEM  | CHB-C4A-NA  | 3.49  | 130.19      | 123.86   |
| 6   | E     | 813 | HEM  | CHA-C4D-ND  | 3.49  | 128.68      | 124.37   |
| 6   | I     | 811 | HEM  | C2B-C1B-NB  | -3.49 | 105.83      | 109.84   |
| 6   | B     | 810 | HEM  | C2B-C1B-NB  | -3.48 | 105.84      | 109.84   |
| 6   | J     | 812 | HEM  | C2B-C1B-NB  | -3.48 | 105.84      | 109.84   |
| 6   | L     | 811 | HEM  | CHB-C4A-NA  | 3.48  | 130.16      | 123.86   |
| 6   | F     | 811 | HEM  | CHA-C4D-ND  | 3.47  | 128.66      | 124.37   |
| 6   | L     | 810 | HEM  | CHA-C4D-ND  | 3.47  | 128.66      | 124.37   |
| 6   | A     | 810 | HEM  | C2B-C1B-NB  | -3.46 | 105.86      | 109.84   |
| 6   | A     | 810 | HEM  | CHA-C4D-ND  | 3.46  | 128.65      | 124.37   |
| 6   | J     | 807 | HEM  | CHB-C4A-NA  | 3.46  | 130.14      | 123.86   |
| 6   | B     | 811 | HEM  | C2B-C1B-NB  | -3.46 | 105.86      | 109.84   |
| 6   | J     | 806 | HEM  | CHD-C1D-ND  | 3.46  | 128.15      | 124.42   |
| 6   | I     | 810 | HEM  | CHD-C1D-C2D | -3.46 | 119.57      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | A     | 813 | HEM  | CHA-C4D-ND  | 3.46  | 128.64      | 124.37   |
| 6   | J     | 811 | HEM  | CHA-C4D-ND  | 3.45  | 128.64      | 124.37   |
| 6   | F     | 811 | HEM  | CHD-C1D-C2D | -3.45 | 119.58      | 125.03   |
| 6   | C     | 807 | HEM  | CHC-C4B-NB  | 3.45  | 128.13      | 124.42   |
| 6   | I     | 810 | HEM  | C2B-C1B-NB  | -3.44 | 105.88      | 109.84   |
| 6   | H     | 810 | HEM  | CHC-C1C-NC  | 3.44  | 128.20      | 124.45   |
| 6   | A     | 812 | HEM  | CHA-C4D-ND  | 3.43  | 128.61      | 124.37   |
| 6   | I     | 813 | HEM  | CHD-C1D-C2D | -3.43 | 119.61      | 125.03   |
| 6   | B     | 807 | HEM  | CHD-C1D-ND  | 3.43  | 128.11      | 124.42   |
| 6   | I     | 813 | HEM  | CHA-C4D-ND  | 3.42  | 128.60      | 124.37   |
| 6   | D     | 812 | HEM  | C2B-C1B-NB  | -3.42 | 105.90      | 109.84   |
| 6   | J     | 812 | HEM  | CHA-C4D-ND  | 3.42  | 128.60      | 124.37   |
| 6   | K     | 812 | HEM  | CHA-C4D-ND  | 3.42  | 128.60      | 124.37   |
| 6   | K     | 810 | HEM  | C2B-C1B-NB  | -3.42 | 105.91      | 109.84   |
| 6   | E     | 809 | HEM  | CHD-C1D-C2D | -3.42 | 119.63      | 125.03   |
| 6   | H     | 808 | HEM  | CHB-C4A-NA  | 3.42  | 130.06      | 123.86   |
| 6   | E     | 810 | HEM  | C2B-C1B-NB  | -3.42 | 105.91      | 109.84   |
| 6   | I     | 808 | HEM  | C2B-C1B-NB  | -3.42 | 105.91      | 109.84   |
| 6   | E     | 813 | HEM  | CHD-C1D-C2D | -3.41 | 119.64      | 125.03   |
| 6   | I     | 809 | HEM  | CHC-C4B-NB  | 3.41  | 128.09      | 124.42   |
| 6   | L     | 808 | HEM  | CHA-C4D-ND  | 3.41  | 128.59      | 124.37   |
| 6   | L     | 812 | HEM  | CHA-C4D-ND  | 3.41  | 128.58      | 124.37   |
| 6   | G     | 809 | HEM  | C2B-C1B-NB  | -3.41 | 105.92      | 109.84   |
| 6   | F     | 809 | HEM  | CHC-C1C-NC  | 3.40  | 128.16      | 124.45   |
| 6   | D     | 807 | HEM  | CHB-C4A-NA  | 3.40  | 130.03      | 123.86   |
| 6   | D     | 807 | HEM  | CHC-C4B-NB  | 3.40  | 128.08      | 124.42   |
| 6   | G     | 808 | HEM  | CHA-C4D-ND  | 3.40  | 128.57      | 124.37   |
| 6   | D     | 806 | HEM  | CHA-C4D-ND  | 3.39  | 128.56      | 124.37   |
| 6   | F     | 809 | HEM  | CHB-C4A-NA  | 3.39  | 130.01      | 123.86   |
| 6   | J     | 807 | HEM  | CHA-C4D-ND  | 3.38  | 128.55      | 124.37   |
| 6   | B     | 810 | HEM  | CHA-C4D-ND  | 3.38  | 128.54      | 124.37   |
| 6   | E     | 807 | HEM  | CHB-C4A-NA  | 3.37  | 129.98      | 123.86   |
| 6   | A     | 808 | HEM  | CHD-C1D-ND  | 3.37  | 128.05      | 124.42   |
| 6   | I     | 807 | HEM  | CHA-C4D-ND  | 3.37  | 128.53      | 124.37   |
| 6   | L     | 808 | HEM  | C2B-C1B-NB  | -3.36 | 105.98      | 109.84   |
| 6   | C     | 809 | HEM  | CHD-C1D-C2D | -3.36 | 119.72      | 125.03   |
| 6   | C     | 810 | HEM  | CHD-C1D-C2D | -3.36 | 119.73      | 125.03   |
| 6   | G     | 807 | HEM  | CHB-C4A-NA  | 3.36  | 129.95      | 123.86   |
| 6   | I     | 806 | HEM  | CHA-C4D-ND  | 3.35  | 128.51      | 124.37   |
| 6   | H     | 811 | HEM  | C2B-C1B-NB  | -3.35 | 105.99      | 109.84   |
| 6   | F     | 813 | HEM  | CHA-C4D-ND  | 3.35  | 128.51      | 124.37   |
| 6   | K     | 811 | HEM  | CHB-C4A-NA  | 3.35  | 129.93      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | K     | 807 | HEM  | CHC-C1C-NC  | 3.34  | 128.09      | 124.45   |
| 6   | K     | 813 | HEM  | CHD-C1D-C2D | -3.34 | 119.75      | 125.03   |
| 6   | A     | 813 | HEM  | CHD-C1D-C2D | -3.34 | 119.75      | 125.03   |
| 6   | I     | 810 | HEM  | CHA-C4D-ND  | 3.34  | 128.50      | 124.37   |
| 6   | A     | 808 | HEM  | CHA-C4D-ND  | 3.34  | 128.50      | 124.37   |
| 6   | L     | 811 | HEM  | CHD-C1D-C2D | -3.34 | 119.76      | 125.03   |
| 6   | G     | 809 | HEM  | CHC-C1C-NC  | 3.33  | 128.08      | 124.45   |
| 6   | A     | 809 | HEM  | CHC-C1C-NC  | 3.33  | 128.08      | 124.45   |
| 6   | E     | 810 | HEM  | CHD-C1D-C2D | -3.33 | 119.77      | 125.03   |
| 6   | E     | 812 | HEM  | C2B-C1B-NB  | -3.33 | 106.02      | 109.84   |
| 6   | G     | 813 | HEM  | C2B-C1B-NB  | -3.33 | 106.02      | 109.84   |
| 6   | J     | 810 | HEM  | C2B-C1B-NB  | -3.32 | 106.02      | 109.84   |
| 6   | L     | 809 | HEM  | CHC-C4B-NB  | 3.32  | 128.00      | 124.42   |
| 6   | I     | 807 | HEM  | CHC-C1C-NC  | 3.32  | 128.07      | 124.45   |
| 6   | B     | 809 | HEM  | CHA-C4D-ND  | 3.32  | 128.47      | 124.37   |
| 6   | C     | 808 | HEM  | CHB-C4A-NA  | 3.32  | 129.88      | 123.86   |
| 6   | F     | 812 | HEM  | CHD-C1D-C2D | -3.32 | 119.79      | 125.03   |
| 6   | K     | 809 | HEM  | CHB-C4A-NA  | 3.32  | 129.87      | 123.86   |
| 6   | K     | 806 | HEM  | CHC-C1C-NC  | 3.31  | 128.06      | 124.45   |
| 6   | G     | 806 | HEM  | CHA-C4D-ND  | 3.31  | 128.46      | 124.37   |
| 6   | K     | 811 | HEM  | C2B-C1B-NB  | -3.31 | 106.03      | 109.84   |
| 6   | J     | 806 | HEM  | CAB-C3B-C2B | -3.31 | 117.67      | 128.43   |
| 6   | A     | 811 | HEM  | CHD-C1D-C2D | -3.31 | 119.80      | 125.03   |
| 6   | H     | 814 | HEM  | C2B-C1B-NB  | -3.31 | 106.04      | 109.84   |
| 6   | J     | 807 | HEM  | CHC-C1C-NC  | 3.31  | 128.05      | 124.45   |
| 6   | E     | 811 | HEM  | CHA-C4D-ND  | 3.31  | 128.46      | 124.37   |
| 6   | A     | 807 | HEM  | CHD-C1D-C2D | -3.30 | 119.82      | 125.03   |
| 6   | K     | 807 | HEM  | CHD-C1D-C2D | -3.30 | 119.82      | 125.03   |
| 6   | D     | 807 | HEM  | CHD-C1D-C2D | -3.30 | 119.82      | 125.03   |
| 6   | E     | 808 | HEM  | CHD-C1D-C2D | -3.29 | 119.83      | 125.03   |
| 6   | L     | 812 | HEM  | CHB-C4A-NA  | 3.29  | 129.82      | 123.86   |
| 6   | J     | 809 | HEM  | CHA-C4D-ND  | 3.29  | 128.43      | 124.37   |
| 6   | J     | 813 | HEM  | CHB-C4A-NA  | 3.29  | 129.82      | 123.86   |
| 6   | G     | 813 | HEM  | CHB-C4A-NA  | 3.28  | 129.81      | 123.86   |
| 6   | D     | 811 | HEM  | CHA-C4D-ND  | 3.28  | 128.43      | 124.37   |
| 6   | G     | 811 | HEM  | CHD-C1D-C2D | -3.28 | 119.84      | 125.03   |
| 6   | E     | 807 | HEM  | CHD-C1D-C2D | -3.28 | 119.85      | 125.03   |
| 6   | I     | 811 | HEM  | CHD-C1D-C2D | -3.27 | 119.86      | 125.03   |
| 6   | I     | 812 | HEM  | CHA-C4D-ND  | 3.27  | 128.41      | 124.37   |
| 6   | L     | 813 | HEM  | CAC-C3C-C2C | -3.27 | 117.80      | 128.43   |
| 6   | K     | 806 | HEM  | CHA-C4D-C3D | -3.27 | 119.20      | 125.23   |
| 6   | J     | 813 | HEM  | CHD-C1D-C2D | -3.27 | 119.87      | 125.03   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | C     | 807 | HEM  | CHA-C4D-ND  | 3.26  | 128.40      | 124.37   |
| 6   | E     | 807 | HEM  | C2B-C1B-NB  | -3.26 | 106.09      | 109.84   |
| 6   | L     | 807 | HEM  | CHC-C4B-NB  | 3.26  | 127.93      | 124.42   |
| 6   | A     | 811 | HEM  | CHC-C4B-NB  | 3.26  | 127.93      | 124.42   |
| 6   | D     | 806 | HEM  | CHD-C1D-C2D | -3.25 | 119.89      | 125.03   |
| 6   | I     | 807 | HEM  | CHC-C4B-NB  | 3.25  | 127.92      | 124.42   |
| 6   | G     | 812 | HEM  | CHA-C4D-ND  | 3.25  | 128.39      | 124.37   |
| 6   | D     | 808 | HEM  | CHB-C4A-NA  | 3.25  | 129.75      | 123.86   |
| 6   | G     | 813 | HEM  | CHA-C4D-ND  | 3.25  | 128.39      | 124.37   |
| 6   | B     | 810 | HEM  | CHD-C1D-C2D | -3.25 | 119.90      | 125.03   |
| 6   | J     | 809 | HEM  | CHC-C1C-NC  | 3.25  | 127.99      | 124.45   |
| 6   | E     | 806 | HEM  | CHA-C4D-ND  | 3.24  | 128.38      | 124.37   |
| 6   | J     | 812 | HEM  | CHB-C4A-NA  | 3.24  | 129.74      | 123.86   |
| 6   | C     | 808 | HEM  | CHD-C1D-C2D | -3.24 | 119.91      | 125.03   |
| 6   | J     | 813 | HEM  | CHA-C4D-ND  | 3.24  | 128.38      | 124.37   |
| 6   | L     | 807 | HEM  | CHC-C1C-NC  | 3.24  | 127.98      | 124.45   |
| 6   | I     | 811 | HEM  | CHA-C4D-ND  | 3.24  | 128.37      | 124.37   |
| 6   | F     | 810 | HEM  | CHC-C4B-NB  | 3.24  | 127.91      | 124.42   |
| 6   | A     | 811 | HEM  | CHA-C4D-ND  | 3.24  | 128.37      | 124.37   |
| 6   | A     | 811 | HEM  | CAB-C3B-C2B | -3.23 | 117.92      | 128.43   |
| 6   | C     | 813 | HEM  | CHD-C1D-C2D | -3.23 | 119.93      | 125.03   |
| 6   | D     | 811 | HEM  | CHD-C1D-C2D | -3.23 | 119.93      | 125.03   |
| 6   | H     | 809 | HEM  | C2B-C1B-NB  | -3.23 | 106.13      | 109.84   |
| 6   | F     | 810 | HEM  | CHB-C4A-NA  | 3.23  | 129.71      | 123.86   |
| 6   | F     | 807 | HEM  | CHD-C1D-C2D | -3.23 | 119.93      | 125.03   |
| 6   | G     | 810 | HEM  | CHA-C4D-ND  | 3.22  | 128.35      | 124.37   |
| 6   | I     | 807 | HEM  | CHB-C4A-NA  | 3.22  | 129.71      | 123.86   |
| 6   | A     | 808 | HEM  | CHC-C1C-NC  | 3.22  | 127.96      | 124.45   |
| 6   | J     | 813 | HEM  | C2B-C1B-NB  | -3.22 | 106.14      | 109.84   |
| 6   | D     | 809 | HEM  | CHB-C4A-NA  | 3.22  | 129.70      | 123.86   |
| 6   | F     | 810 | HEM  | CHD-C1D-C2D | -3.22 | 119.95      | 125.03   |
| 6   | H     | 810 | HEM  | C2B-C1B-NB  | -3.22 | 106.14      | 109.84   |
| 6   | I     | 808 | HEM  | CHC-C1C-NC  | 3.21  | 127.95      | 124.45   |
| 6   | H     | 814 | HEM  | CHB-C4A-NA  | 3.21  | 129.68      | 123.86   |
| 6   | J     | 808 | HEM  | CHD-C1D-C2D | -3.21 | 119.96      | 125.03   |
| 6   | G     | 810 | HEM  | CHD-C1D-C2D | -3.21 | 119.96      | 125.03   |
| 6   | I     | 811 | HEM  | CHB-C4A-NA  | 3.21  | 129.68      | 123.86   |
| 6   | A     | 807 | HEM  | CHA-C4D-ND  | 3.21  | 128.34      | 124.37   |
| 6   | H     | 808 | HEM  | C2B-C1B-NB  | -3.21 | 106.15      | 109.84   |
| 6   | I     | 807 | HEM  | CHD-C1D-C2D | -3.21 | 119.96      | 125.03   |
| 6   | D     | 810 | HEM  | CHD-C1D-C2D | -3.21 | 119.97      | 125.03   |
| 6   | E     | 813 | HEM  | CHB-C4A-NA  | 3.20  | 129.66      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | E     | 812 | HEM  | CHA-C4D-ND  | 3.20  | 128.32      | 124.37   |
| 6   | H     | 811 | HEM  | CHD-C1D-C2D | -3.19 | 119.99      | 125.03   |
| 6   | J     | 813 | HEM  | CHC-C1C-NC  | 3.19  | 127.93      | 124.45   |
| 6   | F     | 811 | HEM  | C2B-C1B-NB  | -3.19 | 106.17      | 109.84   |
| 6   | F     | 809 | HEM  | C4C-NC-C1C  | 3.19  | 111.02      | 105.82   |
| 6   | H     | 811 | HEM  | CHA-C4D-ND  | 3.19  | 128.31      | 124.37   |
| 6   | B     | 814 | HEM  | CHD-C1D-C2D | -3.19 | 120.00      | 125.03   |
| 6   | D     | 809 | HEM  | CHD-C1D-C2D | -3.19 | 120.00      | 125.03   |
| 6   | G     | 811 | HEM  | CHB-C4A-NA  | 3.19  | 129.64      | 123.86   |
| 6   | H     | 814 | HEM  | CHC-C1C-NC  | 3.18  | 127.92      | 124.45   |
| 6   | E     | 806 | HEM  | CHD-C1D-C2D | -3.18 | 120.01      | 125.03   |
| 6   | B     | 807 | HEM  | CHA-C4D-ND  | 3.18  | 128.30      | 124.37   |
| 6   | K     | 809 | HEM  | CHD-C1D-C2D | -3.17 | 120.02      | 125.03   |
| 6   | K     | 806 | HEM  | CHB-C1B-NB  | 3.17  | 128.29      | 124.37   |
| 6   | C     | 812 | HEM  | CHD-C1D-C2D | -3.17 | 120.03      | 125.03   |
| 6   | K     | 812 | HEM  | CHC-C1C-NC  | 3.17  | 127.90      | 124.45   |
| 6   | H     | 809 | HEM  | CHB-C4A-NA  | 3.17  | 129.60      | 123.86   |
| 6   | B     | 814 | HEM  | CHA-C4D-ND  | 3.16  | 128.28      | 124.37   |
| 6   | L     | 811 | HEM  | CHA-C4D-ND  | 3.16  | 128.28      | 124.37   |
| 6   | L     | 812 | HEM  | C2B-C1B-NB  | -3.16 | 106.21      | 109.84   |
| 6   | F     | 810 | HEM  | CHA-C4D-ND  | 3.16  | 128.27      | 124.37   |
| 6   | J     | 808 | HEM  | CHC-C1C-NC  | 3.16  | 127.89      | 124.45   |
| 6   | D     | 811 | HEM  | CHB-C4A-NA  | 3.16  | 129.58      | 123.86   |
| 6   | B     | 812 | HEM  | CHD-C1D-C2D | -3.15 | 120.05      | 125.03   |
| 6   | F     | 808 | HEM  | CHC-C1C-NC  | 3.15  | 127.89      | 124.45   |
| 6   | I     | 809 | HEM  | CHA-C4D-ND  | 3.15  | 128.27      | 124.37   |
| 6   | A     | 809 | HEM  | CHB-C4A-NA  | 3.15  | 129.57      | 123.86   |
| 6   | H     | 810 | HEM  | CHB-C4A-NA  | 3.15  | 129.57      | 123.86   |
| 6   | G     | 807 | HEM  | O2A-CGA-CBA | 3.14  | 123.93      | 114.00   |
| 6   | G     | 809 | HEM  | CHB-C4A-NA  | 3.14  | 129.56      | 123.86   |
| 6   | D     | 808 | HEM  | CHA-C4D-ND  | 3.14  | 128.25      | 124.37   |
| 6   | F     | 807 | HEM  | CHA-C4D-ND  | 3.14  | 128.25      | 124.37   |
| 6   | K     | 807 | HEM  | CHA-C4D-ND  | 3.14  | 128.25      | 124.37   |
| 6   | J     | 808 | HEM  | CHA-C4D-ND  | 3.13  | 128.24      | 124.37   |
| 6   | G     | 809 | HEM  | CHD-C1D-C2D | -3.13 | 120.09      | 125.03   |
| 6   | L     | 806 | HEM  | CHC-C1C-NC  | 3.13  | 127.86      | 124.45   |
| 6   | J     | 806 | HEM  | CHB-C1B-NB  | 3.13  | 128.24      | 124.37   |
| 6   | K     | 813 | HEM  | CHB-C4A-NA  | 3.13  | 129.53      | 123.86   |
| 6   | K     | 810 | HEM  | CHB-C4A-NA  | 3.13  | 129.53      | 123.86   |
| 6   | F     | 808 | HEM  | CHD-C1D-C2D | -3.13 | 120.09      | 125.03   |
| 6   | I     | 808 | HEM  | CHB-C4A-NA  | 3.13  | 129.53      | 123.86   |
| 6   | E     | 809 | HEM  | CHB-C4A-NA  | 3.12  | 129.53      | 123.86   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | H     | 810 | HEM  | CHA-C4D-ND  | 3.12  | 128.23      | 124.37   |
| 6   | E     | 812 | HEM  | CHD-C1D-C2D | -3.12 | 120.11      | 125.03   |
| 6   | B     | 810 | HEM  | CHC-C1C-NC  | 3.12  | 127.85      | 124.45   |
| 6   | C     | 809 | HEM  | CHB-C4A-NA  | 3.12  | 129.51      | 123.86   |
| 6   | A     | 807 | HEM  | CHB-C4A-NA  | 3.12  | 129.51      | 123.86   |
| 6   | H     | 810 | HEM  | CHD-C1D-C2D | -3.11 | 120.11      | 125.03   |
| 6   | D     | 807 | HEM  | CHC-C1C-NC  | 3.11  | 127.84      | 124.45   |
| 6   | I     | 810 | HEM  | CHB-C4A-NA  | 3.11  | 129.50      | 123.86   |
| 6   | I     | 806 | HEM  | CHC-C1C-NC  | 3.11  | 127.83      | 124.45   |
| 6   | E     | 812 | HEM  | CHB-C4A-NA  | 3.10  | 129.49      | 123.86   |
| 6   | L     | 809 | HEM  | CHB-C4A-NA  | 3.10  | 129.49      | 123.86   |
| 6   | L     | 808 | HEM  | CHB-C4A-NA  | 3.10  | 129.48      | 123.86   |
| 6   | F     | 813 | HEM  | CHB-C4A-NA  | 3.10  | 129.48      | 123.86   |
| 6   | L     | 812 | HEM  | CHC-C1C-NC  | 3.10  | 127.83      | 124.45   |
| 6   | B     | 812 | HEM  | CHB-C4A-NA  | 3.10  | 129.48      | 123.86   |
| 6   | C     | 811 | HEM  | CHD-C1D-C2D | -3.10 | 120.14      | 125.03   |
| 6   | A     | 809 | HEM  | CHD-C1D-C2D | -3.10 | 120.14      | 125.03   |
| 6   | D     | 813 | HEM  | CHA-C4D-ND  | 3.09  | 128.19      | 124.37   |
| 6   | H     | 814 | HEM  | CHD-C1D-C2D | -3.09 | 120.15      | 125.03   |
| 6   | J     | 806 | HEM  | C4C-NC-C1C  | 3.09  | 110.86      | 105.82   |
| 6   | C     | 807 | HEM  | CHD-C1D-C2D | -3.09 | 120.15      | 125.03   |
| 6   | J     | 810 | HEM  | CHD-C1D-C2D | -3.09 | 120.15      | 125.03   |
| 6   | E     | 811 | HEM  | CAD-CBD-CGD | -3.09 | 105.47      | 113.67   |
| 6   | B     | 813 | HEM  | CHB-C4A-NA  | 3.09  | 129.46      | 123.86   |
| 6   | K     | 808 | HEM  | CHA-C4D-ND  | 3.08  | 128.18      | 124.37   |
| 6   | H     | 812 | HEM  | CHD-C1D-C2D | -3.08 | 120.17      | 125.03   |
| 6   | E     | 810 | HEM  | CHB-C4A-NA  | 3.07  | 129.44      | 123.86   |
| 6   | C     | 807 | HEM  | C2B-C1B-NB  | -3.07 | 106.31      | 109.84   |
| 6   | D     | 810 | HEM  | CHA-C4D-ND  | 3.06  | 128.16      | 124.37   |
| 6   | B     | 809 | HEM  | CHD-C1D-C2D | -3.06 | 120.19      | 125.03   |
| 6   | K     | 808 | HEM  | CHC-C1C-NC  | 3.06  | 127.79      | 124.45   |
| 6   | L     | 807 | HEM  | CHA-C4D-C3D | -3.06 | 119.59      | 125.23   |
| 6   | D     | 813 | HEM  | CHB-C4A-NA  | 3.06  | 129.41      | 123.86   |
| 6   | D     | 808 | HEM  | C4C-NC-C1C  | 3.06  | 110.81      | 105.82   |
| 6   | J     | 807 | HEM  | CHD-C1D-C2D | -3.05 | 120.21      | 125.03   |
| 6   | L     | 809 | HEM  | CHA-C4D-ND  | 3.05  | 128.14      | 124.37   |
| 6   | L     | 813 | HEM  | C2B-C1B-NB  | -3.05 | 106.33      | 109.84   |
| 6   | C     | 812 | HEM  | CHA-C4D-ND  | 3.04  | 128.13      | 124.37   |
| 6   | A     | 806 | HEM  | CHA-C4D-ND  | 3.04  | 128.13      | 124.37   |
| 6   | B     | 808 | HEM  | C2B-C1B-NB  | -3.04 | 106.35      | 109.84   |
| 6   | F     | 811 | HEM  | CHB-C4A-NA  | 3.04  | 129.37      | 123.86   |
| 6   | J     | 812 | HEM  | CHC-C1C-NC  | 3.04  | 127.76      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | D     | 809 | HEM  | CAD-C3D-C4D | 3.04  | 129.99      | 124.70   |
| 6   | F     | 808 | HEM  | O2A-CGA-CBA | 3.03  | 123.58      | 114.00   |
| 6   | E     | 811 | HEM  | CHD-C1D-C2D | -3.03 | 120.24      | 125.03   |
| 6   | B     | 811 | HEM  | CHB-C4A-NA  | 3.03  | 129.35      | 123.86   |
| 6   | I     | 809 | HEM  | C2B-C1B-NB  | -3.02 | 106.36      | 109.84   |
| 6   | C     | 810 | HEM  | O2D-CGD-CBD | 3.02  | 123.55      | 114.00   |
| 6   | I     | 812 | HEM  | CHD-C1D-C2D | -3.02 | 120.26      | 125.03   |
| 6   | H     | 807 | HEM  | CHB-C4A-NA  | 3.02  | 129.34      | 123.86   |
| 6   | E     | 809 | HEM  | C2B-C1B-NB  | -3.01 | 106.38      | 109.84   |
| 6   | C     | 811 | HEM  | CHA-C4D-ND  | 3.01  | 128.09      | 124.37   |
| 6   | F     | 813 | HEM  | CHD-C1D-C2D | -3.01 | 120.28      | 125.03   |
| 6   | A     | 809 | HEM  | CHC-C4B-NB  | 3.00  | 127.66      | 124.42   |
| 6   | A     | 808 | HEM  | C4C-NC-C1C  | 3.00  | 110.72      | 105.82   |
| 6   | A     | 810 | HEM  | CHB-C4A-NA  | 3.00  | 129.30      | 123.86   |
| 6   | J     | 806 | HEM  | CHC-C1C-NC  | 3.00  | 127.72      | 124.45   |
| 6   | K     | 812 | HEM  | CHB-C4A-NA  | 3.00  | 129.30      | 123.86   |
| 6   | B     | 809 | HEM  | CHB-C4A-NA  | 3.00  | 129.30      | 123.86   |
| 6   | A     | 810 | HEM  | CHD-C1D-C2D | -2.99 | 120.31      | 125.03   |
| 6   | C     | 806 | HEM  | CHA-C4D-ND  | 2.99  | 128.06      | 124.37   |
| 6   | H     | 813 | HEM  | CHD-C1D-C2D | -2.99 | 120.31      | 125.03   |
| 6   | K     | 811 | HEM  | CHD-C1D-C2D | -2.99 | 120.31      | 125.03   |
| 6   | F     | 809 | HEM  | C2B-C1B-NB  | -2.98 | 106.41      | 109.84   |
| 6   | F     | 814 | HEM  | CHB-C4A-NA  | 2.98  | 129.27      | 123.86   |
| 6   | F     | 810 | HEM  | C2B-C1B-NB  | -2.98 | 106.41      | 109.84   |
| 6   | D     | 812 | HEM  | CHC-C1C-NC  | 2.98  | 127.70      | 124.45   |
| 6   | J     | 810 | HEM  | CHB-C4A-NA  | 2.98  | 129.26      | 123.86   |
| 6   | F     | 814 | HEM  | CHD-C1D-C2D | -2.98 | 120.33      | 125.03   |
| 6   | D     | 806 | HEM  | CHB-C4A-NA  | 2.98  | 129.26      | 123.86   |
| 6   | E     | 809 | HEM  | CHA-C4D-ND  | 2.98  | 128.05      | 124.37   |
| 6   | J     | 810 | HEM  | CHC-C1C-NC  | 2.97  | 127.69      | 124.45   |
| 6   | H     | 807 | HEM  | CHA-C4D-C3D | -2.97 | 119.75      | 125.23   |
| 6   | E     | 808 | HEM  | CHB-C4A-NA  | 2.97  | 129.25      | 123.86   |
| 6   | L     | 807 | HEM  | CHD-C1D-C2D | -2.97 | 120.34      | 125.03   |
| 6   | H     | 811 | HEM  | CHB-C4A-NA  | 2.97  | 129.24      | 123.86   |
| 6   | L     | 806 | HEM  | CHB-C4A-NA  | 2.96  | 129.24      | 123.86   |
| 6   | K     | 806 | HEM  | CHC-C4B-C3B | 2.96  | 130.99      | 125.07   |
| 6   | J     | 806 | HEM  | CHA-C4D-C3D | -2.96 | 119.77      | 125.23   |
| 6   | H     | 808 | HEM  | CHC-C1C-NC  | 2.95  | 127.67      | 124.45   |
| 6   | L     | 809 | HEM  | C2B-C1B-NB  | -2.95 | 106.44      | 109.84   |
| 6   | D     | 812 | HEM  | CHD-C1D-C2D | -2.95 | 120.37      | 125.03   |
| 6   | K     | 810 | HEM  | CHA-C4D-ND  | 2.95  | 128.02      | 124.37   |
| 6   | F     | 808 | HEM  | CHC-C4B-NB  | 2.95  | 127.60      | 124.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | J     | 806 | HEM  | CHC-C4B-C3B | 2.95  | 130.96      | 125.07   |
| 6   | K     | 806 | HEM  | C4C-NC-C1C  | 2.95  | 110.63      | 105.82   |
| 6   | L     | 808 | HEM  | CHC-C1C-NC  | 2.95  | 127.66      | 124.45   |
| 6   | G     | 806 | HEM  | CHB-C4A-NA  | 2.95  | 129.20      | 123.86   |
| 6   | D     | 808 | HEM  | CHC-C1C-NC  | 2.94  | 127.66      | 124.45   |
| 6   | H     | 813 | HEM  | CHB-C4A-NA  | 2.94  | 129.19      | 123.86   |
| 6   | C     | 809 | HEM  | CHA-C4D-ND  | 2.94  | 128.00      | 124.37   |
| 6   | C     | 806 | HEM  | CHD-C1D-C2D | -2.94 | 120.39      | 125.03   |
| 6   | J     | 807 | HEM  | O2A-CGA-CBA | 2.94  | 123.27      | 114.00   |
| 6   | I     | 813 | HEM  | CHB-C4A-NA  | 2.93  | 129.18      | 123.86   |
| 6   | C     | 810 | HEM  | CAD-C3D-C4D | 2.93  | 129.80      | 124.70   |
| 6   | I     | 812 | HEM  | CHB-C4A-NA  | 2.93  | 129.17      | 123.86   |
| 6   | I     | 809 | HEM  | CHD-C1D-C2D | -2.93 | 120.41      | 125.03   |
| 6   | I     | 807 | HEM  | CHA-C4D-C3D | -2.93 | 119.83      | 125.23   |
| 6   | K     | 808 | HEM  | CHB-C4A-NA  | 2.93  | 129.17      | 123.86   |
| 6   | I     | 807 | HEM  | C2B-C1B-NB  | -2.92 | 106.48      | 109.84   |
| 6   | C     | 812 | HEM  | CHB-C4A-NA  | 2.92  | 129.15      | 123.86   |
| 6   | F     | 809 | HEM  | CHA-C4D-C3D | -2.92 | 119.85      | 125.23   |
| 6   | G     | 810 | HEM  | CHB-C4A-NA  | 2.91  | 129.14      | 123.86   |
| 6   | B     | 811 | HEM  | CHA-C4D-ND  | 2.91  | 127.97      | 124.37   |
| 6   | C     | 808 | HEM  | CBA-CAA-C2A | -2.91 | 104.50      | 112.53   |
| 6   | J     | 807 | HEM  | C4C-NC-C1C  | 2.90  | 110.56      | 105.82   |
| 6   | J     | 807 | HEM  | CHC-C4B-NB  | 2.90  | 127.55      | 124.42   |
| 6   | D     | 808 | HEM  | CHA-C4D-C3D | -2.90 | 119.88      | 125.23   |
| 6   | B     | 808 | HEM  | CHA-C4D-ND  | 2.90  | 127.96      | 124.37   |
| 6   | C     | 808 | HEM  | CHA-C4D-ND  | 2.90  | 127.95      | 124.37   |
| 6   | L     | 811 | HEM  | CBB-CAB-C3B | -2.90 | 113.04      | 127.53   |
| 6   | C     | 807 | HEM  | CHA-C4D-C3D | -2.90 | 119.88      | 125.23   |
| 6   | A     | 806 | HEM  | CHB-C4A-NA  | 2.90  | 129.11      | 123.86   |
| 6   | H     | 809 | HEM  | CBA-CAA-C2A | -2.89 | 104.53      | 112.53   |
| 6   | D     | 809 | HEM  | C2B-C1B-NB  | -2.89 | 106.52      | 109.84   |
| 6   | I     | 807 | HEM  | C4C-NC-C1C  | 2.89  | 110.53      | 105.82   |
| 6   | D     | 808 | HEM  | CHD-C1D-ND  | 2.89  | 127.53      | 124.42   |
| 6   | K     | 812 | HEM  | CHA-C4D-C3D | -2.88 | 119.91      | 125.23   |
| 6   | H     | 809 | HEM  | CHA-C4D-C3D | -2.88 | 119.91      | 125.23   |
| 6   | C     | 813 | HEM  | CHB-C4A-NA  | 2.88  | 129.09      | 123.86   |
| 6   | D     | 810 | HEM  | O2D-CGD-CBD | 2.88  | 123.10      | 114.00   |
| 6   | H     | 807 | HEM  | CHD-C1D-C2D | -2.88 | 120.48      | 125.03   |
| 6   | F     | 810 | HEM  | C4C-NC-C1C  | 2.88  | 110.52      | 105.82   |
| 6   | F     | 811 | HEM  | CHC-C1C-NC  | 2.88  | 127.59      | 124.45   |
| 6   | L     | 806 | HEM  | CHD-C1D-C2D | -2.88 | 120.48      | 125.03   |
| 6   | A     | 810 | HEM  | CHC-C1C-NC  | 2.88  | 127.59      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | I     | 809 | HEM  | CHB-C4A-NA  | 2.88  | 129.08      | 123.86   |
| 6   | G     | 807 | HEM  | CHC-C4B-NB  | 2.87  | 127.52      | 124.42   |
| 6   | D     | 807 | HEM  | O2A-CGA-CBA | 2.87  | 123.08      | 114.00   |
| 6   | H     | 812 | HEM  | CHB-C4A-NA  | 2.87  | 129.07      | 123.86   |
| 6   | B     | 811 | HEM  | CHC-C1C-NC  | 2.87  | 127.58      | 124.45   |
| 6   | K     | 812 | HEM  | C4C-NC-C1C  | 2.87  | 110.49      | 105.82   |
| 6   | E     | 810 | HEM  | CHC-C1C-NC  | 2.87  | 127.57      | 124.45   |
| 6   | D     | 807 | HEM  | CHA-C4D-ND  | 2.87  | 127.91      | 124.37   |
| 6   | H     | 808 | HEM  | CHA-C4D-ND  | 2.87  | 127.91      | 124.37   |
| 6   | K     | 809 | HEM  | CHC-C4B-NB  | 2.86  | 127.50      | 124.42   |
| 6   | G     | 808 | HEM  | CBA-CAA-C2A | -2.86 | 104.63      | 112.53   |
| 6   | A     | 812 | HEM  | CHB-C4A-NA  | 2.85  | 129.03      | 123.86   |
| 6   | C     | 807 | HEM  | CHC-C1C-NC  | 2.85  | 127.55      | 124.45   |
| 6   | A     | 807 | HEM  | CHA-C4D-C3D | -2.84 | 119.98      | 125.23   |
| 6   | K     | 811 | HEM  | CHC-C1C-NC  | 2.84  | 127.54      | 124.45   |
| 6   | J     | 807 | HEM  | CHA-C4D-C3D | -2.84 | 120.00      | 125.23   |
| 6   | A     | 809 | HEM  | C4C-NC-C1C  | 2.84  | 110.45      | 105.82   |
| 6   | I     | 806 | HEM  | CHA-C4D-C3D | -2.84 | 120.00      | 125.23   |
| 6   | I     | 806 | HEM  | CHB-C4A-NA  | 2.83  | 128.99      | 123.86   |
| 6   | K     | 810 | HEM  | CHC-C1C-NC  | 2.83  | 127.53      | 124.45   |
| 6   | A     | 810 | HEM  | O2D-CGD-CBD | 2.83  | 122.94      | 114.00   |
| 6   | K     | 810 | HEM  | O2D-CGD-CBD | 2.83  | 122.94      | 114.00   |
| 6   | G     | 808 | HEM  | CHD-C1D-C2D | -2.83 | 120.56      | 125.03   |
| 6   | J     | 812 | HEM  | CHD-C1D-C2D | -2.83 | 120.57      | 125.03   |
| 6   | A     | 806 | HEM  | CHA-C4D-C3D | -2.82 | 120.02      | 125.23   |
| 6   | G     | 808 | HEM  | CHB-C4A-NA  | 2.82  | 128.98      | 123.86   |
| 6   | L     | 810 | HEM  | CHB-C4A-NA  | 2.82  | 128.98      | 123.86   |
| 6   | G     | 811 | HEM  | CHC-C1C-NC  | 2.82  | 127.52      | 124.45   |
| 6   | F     | 812 | HEM  | CAD-CBD-CGD | -2.82 | 106.19      | 113.67   |
| 6   | J     | 809 | HEM  | CHB-C4A-NA  | 2.82  | 128.97      | 123.86   |
| 6   | L     | 807 | HEM  | C4C-NC-C1C  | 2.82  | 110.41      | 105.82   |
| 6   | G     | 806 | HEM  | CHA-C4D-C3D | -2.81 | 120.04      | 125.23   |
| 6   | D     | 812 | HEM  | CHB-C4A-NA  | 2.81  | 128.96      | 123.86   |
| 6   | K     | 813 | HEM  | CHC-C1C-NC  | 2.81  | 127.52      | 124.45   |
| 6   | E     | 811 | HEM  | CHB-C4A-NA  | 2.81  | 128.96      | 123.86   |
| 6   | B     | 812 | HEM  | CHA-C4D-ND  | 2.81  | 127.84      | 124.37   |
| 6   | F     | 808 | HEM  | CHA-C4D-ND  | 2.81  | 127.84      | 124.37   |
| 6   | I     | 806 | HEM  | O2D-CGD-CBD | 2.81  | 122.87      | 114.00   |
| 6   | G     | 808 | HEM  | CHA-C4D-C3D | -2.80 | 120.06      | 125.23   |
| 6   | I     | 808 | HEM  | C4C-NC-C1C  | 2.80  | 110.39      | 105.82   |
| 6   | A     | 807 | HEM  | C4C-NC-C1C  | 2.80  | 110.39      | 105.82   |
| 6   | H     | 811 | HEM  | CHC-C1C-NC  | 2.80  | 127.50      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 807 | HEM  | CHA-C4D-C3D | -2.80 | 120.06      | 125.23   |
| 6   | C     | 808 | HEM  | C4C-NC-C1C  | 2.80  | 110.39      | 105.82   |
| 6   | J     | 813 | HEM  | CHA-C4D-C3D | -2.80 | 120.07      | 125.23   |
| 6   | A     | 811 | HEM  | CAD-CBD-CGD | -2.80 | 106.24      | 113.67   |
| 6   | H     | 809 | HEM  | C4C-NC-C1C  | 2.79  | 110.38      | 105.82   |
| 6   | G     | 809 | HEM  | CHA-C4D-ND  | 2.79  | 127.82      | 124.37   |
| 6   | I     | 811 | HEM  | CAD-CBD-CGD | -2.79 | 106.26      | 113.67   |
| 6   | A     | 807 | HEM  | CHC-C4B-NB  | 2.79  | 127.43      | 124.42   |
| 6   | F     | 808 | HEM  | C4C-NC-C1C  | 2.79  | 110.37      | 105.82   |
| 6   | B     | 808 | HEM  | O2A-CGA-CBA | 2.79  | 122.81      | 114.00   |
| 6   | B     | 813 | HEM  | CHD-C1D-C2D | -2.79 | 120.63      | 125.03   |
| 6   | C     | 813 | HEM  | CHA-C4D-C3D | -2.78 | 120.10      | 125.23   |
| 6   | A     | 811 | HEM  | CHC-C1C-NC  | 2.78  | 127.48      | 124.45   |
| 6   | G     | 807 | HEM  | CHA-C4D-ND  | 2.78  | 127.80      | 124.37   |
| 6   | J     | 811 | HEM  | C4C-NC-C1C  | 2.78  | 110.35      | 105.82   |
| 6   | L     | 811 | HEM  | CAD-CBD-CGD | -2.78 | 106.30      | 113.67   |
| 6   | G     | 807 | HEM  | C4C-NC-C1C  | 2.77  | 110.34      | 105.82   |
| 6   | G     | 807 | HEM  | CHC-C1C-NC  | 2.77  | 127.47      | 124.45   |
| 6   | D     | 812 | HEM  | CHA-C4D-C3D | -2.77 | 120.11      | 125.23   |
| 6   | G     | 807 | HEM  | C2B-C1B-NB  | -2.77 | 106.65      | 109.84   |
| 6   | I     | 810 | HEM  | CHC-C1C-NC  | 2.77  | 127.47      | 124.45   |
| 6   | I     | 806 | HEM  | CHD-C1D-C2D | -2.77 | 120.65      | 125.03   |
| 6   | A     | 811 | HEM  | CHB-C4A-NA  | 2.77  | 128.88      | 123.86   |
| 6   | L     | 812 | HEM  | C4C-NC-C1C  | 2.76  | 110.33      | 105.82   |
| 6   | H     | 807 | HEM  | CHC-C1C-NC  | 2.76  | 127.46      | 124.45   |
| 6   | J     | 808 | HEM  | CBA-CAA-C2A | -2.76 | 104.91      | 112.53   |
| 6   | G     | 806 | HEM  | CHD-C1D-C2D | -2.76 | 120.67      | 125.03   |
| 6   | D     | 808 | HEM  | CBB-CAB-C3B | -2.76 | 113.75      | 127.53   |
| 6   | E     | 808 | HEM  | CBA-CAA-C2A | -2.76 | 104.91      | 112.53   |
| 6   | D     | 810 | HEM  | CAD-C3D-C4D | 2.75  | 129.50      | 124.70   |
| 6   | G     | 812 | HEM  | CHD-C1D-C2D | -2.75 | 120.68      | 125.03   |
| 6   | K     | 810 | HEM  | CAD-C3D-C4D | 2.75  | 129.49      | 124.70   |
| 6   | L     | 808 | HEM  | CBA-CAA-C2A | -2.74 | 104.95      | 112.53   |
| 6   | E     | 807 | HEM  | CHA-C4D-ND  | 2.74  | 127.76      | 124.37   |
| 6   | L     | 809 | HEM  | C4C-NC-C1C  | 2.74  | 110.29      | 105.82   |
| 6   | A     | 807 | HEM  | CHC-C1C-NC  | 2.74  | 127.44      | 124.45   |
| 6   | L     | 811 | HEM  | CHC-C1C-NC  | 2.74  | 127.44      | 124.45   |
| 6   | D     | 812 | HEM  | C4C-NC-C1C  | 2.74  | 110.28      | 105.82   |
| 6   | C     | 811 | HEM  | CHB-C4A-NA  | 2.74  | 128.82      | 123.86   |
| 6   | H     | 811 | HEM  | CHA-C4D-C3D | -2.73 | 120.19      | 125.23   |
| 6   | L     | 808 | HEM  | CHD-C1D-C2D | -2.73 | 120.71      | 125.03   |
| 6   | E     | 806 | HEM  | O2D-CGD-CBD | 2.73  | 122.62      | 114.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | I     | 811 | HEM  | O2A-CGA-CBA | 2.73  | 122.62      | 114.00   |
| 6   | J     | 811 | HEM  | CHA-C4D-C3D | -2.73 | 120.20      | 125.23   |
| 6   | L     | 808 | HEM  | CHA-C4D-C3D | -2.73 | 120.20      | 125.23   |
| 6   | H     | 808 | HEM  | C4C-NC-C1C  | 2.73  | 110.27      | 105.82   |
| 6   | K     | 807 | HEM  | C2B-C1B-NB  | -2.73 | 106.71      | 109.84   |
| 6   | G     | 813 | HEM  | CHC-C1C-NC  | 2.72  | 127.42      | 124.45   |
| 6   | L     | 807 | HEM  | C1A-CHA-C4D | -2.72 | 119.84      | 126.25   |
| 6   | H     | 813 | HEM  | CHA-C4D-C3D | -2.72 | 120.20      | 125.23   |
| 6   | I     | 809 | HEM  | C4C-NC-C1C  | 2.72  | 110.25      | 105.82   |
| 6   | A     | 806 | HEM  | O2D-CGD-CBD | 2.72  | 122.58      | 114.00   |
| 6   | K     | 806 | HEM  | CHD-C1D-C2D | -2.71 | 120.74      | 125.03   |
| 6   | L     | 813 | HEM  | CHD-C1D-C2D | -2.71 | 120.75      | 125.03   |
| 6   | B     | 807 | HEM  | CHB-C4A-NA  | 2.71  | 128.78      | 123.86   |
| 6   | G     | 810 | HEM  | CHC-C1C-NC  | 2.71  | 127.40      | 124.45   |
| 6   | C     | 810 | HEM  | CHB-C4A-NA  | 2.71  | 128.77      | 123.86   |
| 6   | E     | 807 | HEM  | CHA-C4D-C3D | -2.71 | 120.24      | 125.23   |
| 6   | L     | 812 | HEM  | CHD-C1D-C2D | -2.70 | 120.76      | 125.03   |
| 6   | A     | 811 | HEM  | C4C-NC-C1C  | 2.70  | 110.22      | 105.82   |
| 6   | A     | 809 | HEM  | CHA-C4D-ND  | 2.70  | 127.71      | 124.37   |
| 6   | K     | 806 | HEM  | CHC-C4B-NB  | 2.70  | 127.33      | 124.42   |
| 6   | A     | 811 | HEM  | CHB-C1B-NB  | 2.70  | 127.71      | 124.37   |
| 6   | K     | 809 | HEM  | C4C-NC-C1C  | 2.70  | 110.22      | 105.82   |
| 6   | A     | 810 | HEM  | CHA-C4D-C3D | -2.70 | 120.25      | 125.23   |
| 6   | A     | 808 | HEM  | CHA-C4D-C3D | -2.70 | 120.26      | 125.23   |
| 6   | A     | 806 | HEM  | CHD-C1D-C2D | -2.69 | 120.78      | 125.03   |
| 6   | A     | 813 | HEM  | CHB-C4A-NA  | 2.69  | 128.75      | 123.86   |
| 6   | F     | 814 | HEM  | C4C-NC-C1C  | 2.69  | 110.21      | 105.82   |
| 6   | D     | 806 | HEM  | CHA-C4D-C3D | -2.69 | 120.27      | 125.23   |
| 6   | L     | 806 | HEM  | CHA-C4D-C3D | -2.69 | 120.27      | 125.23   |
| 6   | F     | 814 | HEM  | CHA-C4D-C3D | -2.69 | 120.27      | 125.23   |
| 6   | E     | 809 | HEM  | C4C-NC-C1C  | 2.69  | 110.20      | 105.82   |
| 6   | E     | 811 | HEM  | C4C-NC-C1C  | 2.69  | 110.20      | 105.82   |
| 6   | B     | 807 | HEM  | CHD-C1D-C2D | -2.68 | 120.79      | 125.03   |
| 6   | A     | 808 | HEM  | CHB-C4A-NA  | 2.68  | 128.73      | 123.86   |
| 6   | C     | 806 | HEM  | CHA-C4D-C3D | -2.68 | 120.28      | 125.23   |
| 6   | J     | 812 | HEM  | CHA-C4D-C3D | -2.68 | 120.28      | 125.23   |
| 6   | L     | 810 | HEM  | CHA-C4D-C3D | -2.68 | 120.28      | 125.23   |
| 6   | B     | 809 | HEM  | C4C-NC-C1C  | 2.68  | 110.19      | 105.82   |
| 6   | G     | 812 | HEM  | CHC-C1C-NC  | 2.68  | 127.37      | 124.45   |
| 6   | B     | 810 | HEM  | CHB-C4A-NA  | 2.68  | 128.71      | 123.86   |
| 6   | A     | 809 | HEM  | CAD-C3D-C4D | 2.68  | 129.36      | 124.70   |
| 6   | E     | 813 | HEM  | CHC-C1C-NC  | 2.68  | 127.37      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 812 | HEM  | O2A-CGA-CBA | 2.68  | 122.45      | 114.00   |
| 6   | E     | 812 | HEM  | CHC-C1C-NC  | 2.68  | 127.37      | 124.45   |
| 6   | K     | 811 | HEM  | C4C-NC-C1C  | 2.67  | 110.18      | 105.82   |
| 6   | B     | 808 | HEM  | CHC-C1C-NC  | 2.67  | 127.36      | 124.45   |
| 6   | J     | 808 | HEM  | C4C-NC-C1C  | 2.67  | 110.17      | 105.82   |
| 6   | I     | 811 | HEM  | CHC-C1C-NC  | 2.67  | 127.36      | 124.45   |
| 6   | F     | 807 | HEM  | CHB-C4A-NA  | 2.67  | 128.69      | 123.86   |
| 6   | K     | 807 | HEM  | C4C-NC-C1C  | 2.66  | 110.16      | 105.82   |
| 6   | J     | 810 | HEM  | CHA-C4D-C3D | -2.66 | 120.32      | 125.23   |
| 6   | B     | 813 | HEM  | CHC-C1C-NC  | 2.66  | 127.35      | 124.45   |
| 6   | E     | 808 | HEM  | CHC-C1C-NC  | 2.66  | 127.35      | 124.45   |
| 6   | E     | 813 | HEM  | CHA-C4D-C3D | -2.66 | 120.32      | 125.23   |
| 6   | F     | 813 | HEM  | CHA-C4D-C3D | -2.66 | 120.33      | 125.23   |
| 6   | B     | 813 | HEM  | CHA-C4D-C3D | -2.66 | 120.33      | 125.23   |
| 6   | E     | 806 | HEM  | CHB-C4A-NA  | 2.66  | 128.68      | 123.86   |
| 6   | C     | 806 | HEM  | CBB-CAB-C3B | -2.66 | 114.26      | 127.53   |
| 6   | J     | 811 | HEM  | CHD-C1D-C2D | -2.65 | 120.84      | 125.03   |
| 6   | C     | 812 | HEM  | C4C-NC-C1C  | 2.65  | 110.15      | 105.82   |
| 6   | I     | 812 | HEM  | CHA-C4D-C3D | -2.65 | 120.34      | 125.23   |
| 6   | E     | 807 | HEM  | CHC-C1C-NC  | 2.65  | 127.34      | 124.45   |
| 6   | D     | 808 | HEM  | CBA-CAA-C2A | -2.65 | 105.21      | 112.53   |
| 6   | H     | 814 | HEM  | CHA-C4D-C3D | -2.65 | 120.34      | 125.23   |
| 6   | D     | 809 | HEM  | CHA-C4D-ND  | 2.65  | 127.64      | 124.37   |
| 6   | B     | 813 | HEM  | C4C-NC-C1C  | 2.64  | 110.13      | 105.82   |
| 6   | K     | 809 | HEM  | CBD-CAD-C3D | -2.64 | 105.22      | 112.53   |
| 6   | C     | 806 | HEM  | CHC-C1C-NC  | 2.64  | 127.33      | 124.45   |
| 6   | F     | 808 | HEM  | CHA-C4D-C3D | -2.64 | 120.36      | 125.23   |
| 6   | E     | 806 | HEM  | CHA-C4D-C3D | -2.64 | 120.36      | 125.23   |
| 6   | L     | 813 | HEM  | C4C-NC-C1C  | 2.64  | 110.12      | 105.82   |
| 6   | D     | 810 | HEM  | CHB-C4A-NA  | 2.64  | 128.65      | 123.86   |
| 6   | G     | 808 | HEM  | C4C-NC-C1C  | 2.64  | 110.12      | 105.82   |
| 6   | F     | 812 | HEM  | CHB-C4A-NA  | 2.64  | 128.65      | 123.86   |
| 6   | B     | 807 | HEM  | O2D-CGD-CBD | 2.64  | 122.33      | 114.00   |
| 6   | L     | 806 | HEM  | O2D-CGD-CBD | 2.64  | 122.33      | 114.00   |
| 6   | F     | 811 | HEM  | O2D-CGD-CBD | 2.64  | 122.33      | 114.00   |
| 6   | L     | 810 | HEM  | CHC-C1C-NC  | 2.63  | 127.32      | 124.45   |
| 6   | C     | 809 | HEM  | CAD-C3D-C4D | 2.63  | 129.28      | 124.70   |
| 6   | L     | 812 | HEM  | CHA-C4D-C3D | -2.63 | 120.38      | 125.23   |
| 6   | A     | 809 | HEM  | C2B-C1B-NB  | -2.63 | 106.82      | 109.84   |
| 6   | F     | 808 | HEM  | C2B-C1B-NB  | -2.62 | 106.82      | 109.84   |
| 6   | I     | 807 | HEM  | C1A-CHA-C4D | -2.62 | 120.08      | 126.25   |
| 6   | C     | 809 | HEM  | CHC-C1C-NC  | 2.62  | 127.31      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | B     | 814 | HEM  | CHC-C1C-NC  | 2.62  | 127.31      | 124.45   |
| 6   | B     | 809 | HEM  | CHC-C1C-NC  | 2.62  | 127.31      | 124.45   |
| 6   | K     | 812 | HEM  | CHD-C1D-C2D | -2.62 | 120.90      | 125.03   |
| 6   | G     | 808 | HEM  | CHC-C1C-NC  | 2.61  | 127.30      | 124.45   |
| 6   | J     | 806 | HEM  | CHB-C4A-NA  | 2.61  | 128.60      | 123.86   |
| 6   | H     | 813 | HEM  | CHC-C1C-NC  | 2.61  | 127.30      | 124.45   |
| 6   | B     | 809 | HEM  | CBA-CAA-C2A | -2.61 | 105.31      | 112.53   |
| 6   | I     | 808 | HEM  | CHA-C4D-C3D | -2.61 | 120.42      | 125.23   |
| 6   | D     | 812 | HEM  | CMD-C2D-C1D | 2.61  | 129.11      | 125.03   |
| 6   | C     | 812 | HEM  | CHD-C4C-NC  | 2.61  | 127.29      | 124.45   |
| 6   | D     | 807 | HEM  | C4C-NC-C1C  | 2.60  | 110.06      | 105.82   |
| 6   | K     | 808 | HEM  | CHD-C1D-C2D | -2.60 | 120.93      | 125.03   |
| 6   | F     | 807 | HEM  | CHA-C4D-C3D | -2.60 | 120.44      | 125.23   |
| 6   | C     | 806 | HEM  | O2D-CGD-CBD | 2.59  | 122.19      | 114.00   |
| 6   | D     | 809 | HEM  | C4C-NC-C1C  | 2.59  | 110.04      | 105.82   |
| 6   | D     | 806 | HEM  | O2D-CGD-CBD | 2.59  | 122.18      | 114.00   |
| 6   | B     | 809 | HEM  | CHA-C4D-C3D | -2.59 | 120.45      | 125.23   |
| 6   | B     | 807 | HEM  | CHC-C1C-NC  | 2.59  | 127.27      | 124.45   |
| 6   | A     | 811 | HEM  | CHC-C4B-C3B | 2.58  | 130.23      | 125.07   |
| 6   | D     | 807 | HEM  | C2B-C1B-NB  | -2.58 | 106.87      | 109.84   |
| 6   | K     | 813 | HEM  | C4C-NC-C1C  | 2.58  | 110.03      | 105.82   |
| 6   | A     | 806 | HEM  | CHC-C1C-NC  | 2.58  | 127.26      | 124.45   |
| 6   | C     | 810 | HEM  | CHC-C1C-NC  | 2.58  | 127.26      | 124.45   |
| 6   | G     | 806 | HEM  | CHC-C1C-NC  | 2.58  | 127.26      | 124.45   |
| 6   | E     | 811 | HEM  | O2A-CGA-CBA | 2.58  | 122.14      | 114.00   |
| 6   | K     | 808 | HEM  | CBA-CAA-C2A | -2.58 | 105.41      | 112.53   |
| 6   | J     | 811 | HEM  | CAD-CBD-CGD | -2.58 | 106.83      | 113.67   |
| 6   | A     | 806 | HEM  | C4C-NC-C1C  | 2.58  | 110.02      | 105.82   |
| 6   | I     | 808 | HEM  | CHD-C1D-C2D | -2.57 | 120.96      | 125.03   |
| 6   | K     | 808 | HEM  | C4C-NC-C1C  | 2.57  | 110.02      | 105.82   |
| 6   | L     | 809 | HEM  | CAD-C3D-C4D | 2.57  | 129.18      | 124.70   |
| 6   | K     | 809 | HEM  | C2B-C1B-NB  | -2.57 | 106.88      | 109.84   |
| 6   | C     | 808 | HEM  | CHD-C4C-NC  | 2.57  | 127.25      | 124.45   |
| 6   | C     | 812 | HEM  | CHA-C4D-C3D | -2.57 | 120.49      | 125.23   |
| 6   | J     | 807 | HEM  | C2B-C1B-NB  | -2.57 | 106.89      | 109.84   |
| 6   | K     | 806 | HEM  | C3B-C2B-C1B | 2.57  | 108.34      | 106.41   |
| 6   | E     | 808 | HEM  | C4C-NC-C1C  | 2.57  | 110.00      | 105.82   |
| 6   | B     | 811 | HEM  | CAD-C3D-C4D | 2.57  | 129.17      | 124.70   |
| 6   | I     | 806 | HEM  | C4C-NC-C1C  | 2.57  | 110.00      | 105.82   |
| 6   | F     | 814 | HEM  | CHC-C1C-NC  | 2.57  | 127.25      | 124.45   |
| 6   | H     | 814 | HEM  | C4C-NC-C1C  | 2.56  | 110.00      | 105.82   |
| 6   | H     | 812 | HEM  | CAD-CBD-CGD | -2.56 | 106.88      | 113.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | A     | 807 | HEM  | O2A-CGA-CBA | 2.56  | 122.09      | 114.00   |
| 6   | K     | 806 | HEM  | CHB-C4A-NA  | 2.56  | 128.50      | 123.86   |
| 6   | G     | 812 | HEM  | C1A-CHA-C4D | -2.56 | 120.23      | 126.25   |
| 6   | D     | 806 | HEM  | CHC-C1C-NC  | 2.55  | 127.23      | 124.45   |
| 6   | E     | 807 | HEM  | C1A-CHA-C4D | -2.55 | 120.24      | 126.25   |
| 6   | G     | 809 | HEM  | C4C-NC-C1C  | 2.55  | 109.98      | 105.82   |
| 6   | F     | 809 | HEM  | CBA-CAA-C2A | -2.55 | 105.48      | 112.53   |
| 6   | K     | 811 | HEM  | CHA-C4D-C3D | -2.55 | 120.52      | 125.23   |
| 6   | L     | 808 | HEM  | C4C-NC-C1C  | 2.55  | 109.98      | 105.82   |
| 6   | J     | 812 | HEM  | C4C-NC-C1C  | 2.55  | 109.97      | 105.82   |
| 6   | B     | 807 | HEM  | CMD-C2D-C1D | 2.54  | 129.01      | 125.03   |
| 6   | B     | 810 | HEM  | CHA-C4D-C3D | -2.54 | 120.53      | 125.23   |
| 6   | A     | 813 | HEM  | C4C-NC-C1C  | 2.54  | 109.97      | 105.82   |
| 6   | H     | 810 | HEM  | CHA-C4D-C3D | -2.54 | 120.54      | 125.23   |
| 6   | J     | 809 | HEM  | CBD-CAD-C3D | -2.54 | 105.51      | 112.53   |
| 6   | H     | 811 | HEM  | C4C-NC-C1C  | 2.54  | 109.96      | 105.82   |
| 6   | L     | 807 | HEM  | C2B-C1B-NB  | -2.54 | 106.92      | 109.84   |
| 6   | J     | 813 | HEM  | C4C-NC-C1C  | 2.54  | 109.96      | 105.82   |
| 6   | C     | 807 | HEM  | C4C-NC-C1C  | 2.54  | 109.96      | 105.82   |
| 6   | B     | 811 | HEM  | O2D-CGD-CBD | 2.54  | 122.01      | 114.00   |
| 6   | F     | 812 | HEM  | O2A-CGA-CBA | 2.53  | 121.99      | 114.00   |
| 6   | J     | 806 | HEM  | CHC-C4B-NB  | 2.53  | 127.14      | 124.42   |
| 6   | D     | 810 | HEM  | CHA-C4D-C3D | -2.53 | 120.57      | 125.23   |
| 6   | L     | 809 | HEM  | C1A-CHA-C4D | -2.53 | 120.31      | 126.25   |
| 6   | D     | 808 | HEM  | CHD-C1D-C2D | -2.52 | 121.04      | 125.03   |
| 6   | A     | 808 | HEM  | CBA-CAA-C2A | -2.52 | 105.56      | 112.53   |
| 6   | G     | 811 | HEM  | C4C-NC-C1C  | 2.52  | 109.93      | 105.82   |
| 6   | H     | 811 | HEM  | O2D-CGD-CBD | 2.51  | 121.94      | 114.00   |
| 6   | K     | 808 | HEM  | CHA-C4D-C3D | -2.51 | 120.60      | 125.23   |
| 6   | F     | 807 | HEM  | O2D-CGD-CBD | 2.51  | 121.92      | 114.00   |
| 6   | H     | 811 | HEM  | CAD-C3D-C4D | 2.50  | 129.06      | 124.70   |
| 6   | D     | 811 | HEM  | CHC-C1C-NC  | 2.50  | 127.18      | 124.45   |
| 6   | I     | 813 | HEM  | CAD-CBD-CGD | -2.50 | 107.03      | 113.67   |
| 6   | J     | 809 | HEM  | CMD-C2D-C1D | 2.50  | 128.94      | 125.03   |
| 6   | C     | 810 | HEM  | CMD-C2D-C1D | 2.49  | 128.93      | 125.03   |
| 6   | J     | 811 | HEM  | CHB-C4A-NA  | 2.49  | 128.37      | 123.86   |
| 6   | L     | 809 | HEM  | CHA-C4D-C3D | -2.49 | 120.64      | 125.23   |
| 6   | J     | 811 | HEM  | CHC-C1C-NC  | 2.49  | 127.16      | 124.45   |
| 6   | H     | 812 | HEM  | CHA-C4D-C3D | -2.49 | 120.64      | 125.23   |
| 6   | J     | 811 | HEM  | O2A-CGA-CBA | 2.48  | 121.85      | 114.00   |
| 6   | J     | 808 | HEM  | CHA-C4D-C3D | -2.48 | 120.65      | 125.23   |
| 6   | K     | 809 | HEM  | CHA-C4D-C3D | -2.48 | 120.65      | 125.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | G     | 806 | HEM  | C4C-NC-C1C  | 2.48  | 109.87      | 105.82   |
| 6   | E     | 809 | HEM  | CMD-C2D-C1D | 2.48  | 128.91      | 125.03   |
| 6   | G     | 811 | HEM  | C1A-CHA-C4D | -2.48 | 120.42      | 126.25   |
| 6   | C     | 811 | HEM  | CAD-CBD-CGD | -2.48 | 107.10      | 113.67   |
| 6   | E     | 807 | HEM  | C4C-NC-C1C  | 2.47  | 109.85      | 105.82   |
| 6   | I     | 813 | HEM  | CMD-C2D-C1D | 2.47  | 128.89      | 125.03   |
| 6   | K     | 813 | HEM  | C1A-CHA-C4D | -2.47 | 120.45      | 126.25   |
| 6   | E     | 810 | HEM  | CAD-C3D-C4D | 2.46  | 128.99      | 124.70   |
| 6   | C     | 812 | HEM  | C1A-CHA-C4D | -2.46 | 120.46      | 126.25   |
| 6   | I     | 807 | HEM  | O2A-CGA-CBA | 2.46  | 121.78      | 114.00   |
| 6   | G     | 806 | HEM  | O2D-CGD-CBD | 2.46  | 121.78      | 114.00   |
| 6   | H     | 813 | HEM  | C4C-NC-C1C  | 2.46  | 109.83      | 105.82   |
| 6   | A     | 813 | HEM  | CHA-C4D-C3D | -2.46 | 120.69      | 125.23   |
| 6   | C     | 810 | HEM  | CHA-C4D-ND  | 2.46  | 127.41      | 124.37   |
| 6   | L     | 813 | HEM  | CHA-C4D-C3D | -2.46 | 120.70      | 125.23   |
| 6   | E     | 812 | HEM  | CHA-C4D-C3D | -2.45 | 120.70      | 125.23   |
| 6   | J     | 806 | HEM  | CHD-C1D-C2D | -2.45 | 121.15      | 125.03   |
| 6   | L     | 807 | HEM  | O2A-CGA-CBA | 2.45  | 121.75      | 114.00   |
| 6   | E     | 810 | HEM  | CHA-C4D-C3D | -2.45 | 120.71      | 125.23   |
| 6   | F     | 813 | HEM  | C4C-NC-C1C  | 2.45  | 109.81      | 105.82   |
| 6   | I     | 812 | HEM  | C4C-NC-C1C  | 2.45  | 109.81      | 105.82   |
| 6   | E     | 811 | HEM  | C1A-CHA-C4D | -2.45 | 120.49      | 126.25   |
| 6   | K     | 806 | HEM  | O2D-CGD-CBD | 2.45  | 121.73      | 114.00   |
| 6   | J     | 812 | HEM  | C1A-CHA-C4D | -2.45 | 120.49      | 126.25   |
| 6   | A     | 809 | HEM  | CHA-C4D-C3D | -2.45 | 120.72      | 125.23   |
| 6   | K     | 813 | HEM  | CHA-C4D-C3D | -2.45 | 120.72      | 125.23   |
| 6   | I     | 812 | HEM  | CAD-C3D-C4D | 2.44  | 128.96      | 124.70   |
| 6   | D     | 807 | HEM  | C1A-CHA-C4D | -2.44 | 120.50      | 126.25   |
| 6   | B     | 812 | HEM  | C4C-NC-C1C  | 2.44  | 109.80      | 105.82   |
| 6   | K     | 807 | HEM  | C1A-CHA-C4D | -2.44 | 120.51      | 126.25   |
| 6   | H     | 810 | HEM  | C4C-NC-C1C  | 2.44  | 109.80      | 105.82   |
| 6   | K     | 807 | HEM  | CHA-C4D-C3D | -2.44 | 120.73      | 125.23   |
| 6   | D     | 811 | HEM  | C4C-NC-C1C  | 2.44  | 109.80      | 105.82   |
| 6   | A     | 807 | HEM  | C2B-C1B-NB  | -2.44 | 107.04      | 109.84   |
| 6   | G     | 812 | HEM  | CMD-C2D-C1D | 2.43  | 128.84      | 125.03   |
| 6   | F     | 811 | HEM  | CHA-C4D-C3D | -2.43 | 120.74      | 125.23   |
| 6   | J     | 809 | HEM  | C4C-NC-C1C  | 2.43  | 109.78      | 105.82   |
| 6   | E     | 808 | HEM  | CHA-C4D-ND  | 2.43  | 127.37      | 124.37   |
| 6   | C     | 811 | HEM  | C4C-NC-C1C  | 2.43  | 109.78      | 105.82   |
| 6   | K     | 806 | HEM  | CAB-C3B-C4B | 2.43  | 135.12      | 124.39   |
| 6   | A     | 812 | HEM  | CAD-CBD-CGD | -2.43 | 107.23      | 113.67   |
| 6   | C     | 809 | HEM  | CHA-C4D-C3D | -2.43 | 120.75      | 125.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | C     | 806 | HEM  | CHB-C4A-NA  | 2.42  | 128.25      | 123.86   |
| 6   | F     | 811 | HEM  | CMD-C2D-C1D | 2.42  | 128.81      | 125.03   |
| 6   | C     | 809 | HEM  | C4C-NC-C1C  | 2.42  | 109.76      | 105.82   |
| 6   | B     | 807 | HEM  | C4C-NC-C1C  | 2.41  | 109.76      | 105.82   |
| 6   | D     | 810 | HEM  | O2D-CGD-O1D | -2.41 | 117.13      | 123.33   |
| 6   | F     | 810 | HEM  | CMD-C2D-C1D | 2.41  | 128.80      | 125.03   |
| 6   | G     | 807 | HEM  | CHA-C4D-C3D | -2.41 | 120.78      | 125.23   |
| 6   | E     | 809 | HEM  | CAD-C3D-C4D | 2.41  | 128.89      | 124.70   |
| 6   | A     | 810 | HEM  | O2D-CGD-O1D | -2.41 | 117.14      | 123.33   |
| 6   | E     | 810 | HEM  | O2D-CGD-CBD | 2.40  | 121.59      | 114.00   |
| 6   | G     | 810 | HEM  | O2D-CGD-CBD | 2.40  | 121.59      | 114.00   |
| 6   | H     | 814 | HEM  | CAA-CBA-CGA | -2.40 | 107.30      | 113.67   |
| 6   | L     | 810 | HEM  | CAD-C3D-C4D | 2.40  | 128.88      | 124.70   |
| 6   | J     | 806 | HEM  | O2D-CGD-CBD | 2.40  | 121.58      | 114.00   |
| 6   | A     | 806 | HEM  | CBB-CAB-C3B | -2.40 | 115.54      | 127.53   |
| 6   | F     | 813 | HEM  | C1A-CHA-C4D | -2.40 | 120.61      | 126.25   |
| 6   | F     | 810 | HEM  | CAD-C3D-C4D | 2.40  | 128.87      | 124.70   |
| 6   | A     | 813 | HEM  | CHC-C1C-NC  | 2.40  | 127.06      | 124.45   |
| 6   | E     | 808 | HEM  | CAD-C3D-C4D | 2.40  | 128.87      | 124.70   |
| 6   | C     | 808 | HEM  | CHC-C1C-NC  | 2.40  | 127.06      | 124.45   |
| 6   | C     | 812 | HEM  | CHC-C1C-NC  | 2.40  | 127.06      | 124.45   |
| 6   | L     | 813 | HEM  | CHD-C4C-C3C | 2.39  | 129.25      | 125.21   |
| 6   | A     | 808 | HEM  | C1A-CHA-C4D | -2.39 | 120.62      | 126.25   |
| 6   | B     | 808 | HEM  | C1A-CHA-C4D | -2.39 | 120.62      | 126.25   |
| 6   | A     | 810 | HEM  | CBB-CAB-C3B | -2.39 | 115.58      | 127.53   |
| 6   | F     | 808 | HEM  | C1A-CHA-C4D | -2.39 | 120.63      | 126.25   |
| 6   | B     | 810 | HEM  | C4C-NC-C1C  | 2.39  | 109.72      | 105.82   |
| 6   | C     | 812 | HEM  | CAD-C3D-C4D | 2.39  | 128.86      | 124.70   |
| 6   | D     | 813 | HEM  | CHA-C4D-C3D | -2.39 | 120.82      | 125.23   |
| 6   | I     | 810 | HEM  | CAA-CBA-CGA | -2.39 | 107.33      | 113.67   |
| 6   | F     | 807 | HEM  | CHC-C1C-NC  | 2.39  | 127.05      | 124.45   |
| 6   | I     | 812 | HEM  | CHC-C1C-NC  | 2.39  | 127.05      | 124.45   |
| 6   | I     | 811 | HEM  | C4C-NC-C1C  | 2.39  | 109.71      | 105.82   |
| 6   | J     | 807 | HEM  | C1A-CHA-C4D | -2.39 | 120.64      | 126.25   |
| 6   | G     | 811 | HEM  | CHA-C4D-C3D | -2.39 | 120.83      | 125.23   |
| 6   | D     | 808 | HEM  | CHD-C4C-NC  | 2.39  | 127.05      | 124.45   |
| 6   | C     | 806 | HEM  | C4C-NC-C1C  | 2.38  | 109.71      | 105.82   |
| 6   | L     | 810 | HEM  | O2D-CGD-CBD | 2.38  | 121.53      | 114.00   |
| 6   | B     | 814 | HEM  | C3A-C4A-NA  | -2.38 | 106.32      | 110.14   |
| 6   | F     | 810 | HEM  | CHD-C4C-NC  | 2.38  | 127.05      | 124.45   |
| 6   | H     | 808 | HEM  | O2A-CGA-CBA | 2.38  | 121.52      | 114.00   |
| 6   | B     | 810 | HEM  | C1A-CHA-C4D | -2.38 | 120.66      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | C     | 813 | HEM  | C1A-CHA-C4D | -2.38 | 120.66      | 126.25   |
| 6   | F     | 814 | HEM  | C1A-CHA-C4D | -2.38 | 120.66      | 126.25   |
| 6   | E     | 806 | HEM  | C4C-NC-C1C  | 2.38  | 109.69      | 105.82   |
| 6   | E     | 812 | HEM  | C4C-NC-C1C  | 2.37  | 109.69      | 105.82   |
| 6   | K     | 806 | HEM  | CMD-C2D-C1D | 2.37  | 128.74      | 125.03   |
| 6   | G     | 813 | HEM  | CAA-CBA-CGA | -2.37 | 107.38      | 113.67   |
| 6   | K     | 810 | HEM  | CAA-CBA-CGA | -2.37 | 107.38      | 113.67   |
| 6   | F     | 810 | HEM  | CHA-C4D-C3D | -2.37 | 120.86      | 125.23   |
| 6   | G     | 812 | HEM  | CAD-C3D-C4D | 2.37  | 128.82      | 124.70   |
| 6   | D     | 811 | HEM  | C1A-CHA-C4D | -2.37 | 120.68      | 126.25   |
| 6   | H     | 812 | HEM  | CHC-C1C-NC  | 2.37  | 127.03      | 124.45   |
| 6   | H     | 812 | HEM  | C4C-NC-C1C  | 2.36  | 109.68      | 105.82   |
| 6   | F     | 811 | HEM  | C1A-CHA-C4D | -2.36 | 120.69      | 126.25   |
| 6   | I     | 813 | HEM  | C1A-CHA-C4D | -2.36 | 120.69      | 126.25   |
| 6   | A     | 810 | HEM  | C4C-NC-C1C  | 2.36  | 109.67      | 105.82   |
| 6   | I     | 810 | HEM  | CMD-C2D-C1D | 2.36  | 128.73      | 125.03   |
| 6   | L     | 811 | HEM  | C4C-NC-C1C  | 2.36  | 109.67      | 105.82   |
| 6   | L     | 813 | HEM  | CAA-CBA-CGA | -2.36 | 107.40      | 113.67   |
| 6   | B     | 813 | HEM  | CMD-C2D-C1D | 2.36  | 128.72      | 125.03   |
| 6   | A     | 811 | HEM  | CHA-C4D-C3D | -2.36 | 120.88      | 125.23   |
| 6   | A     | 812 | HEM  | CMD-C2D-C1D | 2.36  | 128.72      | 125.03   |
| 6   | F     | 810 | HEM  | C1A-CHA-C4D | -2.36 | 120.70      | 126.25   |
| 6   | E     | 806 | HEM  | CHC-C1C-NC  | 2.36  | 127.02      | 124.45   |
| 6   | F     | 811 | HEM  | CAA-CBA-CGA | -2.35 | 107.42      | 113.67   |
| 6   | G     | 807 | HEM  | CHD-C4C-NC  | 2.35  | 127.01      | 124.45   |
| 6   | J     | 809 | HEM  | C1A-CHA-C4D | -2.35 | 120.72      | 126.25   |
| 6   | H     | 808 | HEM  | C1A-CHA-C4D | -2.35 | 120.72      | 126.25   |
| 6   | G     | 812 | HEM  | C4C-NC-C1C  | 2.35  | 109.65      | 105.82   |
| 6   | C     | 810 | HEM  | C3A-C4A-NA  | -2.35 | 106.38      | 110.14   |
| 6   | A     | 811 | HEM  | C1A-CHA-C4D | -2.35 | 120.72      | 126.25   |
| 6   | K     | 811 | HEM  | C1A-CHA-C4D | -2.35 | 120.73      | 126.25   |
| 6   | I     | 809 | HEM  | CHA-C4D-C3D | -2.35 | 120.90      | 125.23   |
| 6   | H     | 812 | HEM  | O2A-CGA-CBA | 2.34  | 121.40      | 114.00   |
| 6   | G     | 809 | HEM  | CHA-C4D-C3D | -2.34 | 120.91      | 125.23   |
| 6   | D     | 809 | HEM  | C1A-CHA-C4D | -2.34 | 120.75      | 126.25   |
| 6   | J     | 809 | HEM  | CAD-C3D-C4D | 2.33  | 128.76      | 124.70   |
| 6   | C     | 808 | HEM  | CHA-C4D-C3D | -2.33 | 120.93      | 125.23   |
| 6   | J     | 809 | HEM  | CHA-C4D-C3D | -2.33 | 120.93      | 125.23   |
| 6   | J     | 810 | HEM  | C4C-NC-C1C  | 2.33  | 109.62      | 105.82   |
| 6   | G     | 813 | HEM  | CHA-C4D-C3D | -2.33 | 120.94      | 125.23   |
| 6   | K     | 812 | HEM  | O2D-CGD-CBD | 2.33  | 121.35      | 114.00   |
| 6   | D     | 813 | HEM  | CHC-C1C-NC  | 2.33  | 126.98      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | A     | 807 | HEM  | C1A-CHA-C4D | -2.32 | 120.78      | 126.25   |
| 6   | H     | 807 | HEM  | C4C-NC-C1C  | 2.32  | 109.61      | 105.82   |
| 6   | F     | 812 | HEM  | C1A-CHA-C4D | -2.32 | 120.79      | 126.25   |
| 6   | I     | 810 | HEM  | O2D-CGD-CBD | 2.32  | 121.33      | 114.00   |
| 6   | L     | 806 | HEM  | C4C-NC-C1C  | 2.32  | 109.60      | 105.82   |
| 6   | F     | 812 | HEM  | CHA-C4D-C3D | -2.32 | 120.96      | 125.23   |
| 6   | I     | 811 | HEM  | C1A-CHA-C4D | -2.32 | 120.80      | 126.25   |
| 6   | E     | 811 | HEM  | CHA-C4D-C3D | -2.31 | 120.96      | 125.23   |
| 6   | F     | 809 | HEM  | CMD-C2D-C1D | 2.31  | 128.65      | 125.03   |
| 6   | D     | 808 | HEM  | C1A-CHA-C4D | -2.31 | 120.81      | 126.25   |
| 6   | G     | 812 | HEM  | CHA-C4D-C3D | -2.31 | 120.97      | 125.23   |
| 6   | H     | 812 | HEM  | C1A-CHA-C4D | -2.31 | 120.81      | 126.25   |
| 6   | H     | 808 | HEM  | CHA-C4D-C3D | -2.31 | 120.97      | 125.23   |
| 6   | D     | 809 | HEM  | CMD-C2D-C1D | 2.31  | 128.64      | 125.03   |
| 6   | L     | 812 | HEM  | O2D-CGD-CBD | 2.31  | 121.29      | 114.00   |
| 6   | C     | 807 | HEM  | C1A-CHA-C4D | -2.30 | 120.83      | 126.25   |
| 6   | I     | 813 | HEM  | CHA-C4D-C3D | -2.30 | 120.98      | 125.23   |
| 6   | E     | 812 | HEM  | O2D-CGD-CBD | 2.30  | 121.28      | 114.00   |
| 6   | H     | 810 | HEM  | C1A-CHA-C4D | -2.30 | 120.84      | 126.25   |
| 6   | G     | 811 | HEM  | O2A-CGA-CBA | 2.30  | 121.27      | 114.00   |
| 6   | H     | 814 | HEM  | C1A-CHA-C4D | -2.30 | 120.84      | 126.25   |
| 6   | I     | 806 | HEM  | O2A-CGA-O1A | -2.30 | 117.42      | 123.33   |
| 6   | D     | 810 | HEM  | CMD-C2D-C1D | 2.30  | 128.62      | 125.03   |
| 6   | G     | 810 | HEM  | CAD-C3D-C4D | 2.30  | 128.70      | 124.70   |
| 6   | E     | 811 | HEM  | O2A-CGA-O1A | -2.30 | 117.43      | 123.33   |
| 6   | B     | 812 | HEM  | CHC-C1C-NC  | 2.30  | 126.95      | 124.45   |
| 6   | E     | 813 | HEM  | C4C-NC-C1C  | 2.29  | 109.56      | 105.82   |
| 6   | I     | 809 | HEM  | C1A-CHA-C4D | -2.29 | 120.85      | 126.25   |
| 6   | D     | 807 | HEM  | CHA-C4D-C3D | -2.29 | 121.00      | 125.23   |
| 6   | A     | 812 | HEM  | C1A-CHA-C4D | -2.29 | 120.86      | 126.25   |
| 6   | K     | 810 | HEM  | CHA-C4D-C3D | -2.29 | 121.00      | 125.23   |
| 6   | F     | 813 | HEM  | CMD-C2D-C1D | 2.29  | 128.61      | 125.03   |
| 6   | J     | 806 | HEM  | C3B-C2B-C1B | 2.29  | 108.13      | 106.41   |
| 6   | L     | 811 | HEM  | C1A-CHA-C4D | -2.29 | 120.86      | 126.25   |
| 6   | K     | 813 | HEM  | CMD-C2D-C1D | 2.28  | 128.60      | 125.03   |
| 6   | I     | 813 | HEM  | C4C-NC-C1C  | 2.28  | 109.54      | 105.82   |
| 6   | A     | 813 | HEM  | CHD-C4C-NC  | 2.28  | 126.94      | 124.45   |
| 6   | G     | 812 | HEM  | O2A-CGA-CBA | 2.28  | 121.21      | 114.00   |
| 6   | B     | 810 | HEM  | CMD-C2D-C1D | 2.28  | 128.60      | 125.03   |
| 6   | B     | 811 | HEM  | CBB-CAB-C3B | -2.28 | 116.13      | 127.53   |
| 6   | B     | 814 | HEM  | C4C-NC-C1C  | 2.28  | 109.54      | 105.82   |
| 6   | A     | 812 | HEM  | CBB-CAB-C3B | -2.28 | 116.14      | 127.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | I     | 813 | HEM  | CHC-C1C-NC  | 2.28  | 126.93      | 124.45   |
| 6   | F     | 809 | HEM  | CHD-C4C-NC  | 2.28  | 126.93      | 124.45   |
| 6   | A     | 813 | HEM  | C3A-C4A-NA  | -2.28 | 106.50      | 110.14   |
| 6   | L     | 810 | HEM  | C4C-NC-C1C  | 2.27  | 109.52      | 105.82   |
| 6   | C     | 808 | HEM  | C1A-CHA-C4D | -2.27 | 120.91      | 126.25   |
| 6   | A     | 809 | HEM  | CMD-C2D-C1D | 2.27  | 128.58      | 125.03   |
| 6   | H     | 810 | HEM  | CMD-C2D-C1D | 2.27  | 128.58      | 125.03   |
| 6   | G     | 809 | HEM  | C1A-CHA-C4D | -2.27 | 120.91      | 126.25   |
| 6   | G     | 809 | HEM  | O2A-CGA-O1A | -2.27 | 117.50      | 123.33   |
| 6   | B     | 814 | HEM  | CHA-C4D-C3D | -2.26 | 121.05      | 125.23   |
| 6   | E     | 810 | HEM  | C4C-NC-C1C  | 2.26  | 109.51      | 105.82   |
| 6   | J     | 808 | HEM  | C1A-CHA-C4D | -2.26 | 120.93      | 126.25   |
| 6   | F     | 813 | HEM  | CBB-CAB-C3B | -2.26 | 116.23      | 127.53   |
| 6   | J     | 808 | HEM  | C3A-C4A-NA  | -2.26 | 106.52      | 110.14   |
| 6   | G     | 810 | HEM  | C1A-CHA-C4D | -2.26 | 120.93      | 126.25   |
| 6   | D     | 808 | HEM  | CMD-C2D-C1D | 2.26  | 128.57      | 125.03   |
| 6   | J     | 810 | HEM  | O2D-CGD-CBD | 2.26  | 121.14      | 114.00   |
| 6   | E     | 806 | HEM  | CBB-CAB-C3B | -2.26 | 116.23      | 127.53   |
| 6   | H     | 807 | HEM  | O2D-CGD-CBD | 2.26  | 121.14      | 114.00   |
| 6   | F     | 809 | HEM  | CHD-C1D-C2D | -2.26 | 121.47      | 125.03   |
| 6   | D     | 809 | HEM  | CHA-C4D-C3D | -2.26 | 121.07      | 125.23   |
| 6   | B     | 813 | HEM  | CAD-C3D-C4D | 2.26  | 128.63      | 124.70   |
| 6   | C     | 811 | HEM  | CHC-C1C-NC  | 2.25  | 126.91      | 124.45   |
| 6   | A     | 812 | HEM  | CAD-C3D-C4D | 2.25  | 128.63      | 124.70   |
| 6   | A     | 812 | HEM  | C4C-NC-C1C  | 2.25  | 109.50      | 105.82   |
| 6   | H     | 813 | HEM  | C1A-CHA-C4D | -2.25 | 120.95      | 126.25   |
| 6   | B     | 812 | HEM  | CHA-C4D-C3D | -2.25 | 121.07      | 125.23   |
| 6   | K     | 812 | HEM  | C1A-CHA-C4D | -2.25 | 120.95      | 126.25   |
| 6   | L     | 810 | HEM  | C1A-CHA-C4D | -2.25 | 120.95      | 126.25   |
| 6   | E     | 810 | HEM  | CMD-C2D-C1D | 2.25  | 128.55      | 125.03   |
| 6   | C     | 811 | HEM  | O2A-CGA-CBA | 2.25  | 121.11      | 114.00   |
| 6   | G     | 807 | HEM  | C1A-CHA-C4D | -2.25 | 120.96      | 126.25   |
| 6   | A     | 810 | HEM  | C1A-CHA-C4D | -2.25 | 120.97      | 126.25   |
| 6   | F     | 808 | HEM  | O2A-CGA-O1A | -2.24 | 117.56      | 123.33   |
| 6   | G     | 809 | HEM  | CAD-C3D-C4D | 2.24  | 128.61      | 124.70   |
| 6   | I     | 809 | HEM  | CMD-C2D-C1D | 2.24  | 128.54      | 125.03   |
| 6   | K     | 806 | HEM  | C1A-CHA-C4D | -2.24 | 120.97      | 126.25   |
| 6   | B     | 808 | HEM  | C4C-NC-C1C  | 2.24  | 109.47      | 105.82   |
| 6   | C     | 810 | HEM  | CHA-C4D-C3D | -2.24 | 121.09      | 125.23   |
| 6   | E     | 812 | HEM  | O2A-CGA-CBA | 2.24  | 121.08      | 114.00   |
| 6   | E     | 809 | HEM  | C1A-CHA-C4D | -2.24 | 120.98      | 126.25   |
| 6   | L     | 811 | HEM  | C3A-C4A-NA  | -2.24 | 106.56      | 110.14   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | G     | 809 | HEM  | O2A-CGA-CBA | 2.24  | 121.07      | 114.00   |
| 6   | A     | 808 | HEM  | CHD-C4C-NC  | 2.24  | 126.89      | 124.45   |
| 6   | B     | 807 | HEM  | CAD-C3D-C4D | 2.24  | 128.60      | 124.70   |
| 6   | L     | 806 | HEM  | C1A-CHA-C4D | -2.23 | 120.99      | 126.25   |
| 6   | F     | 811 | HEM  | C4C-NC-C1C  | 2.23  | 109.46      | 105.82   |
| 6   | J     | 806 | HEM  | CMD-C2D-C1D | 2.23  | 128.52      | 125.03   |
| 6   | A     | 810 | HEM  | O2A-CGA-CBA | 2.23  | 121.04      | 114.00   |
| 6   | D     | 812 | HEM  | C4C-CHD-C1D | -2.23 | 121.28      | 126.02   |
| 6   | A     | 808 | HEM  | CHD-C1D-C2D | -2.23 | 121.51      | 125.03   |
| 6   | B     | 813 | HEM  | C1A-CHA-C4D | -2.22 | 121.02      | 126.25   |
| 6   | L     | 809 | HEM  | O2A-CGA-CBA | 2.22  | 121.03      | 114.00   |
| 6   | E     | 809 | HEM  | CHA-C4D-C3D | -2.22 | 121.13      | 125.23   |
| 6   | K     | 807 | HEM  | O2A-CGA-CBA | 2.22  | 121.01      | 114.00   |
| 6   | D     | 811 | HEM  | CAD-CBD-CGD | -2.22 | 107.78      | 113.67   |
| 6   | H     | 811 | HEM  | CMD-C2D-C1D | 2.22  | 128.50      | 125.03   |
| 6   | A     | 811 | HEM  | CAB-C3B-C4B | 2.22  | 134.18      | 124.39   |
| 6   | D     | 813 | HEM  | C1A-CHA-C4D | -2.21 | 121.04      | 126.25   |
| 6   | G     | 810 | HEM  | CHA-C4D-C3D | -2.21 | 121.14      | 125.23   |
| 6   | G     | 813 | HEM  | C4C-NC-C1C  | 2.21  | 109.43      | 105.82   |
| 6   | C     | 808 | HEM  | CBB-CAB-C3B | -2.21 | 116.48      | 127.53   |
| 6   | L     | 811 | HEM  | O2D-CGD-CBD | 2.21  | 120.98      | 114.00   |
| 6   | G     | 808 | HEM  | C1A-CHA-C4D | -2.21 | 121.06      | 126.25   |
| 6   | C     | 809 | HEM  | C3A-C4A-NA  | -2.21 | 106.61      | 110.14   |
| 6   | F     | 812 | HEM  | C4C-NC-C1C  | 2.21  | 109.42      | 105.82   |
| 6   | H     | 811 | HEM  | O2A-CGA-CBA | 2.21  | 120.97      | 114.00   |
| 6   | I     | 810 | HEM  | O2A-CGA-CBA | 2.21  | 120.97      | 114.00   |
| 6   | K     | 808 | HEM  | C1A-CHA-C4D | -2.20 | 121.06      | 126.25   |
| 6   | A     | 813 | HEM  | C1A-CHA-C4D | -2.20 | 121.06      | 126.25   |
| 6   | B     | 809 | HEM  | C1A-CHA-C4D | -2.20 | 121.07      | 126.25   |
| 6   | J     | 806 | HEM  | CAB-C3B-C4B | 2.20  | 134.12      | 124.39   |
| 6   | B     | 810 | HEM  | CAD-C3D-C4D | 2.20  | 128.53      | 124.70   |
| 6   | I     | 806 | HEM  | C3A-C4A-NA  | -2.20 | 106.62      | 110.14   |
| 6   | E     | 809 | HEM  | O2A-CGA-CBA | 2.20  | 120.94      | 114.00   |
| 6   | I     | 813 | HEM  | CAD-C3D-C4D | 2.20  | 128.52      | 124.70   |
| 6   | C     | 810 | HEM  | C4C-NC-C1C  | 2.19  | 109.40      | 105.82   |
| 6   | E     | 811 | HEM  | CHC-C1C-NC  | 2.19  | 126.84      | 124.45   |
| 6   | G     | 811 | HEM  | CAD-CBD-CGD | -2.19 | 107.86      | 113.67   |
| 6   | C     | 811 | HEM  | CHA-C4D-C3D | -2.19 | 121.19      | 125.23   |
| 6   | D     | 806 | HEM  | CBB-CAB-C3B | -2.19 | 116.58      | 127.53   |
| 6   | G     | 806 | HEM  | CMD-C2D-C1D | 2.19  | 128.46      | 125.03   |
| 6   | J     | 809 | HEM  | O2A-CGA-CBA | 2.18  | 120.90      | 114.00   |
| 6   | L     | 808 | HEM  | C1A-CHA-C4D | -2.18 | 121.11      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | J     | 810 | HEM  | CMD-C2D-C1D | 2.18  | 128.44      | 125.03   |
| 6   | E     | 809 | HEM  | O2A-CGA-O1A | -2.18 | 117.72      | 123.33   |
| 6   | I     | 812 | HEM  | CMD-C2D-C1D | 2.18  | 128.44      | 125.03   |
| 6   | J     | 811 | HEM  | C1A-CHA-C4D | -2.18 | 121.12      | 126.25   |
| 6   | C     | 811 | HEM  | C1A-CHA-C4D | -2.18 | 121.12      | 126.25   |
| 6   | K     | 813 | HEM  | C3A-C4A-NA  | -2.18 | 106.65      | 110.14   |
| 6   | A     | 812 | HEM  | CHC-C1C-NC  | 2.18  | 126.82      | 124.45   |
| 6   | J     | 806 | HEM  | C1A-CHA-C4D | -2.18 | 121.13      | 126.25   |
| 6   | B     | 813 | HEM  | O2D-CGD-CBD | 2.18  | 120.88      | 114.00   |
| 6   | D     | 813 | HEM  | C4C-NC-C1C  | 2.18  | 109.37      | 105.82   |
| 6   | D     | 806 | HEM  | C1A-CHA-C4D | -2.18 | 121.13      | 126.25   |
| 6   | E     | 813 | HEM  | C1A-CHA-C4D | -2.17 | 121.13      | 126.25   |
| 6   | I     | 806 | HEM  | CMD-C2D-C1D | 2.17  | 128.43      | 125.03   |
| 6   | L     | 811 | HEM  | CAB-C3B-C2B | 2.17  | 135.50      | 128.43   |
| 6   | J     | 809 | HEM  | C3A-C4A-NA  | -2.17 | 106.66      | 110.14   |
| 6   | D     | 806 | HEM  | C3A-C4A-NA  | -2.17 | 106.66      | 110.14   |
| 6   | F     | 807 | HEM  | C4C-NC-C1C  | 2.17  | 109.36      | 105.82   |
| 6   | H     | 809 | HEM  | CMD-C2D-C1D | 2.17  | 128.42      | 125.03   |
| 6   | F     | 807 | HEM  | C3A-C4A-NA  | -2.17 | 106.67      | 110.14   |
| 6   | H     | 807 | HEM  | CBB-CAB-C3B | -2.17 | 116.69      | 127.53   |
| 6   | J     | 810 | HEM  | C1A-CHA-C4D | -2.17 | 121.15      | 126.25   |
| 6   | F     | 814 | HEM  | O2D-CGD-CBD | 2.17  | 120.85      | 114.00   |
| 6   | B     | 811 | HEM  | CHA-C4D-C3D | -2.17 | 121.23      | 125.23   |
| 6   | B     | 812 | HEM  | C1A-CHA-C4D | -2.17 | 121.15      | 126.25   |
| 6   | A     | 812 | HEM  | CHA-C4D-C3D | -2.17 | 121.23      | 125.23   |
| 6   | H     | 809 | HEM  | C1A-CHA-C4D | -2.16 | 121.16      | 126.25   |
| 6   | H     | 809 | HEM  | CHD-C1D-C2D | -2.16 | 121.61      | 125.03   |
| 6   | E     | 813 | HEM  | C3A-C4A-NA  | -2.16 | 106.68      | 110.14   |
| 6   | L     | 810 | HEM  | O2A-CGA-CBA | 2.16  | 120.82      | 114.00   |
| 6   | A     | 811 | HEM  | CMB-C2B-C1B | 2.16  | 128.41      | 125.03   |
| 6   | D     | 806 | HEM  | C4C-NC-C1C  | 2.16  | 109.34      | 105.82   |
| 6   | C     | 812 | HEM  | O2D-CGD-CBD | 2.16  | 120.82      | 114.00   |
| 6   | J     | 808 | HEM  | O2A-CGA-CBA | 2.16  | 120.81      | 114.00   |
| 6   | G     | 810 | HEM  | O2A-CGA-CBA | 2.16  | 120.81      | 114.00   |
| 6   | L     | 811 | HEM  | CHA-C4D-C3D | -2.15 | 121.25      | 125.23   |
| 6   | F     | 808 | HEM  | CHD-C4C-NC  | 2.15  | 126.80      | 124.45   |
| 6   | D     | 811 | HEM  | O2A-CGA-CBA | 2.15  | 120.80      | 114.00   |
| 6   | I     | 808 | HEM  | O2A-CGA-CBA | 2.15  | 120.80      | 114.00   |
| 6   | A     | 811 | HEM  | C3B-C2B-C1B | 2.15  | 108.03      | 106.41   |
| 6   | B     | 811 | HEM  | O2A-CGA-CBA | 2.15  | 120.80      | 114.00   |
| 6   | D     | 809 | HEM  | O2A-CGA-O1A | -2.15 | 117.80      | 123.33   |
| 6   | G     | 813 | HEM  | C1A-CHA-C4D | -2.15 | 121.19      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | D     | 810 | HEM  | CBB-CAB-C3B | -2.15 | 116.80      | 127.53   |
| 6   | C     | 806 | HEM  | CAD-C3D-C4D | 2.15  | 128.44      | 124.70   |
| 6   | D     | 810 | HEM  | O2A-CGA-CBA | 2.14  | 120.77      | 114.00   |
| 6   | I     | 809 | HEM  | CAD-C3D-C4D | 2.14  | 128.43      | 124.70   |
| 6   | H     | 811 | HEM  | C1A-CHA-C4D | -2.14 | 121.21      | 126.25   |
| 6   | D     | 812 | HEM  | CAD-C3D-C4D | 2.14  | 128.43      | 124.70   |
| 6   | K     | 810 | HEM  | C4C-NC-C1C  | 2.14  | 109.31      | 105.82   |
| 6   | I     | 810 | HEM  | CHA-C4D-C3D | -2.14 | 121.28      | 125.23   |
| 6   | I     | 808 | HEM  | CHD-C4C-NC  | 2.14  | 126.78      | 124.45   |
| 6   | F     | 808 | HEM  | C4A-C3A-C2A | 2.13  | 109.26      | 106.82   |
| 6   | G     | 812 | HEM  | O2D-CGD-CBD | 2.13  | 120.73      | 114.00   |
| 6   | I     | 812 | HEM  | C4C-CHD-C1D | -2.13 | 121.49      | 126.02   |
| 6   | B     | 811 | HEM  | C4C-NC-C1C  | 2.13  | 109.30      | 105.82   |
| 6   | H     | 810 | HEM  | O2A-CGA-O1A | -2.13 | 117.86      | 123.33   |
| 6   | H     | 810 | HEM  | CAD-C3D-C4D | 2.13  | 128.41      | 124.70   |
| 6   | E     | 812 | HEM  | CAD-C3D-C4D | 2.13  | 128.40      | 124.70   |
| 6   | C     | 810 | HEM  | O2D-CGD-O1D | -2.13 | 117.86      | 123.33   |
| 6   | L     | 812 | HEM  | C1A-CHA-C4D | -2.12 | 121.25      | 126.25   |
| 6   | L     | 806 | HEM  | C3A-C4A-NA  | -2.12 | 106.74      | 110.14   |
| 6   | B     | 809 | HEM  | O2A-CGA-CBA | 2.12  | 120.70      | 114.00   |
| 6   | L     | 811 | HEM  | C2A-C1A-NA  | -2.12 | 107.80      | 110.15   |
| 6   | C     | 809 | HEM  | O2A-CGA-CBA | 2.12  | 120.70      | 114.00   |
| 6   | D     | 810 | HEM  | CHC-C1C-NC  | 2.12  | 126.76      | 124.45   |
| 6   | A     | 813 | HEM  | O2A-CGA-CBA | 2.12  | 120.69      | 114.00   |
| 6   | L     | 811 | HEM  | O2A-CGA-CBA | 2.12  | 120.69      | 114.00   |
| 6   | C     | 810 | HEM  | CHD-C4C-NC  | 2.12  | 126.76      | 124.45   |
| 6   | D     | 806 | HEM  | CAB-C3B-C2B | 2.12  | 135.31      | 128.43   |
| 6   | D     | 813 | HEM  | O2A-CGA-CBA | 2.11  | 120.68      | 114.00   |
| 6   | G     | 813 | HEM  | CAD-C3D-C4D | 2.11  | 128.38      | 124.70   |
| 6   | A     | 812 | HEM  | O2D-CGD-CBD | 2.11  | 120.68      | 114.00   |
| 6   | K     | 810 | HEM  | CMD-C2D-C1D | 2.11  | 128.34      | 125.03   |
| 6   | G     | 813 | HEM  | CMD-C2D-C1D | 2.11  | 128.34      | 125.03   |
| 6   | B     | 811 | HEM  | C1A-CHA-C4D | -2.11 | 121.28      | 126.25   |
| 6   | F     | 809 | HEM  | C1A-CHA-C4D | -2.11 | 121.28      | 126.25   |
| 6   | A     | 806 | HEM  | CAD-C3D-C4D | 2.11  | 128.38      | 124.70   |
| 6   | D     | 813 | HEM  | C3A-C4A-NA  | -2.11 | 106.76      | 110.14   |
| 6   | F     | 811 | HEM  | CAD-C3D-C4D | 2.11  | 128.37      | 124.70   |
| 6   | B     | 811 | HEM  | O2D-CGD-O1D | -2.11 | 117.91      | 123.33   |
| 6   | B     | 814 | HEM  | C4A-NA-C1A  | 2.11  | 109.26      | 105.82   |
| 6   | C     | 813 | HEM  | C4C-NC-C1C  | 2.11  | 109.26      | 105.82   |
| 6   | G     | 812 | HEM  | CBB-CAB-C3B | -2.11 | 117.00      | 127.53   |
| 6   | J     | 810 | HEM  | CAD-C3D-C4D | 2.11  | 128.37      | 124.70   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | F     | 807 | HEM  | C1A-CHA-C4D | -2.10 | 121.30      | 126.25   |
| 6   | B     | 809 | HEM  | C3A-C4A-NA  | -2.10 | 106.77      | 110.14   |
| 6   | E     | 808 | HEM  | C3A-C4A-NA  | -2.10 | 106.77      | 110.14   |
| 6   | I     | 810 | HEM  | C4C-NC-C1C  | 2.10  | 109.25      | 105.82   |
| 6   | K     | 809 | HEM  | C1A-CHA-C4D | -2.10 | 121.30      | 126.25   |
| 6   | E     | 809 | HEM  | CHD-C4C-NC  | 2.10  | 126.74      | 124.45   |
| 6   | E     | 812 | HEM  | C1A-CHA-C4D | -2.10 | 121.31      | 126.25   |
| 6   | F     | 809 | HEM  | C4C-CHD-C1D | -2.10 | 121.56      | 126.02   |
| 6   | K     | 812 | HEM  | CHD-C4C-NC  | 2.10  | 126.74      | 124.45   |
| 6   | E     | 808 | HEM  | C4C-CHD-C1D | -2.10 | 121.56      | 126.02   |
| 6   | D     | 810 | HEM  | C4C-NC-C1C  | 2.10  | 109.24      | 105.82   |
| 6   | H     | 813 | HEM  | O2D-CGD-CBD | 2.10  | 120.62      | 114.00   |
| 6   | C     | 811 | HEM  | CAD-C3D-C4D | 2.10  | 128.35      | 124.70   |
| 6   | K     | 811 | HEM  | O2A-CGA-CBA | 2.09  | 120.62      | 114.00   |
| 6   | A     | 811 | HEM  | CAD-C3D-C4D | 2.09  | 128.35      | 124.70   |
| 6   | I     | 809 | HEM  | O2D-CGD-CBD | 2.09  | 120.61      | 114.00   |
| 6   | A     | 812 | HEM  | C4C-CHD-C1D | -2.09 | 121.57      | 126.02   |
| 6   | C     | 813 | HEM  | O2D-CGD-CBD | 2.09  | 120.61      | 114.00   |
| 6   | I     | 808 | HEM  | C1A-CHA-C4D | -2.09 | 121.33      | 126.25   |
| 6   | I     | 810 | HEM  | C1A-CHA-C4D | -2.09 | 121.34      | 126.25   |
| 6   | F     | 813 | HEM  | CHC-C1C-NC  | 2.09  | 126.73      | 124.45   |
| 6   | C     | 813 | HEM  | O2A-CGA-CBA | 2.09  | 120.60      | 114.00   |
| 6   | H     | 813 | HEM  | C3A-C4A-NA  | -2.09 | 106.80      | 110.14   |
| 6   | J     | 811 | HEM  | C3A-C4A-NA  | -2.09 | 106.80      | 110.14   |
| 6   | K     | 809 | HEM  | CMD-C2D-C1D | 2.09  | 128.29      | 125.03   |
| 6   | B     | 811 | HEM  | C3A-C4A-NA  | -2.09 | 106.80      | 110.14   |
| 6   | E     | 806 | HEM  | C1A-CHA-C4D | -2.09 | 121.34      | 126.25   |
| 6   | F     | 810 | HEM  | O2A-CGA-CBA | 2.08  | 120.59      | 114.00   |
| 6   | B     | 807 | HEM  | CBB-CAB-C3B | -2.08 | 117.11      | 127.53   |
| 6   | C     | 807 | HEM  | O2A-CGA-CBA | 2.08  | 120.58      | 114.00   |
| 6   | L     | 809 | HEM  | CHD-C4C-NC  | 2.08  | 126.72      | 124.45   |
| 6   | H     | 813 | HEM  | CMD-C2D-C1D | 2.08  | 128.29      | 125.03   |
| 6   | A     | 809 | HEM  | O2A-CGA-O1A | -2.08 | 117.99      | 123.33   |
| 6   | G     | 810 | HEM  | CAA-CBA-CGA | -2.08 | 108.15      | 113.67   |
| 6   | I     | 813 | HEM  | C3A-C4A-NA  | -2.08 | 106.81      | 110.14   |
| 6   | I     | 811 | HEM  | C4C-CHD-C1D | -2.08 | 121.61      | 126.02   |
| 6   | C     | 808 | HEM  | CAD-C3D-C4D | 2.07  | 128.31      | 124.70   |
| 6   | K     | 813 | HEM  | CAD-CBD-CGD | -2.07 | 108.17      | 113.67   |
| 6   | I     | 812 | HEM  | O2D-CGD-CBD | 2.07  | 120.54      | 114.00   |
| 6   | E     | 810 | HEM  | C1A-CHA-C4D | -2.07 | 121.38      | 126.25   |
| 6   | J     | 813 | HEM  | C1A-CHA-C4D | -2.07 | 121.38      | 126.25   |
| 6   | I     | 806 | HEM  | CBB-CAB-C3B | -2.07 | 117.18      | 127.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | D     | 811 | HEM  | CAD-C3D-C4D | 2.07  | 128.30      | 124.70   |
| 6   | J     | 812 | HEM  | O2D-CGD-CBD | 2.07  | 120.53      | 114.00   |
| 6   | L     | 811 | HEM  | C4A-NA-C1A  | 2.07  | 109.19      | 105.82   |
| 6   | F     | 813 | HEM  | CHD-C4C-NC  | 2.06  | 126.70      | 124.45   |
| 6   | L     | 813 | HEM  | C1A-CHA-C4D | -2.06 | 121.39      | 126.25   |
| 6   | G     | 813 | HEM  | C2A-C1A-NA  | -2.06 | 107.86      | 110.15   |
| 6   | A     | 806 | HEM  | O2D-CGD-O1D | -2.06 | 118.03      | 123.33   |
| 6   | A     | 809 | HEM  | C1A-CHA-C4D | -2.06 | 121.40      | 126.25   |
| 6   | C     | 812 | HEM  | CMD-C2D-C1D | 2.06  | 128.25      | 125.03   |
| 6   | B     | 814 | HEM  | C1A-CHA-C4D | -2.06 | 121.41      | 126.25   |
| 6   | H     | 807 | HEM  | O2A-CGA-O1A | -2.06 | 118.04      | 123.33   |
| 6   | G     | 811 | HEM  | C4C-CHD-C1D | -2.06 | 121.65      | 126.02   |
| 6   | I     | 810 | HEM  | CAD-C3D-C4D | 2.06  | 128.28      | 124.70   |
| 6   | B     | 812 | HEM  | C3A-C4A-NA  | -2.06 | 106.85      | 110.14   |
| 6   | L     | 812 | HEM  | C4C-CHD-C1D | -2.05 | 121.65      | 126.02   |
| 6   | E     | 812 | HEM  | O2A-CGA-O1A | -2.05 | 118.05      | 123.33   |
| 6   | H     | 807 | HEM  | C3A-C4A-NA  | -2.05 | 106.85      | 110.14   |
| 6   | A     | 812 | HEM  | CHD-C4C-NC  | 2.05  | 126.69      | 124.45   |
| 6   | G     | 813 | HEM  | O2A-CGA-CBA | 2.05  | 120.48      | 114.00   |
| 6   | B     | 813 | HEM  | CBB-CAB-C3B | -2.05 | 117.28      | 127.53   |
| 6   | J     | 813 | HEM  | C3A-C4A-NA  | -2.05 | 106.86      | 110.14   |
| 6   | J     | 813 | HEM  | O2A-CGA-CBA | 2.05  | 120.47      | 114.00   |
| 6   | H     | 811 | HEM  | CBB-CAB-C3B | -2.05 | 117.30      | 127.53   |
| 6   | K     | 810 | HEM  | C3A-C4A-NA  | -2.05 | 106.86      | 110.14   |
| 6   | B     | 812 | HEM  | CAD-CBD-CGD | -2.05 | 108.24      | 113.67   |
| 6   | G     | 810 | HEM  | O2D-CGD-O1D | -2.04 | 118.07      | 123.33   |
| 6   | K     | 806 | HEM  | CMB-C2B-C3B | -2.04 | 123.48      | 128.43   |
| 6   | E     | 812 | HEM  | CBB-CAB-C3B | -2.04 | 117.31      | 127.53   |
| 6   | B     | 807 | HEM  | O2D-CGD-O1D | -2.04 | 118.08      | 123.33   |
| 6   | C     | 812 | HEM  | CBB-CAB-C3B | -2.04 | 117.33      | 127.53   |
| 6   | F     | 811 | HEM  | O2A-CGA-CBA | 2.04  | 120.44      | 114.00   |
| 6   | H     | 811 | HEM  | CHD-C4C-NC  | 2.04  | 126.67      | 124.45   |
| 6   | L     | 813 | HEM  | O2A-CGA-CBA | 2.04  | 120.44      | 114.00   |
| 6   | D     | 812 | HEM  | CBB-CAB-C3B | -2.04 | 117.35      | 127.53   |
| 6   | L     | 813 | HEM  | CAD-C3D-C4D | 2.03  | 128.24      | 124.70   |
| 6   | F     | 810 | HEM  | O2D-CGD-CBD | 2.03  | 120.43      | 114.00   |
| 6   | F     | 811 | HEM  | CBB-CAB-C3B | -2.03 | 117.36      | 127.53   |
| 6   | H     | 810 | HEM  | C3A-C4A-NA  | -2.03 | 106.88      | 110.14   |
| 6   | H     | 810 | HEM  | O2D-CGD-CBD | 2.03  | 120.42      | 114.00   |
| 6   | C     | 809 | HEM  | C1A-CHA-C4D | -2.03 | 121.47      | 126.25   |
| 6   | G     | 809 | HEM  | O2D-CGD-CBD | 2.03  | 120.42      | 114.00   |
| 6   | I     | 807 | HEM  | CHD-C4C-NC  | 2.03  | 126.67      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | C     | 810 | HEM  | O2A-CGA-CBA | 2.03  | 120.42      | 114.00   |
| 6   | K     | 808 | HEM  | O2A-CGA-CBA | 2.03  | 120.41      | 114.00   |
| 6   | F     | 814 | HEM  | O2A-CGA-CBA | 2.03  | 120.41      | 114.00   |
| 6   | G     | 811 | HEM  | CBB-CAB-C3B | -2.03 | 117.40      | 127.53   |
| 6   | G     | 809 | HEM  | C3A-C4A-NA  | -2.03 | 106.89      | 110.14   |
| 6   | H     | 814 | HEM  | C4C-CHD-C1D | -2.02 | 121.72      | 126.02   |
| 6   | B     | 814 | HEM  | O2D-CGD-CBD | 2.02  | 120.38      | 114.00   |
| 6   | C     | 808 | HEM  | C3A-C4A-NA  | -2.02 | 106.90      | 110.14   |
| 6   | E     | 813 | HEM  | CAD-CBD-CGD | -2.02 | 108.31      | 113.67   |
| 6   | D     | 811 | HEM  | CHA-C4D-C3D | -2.02 | 121.50      | 125.23   |
| 6   | H     | 812 | HEM  | C3A-C4A-NA  | -2.02 | 106.91      | 110.14   |
| 6   | A     | 812 | HEM  | CHB-C1B-NB  | 2.02  | 126.86      | 124.37   |
| 6   | D     | 812 | HEM  | CHD-C4C-NC  | 2.02  | 126.65      | 124.45   |
| 6   | E     | 810 | HEM  | O2D-CGD-O1D | -2.02 | 118.14      | 123.33   |
| 6   | A     | 806 | HEM  | C3A-C4A-NA  | -2.02 | 106.91      | 110.14   |
| 6   | E     | 813 | HEM  | C4C-CHD-C1D | -2.01 | 121.74      | 126.02   |
| 6   | A     | 811 | HEM  | CMB-C2B-C3B | -2.01 | 123.56      | 128.43   |
| 6   | J     | 810 | HEM  | O2A-CGA-CBA | 2.01  | 120.36      | 114.00   |
| 6   | L     | 812 | HEM  | CMD-C2D-C1D | 2.01  | 128.18      | 125.03   |
| 6   | A     | 810 | HEM  | CAA-CBA-CGA | -2.01 | 108.33      | 113.67   |
| 6   | G     | 813 | HEM  | C3A-C4A-NA  | -2.01 | 106.92      | 110.14   |
| 6   | C     | 810 | HEM  | C1A-CHA-C4D | -2.01 | 121.52      | 126.25   |
| 6   | G     | 812 | HEM  | C3A-C4A-NA  | -2.01 | 106.92      | 110.14   |
| 6   | L     | 813 | HEM  | CMD-C2D-C1D | 2.01  | 128.17      | 125.03   |
| 6   | C     | 813 | HEM  | CBD-CAD-C3D | -2.01 | 106.98      | 112.53   |
| 6   | F     | 814 | HEM  | CMD-C2D-C1D | 2.01  | 128.17      | 125.03   |
| 6   | D     | 811 | HEM  | CBB-CAB-C3B | -2.01 | 117.50      | 127.53   |
| 6   | J     | 810 | HEM  | C3A-C4A-NA  | -2.01 | 106.93      | 110.14   |
| 6   | H     | 808 | HEM  | O2A-CGA-O1A | -2.00 | 118.18      | 123.33   |
| 6   | K     | 810 | HEM  | C1A-CHA-C4D | -2.00 | 121.53      | 126.25   |
| 6   | H     | 814 | HEM  | O2D-CGD-CBD | 2.00  | 120.33      | 114.00   |
| 6   | K     | 806 | HEM  | CMB-C2B-C1B | 2.00  | 128.17      | 125.03   |
| 6   | B     | 811 | HEM  | CAA-CBA-CGA | -2.00 | 108.35      | 113.67   |
| 6   | L     | 808 | HEM  | CMD-C2D-C1D | 2.00  | 128.16      | 125.03   |
| 6   | K     | 813 | HEM  | CAD-C3D-C4D | 2.00  | 128.18      | 124.70   |

There are no chirality outliers.

All (367) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | A     | 803 | BU3  | O5-C2-C3-O6 |
| 4   | A     | 803 | BU3  | C1-C2-C3-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | A     | 803 | BU3  | O5-C2-C3-C4 |
| 4   | A     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | A     | 804 | BU3  | C1-C2-C3-O6 |
| 4   | A     | 804 | BU3  | O5-C2-C3-C4 |
| 4   | A     | 804 | BU3  | C1-C2-C3-C4 |
| 4   | B     | 803 | BU3  | C1-C2-C3-O6 |
| 4   | B     | 803 | BU3  | O5-C2-C3-C4 |
| 4   | B     | 803 | BU3  | C1-C2-C3-C4 |
| 4   | B     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | B     | 804 | BU3  | O5-C2-C3-C4 |
| 4   | B     | 804 | BU3  | C1-C2-C3-C4 |
| 4   | C     | 803 | BU3  | O5-C2-C3-O6 |
| 4   | C     | 803 | BU3  | C1-C2-C3-C4 |
| 4   | C     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | C     | 804 | BU3  | C1-C2-C3-O6 |
| 4   | C     | 804 | BU3  | O5-C2-C3-C4 |
| 4   | C     | 804 | BU3  | C1-C2-C3-C4 |
| 4   | D     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | E     | 803 | BU3  | C1-C2-C3-C4 |
| 4   | F     | 803 | BU3  | O5-C2-C3-O6 |
| 4   | F     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | F     | 804 | BU3  | C1-C2-C3-C4 |
| 4   | F     | 805 | BU3  | O5-C2-C3-O6 |
| 4   | F     | 805 | BU3  | C1-C2-C3-O6 |
| 4   | F     | 805 | BU3  | O5-C2-C3-C4 |
| 4   | F     | 805 | BU3  | C1-C2-C3-C4 |
| 4   | H     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | H     | 804 | BU3  | C1-C2-C3-C4 |
| 4   | I     | 803 | BU3  | O5-C2-C3-O6 |
| 4   | I     | 803 | BU3  | C1-C2-C3-O6 |
| 4   | I     | 803 | BU3  | O5-C2-C3-C4 |
| 4   | I     | 803 | BU3  | C1-C2-C3-C4 |
| 4   | I     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | J     | 803 | BU3  | C1-C2-C3-O6 |
| 4   | J     | 803 | BU3  | O5-C2-C3-C4 |
| 4   | J     | 803 | BU3  | C1-C2-C3-C4 |
| 4   | J     | 804 | BU3  | C1-C2-C3-O6 |
| 4   | J     | 804 | BU3  | O5-C2-C3-C4 |
| 4   | J     | 804 | BU3  | C1-C2-C3-C4 |
| 4   | K     | 804 | BU3  | O5-C2-C3-O6 |
| 4   | K     | 804 | BU3  | C1-C2-C3-C4 |
| 4   | L     | 803 | BU3  | O5-C2-C3-O6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | L     | 803 | BU3  | C1-C2-C3-O6     |
| 4   | L     | 803 | BU3  | O5-C2-C3-C4     |
| 4   | L     | 803 | BU3  | C1-C2-C3-C4     |
| 4   | L     | 804 | BU3  | O5-C2-C3-O6     |
| 4   | L     | 804 | BU3  | C1-C2-C3-C4     |
| 4   | G     | 803 | BU3  | O5-C2-C3-O6     |
| 6   | B     | 808 | HEM  | C2D-C3D-CAD-CBD |
| 6   | D     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | F     | 808 | HEM  | C2D-C3D-CAD-CBD |
| 6   | H     | 808 | HEM  | C2D-C3D-CAD-CBD |
| 6   | I     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | J     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | J     | 813 | HEM  | C2D-C3D-CAD-CBD |
| 6   | J     | 813 | HEM  | C4D-C3D-CAD-CBD |
| 6   | K     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | L     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | G     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | A     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | C     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | E     | 807 | HEM  | C2D-C3D-CAD-CBD |
| 6   | A     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | B     | 808 | HEM  | C4D-C3D-CAD-CBD |
| 6   | C     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | D     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | E     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | F     | 808 | HEM  | C4D-C3D-CAD-CBD |
| 6   | H     | 808 | HEM  | C4D-C3D-CAD-CBD |
| 6   | I     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | J     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | K     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | L     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | G     | 807 | HEM  | C4D-C3D-CAD-CBD |
| 6   | F     | 807 | HEM  | C2A-CAA-CBA-CGA |
| 6   | L     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 6   | L     | 811 | HEM  | C4B-C3B-CAB-CBB |
| 6   | D     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 6   | J     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 6   | A     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 6   | B     | 807 | HEM  | C2A-CAA-CBA-CGA |
| 6   | B     | 812 | HEM  | C3D-CAD-CBD-CGD |
| 6   | C     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 6   | E     | 806 | HEM  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | F     | 809 | HEM  | C3D-CAD-CBD-CGD |
| 6   | H     | 807 | HEM  | C2A-CAA-CBA-CGA |
| 6   | I     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 6   | G     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 4   | B     | 804 | BU3  | C1-C2-C3-O6     |
| 4   | C     | 803 | BU3  | C1-C2-C3-O6     |
| 4   | C     | 803 | BU3  | O5-C2-C3-C4     |
| 4   | D     | 804 | BU3  | C1-C2-C3-O6     |
| 4   | D     | 804 | BU3  | O5-C2-C3-C4     |
| 4   | F     | 803 | BU3  | C1-C2-C3-O6     |
| 4   | F     | 803 | BU3  | O5-C2-C3-C4     |
| 4   | F     | 804 | BU3  | C1-C2-C3-O6     |
| 4   | F     | 804 | BU3  | O5-C2-C3-C4     |
| 4   | H     | 804 | BU3  | C1-C2-C3-O6     |
| 4   | H     | 804 | BU3  | O5-C2-C3-C4     |
| 4   | I     | 804 | BU3  | C1-C2-C3-O6     |
| 4   | I     | 804 | BU3  | O5-C2-C3-C4     |
| 4   | K     | 804 | BU3  | C1-C2-C3-O6     |
| 4   | K     | 804 | BU3  | O5-C2-C3-C4     |
| 4   | L     | 804 | BU3  | C1-C2-C3-O6     |
| 4   | L     | 804 | BU3  | O5-C2-C3-C4     |
| 4   | G     | 803 | BU3  | C1-C2-C3-O6     |
| 4   | G     | 803 | BU3  | O5-C2-C3-C4     |
| 6   | B     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | I     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | K     | 806 | HEM  | C2A-CAA-CBA-CGA |
| 6   | K     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | L     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | G     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 4   | A     | 803 | BU3  | C1-C2-C3-C4     |
| 4   | D     | 804 | BU3  | C1-C2-C3-C4     |
| 4   | F     | 803 | BU3  | C1-C2-C3-C4     |
| 4   | I     | 804 | BU3  | C1-C2-C3-C4     |
| 4   | G     | 803 | BU3  | C1-C2-C3-C4     |
| 4   | B     | 803 | BU3  | O5-C2-C3-O6     |
| 4   | J     | 803 | BU3  | O5-C2-C3-O6     |
| 6   | A     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | C     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | J     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | J     | 806 | HEM  | C2B-C3B-CAB-CBB |
| 6   | K     | 806 | HEM  | C2B-C3B-CAB-CBB |
| 6   | H     | 809 | HEM  | C3D-CAD-CBD-CGD |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | A     | 806 | HEM  | C4B-C3B-CAB-CBB |
| 6   | B     | 811 | HEM  | C4B-C3B-CAB-CBB |
| 6   | C     | 806 | HEM  | C4B-C3B-CAB-CBB |
| 6   | A     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | L     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | D     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | A     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | B     | 814 | HEM  | CAD-CBD-CGD-O2D |
| 6   | G     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | C     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | C     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | F     | 814 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | G     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | H     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | L     | 813 | HEM  | C3D-CAD-CBD-CGD |
| 6   | G     | 807 | HEM  | C3D-CAD-CBD-CGD |
| 6   | B     | 814 | HEM  | CAD-CBD-CGD-O1D |
| 6   | F     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | J     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | K     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | J     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | C     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | F     | 814 | HEM  | CAA-CBA-CGA-O1A |
| 6   | H     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | K     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | A     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | A     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | B     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | K     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | A     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | D     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | E     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | H     | 809 | HEM  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | I     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | J     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | B     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | B     | 814 | HEM  | CAA-CBA-CGA-O2A |
| 6   | C     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | D     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | F     | 814 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | K     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | B     | 809 | HEM  | CAA-CBA-CGA-O1A |
| 6   | E     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | F     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | L     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | G     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | G     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | B     | 809 | HEM  | C3D-CAD-CBD-CGD |
| 6   | A     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | F     | 809 | HEM  | CAA-CBA-CGA-O1A |
| 6   | F     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | J     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | J     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | L     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | A     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | B     | 814 | HEM  | CAA-CBA-CGA-O1A |
| 6   | H     | 811 | HEM  | CAA-CBA-CGA-O1A |
| 6   | H     | 814 | HEM  | CAA-CBA-CGA-O2A |
| 6   | A     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | C     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | D     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | E     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | H     | 811 | HEM  | CAA-CBA-CGA-O2A |
| 6   | H     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | G     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | F     | 814 | HEM  | CAD-CBD-CGD-O2D |
| 6   | L     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | G     | 813 | HEM  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | C     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | H     | 814 | HEM  | CAA-CBA-CGA-O1A |
| 6   | J     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | G     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | B     | 811 | HEM  | CAA-CBA-CGA-O1A |
| 6   | C     | 808 | HEM  | CAA-CBA-CGA-O1A |
| 6   | J     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | B     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | D     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | J     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | G     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | A     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | B     | 809 | HEM  | CAA-CBA-CGA-O2A |
| 6   | F     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | H     | 809 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | L     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | E     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | E     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | F     | 811 | HEM  | CAA-CBA-CGA-O2A |
| 6   | I     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | E     | 808 | HEM  | C2D-C3D-CAD-CBD |
| 6   | A     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | B     | 811 | HEM  | CAA-CBA-CGA-O2A |
| 6   | C     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | D     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | E     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | J     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | A     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | B     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | B     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | C     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | D     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | H     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | H     | 814 | HEM  | CAD-CBD-CGD-O2D |
| 6   | K     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | B     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | D     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | I     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | I     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | G     | 812 | HEM  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | C     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | E     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | E     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | F     | 811 | HEM  | CAA-CBA-CGA-O1A |
| 6   | H     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | C     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | D     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | H     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | J     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 811 | HEM  | CAA-CBA-CGA-O2A |
| 6   | B     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | B     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | B     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | F     | 809 | HEM  | CAA-CBA-CGA-O2A |
| 6   | E     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | H     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | J     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | D     | 813 | HEM  | CAA-CBA-CGA-O1A |
| 6   | H     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | J     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | L     | 811 | HEM  | CAA-CBA-CGA-O2A |
| 6   | L     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | D     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | G     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | A     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | D     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | I     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | L     | 811 | HEM  | C2B-C3B-CAB-CBB |
| 6   | A     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | F     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | H     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | I     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | I     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | E     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | K     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | G     | 808 | HEM  | C2D-C3D-CAD-CBD |
| 6   | A     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | C     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | D     | 810 | HEM  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | H     | 814 | HEM  | CAD-CBD-CGD-O1D |
| 6   | K     | 811 | HEM  | CAA-CBA-CGA-O1A |
| 6   | D     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | I     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | D     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | E     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | I     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | J     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | K     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | A     | 810 | HEM  | C4B-C3B-CAB-CBB |
| 6   | C     | 808 | HEM  | C4B-C3B-CAB-CBB |
| 6   | D     | 806 | HEM  | C4B-C3B-CAB-CBB |
| 6   | D     | 808 | HEM  | C4B-C3B-CAB-CBB |
| 6   | D     | 810 | HEM  | C4B-C3B-CAB-CBB |
| 6   | A     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | A     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | G     | 812 | HEM  | CAD-CBD-CGD-O1D |
| 6   | F     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | E     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | J     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | G     | 810 | HEM  | CAA-CBA-CGA-O1A |
| 6   | B     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | E     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | G     | 810 | HEM  | CAA-CBA-CGA-O2A |
| 6   | A     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | J     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 6   | C     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | A     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | J     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | E     | 808 | HEM  | C3D-CAD-CBD-CGD |
| 6   | D     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | E     | 811 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 811 | HEM  | CAA-CBA-CGA-O1A |
| 6   | E     | 811 | HEM  | CAA-CBA-CGA-O2A |
| 6   | C     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | D     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | C     | 813 | HEM  | CAD-CBD-CGD-O1D |
| 6   | F     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | J     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | K     | 807 | HEM  | CAA-CBA-CGA-O2A |
| 6   | E     | 812 | HEM  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 6   | I     | 810 | HEM  | CAD-CBD-CGD-O1D |
| 6   | L     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | I     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | L     | 809 | HEM  | CAD-CBD-CGD-O2D |
| 6   | J     | 810 | HEM  | CAD-CBD-CGD-O2D |
| 6   | G     | 812 | HEM  | CAD-CBD-CGD-O2D |
| 6   | C     | 808 | HEM  | C4D-C3D-CAD-CBD |
| 6   | C     | 813 | HEM  | CAD-CBD-CGD-O2D |
| 4   | J     | 804 | BU3  | O5-C2-C3-O6     |
| 6   | K     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | L     | 809 | HEM  | CAD-CBD-CGD-O1D |
| 6   | D     | 806 | HEM  | CAD-CBD-CGD-O2D |
| 6   | E     | 808 | HEM  | CAD-CBD-CGD-O2D |
| 6   | H     | 813 | HEM  | CAA-CBA-CGA-O2A |
| 6   | J     | 807 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 807 | HEM  | CAA-CBA-CGA-O1A |
| 6   | B     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | F     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | D     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | F     | 811 | HEM  | CAD-CBD-CGD-O2D |
| 6   | L     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | L     | 807 | HEM  | C3D-CAD-CBD-CGD |
| 6   | B     | 812 | HEM  | CAA-CBA-CGA-O2A |
| 6   | H     | 808 | HEM  | CAA-CBA-CGA-O2A |
| 6   | I     | 807 | HEM  | CAA-CBA-CGA-O2A |
| 6   | K     | 812 | HEM  | CAA-CBA-CGA-O1A |
| 6   | F     | 811 | HEM  | CAD-CBD-CGD-O1D |
| 6   | K     | 806 | HEM  | CAD-CBD-CGD-O2D |
| 6   | D     | 806 | HEM  | CAD-CBD-CGD-O1D |

There are no ring outliers.

101 monomers are involved in 790 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | K     | 806 | HEM  | 10      | 0            |
| 6   | G     | 809 | HEM  | 9       | 0            |
| 6   | F     | 813 | HEM  | 6       | 0            |
| 6   | F     | 814 | HEM  | 7       | 0            |
| 4   | E     | 804 | BU3  | 2       | 0            |
| 6   | K     | 808 | HEM  | 7       | 0            |
| 6   | A     | 812 | HEM  | 8       | 0            |
| 6   | J     | 809 | HEM  | 9       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | I     | 808 | HEM  | 5       | 0            |
| 4   | H     | 803 | BU3  | 1       | 0            |
| 6   | B     | 814 | HEM  | 8       | 0            |
| 6   | I     | 806 | HEM  | 8       | 0            |
| 6   | G     | 811 | HEM  | 6       | 0            |
| 6   | F     | 808 | HEM  | 12      | 0            |
| 6   | G     | 808 | HEM  | 6       | 0            |
| 6   | C     | 813 | HEM  | 9       | 0            |
| 6   | E     | 808 | HEM  | 8       | 0            |
| 6   | L     | 808 | HEM  | 9       | 0            |
| 6   | D     | 813 | HEM  | 8       | 0            |
| 6   | H     | 809 | HEM  | 8       | 0            |
| 6   | F     | 811 | HEM  | 9       | 0            |
| 6   | F     | 812 | HEM  | 6       | 0            |
| 6   | D     | 806 | HEM  | 8       | 0            |
| 6   | L     | 813 | HEM  | 11      | 0            |
| 6   | C     | 809 | HEM  | 6       | 0            |
| 6   | B     | 807 | HEM  | 6       | 0            |
| 6   | E     | 812 | HEM  | 8       | 0            |
| 6   | H     | 812 | HEM  | 7       | 0            |
| 6   | G     | 807 | HEM  | 11      | 0            |
| 6   | K     | 811 | HEM  | 7       | 0            |
| 6   | B     | 809 | HEM  | 7       | 0            |
| 6   | L     | 812 | HEM  | 9       | 0            |
| 6   | J     | 811 | HEM  | 6       | 0            |
| 6   | G     | 813 | HEM  | 8       | 0            |
| 6   | E     | 806 | HEM  | 7       | 0            |
| 6   | A     | 811 | HEM  | 6       | 0            |
| 6   | C     | 811 | HEM  | 7       | 0            |
| 6   | I     | 811 | HEM  | 6       | 0            |
| 6   | K     | 807 | HEM  | 9       | 0            |
| 6   | H     | 810 | HEM  | 8       | 0            |
| 6   | C     | 806 | HEM  | 8       | 0            |
| 6   | B     | 811 | HEM  | 9       | 0            |
| 6   | B     | 812 | HEM  | 7       | 0            |
| 6   | H     | 807 | HEM  | 9       | 0            |
| 6   | J     | 810 | HEM  | 7       | 0            |
| 6   | A     | 813 | HEM  | 7       | 0            |
| 6   | L     | 807 | HEM  | 14      | 0            |
| 6   | K     | 812 | HEM  | 7       | 0            |
| 6   | C     | 810 | HEM  | 8       | 0            |
| 6   | K     | 809 | HEM  | 8       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | D     | 807 | HEM  | 8       | 0            |
| 6   | D     | 811 | HEM  | 6       | 0            |
| 6   | D     | 812 | HEM  | 9       | 0            |
| 6   | E     | 810 | HEM  | 11      | 0            |
| 6   | I     | 810 | HEM  | 8       | 0            |
| 6   | L     | 809 | HEM  | 11      | 0            |
| 6   | D     | 809 | HEM  | 11      | 0            |
| 6   | H     | 811 | HEM  | 10      | 0            |
| 6   | H     | 808 | HEM  | 11      | 0            |
| 6   | L     | 811 | HEM  | 8       | 0            |
| 6   | A     | 810 | HEM  | 10      | 0            |
| 6   | I     | 809 | HEM  | 8       | 0            |
| 6   | J     | 806 | HEM  | 7       | 0            |
| 6   | B     | 808 | HEM  | 13      | 0            |
| 6   | J     | 808 | HEM  | 7       | 0            |
| 6   | F     | 807 | HEM  | 8       | 0            |
| 6   | D     | 808 | HEM  | 8       | 0            |
| 6   | G     | 810 | HEM  | 7       | 0            |
| 6   | C     | 808 | HEM  | 10      | 0            |
| 6   | J     | 807 | HEM  | 12      | 0            |
| 6   | E     | 809 | HEM  | 7       | 0            |
| 6   | J     | 813 | HEM  | 9       | 0            |
| 5   | F     | 806 | ACT  | 1       | 0            |
| 6   | H     | 814 | HEM  | 7       | 0            |
| 6   | E     | 813 | HEM  | 8       | 0            |
| 6   | I     | 813 | HEM  | 7       | 0            |
| 6   | I     | 807 | HEM  | 6       | 0            |
| 6   | A     | 808 | HEM  | 7       | 0            |
| 6   | A     | 806 | HEM  | 7       | 0            |
| 6   | J     | 812 | HEM  | 7       | 0            |
| 6   | F     | 809 | HEM  | 4       | 0            |
| 6   | K     | 813 | HEM  | 7       | 0            |
| 6   | B     | 813 | HEM  | 6       | 0            |
| 6   | C     | 812 | HEM  | 8       | 0            |
| 6   | I     | 812 | HEM  | 10      | 0            |
| 5   | C     | 805 | ACT  | 1       | 0            |
| 6   | E     | 811 | HEM  | 5       | 0            |
| 6   | K     | 810 | HEM  | 8       | 0            |
| 6   | G     | 812 | HEM  | 9       | 0            |
| 6   | B     | 810 | HEM  | 10      | 0            |
| 6   | D     | 810 | HEM  | 10      | 0            |
| 6   | G     | 806 | HEM  | 9       | 0            |

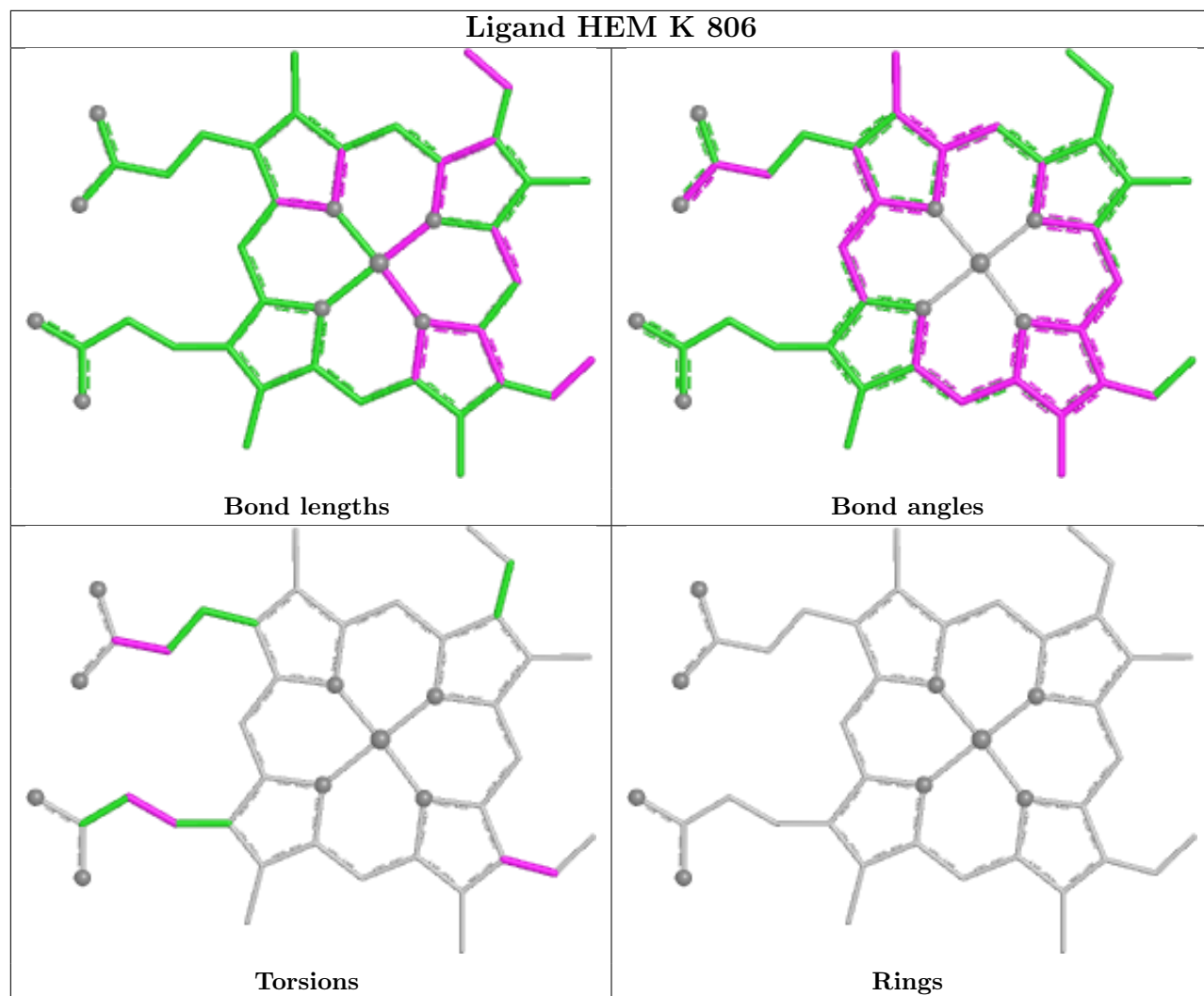
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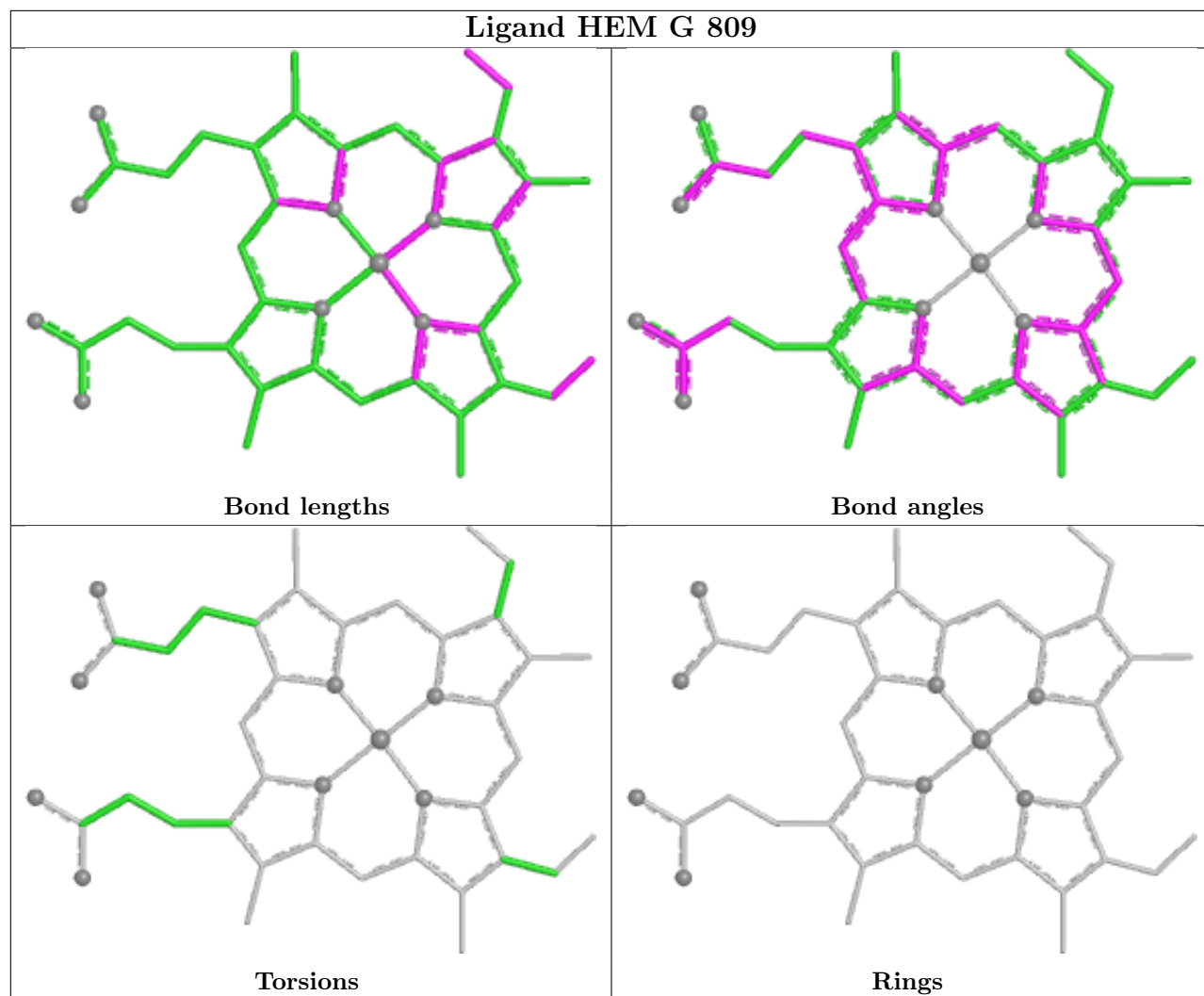
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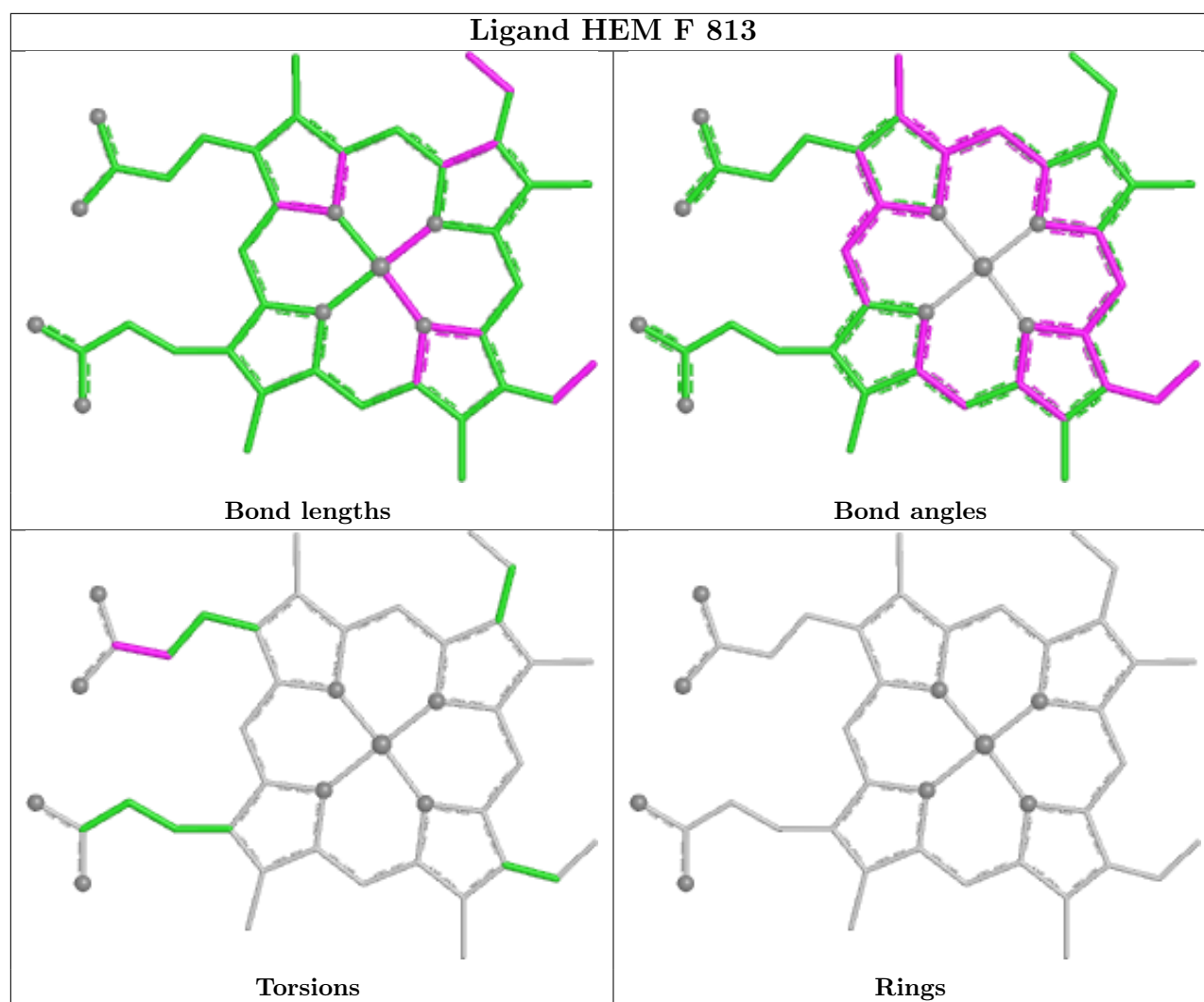
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | E     | 807 | HEM  | 11      | 0            |
| 4   | K     | 803 | BU3  | 1       | 0            |
| 6   | L     | 806 | HEM  | 8       | 0            |
| 6   | A     | 809 | HEM  | 10      | 0            |
| 6   | A     | 807 | HEM  | 9       | 0            |
| 6   | C     | 807 | HEM  | 14      | 0            |
| 6   | H     | 813 | HEM  | 8       | 0            |
| 6   | L     | 810 | HEM  | 6       | 0            |
| 6   | F     | 810 | HEM  | 9       | 0            |

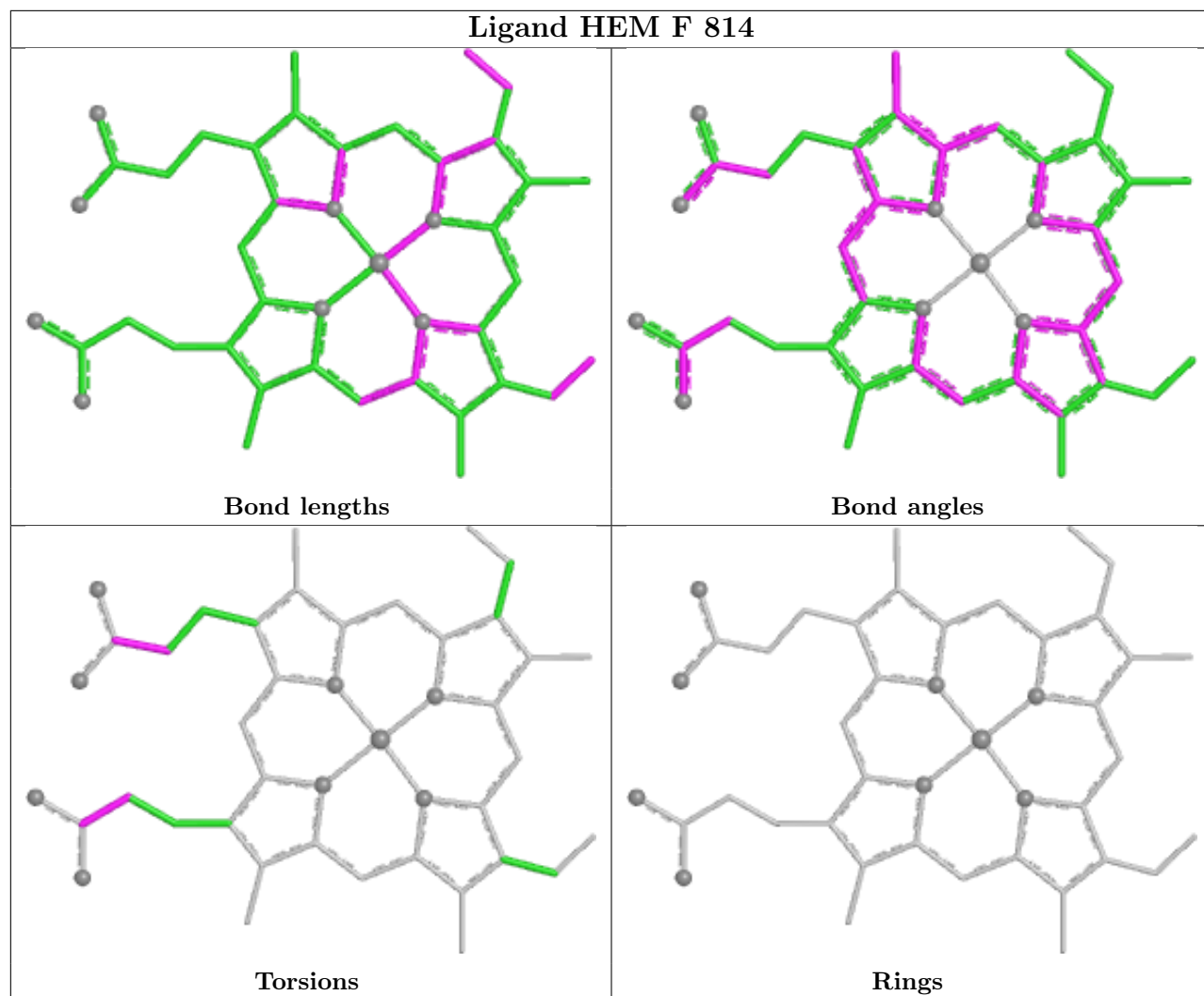
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

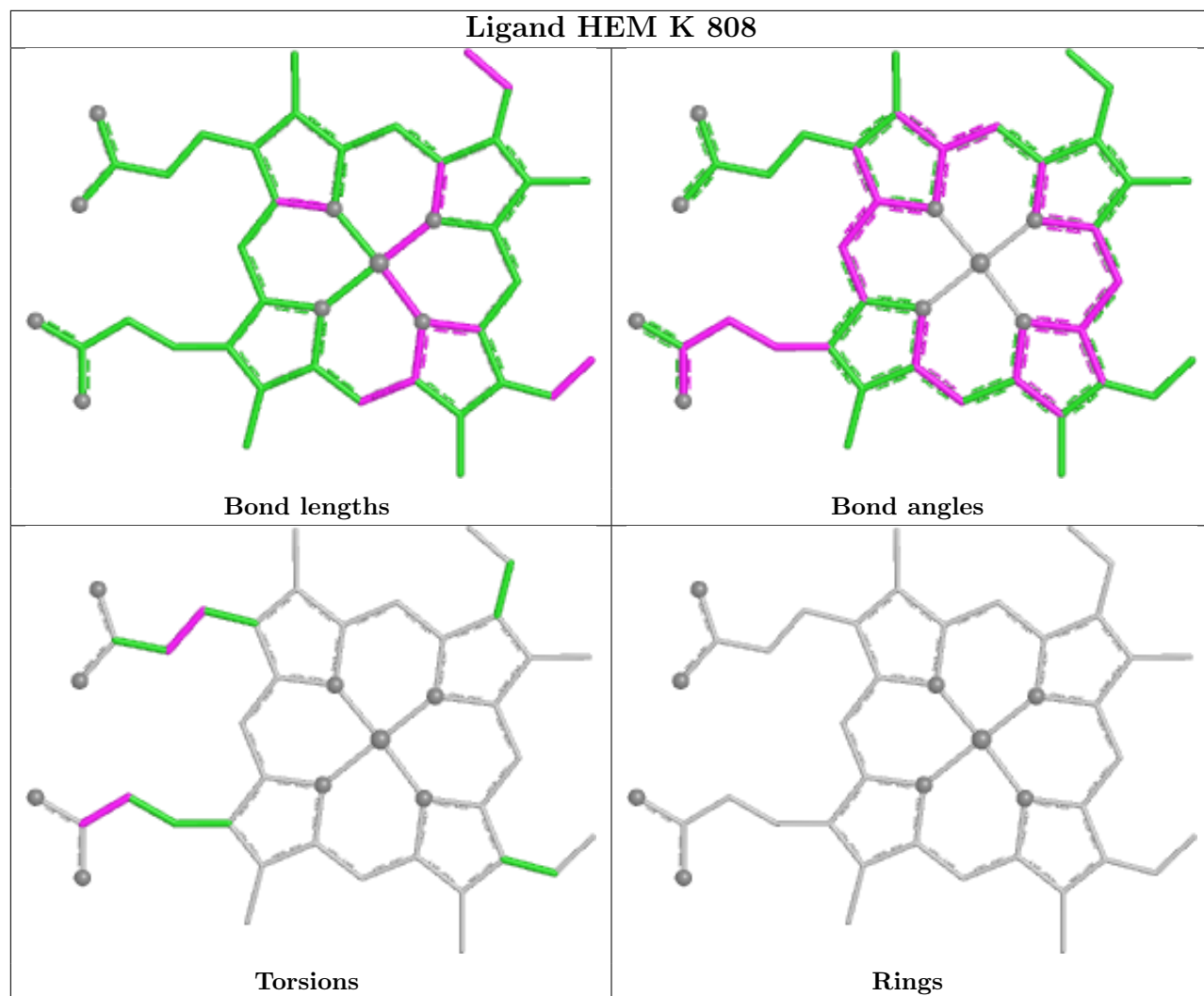


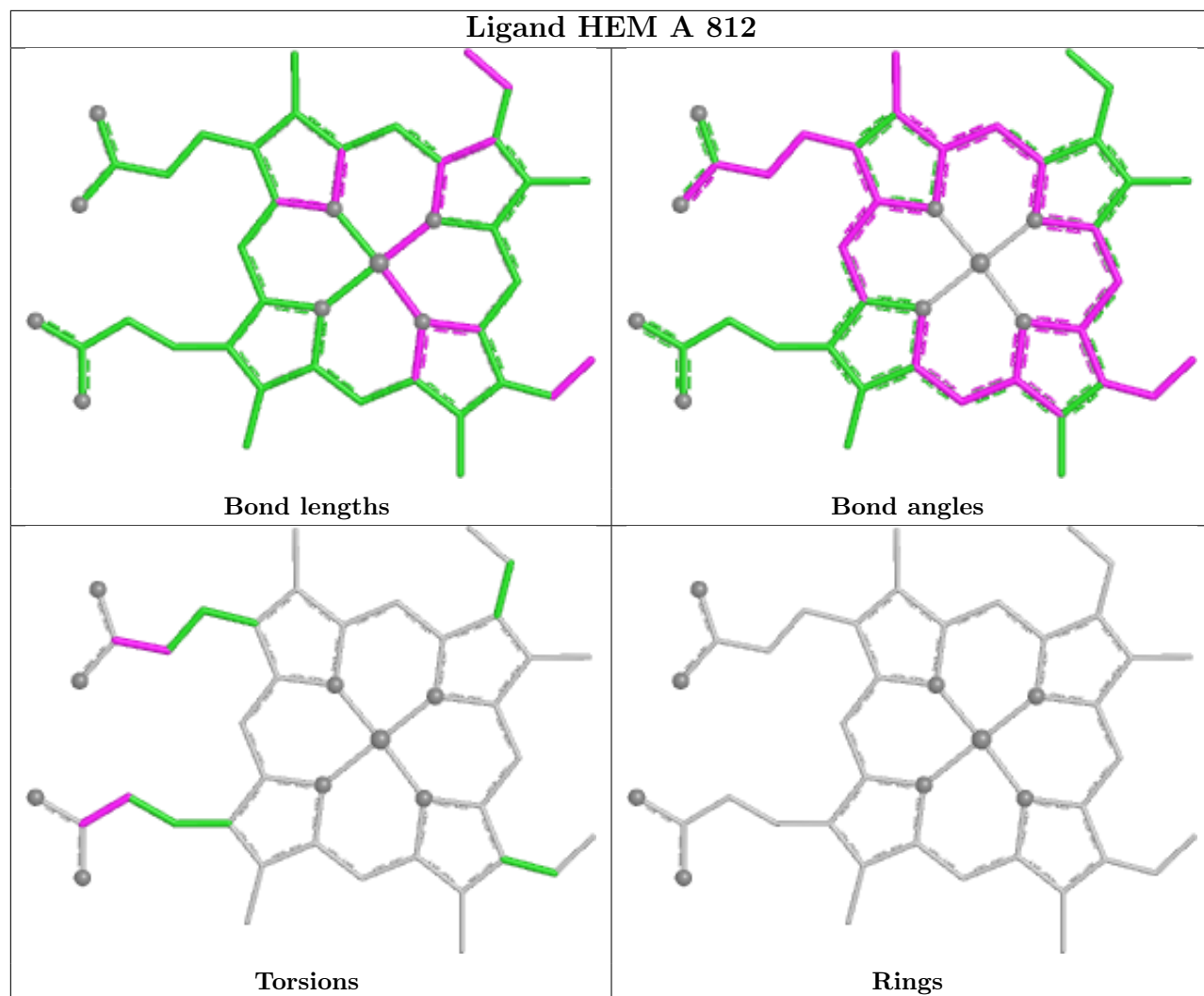


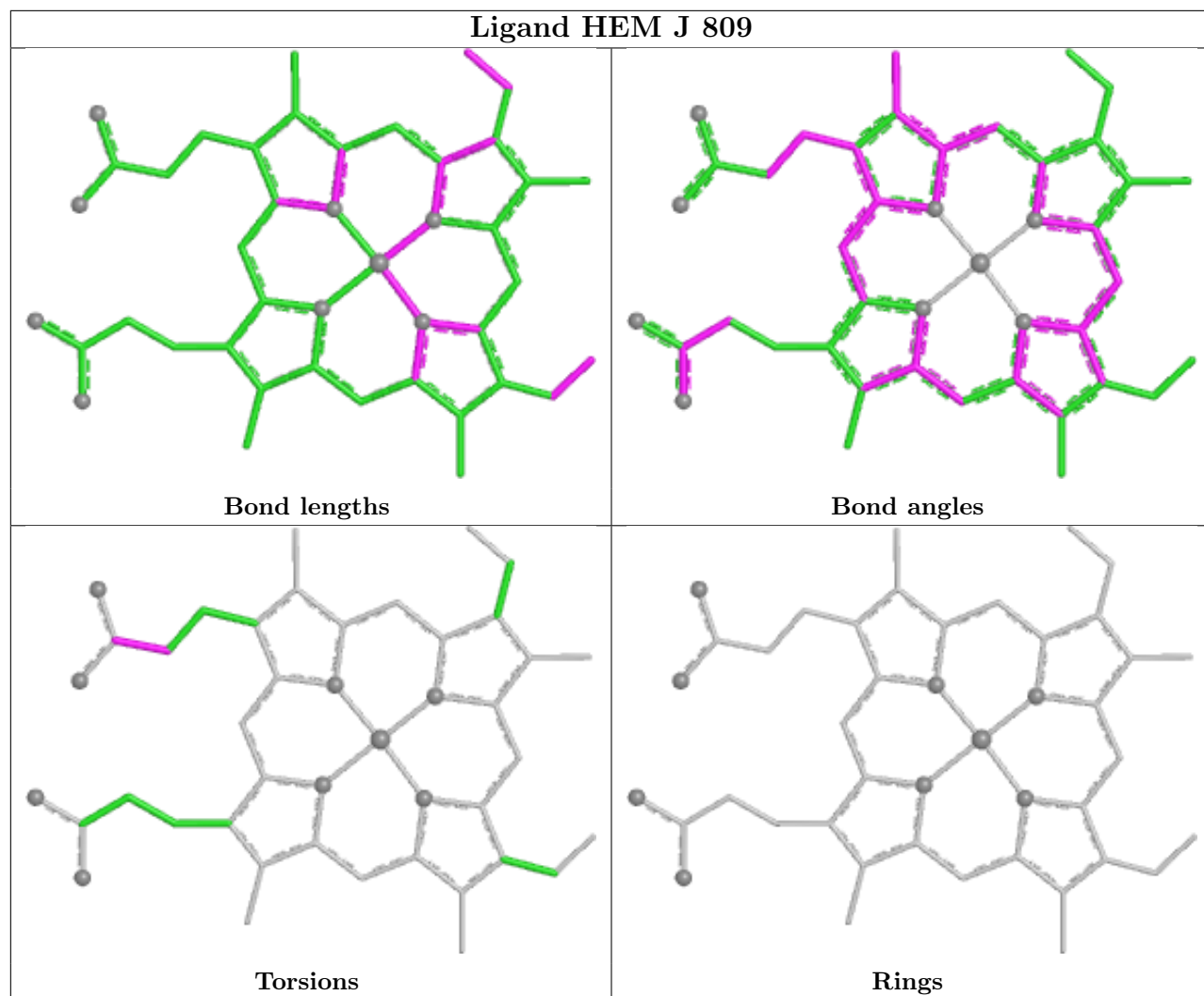






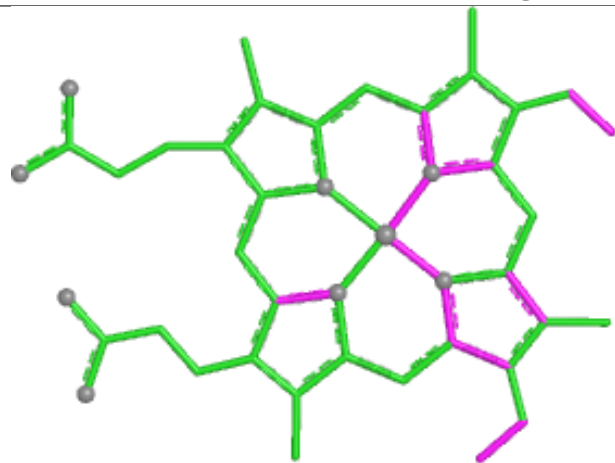




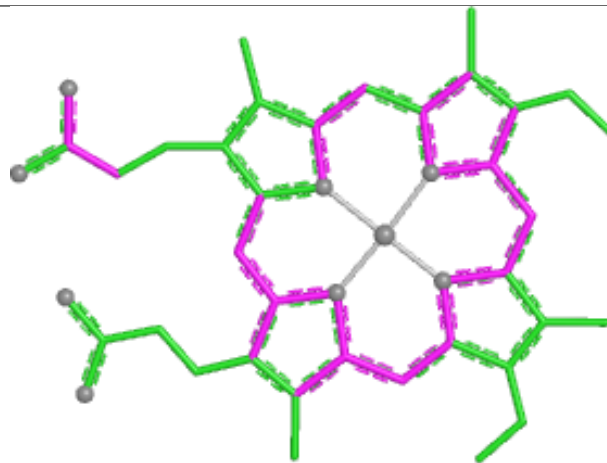




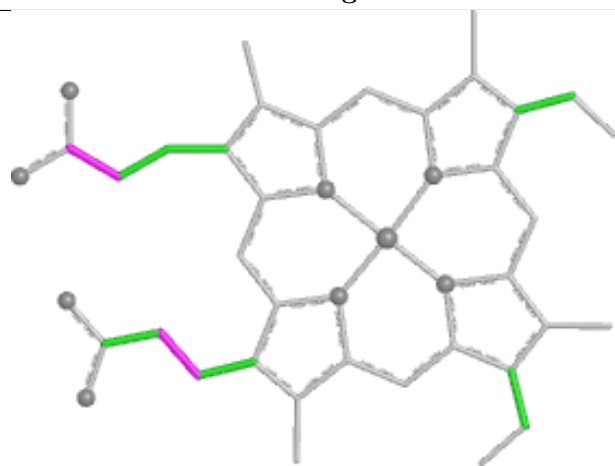
## Ligand HEM I 808



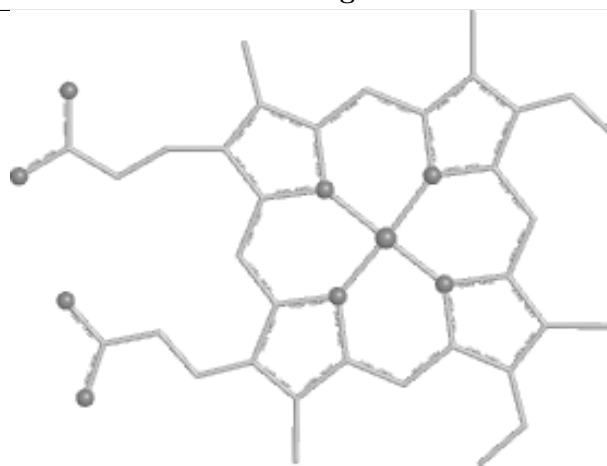
Bond lengths



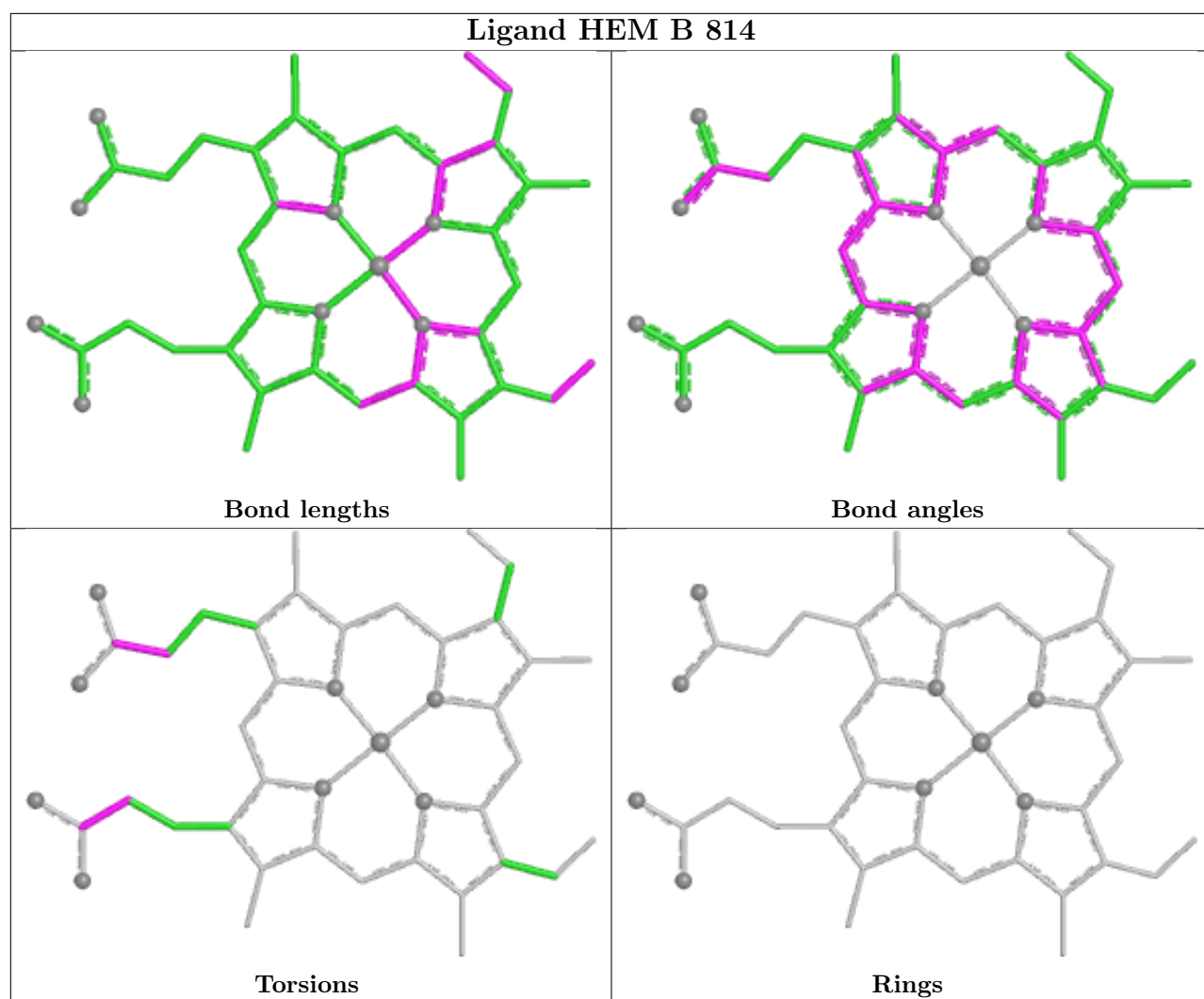
Bond angles



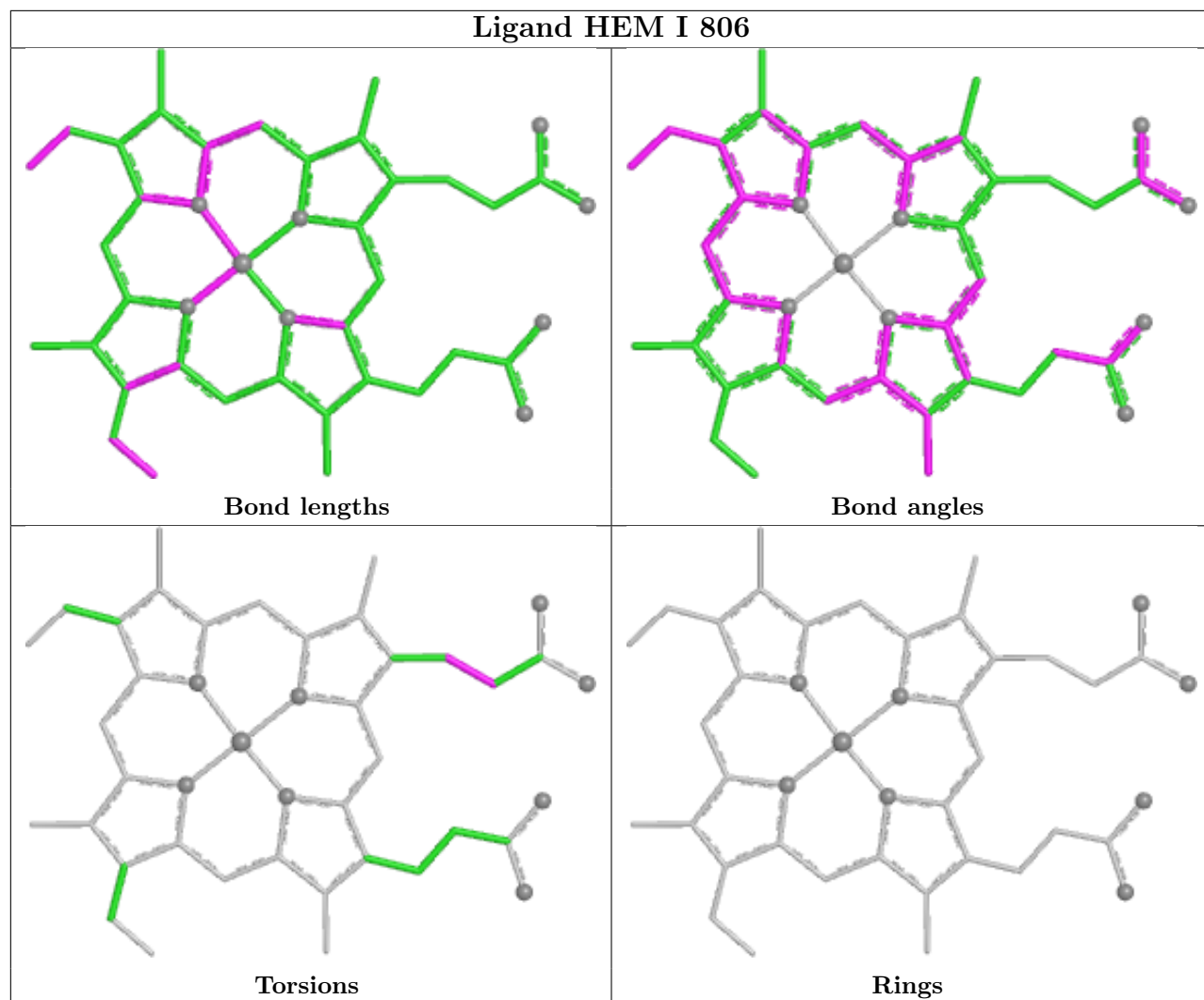
Torsions

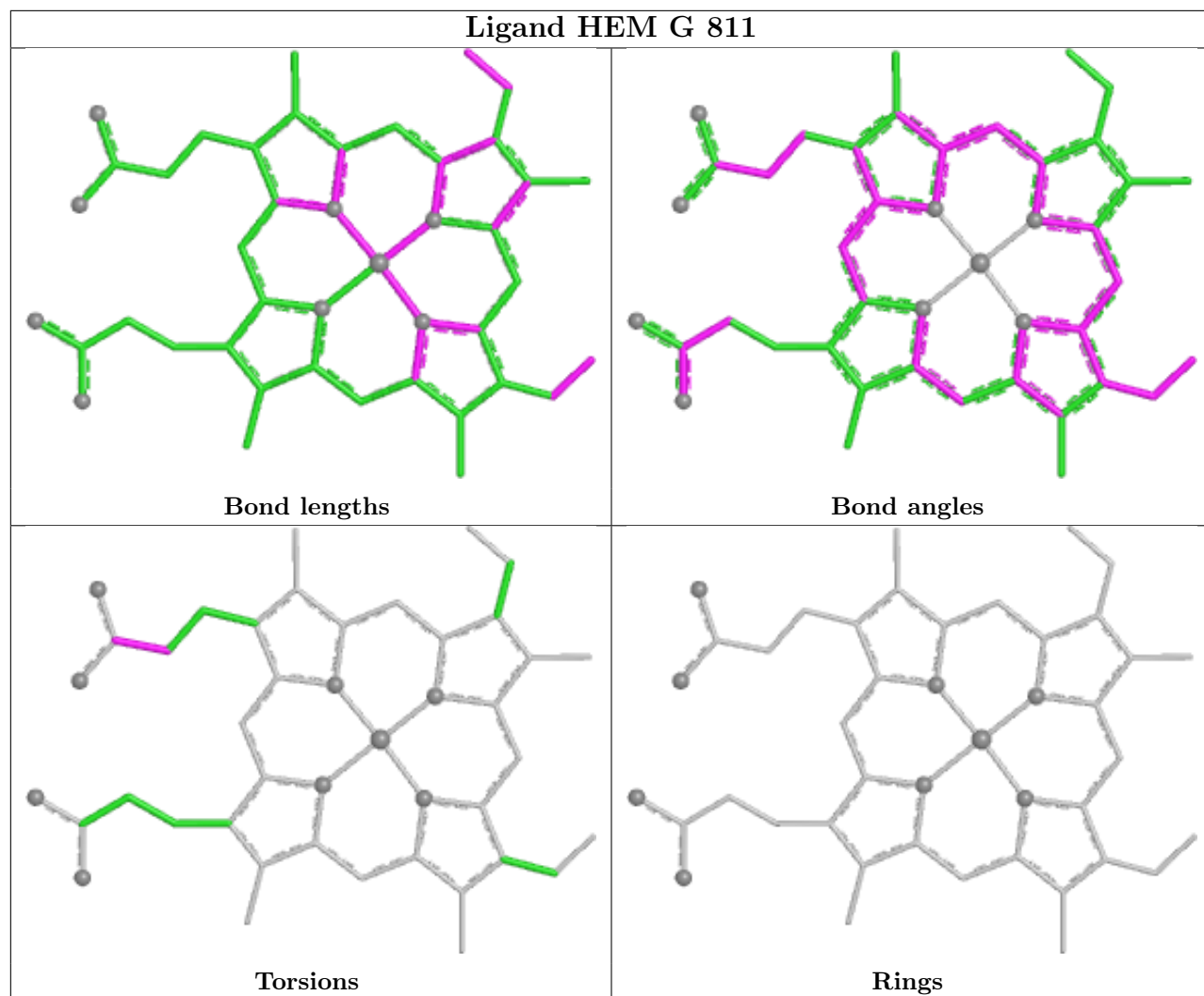


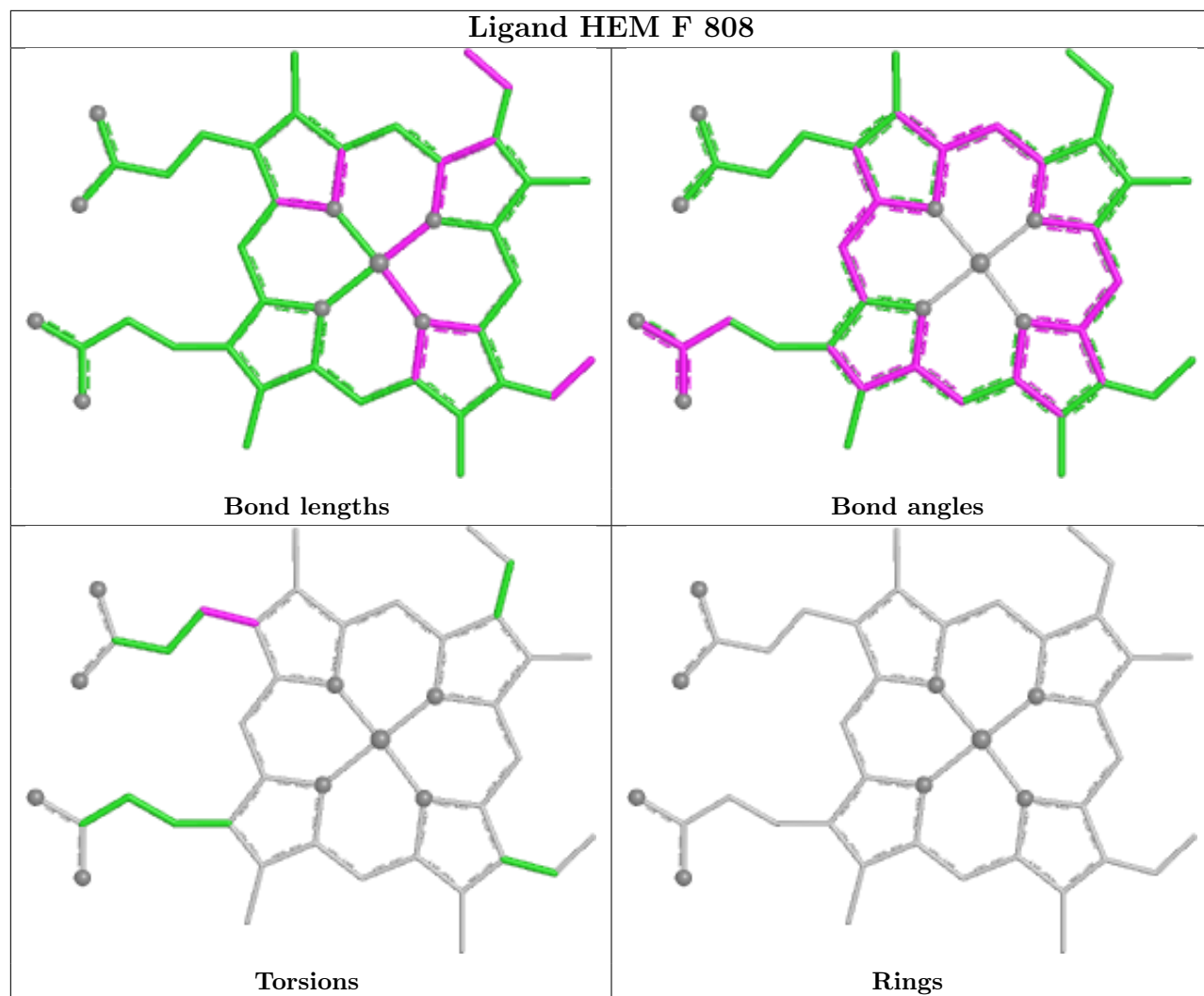
Rings

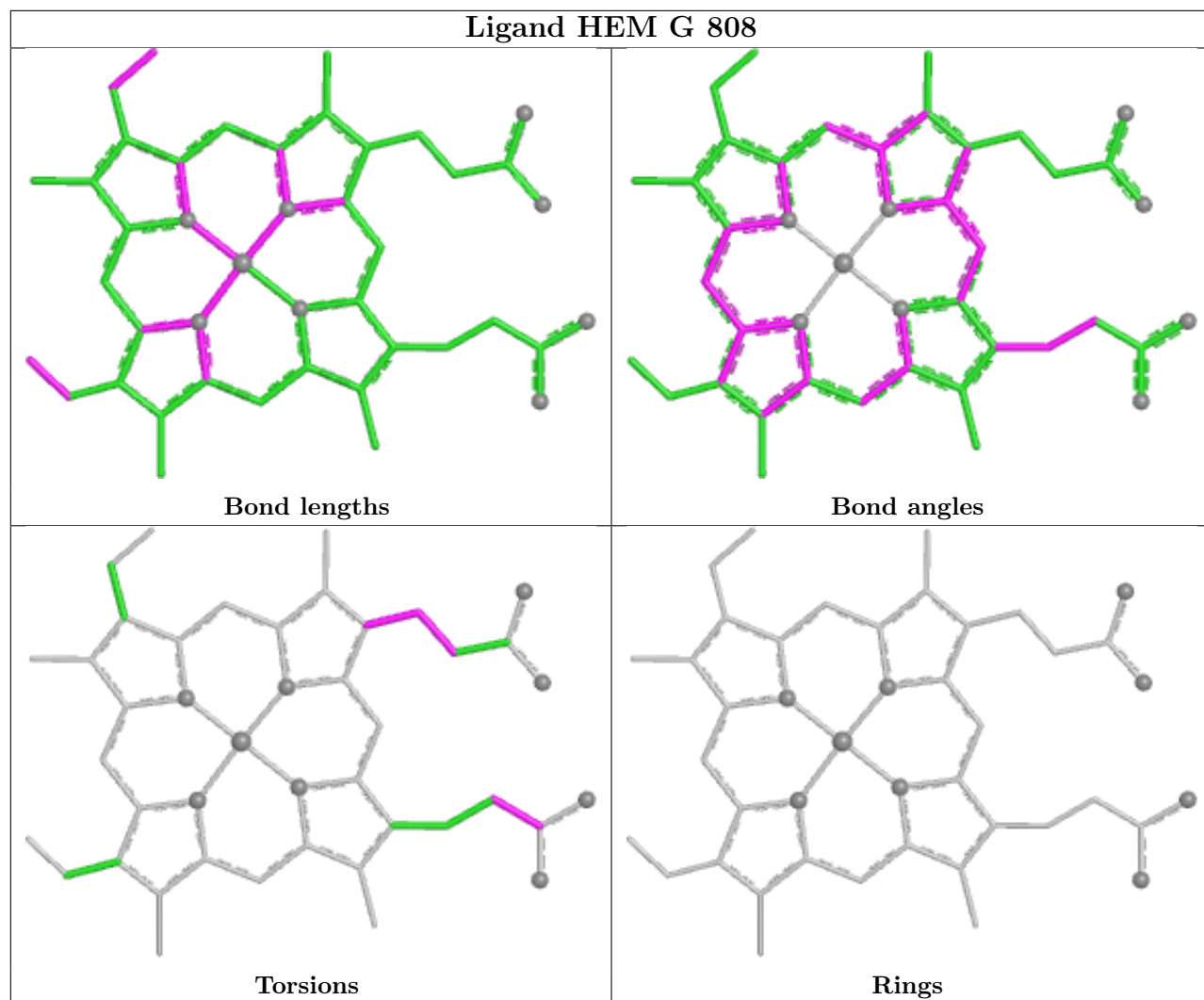


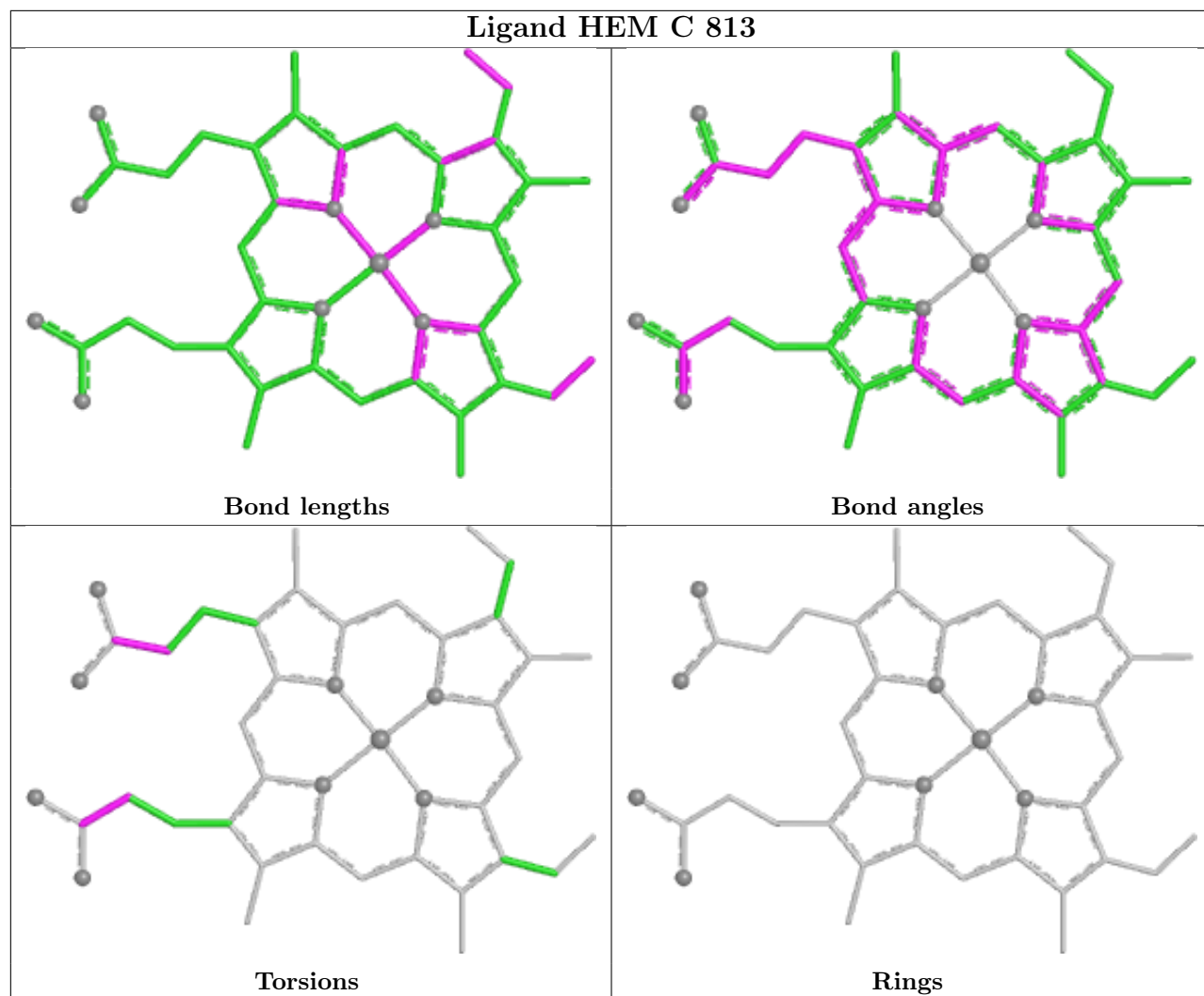
## Ligand HEM I 806

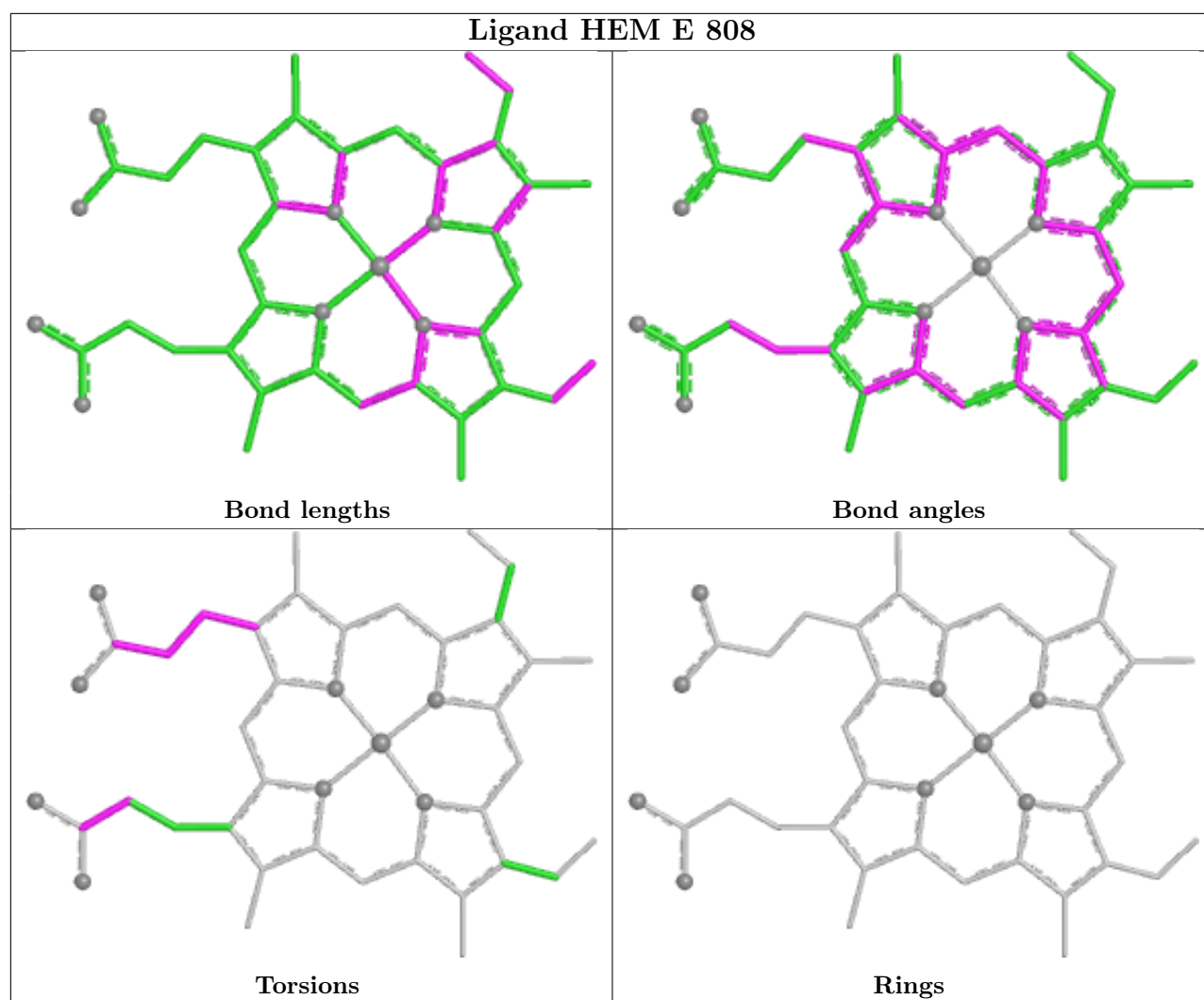




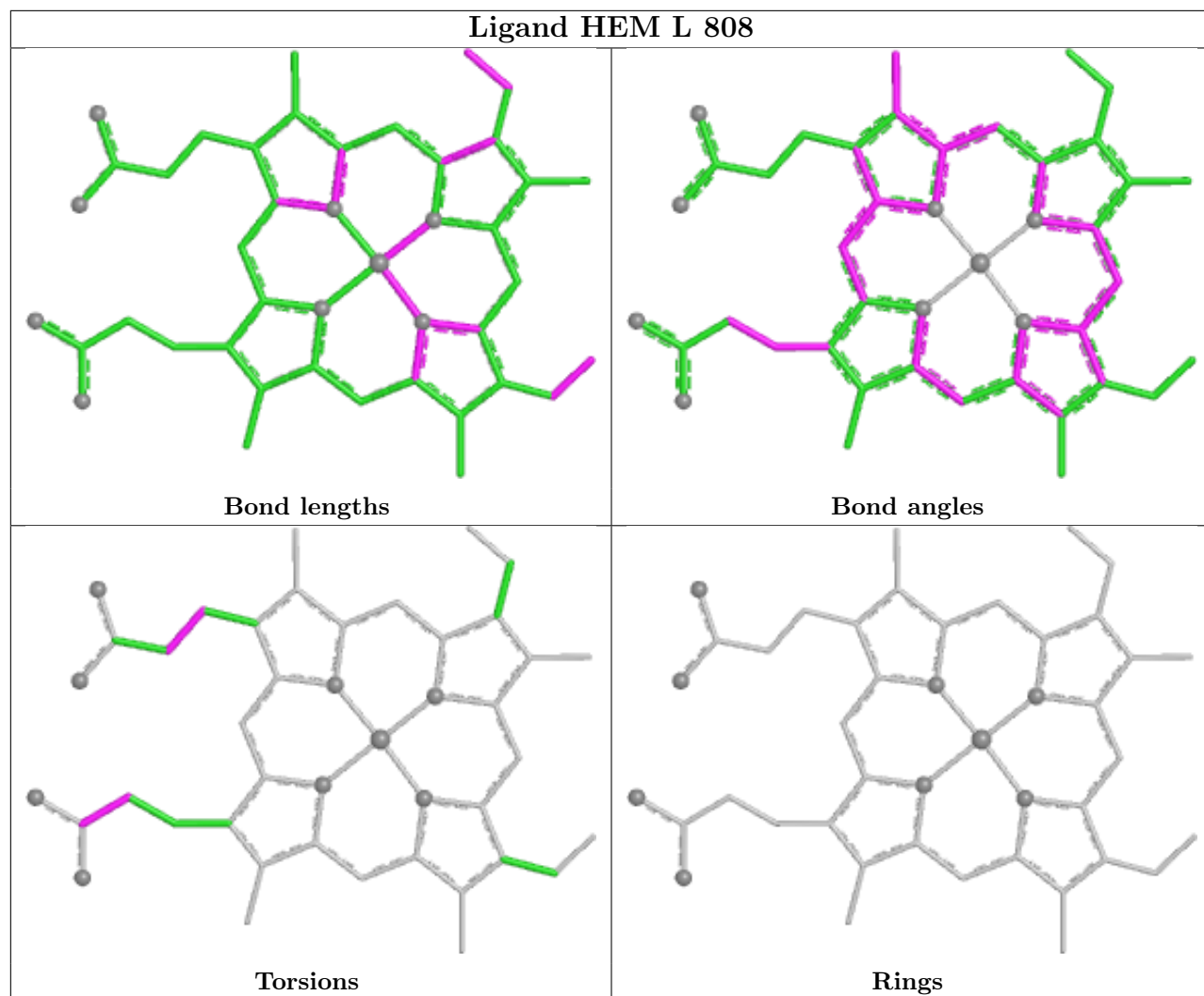


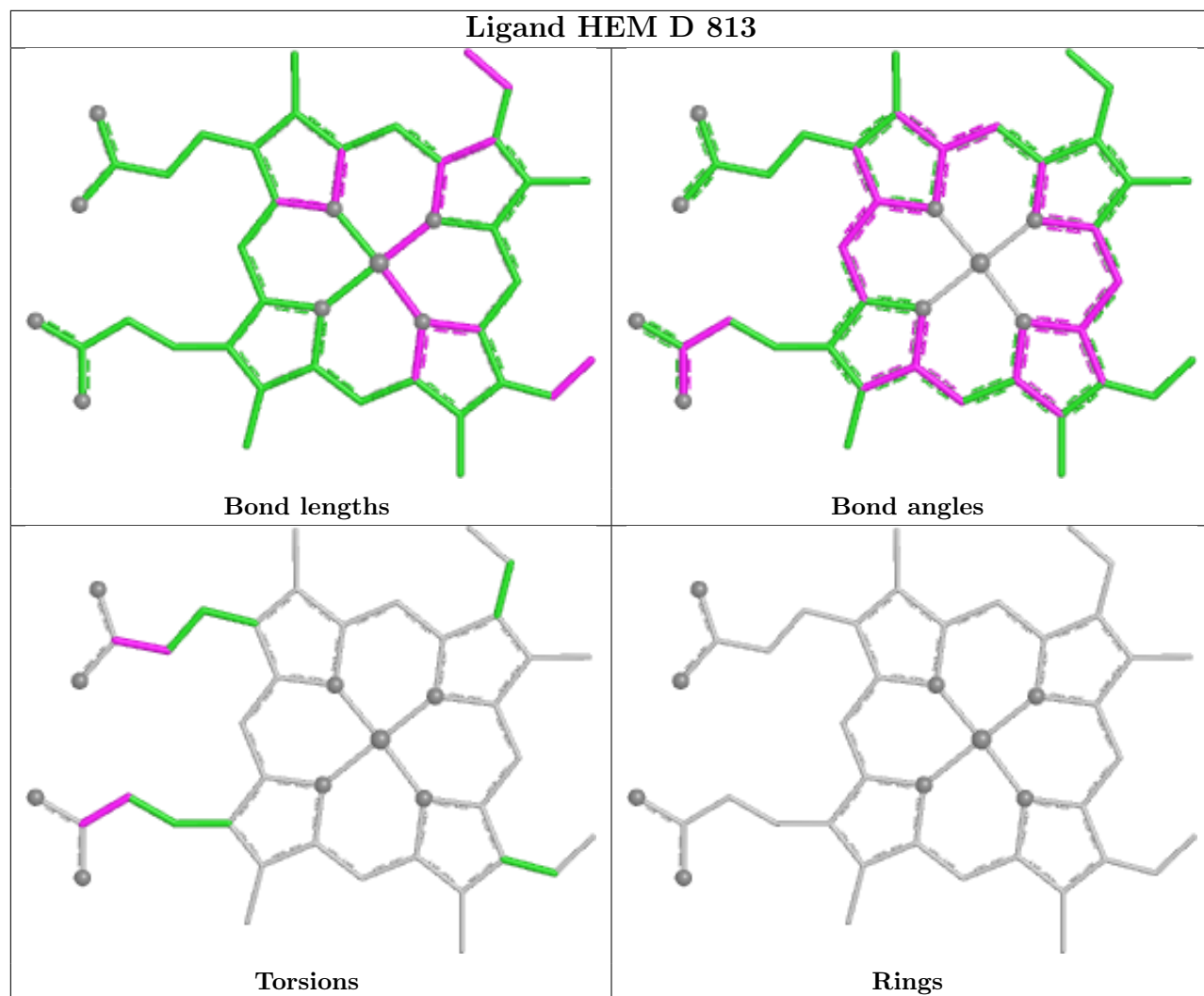


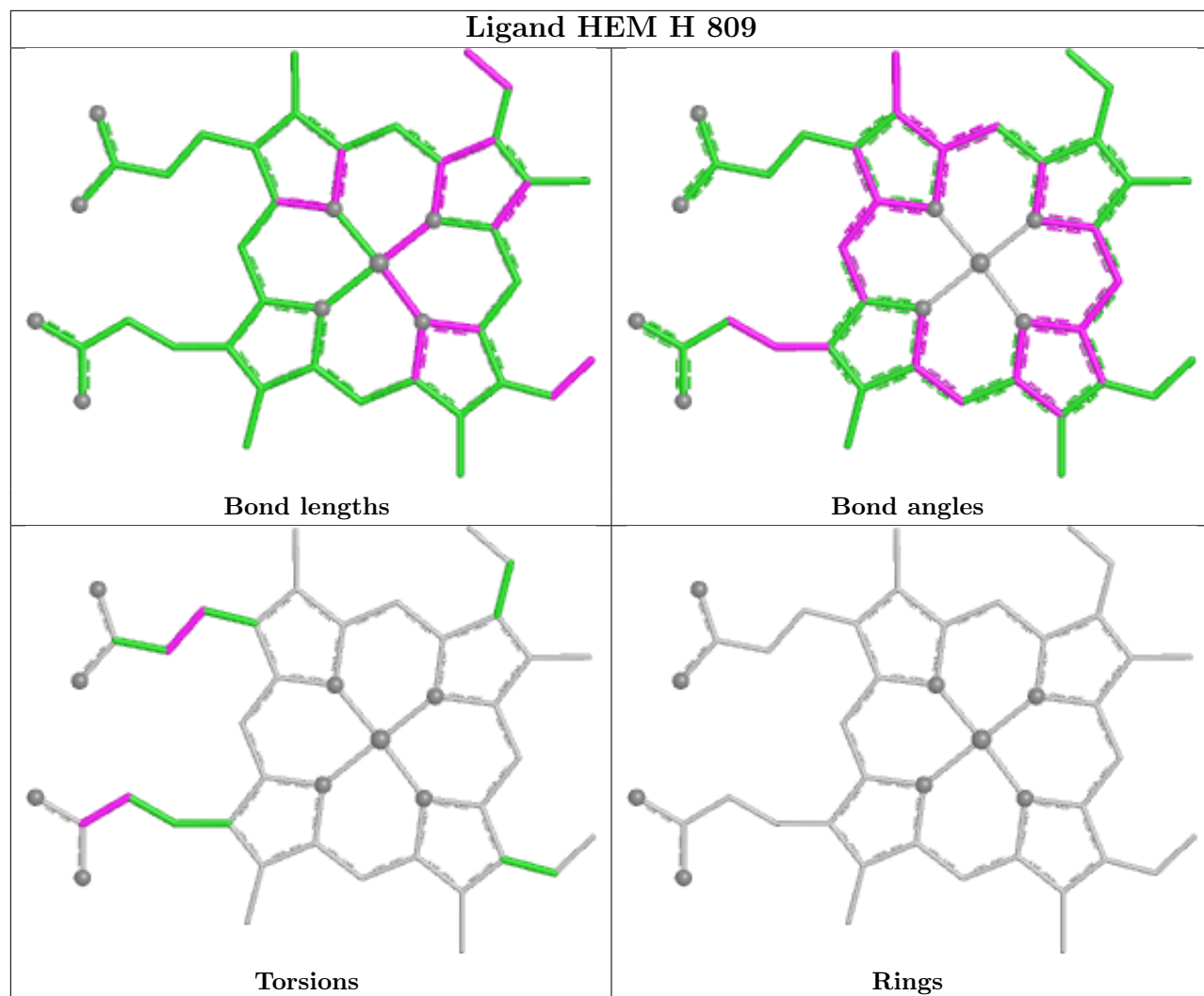


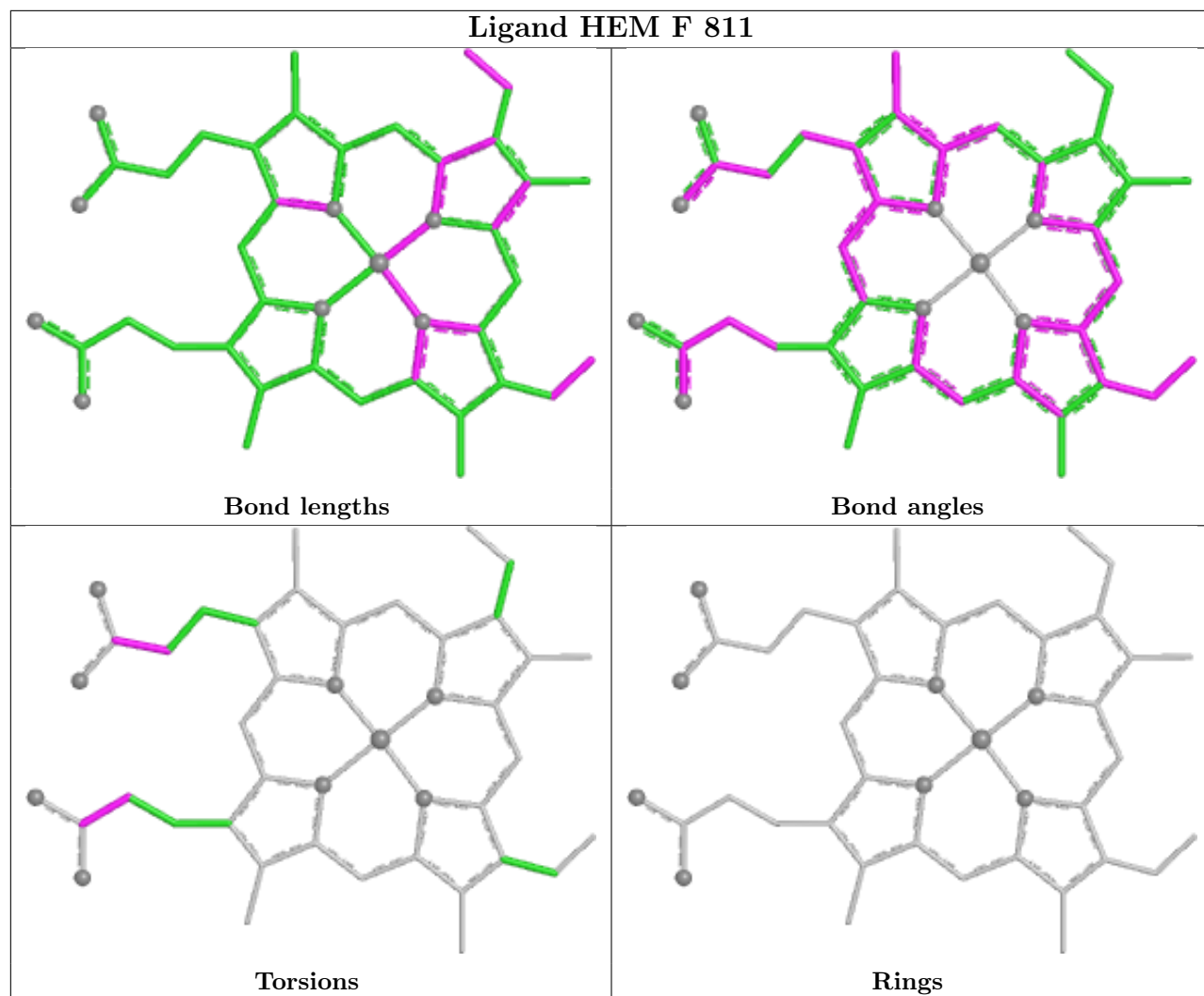


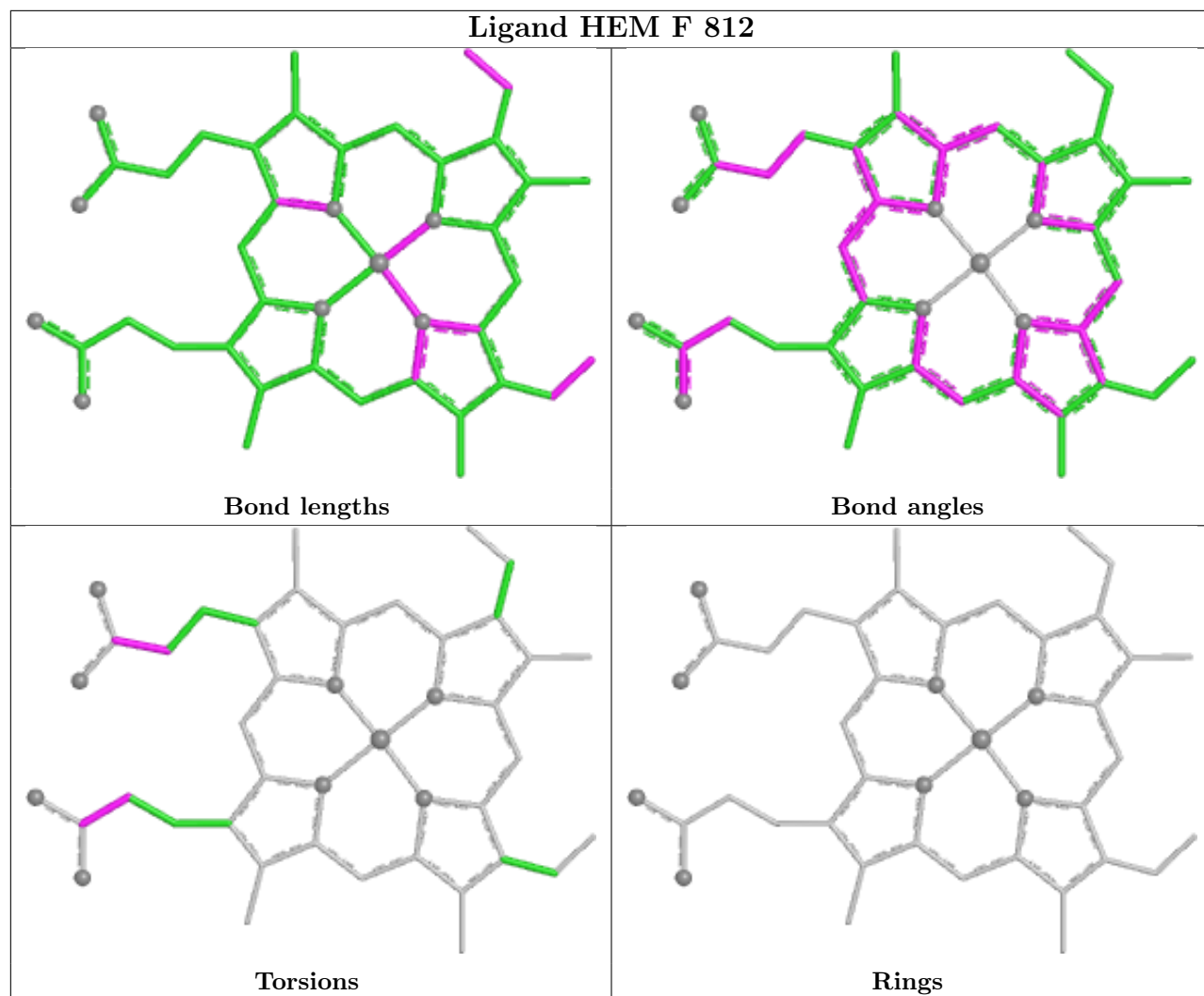


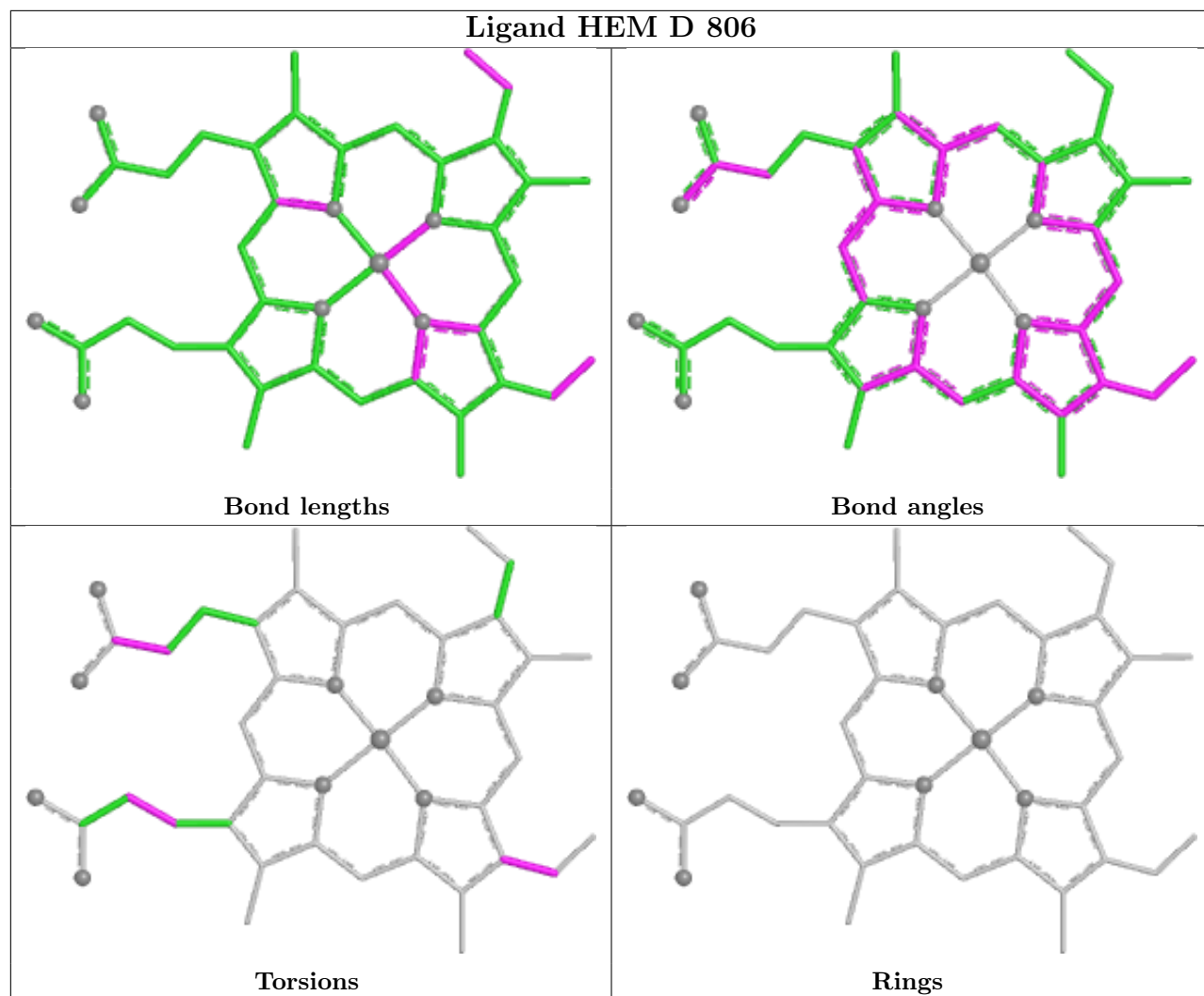


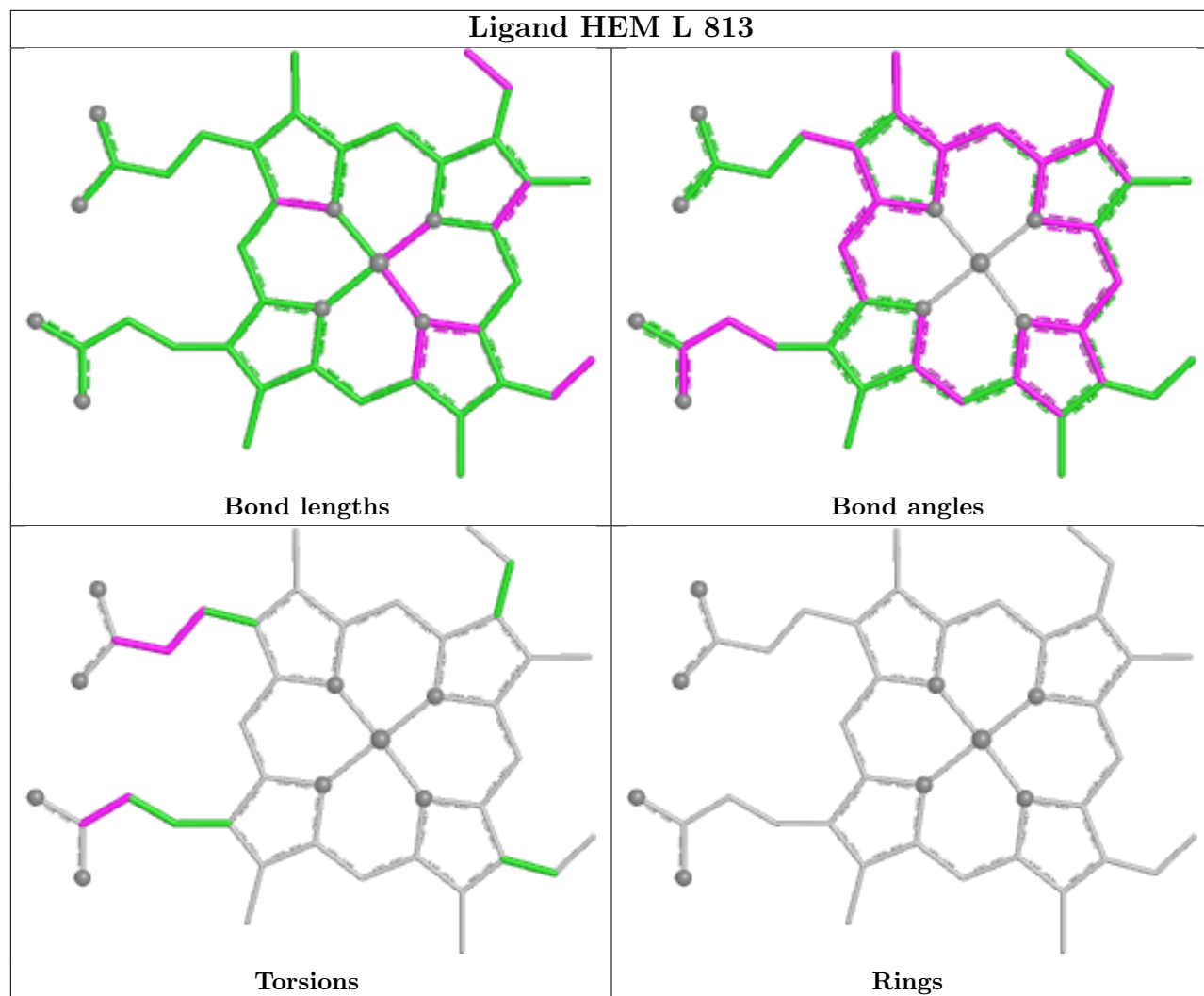


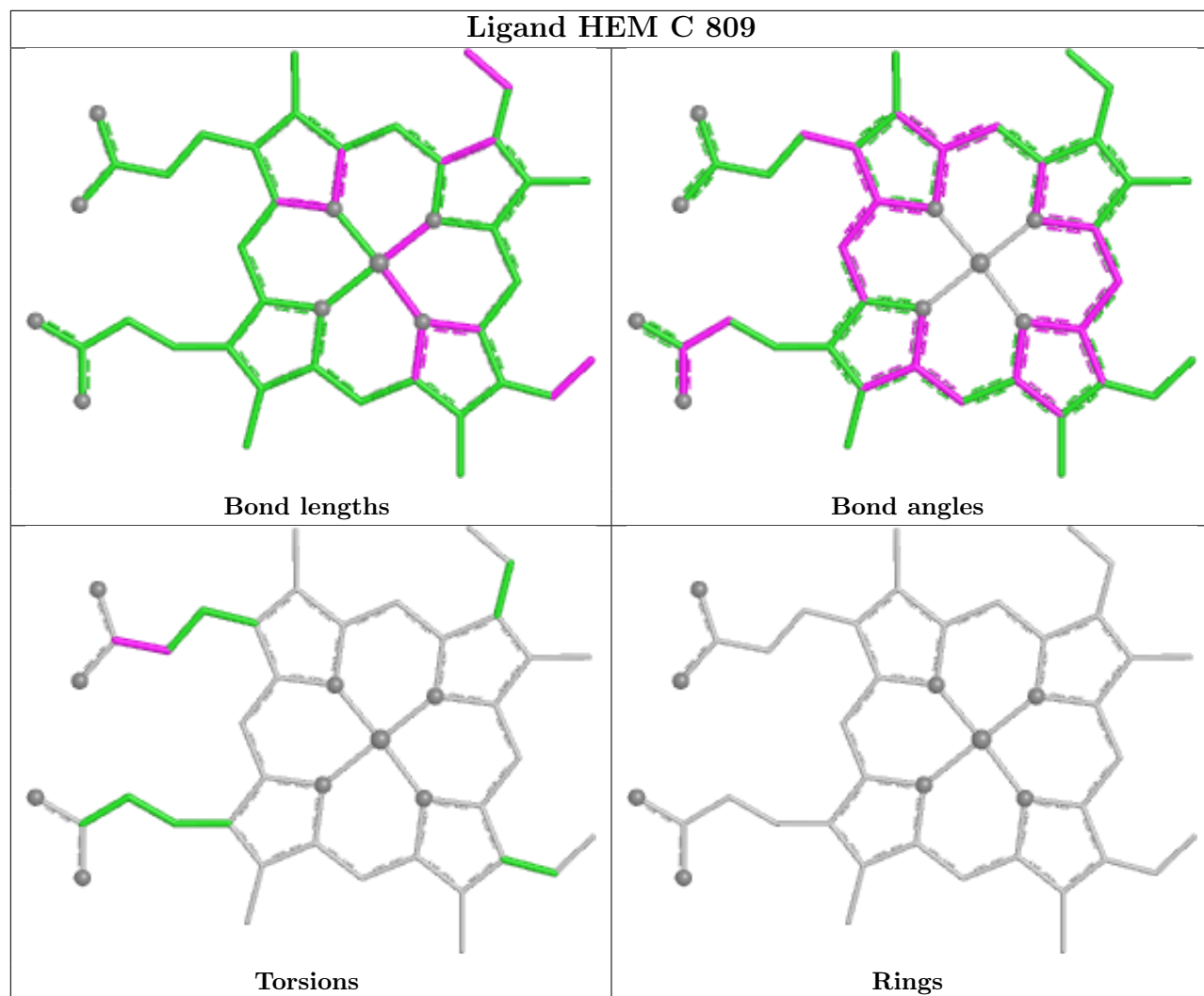




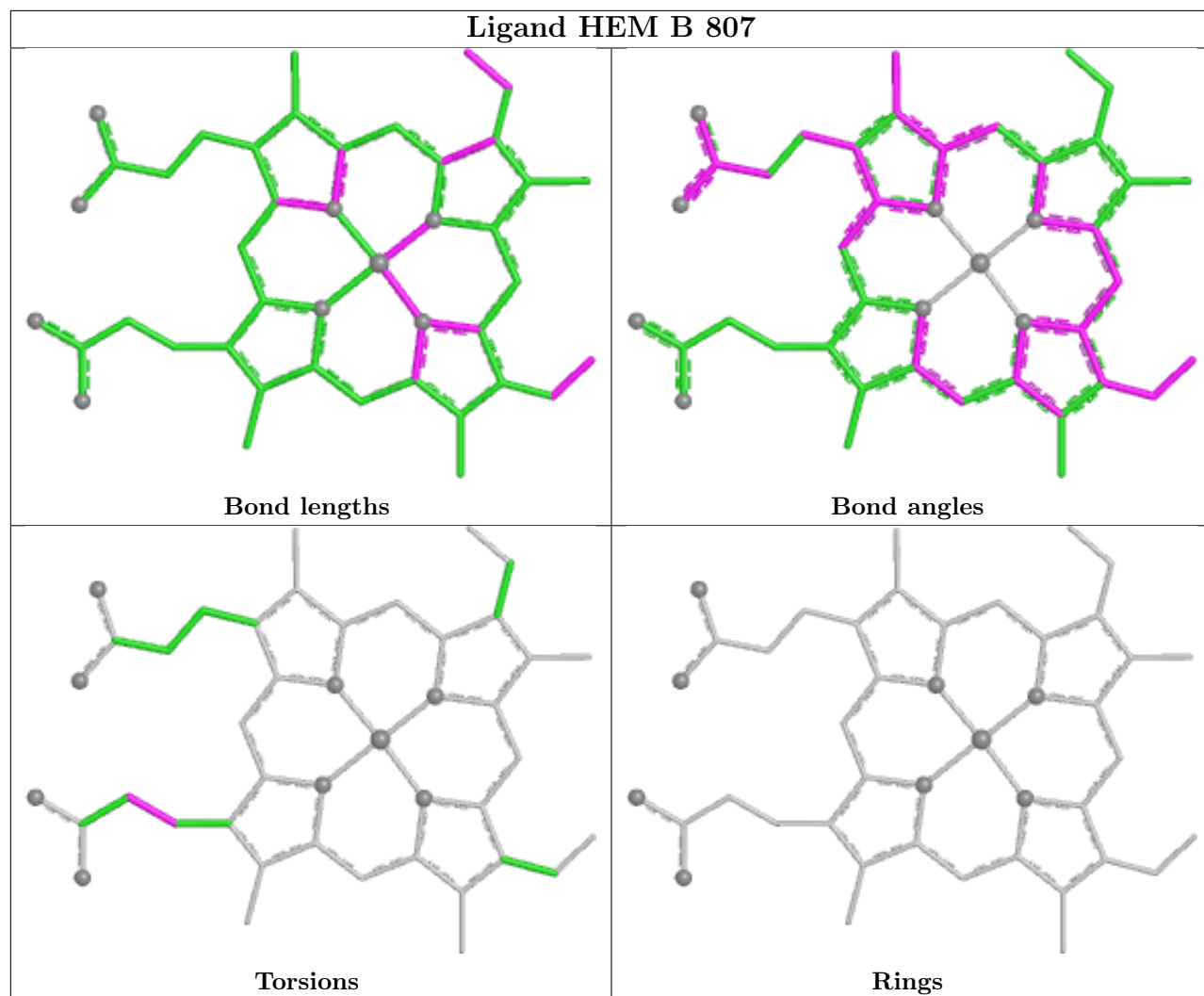


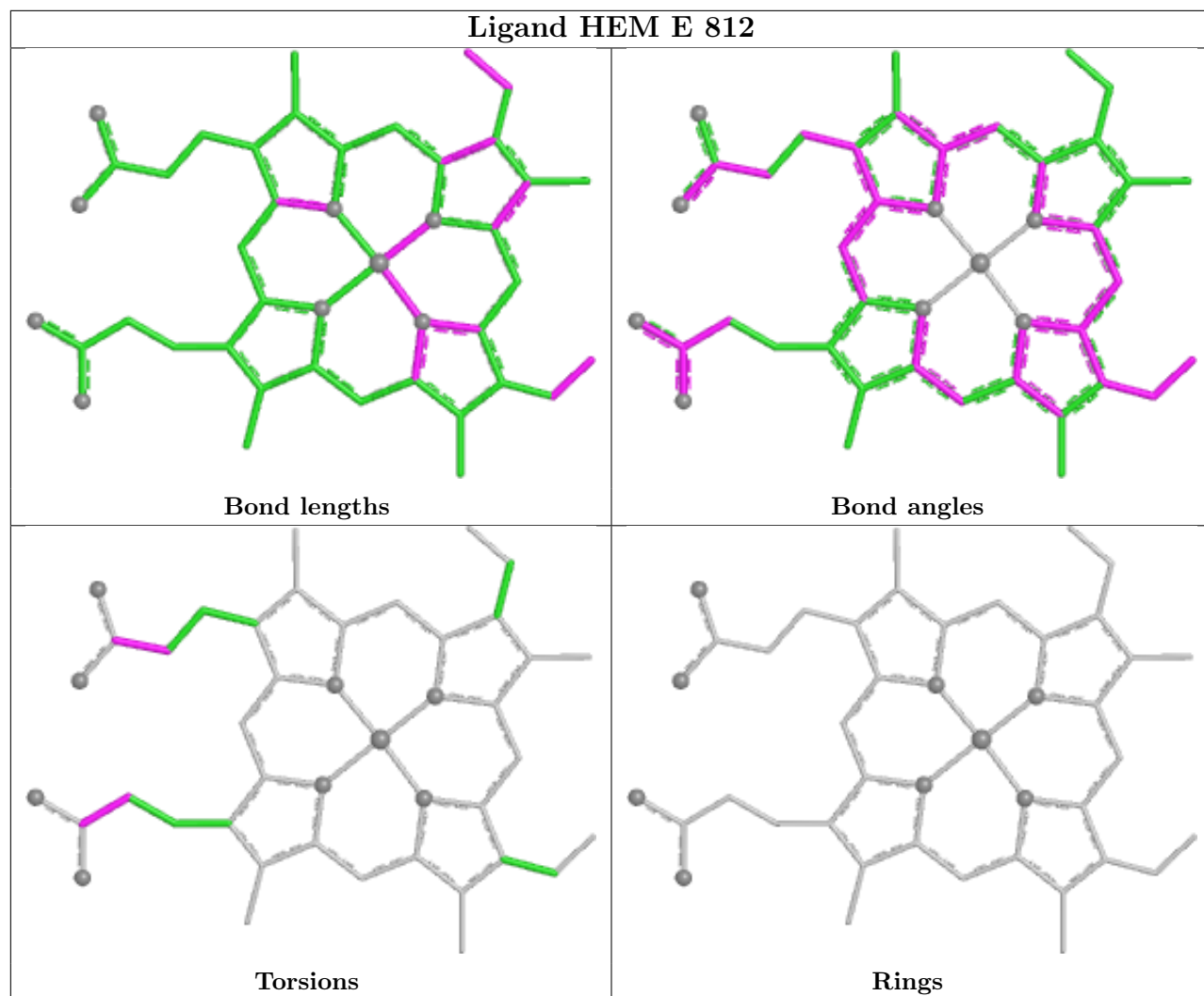


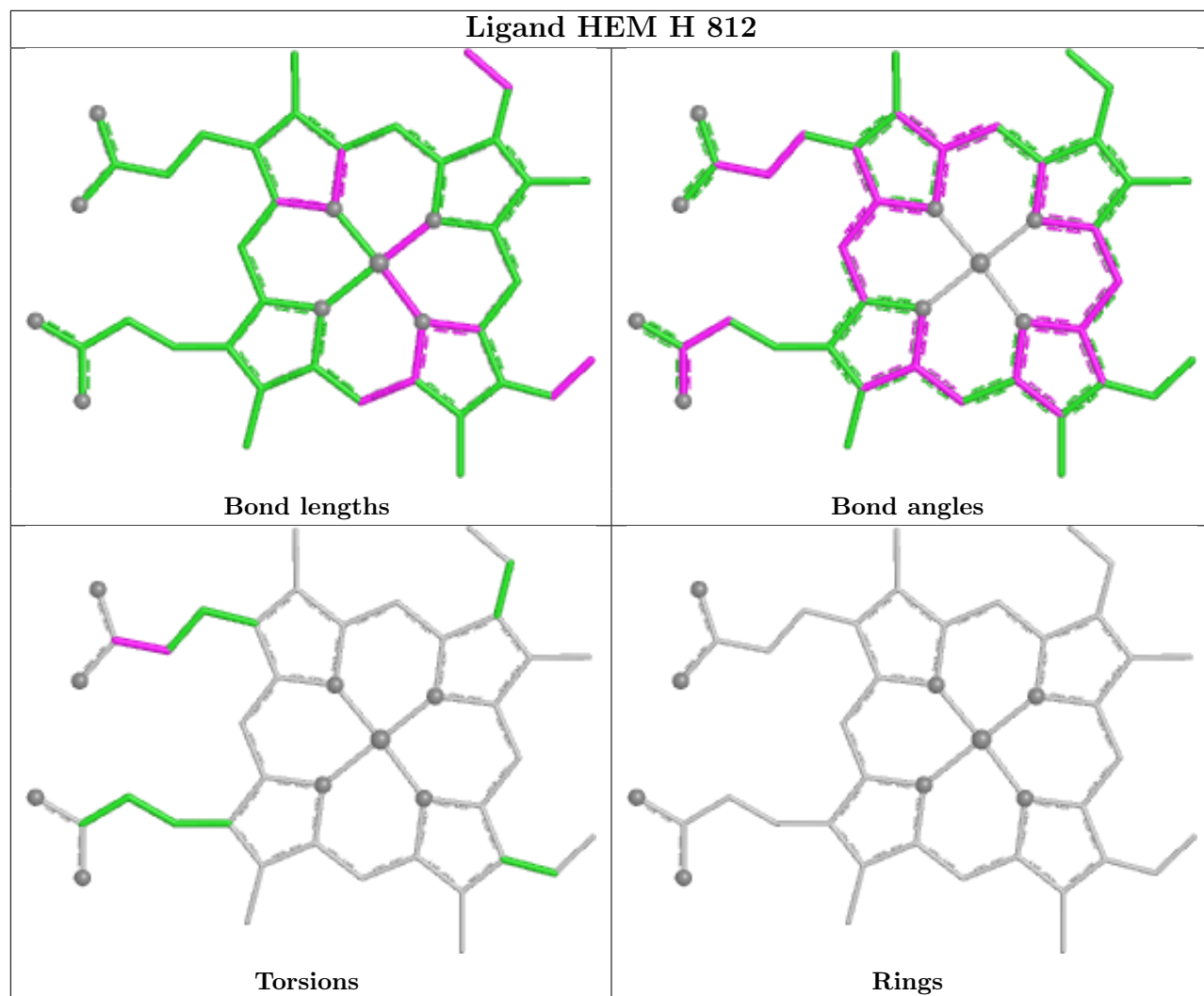


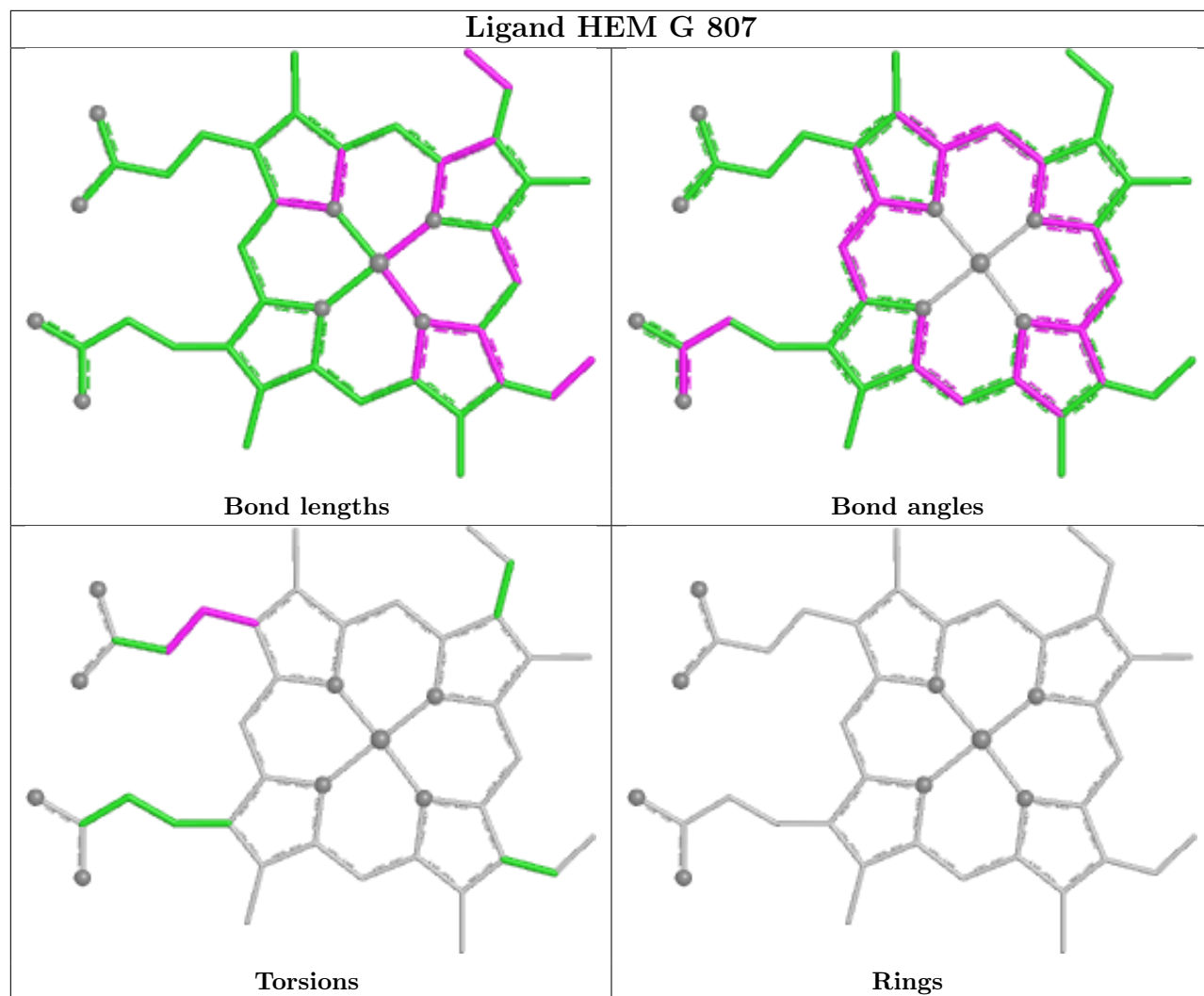


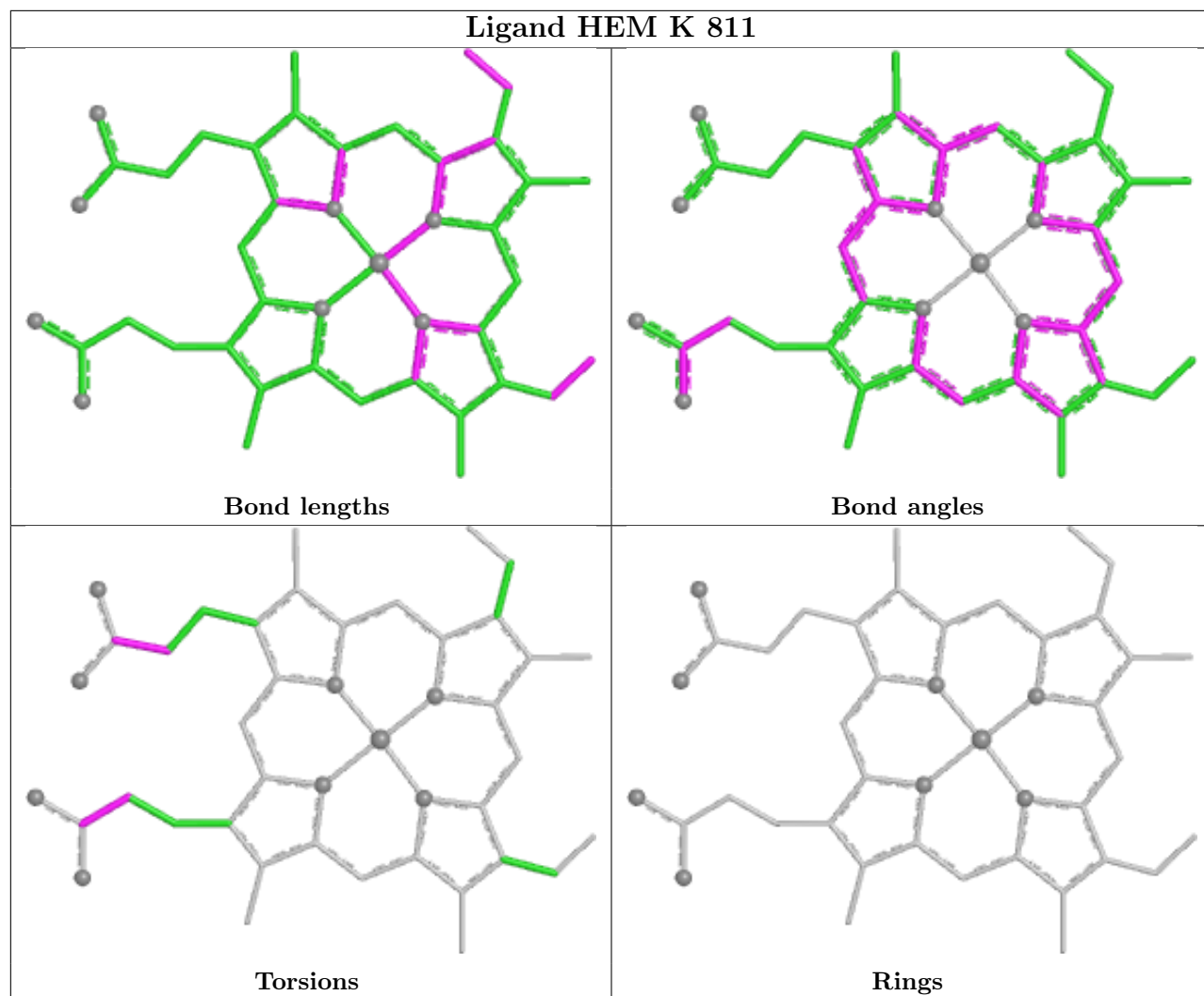


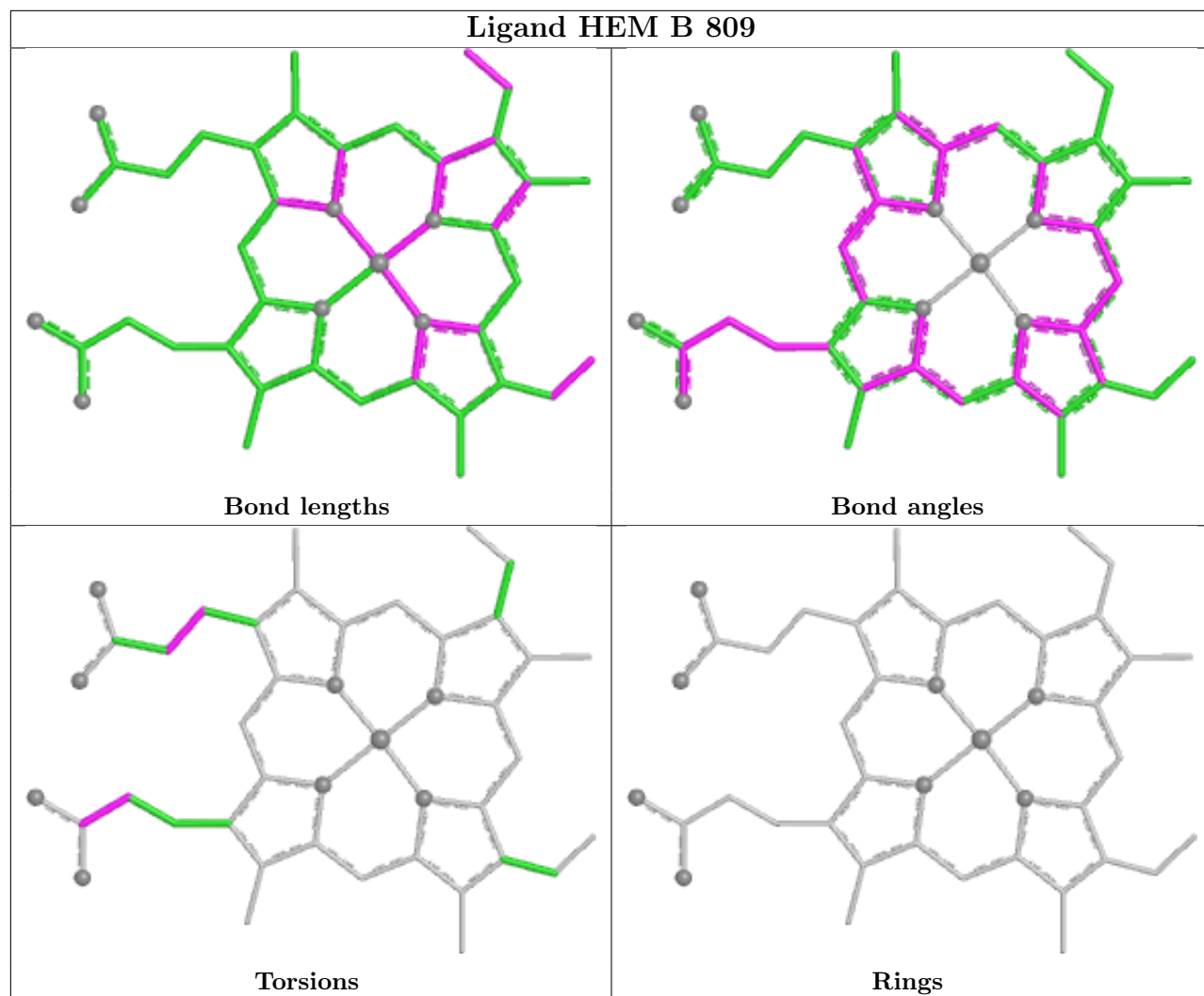


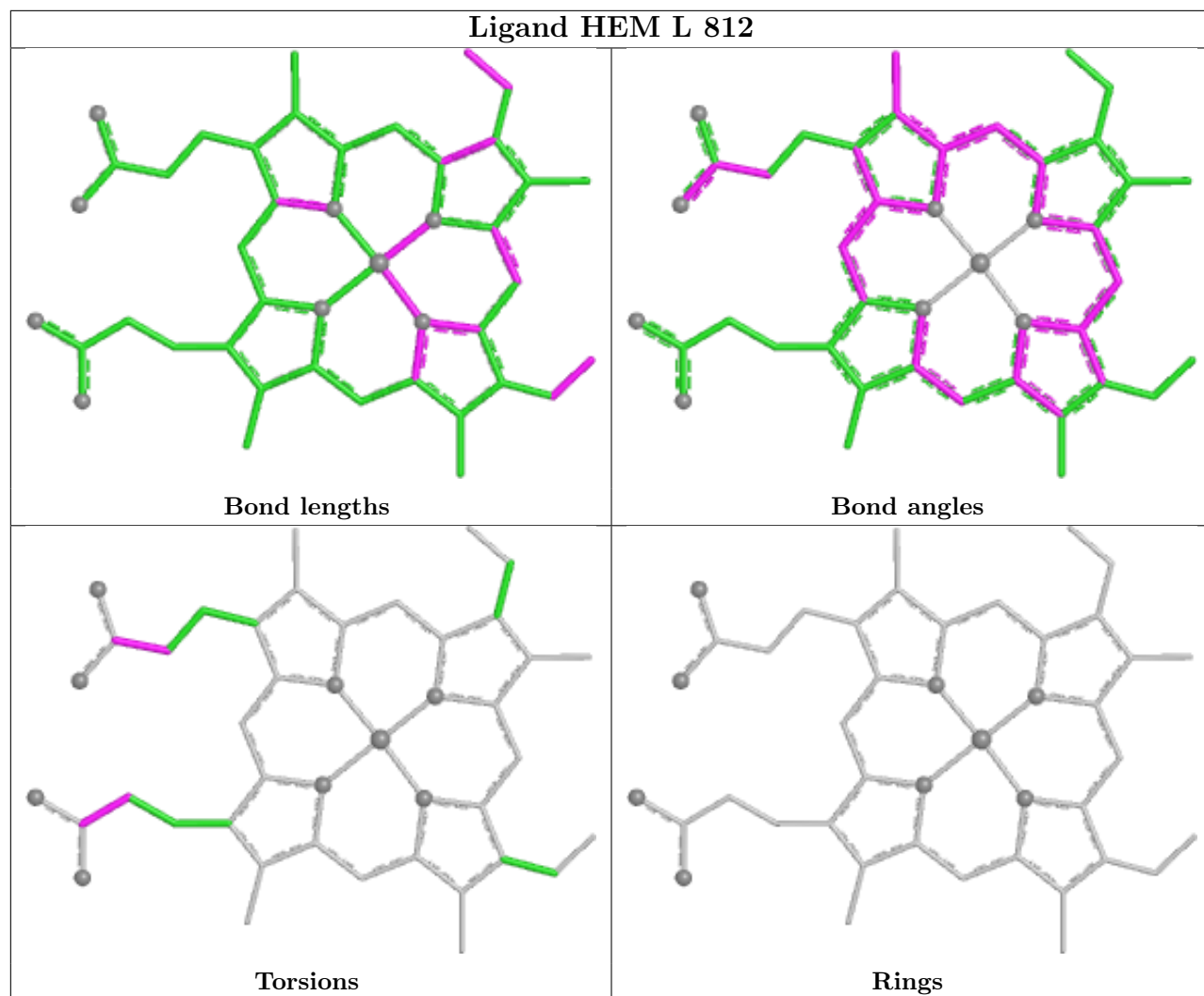


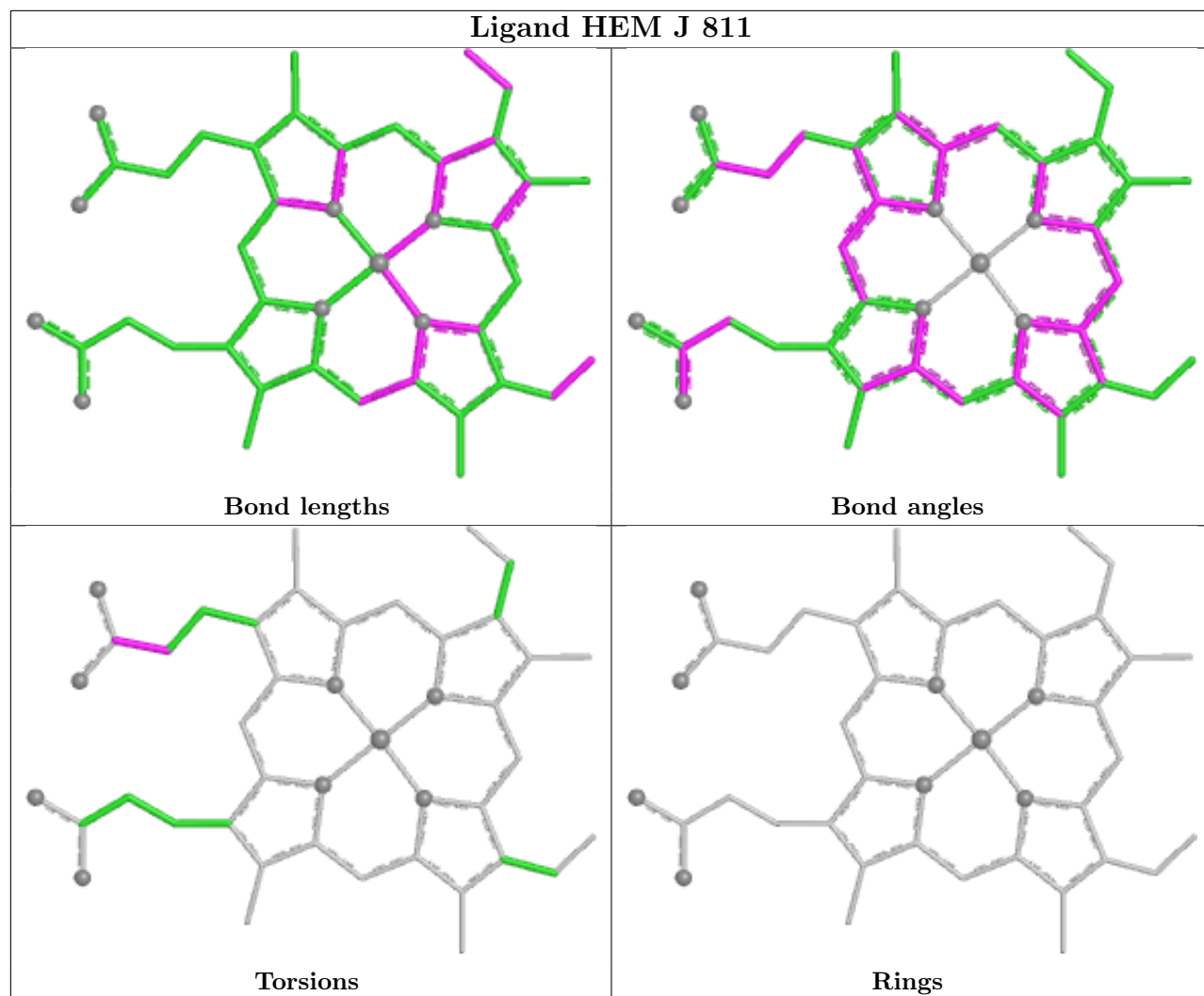




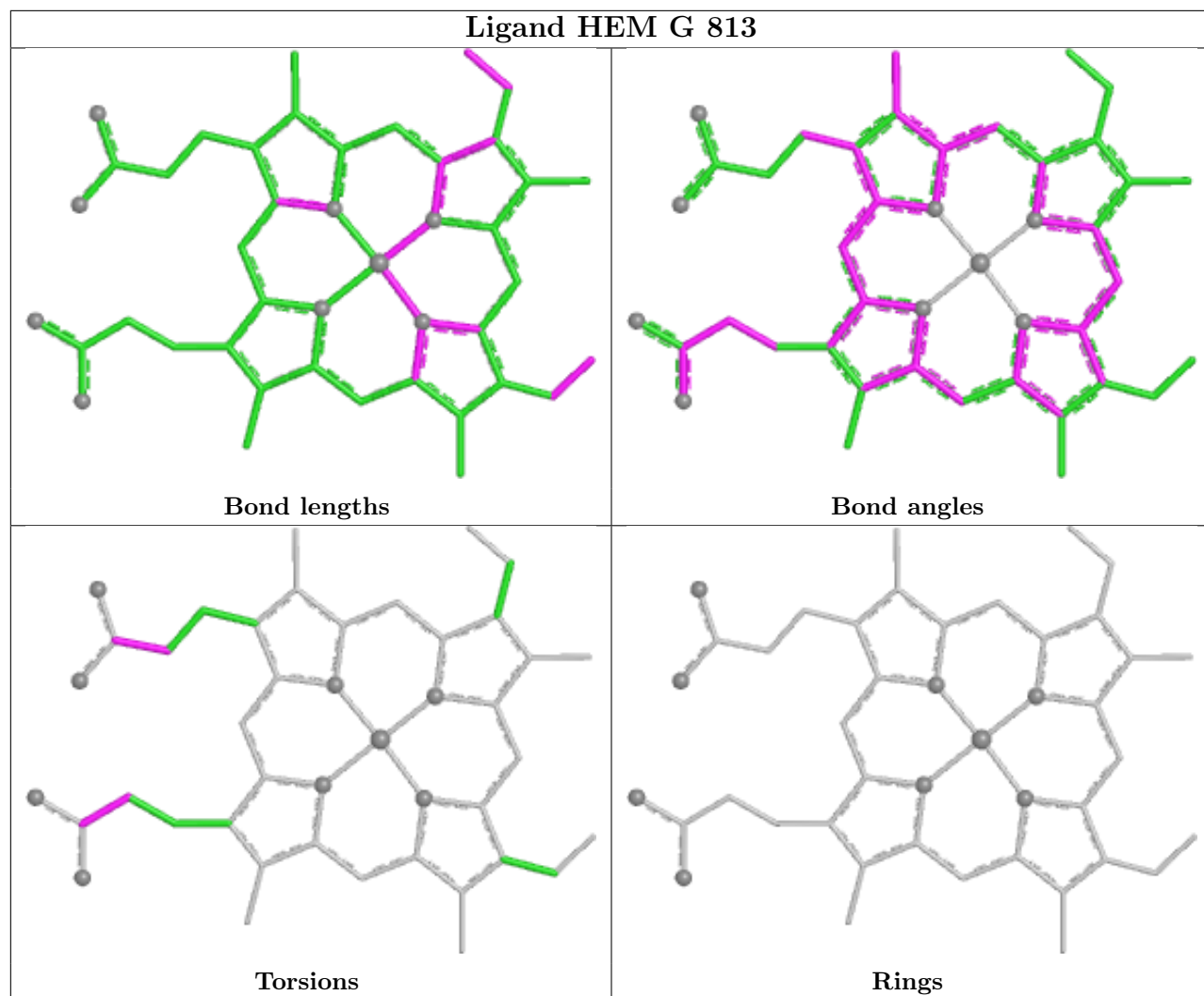


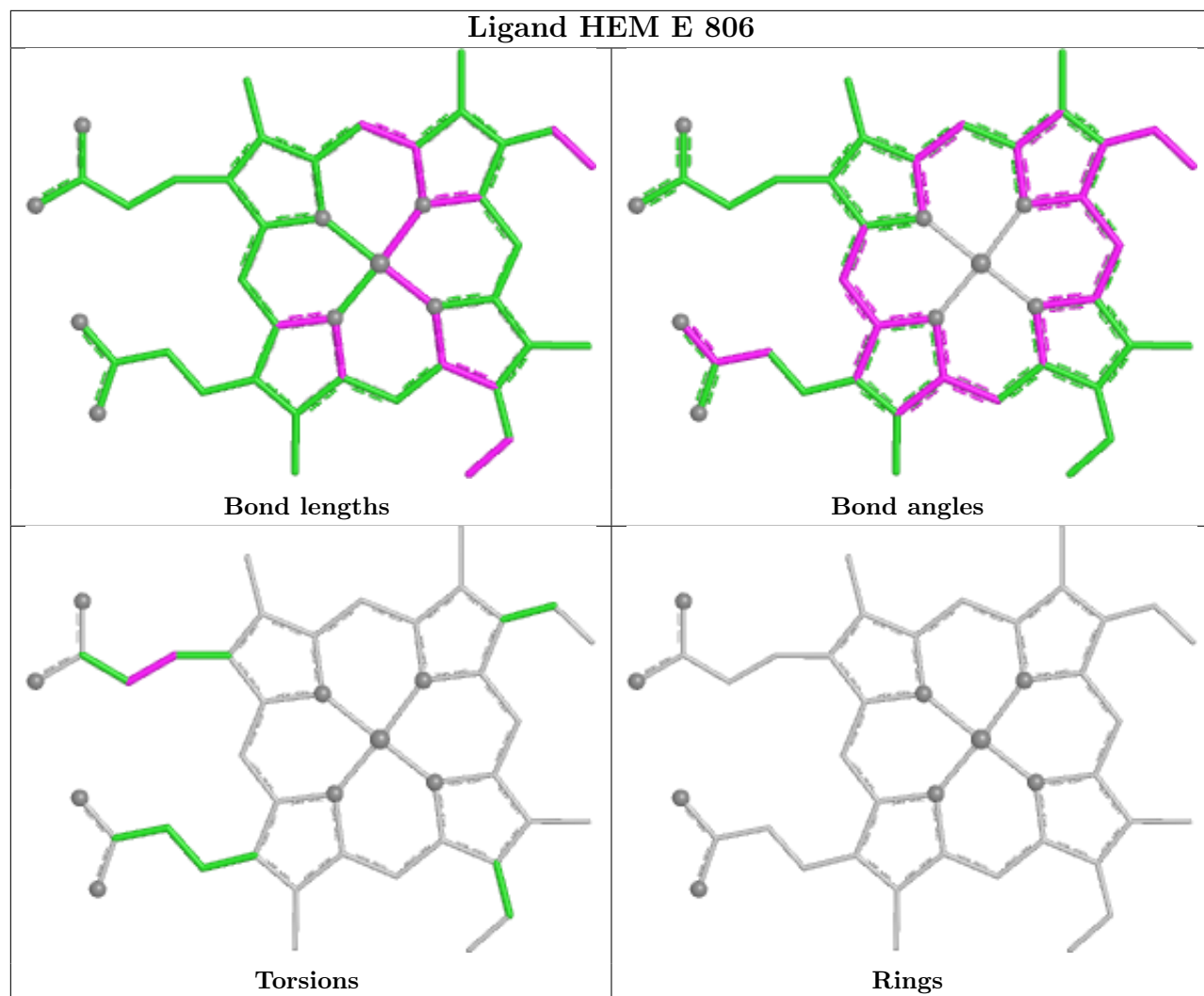


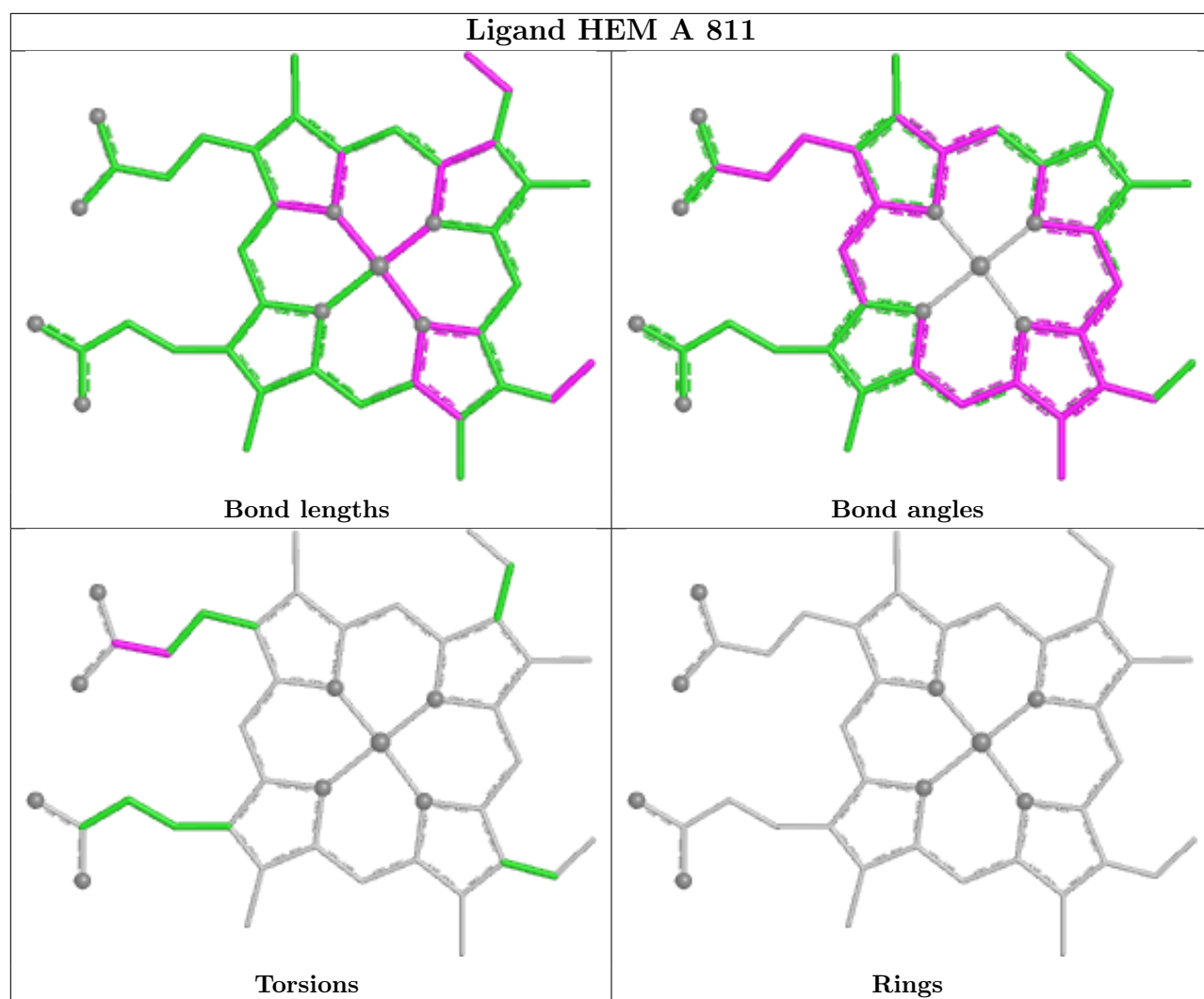




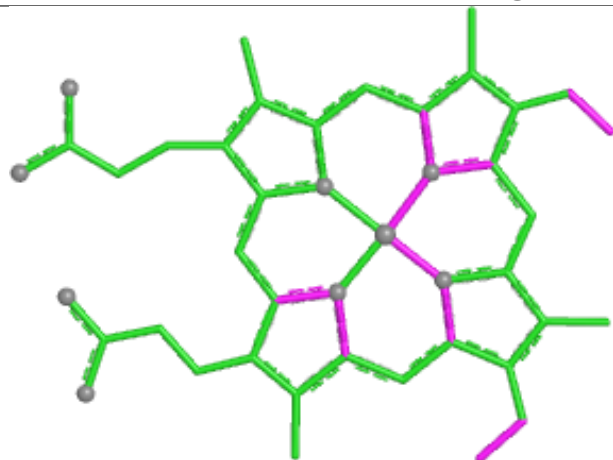




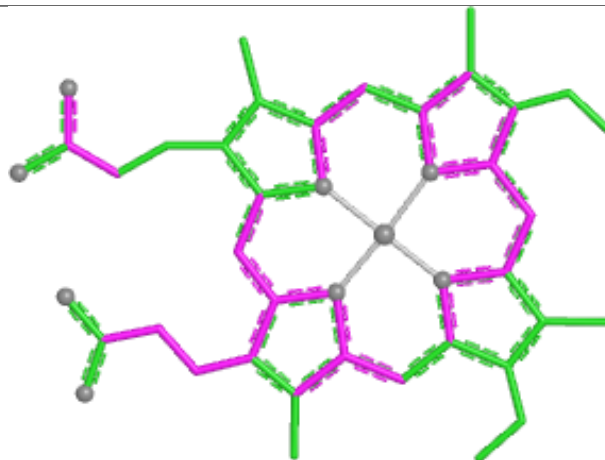




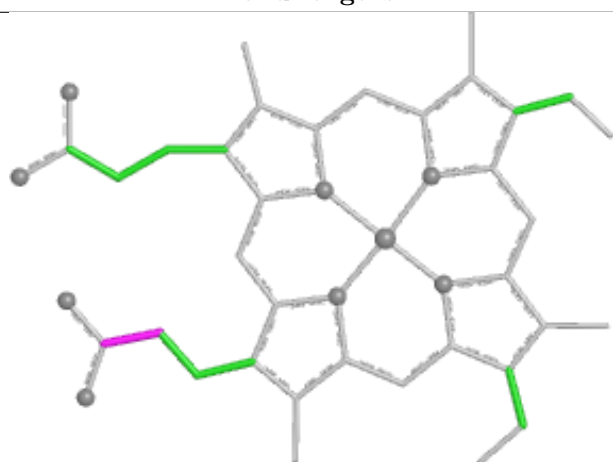
## Ligand HEM C 811



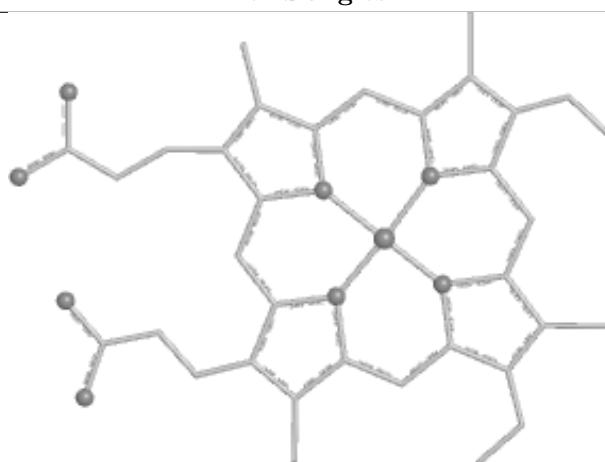
Bond lengths



Bond angles

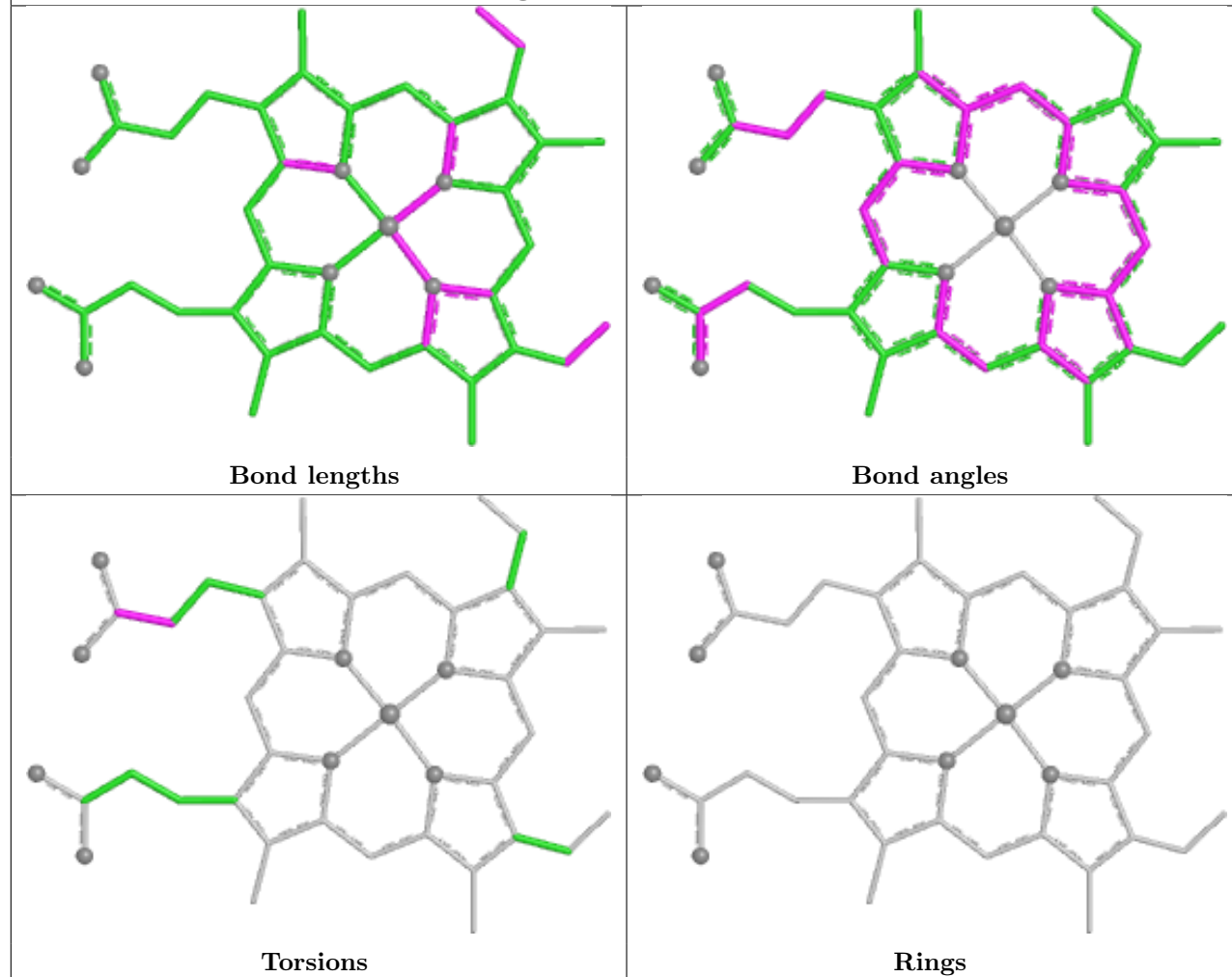


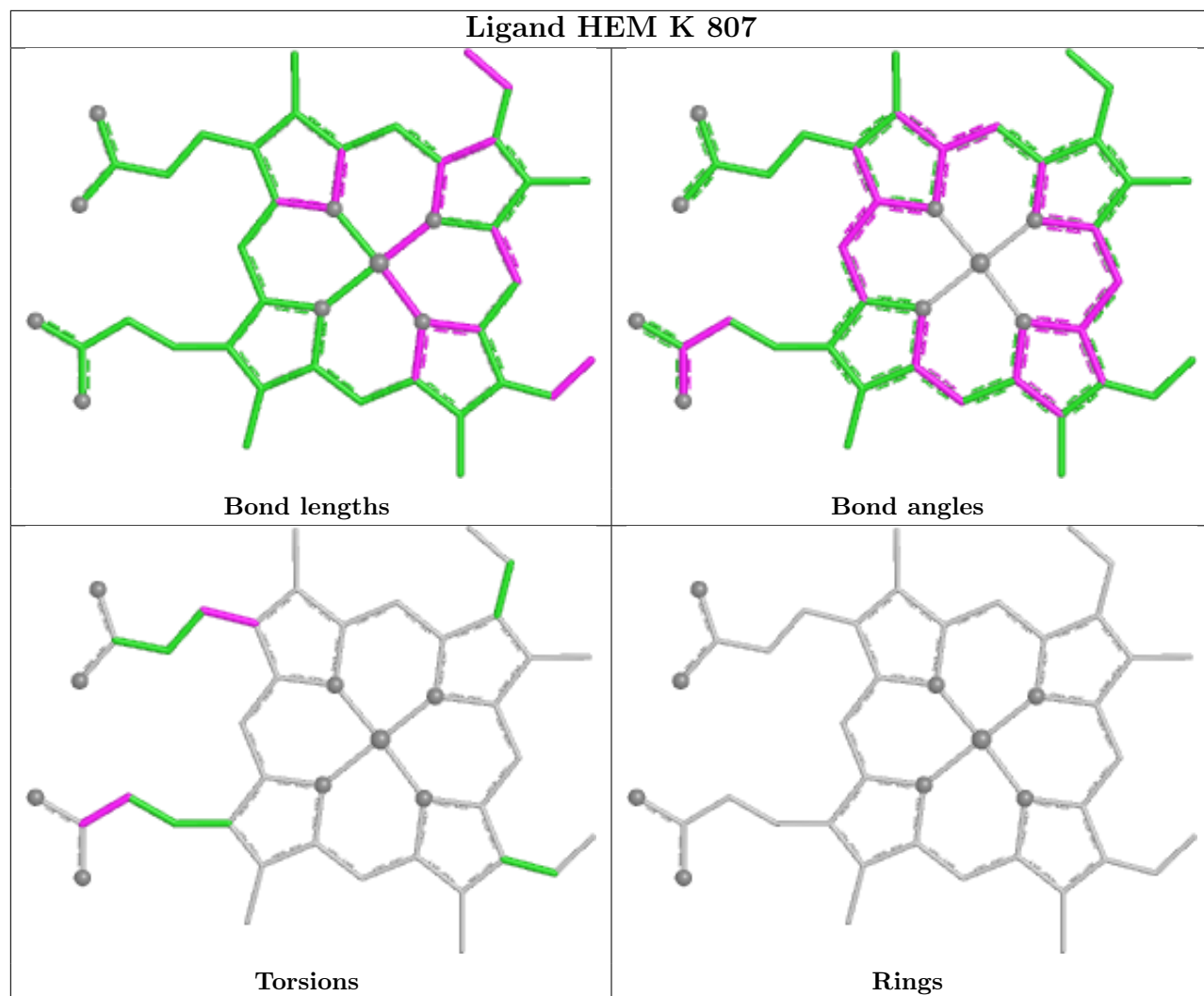
Torsions

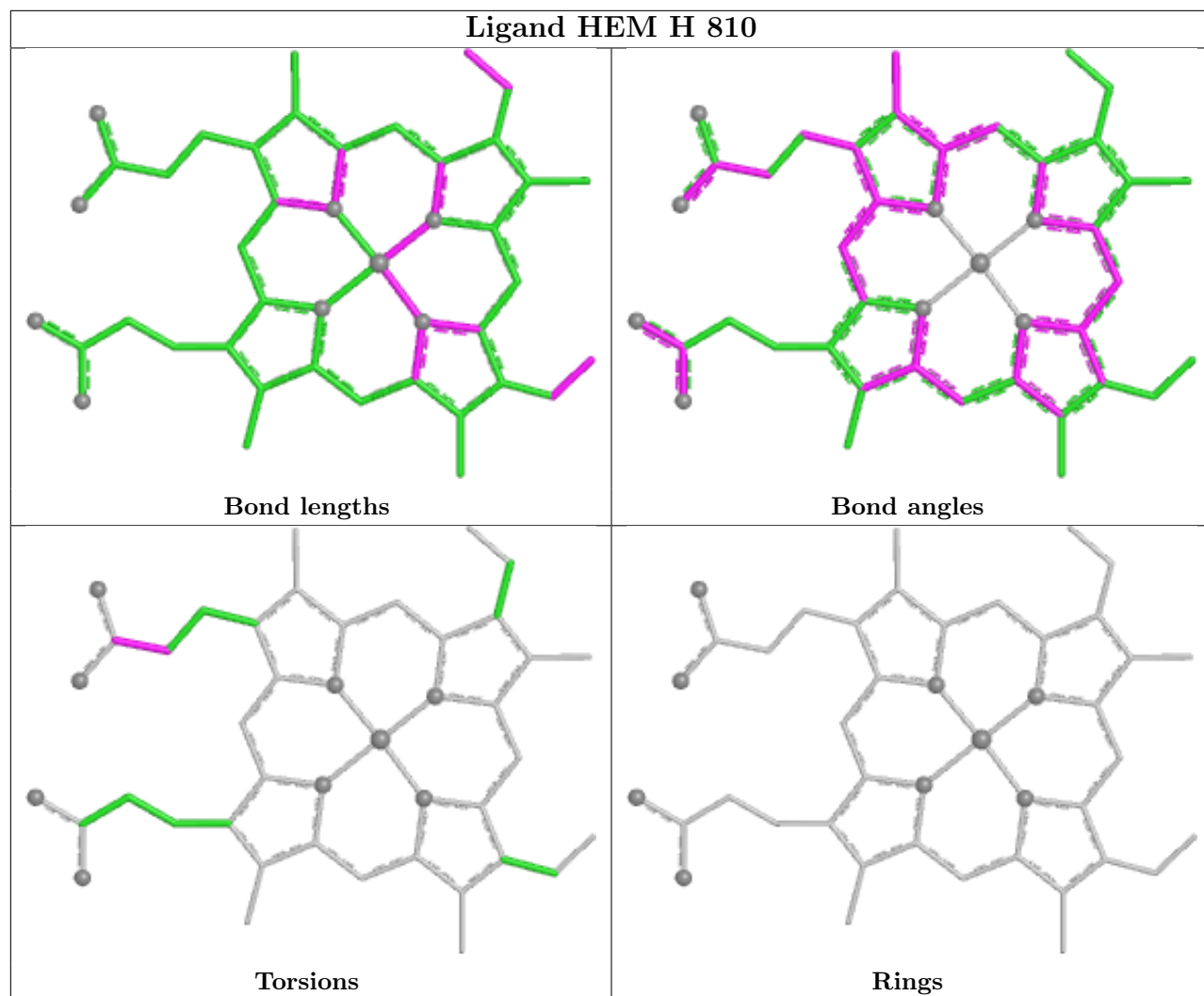


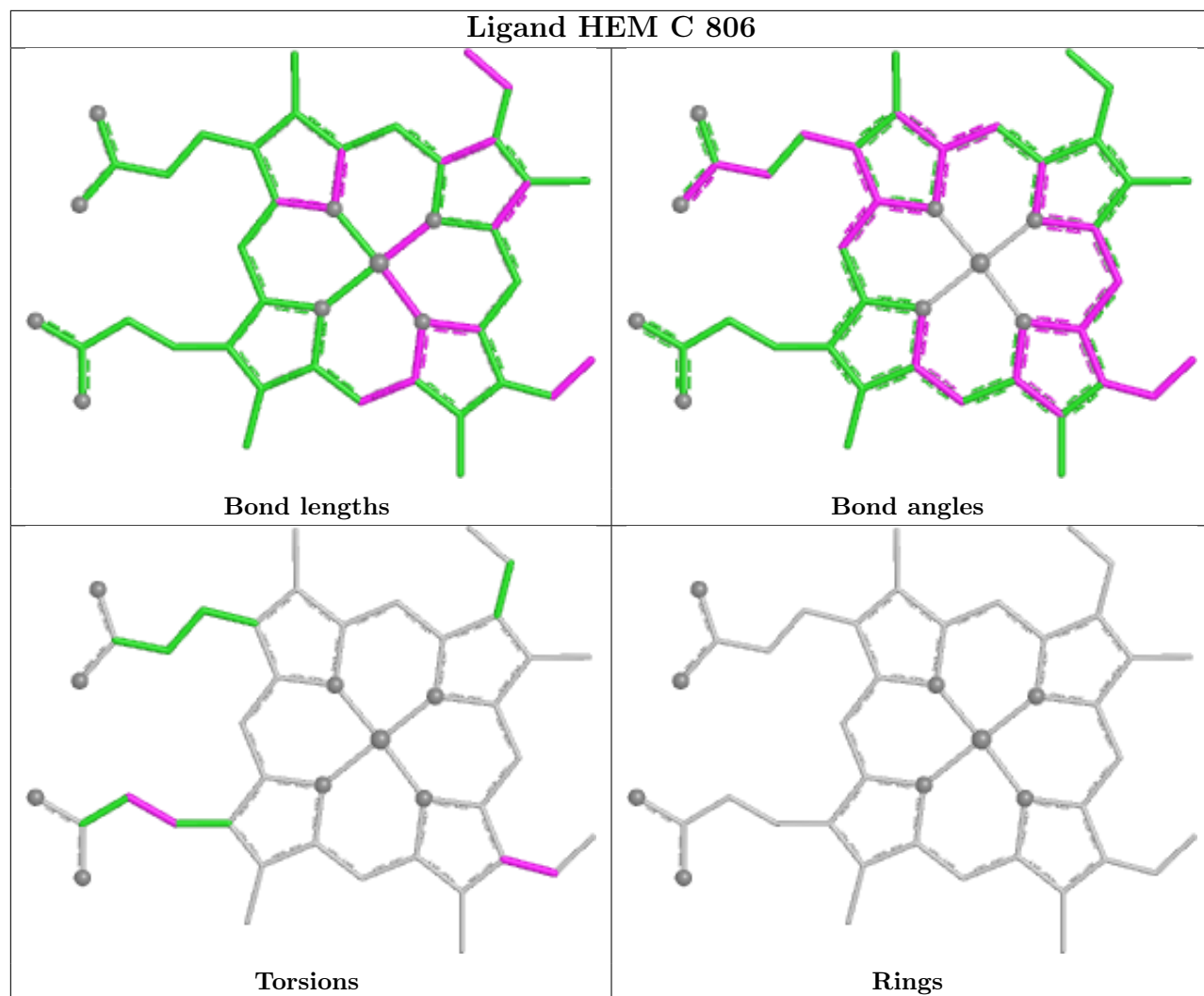
Rings

## Ligand HEM I 811

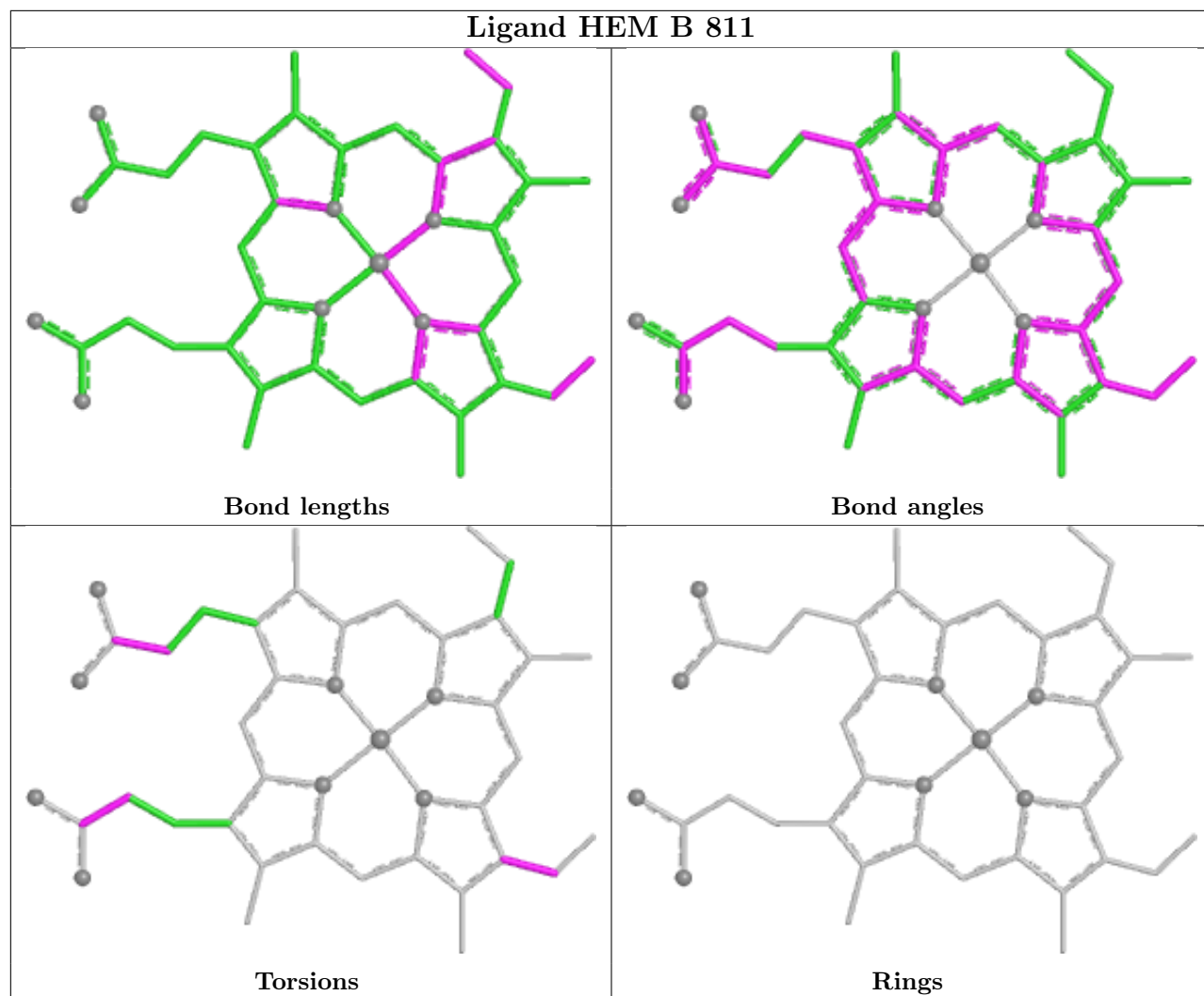


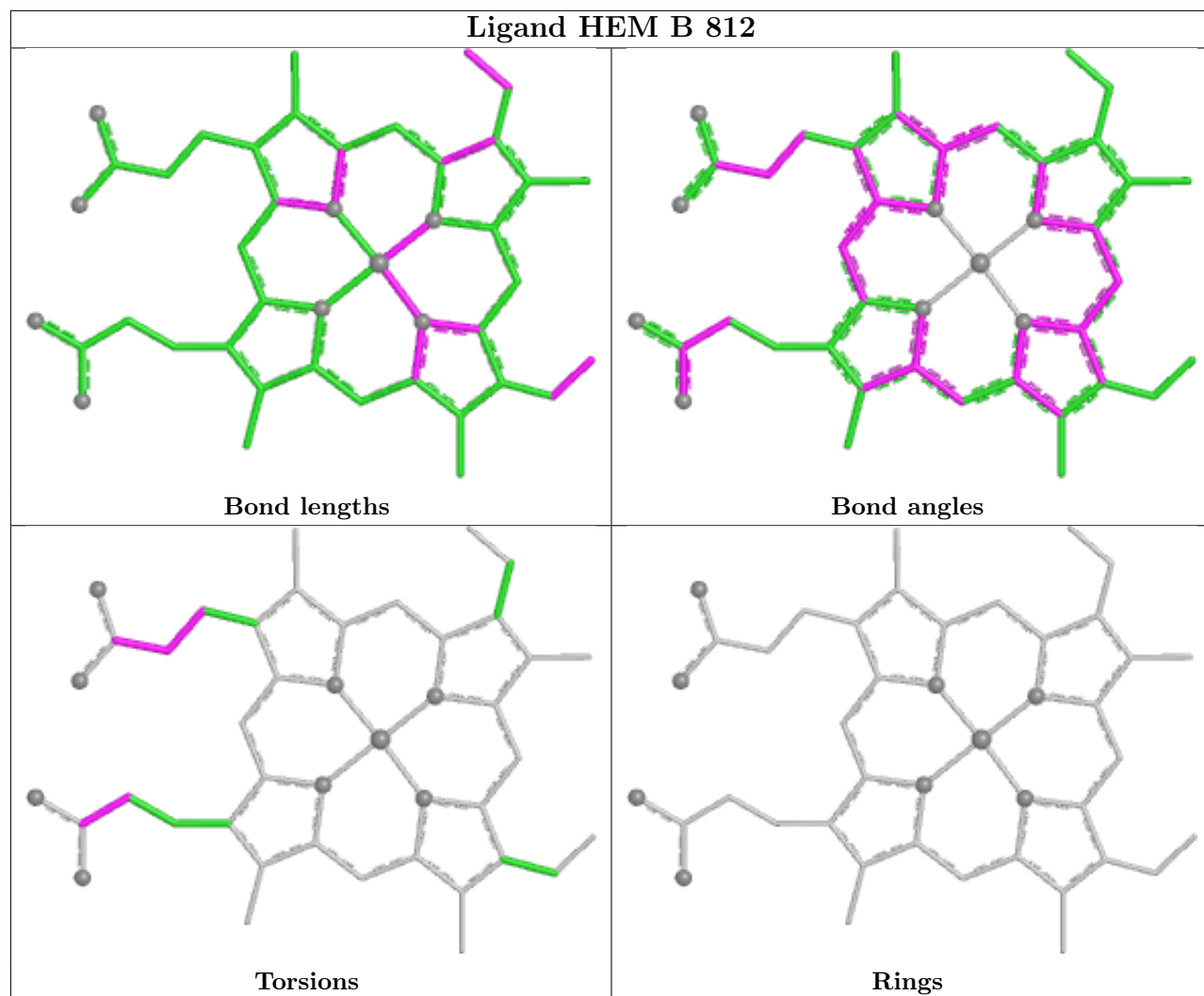


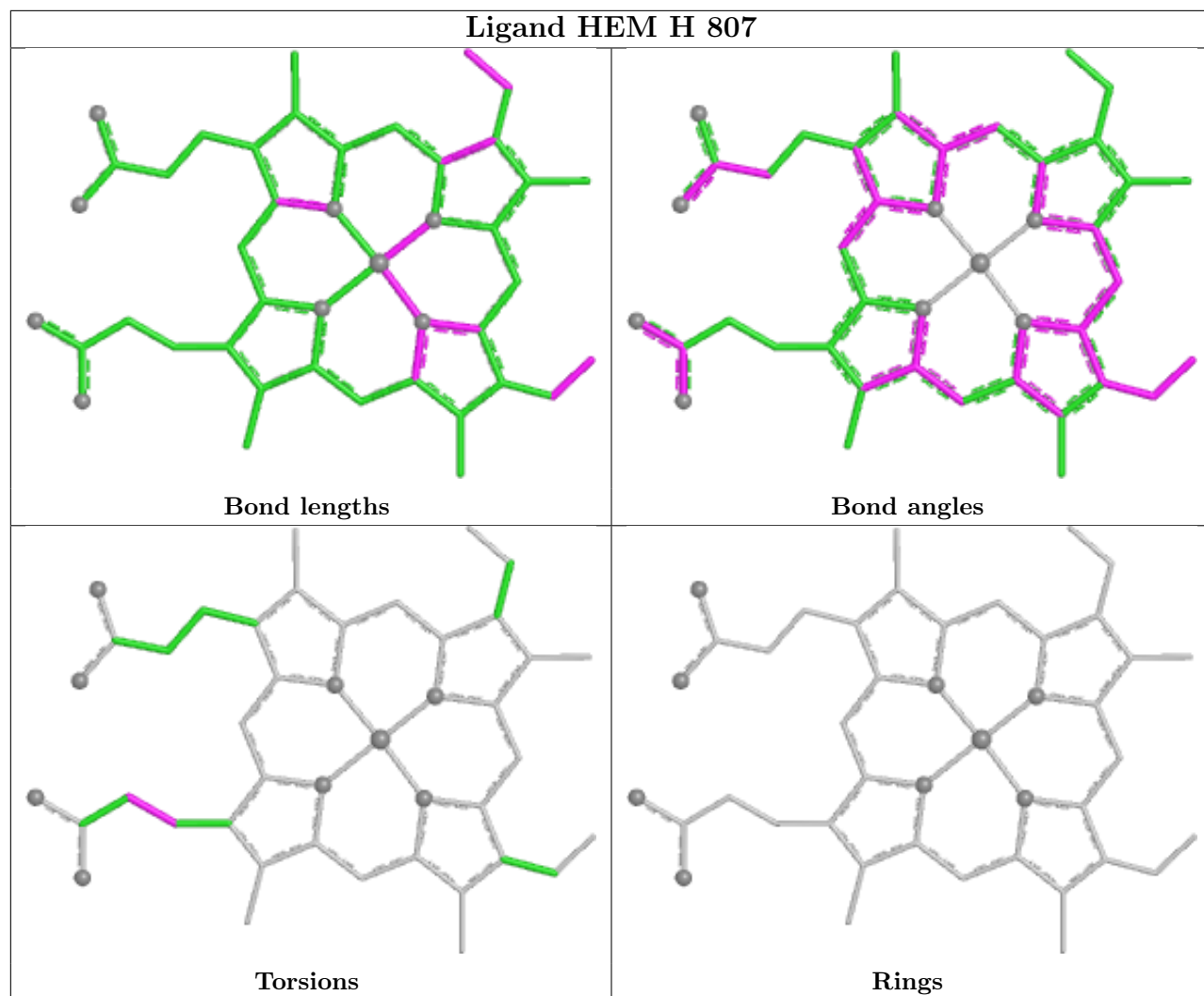


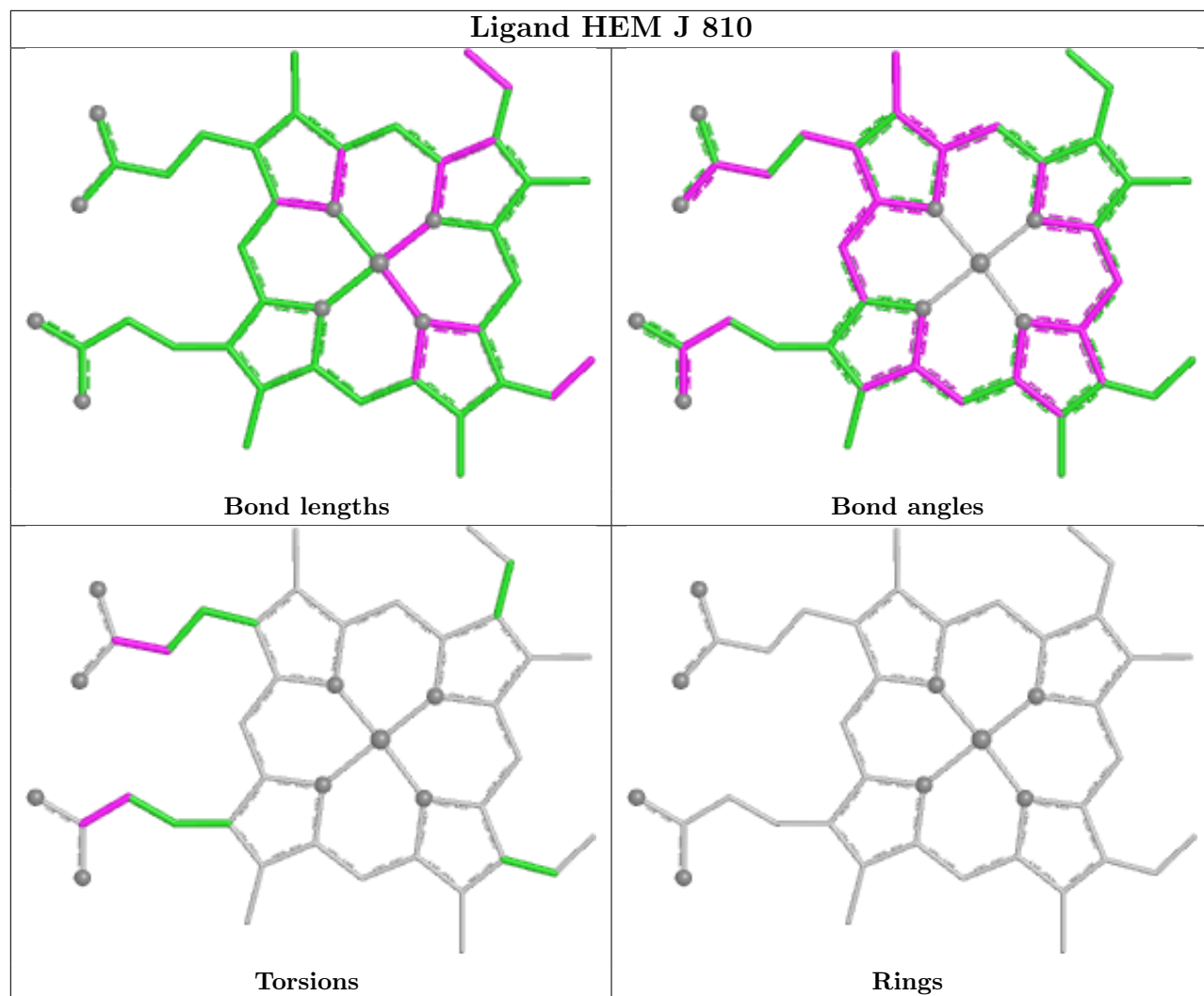


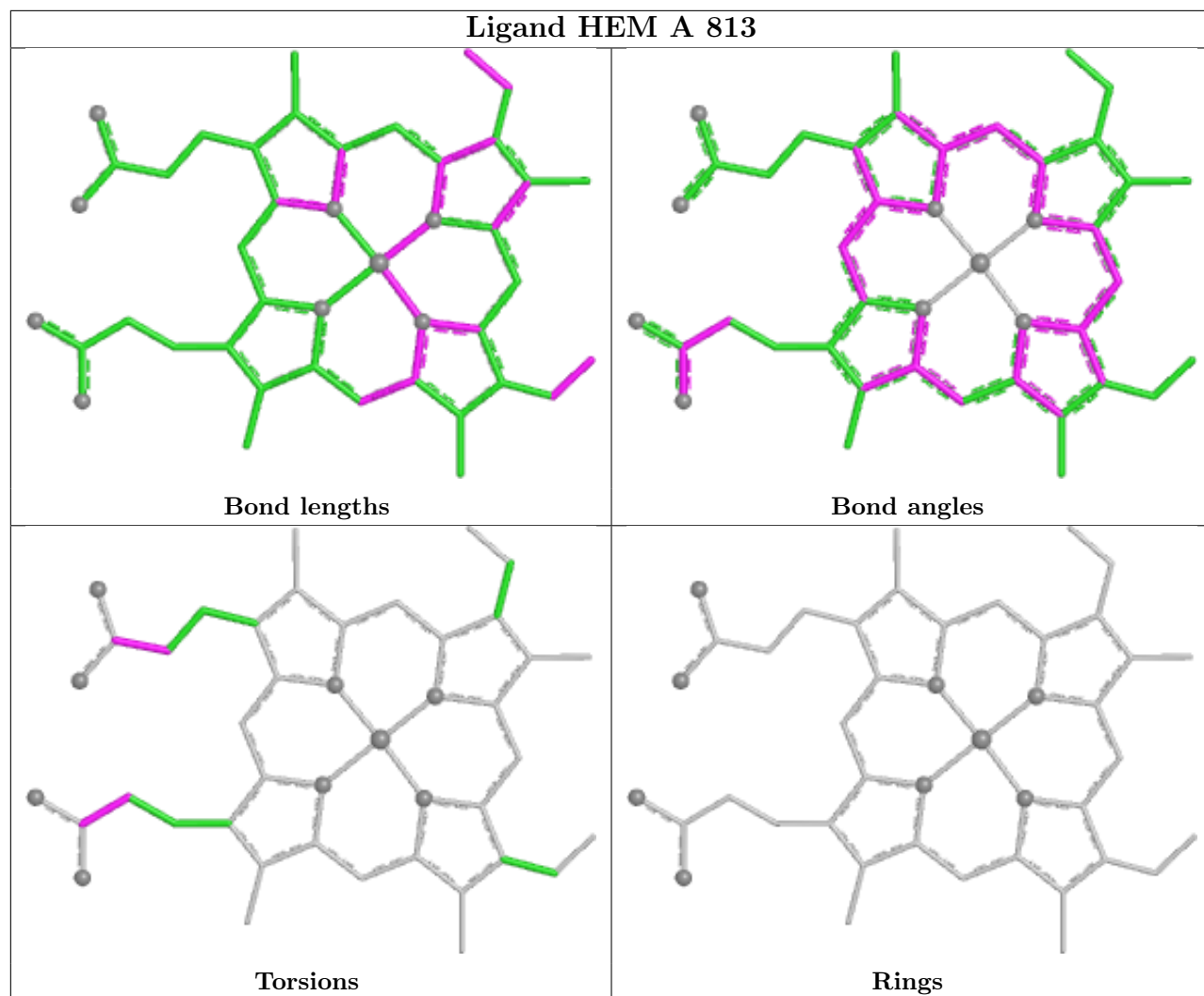


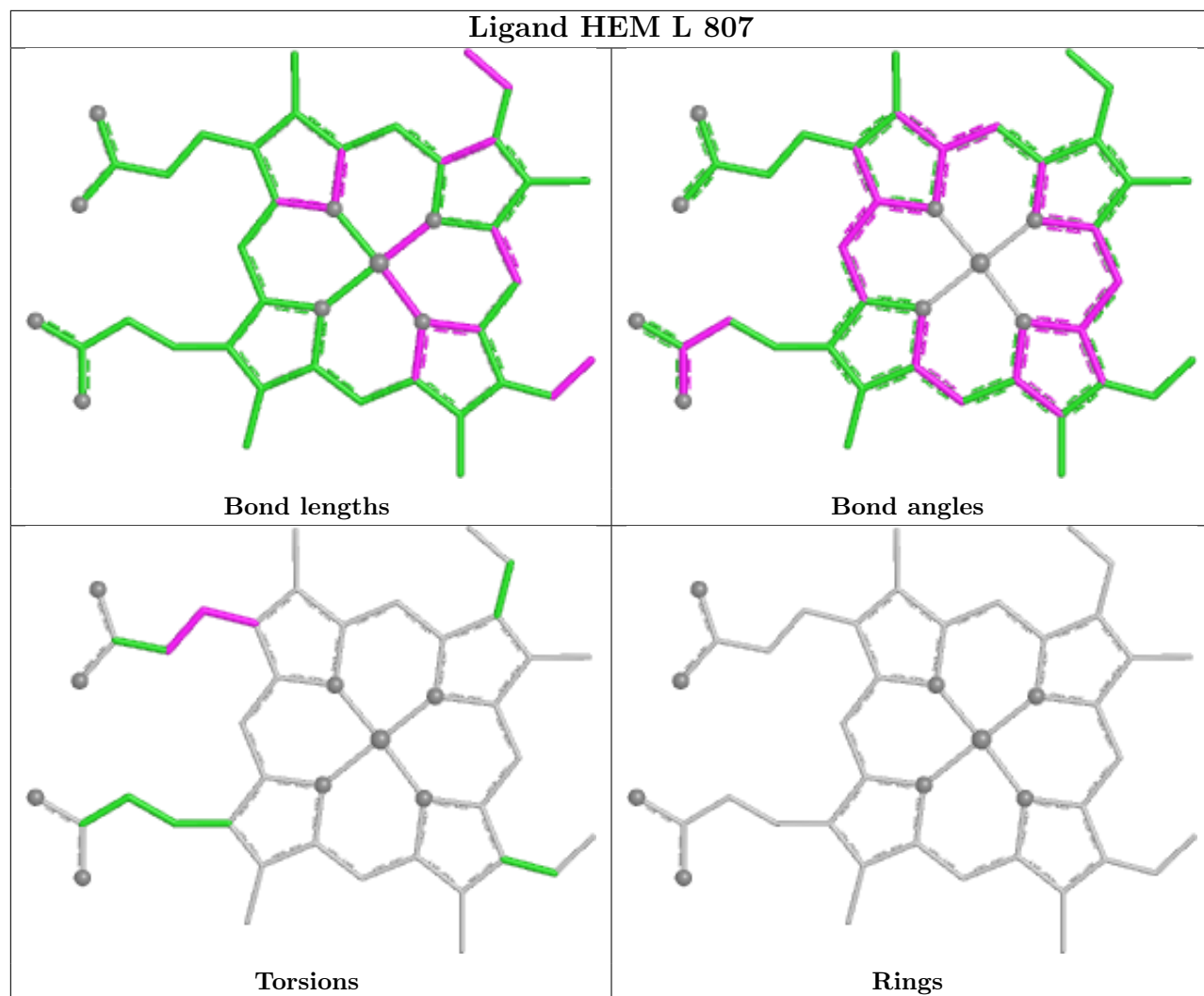


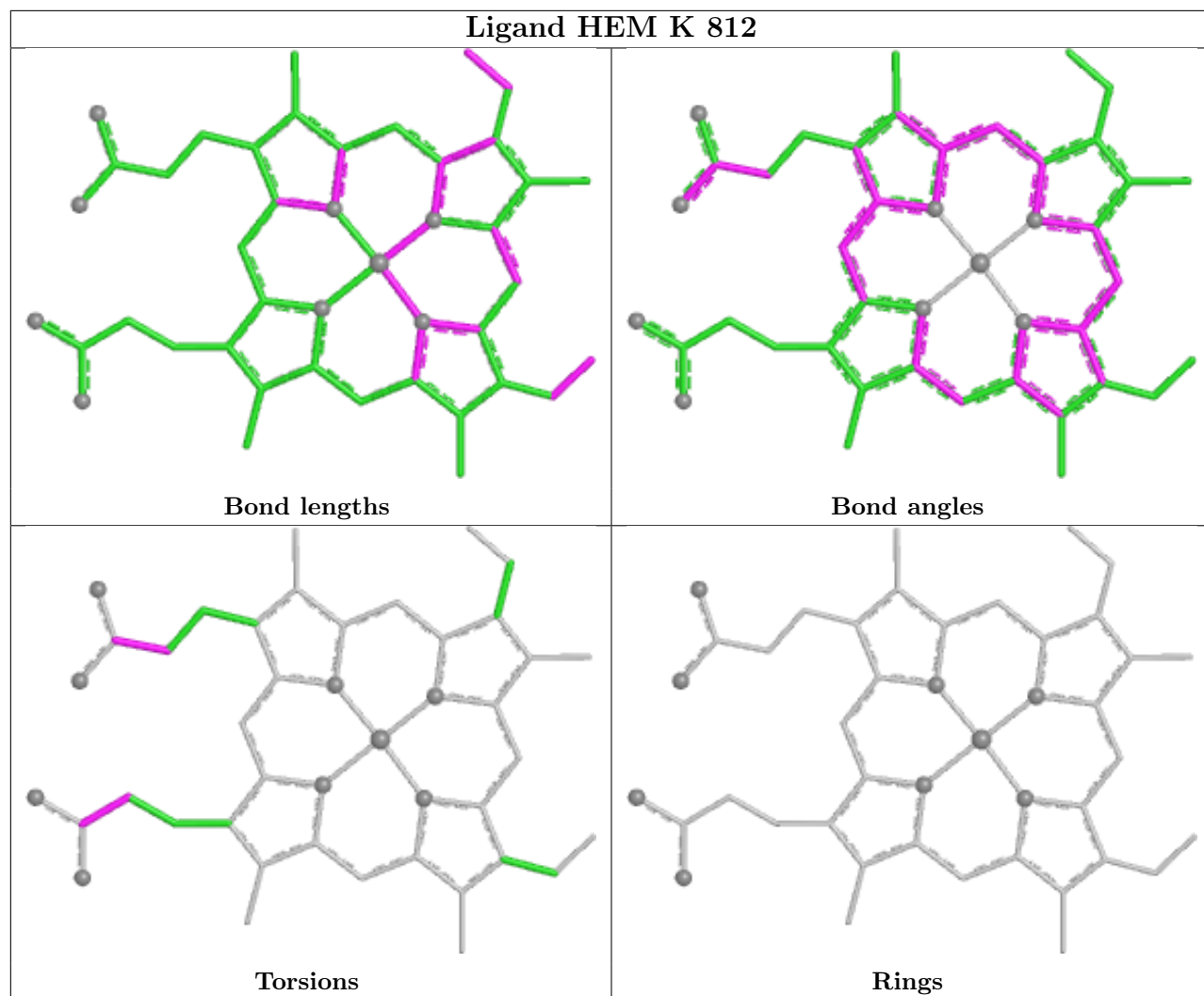


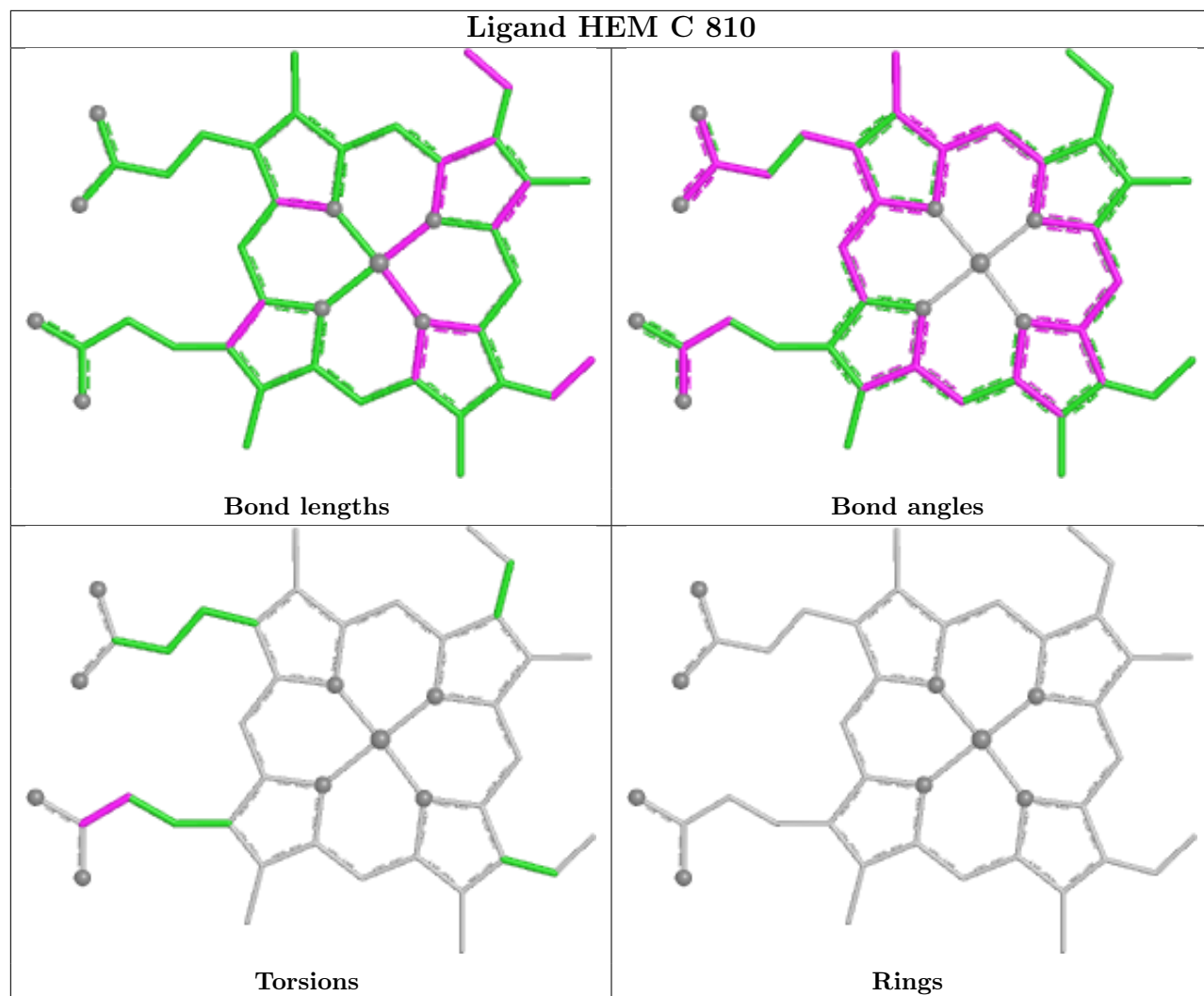






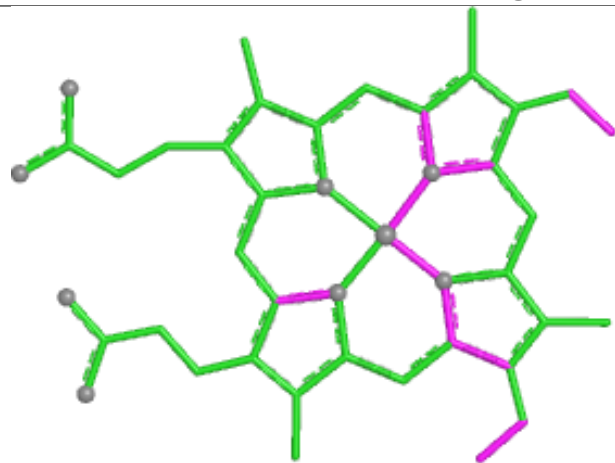




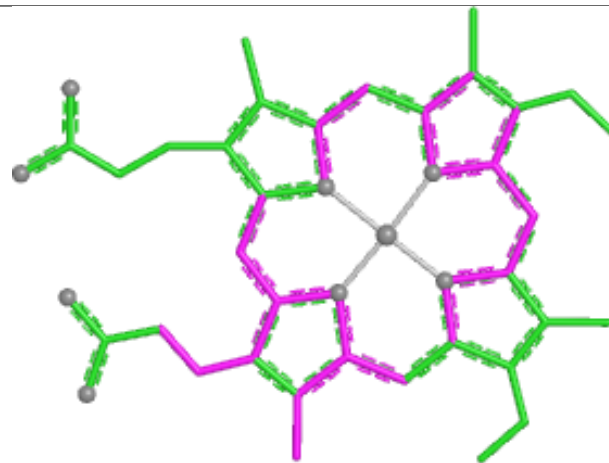




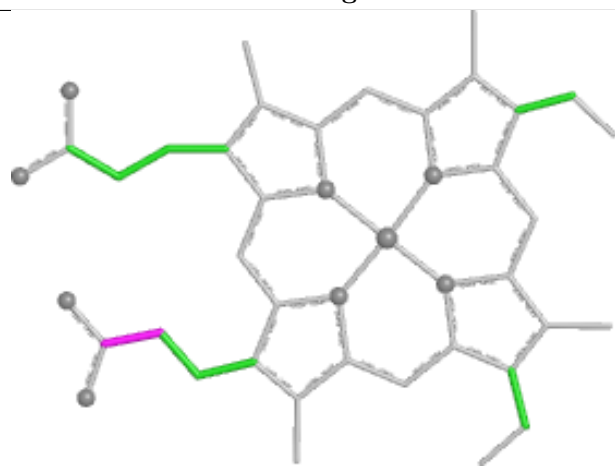
## Ligand HEM K 809



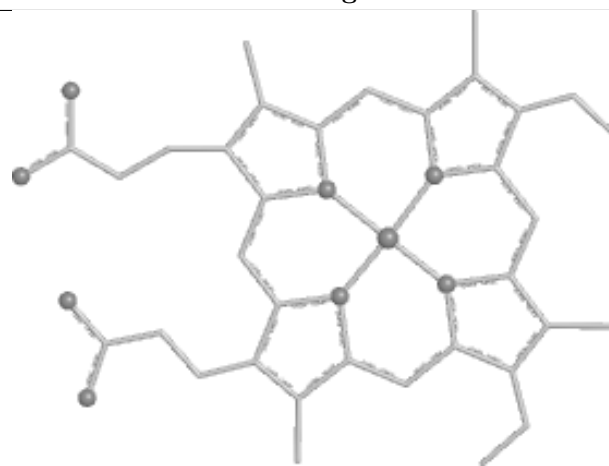
Bond lengths



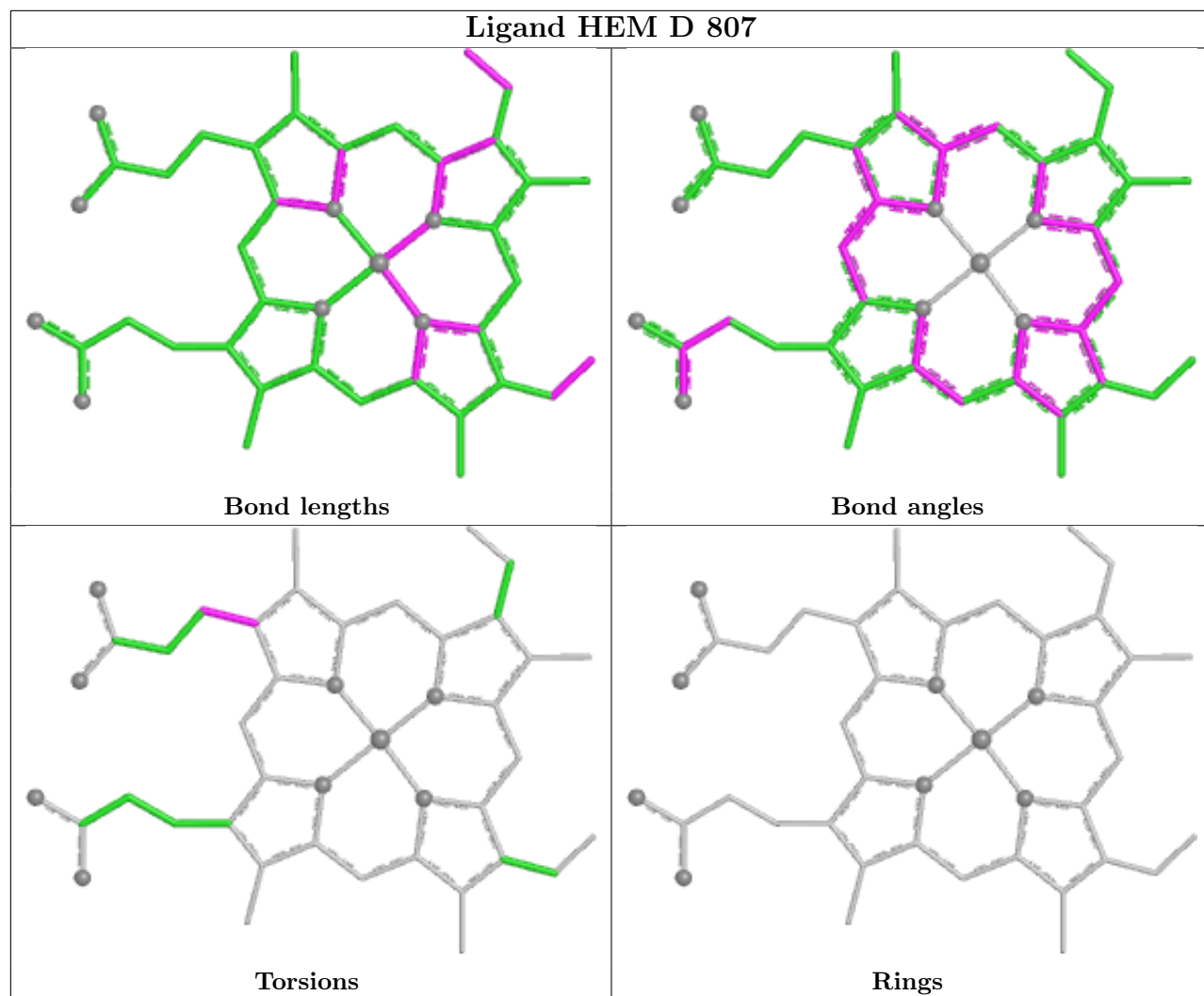
Bond angles

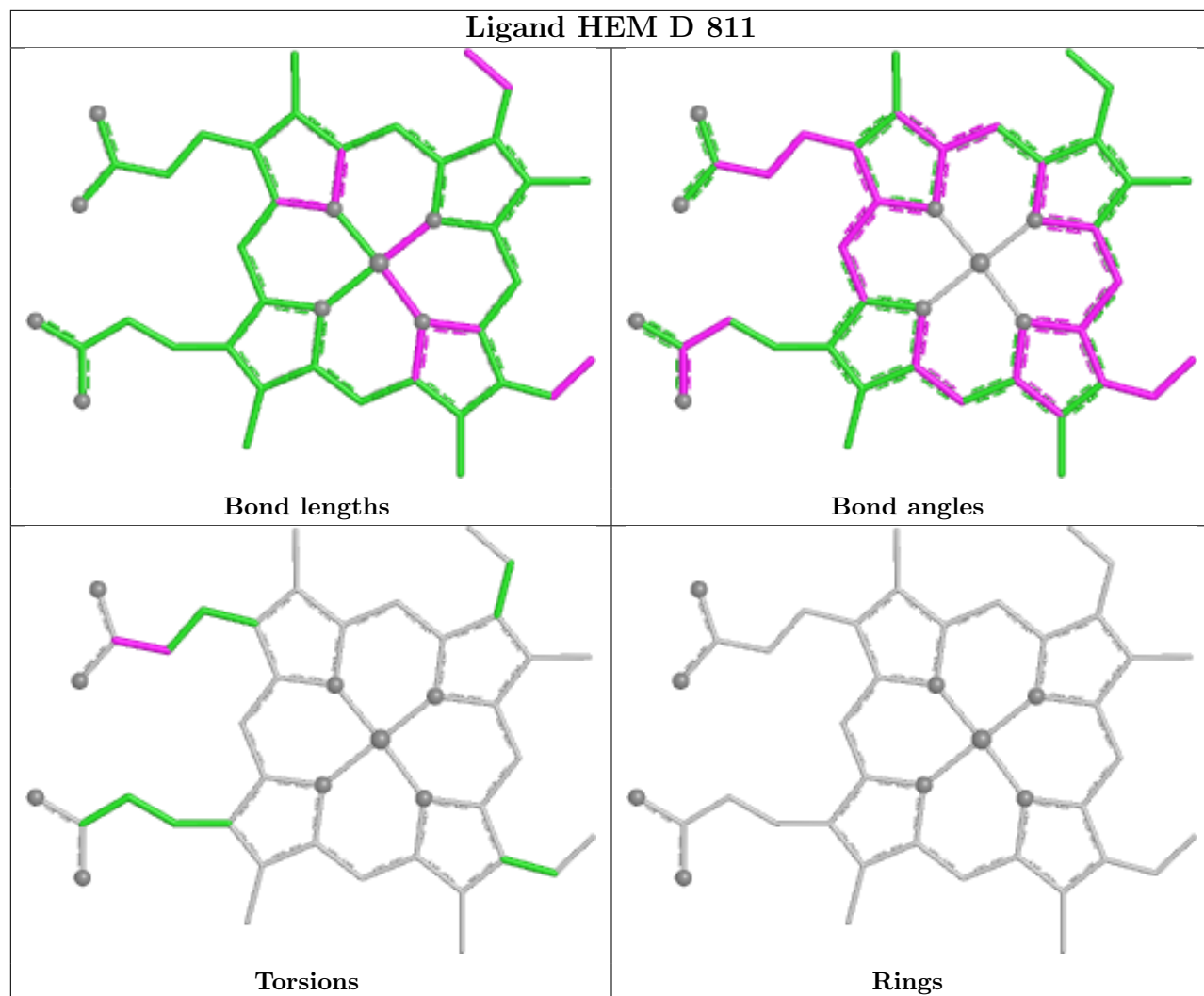


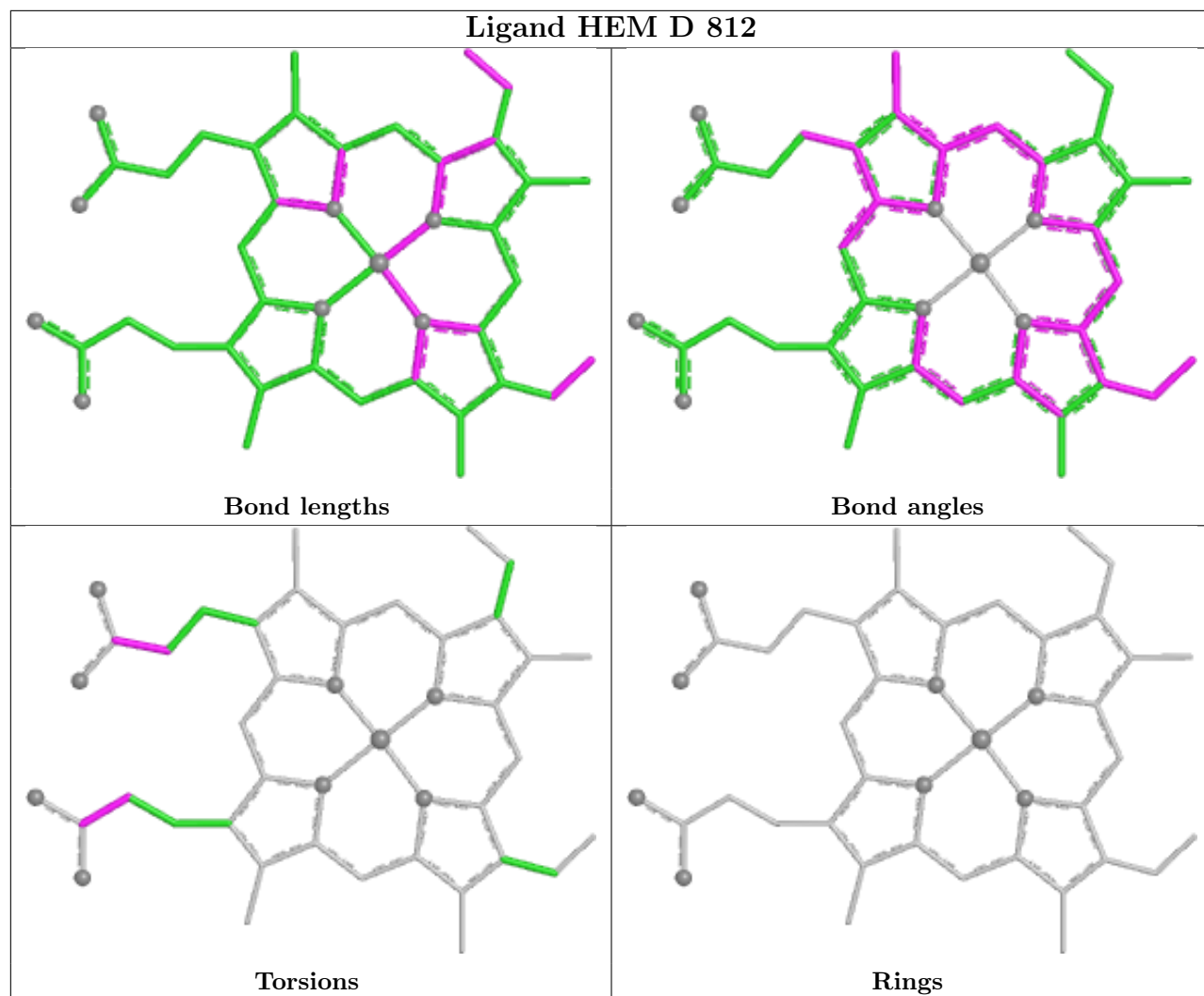
Torsions

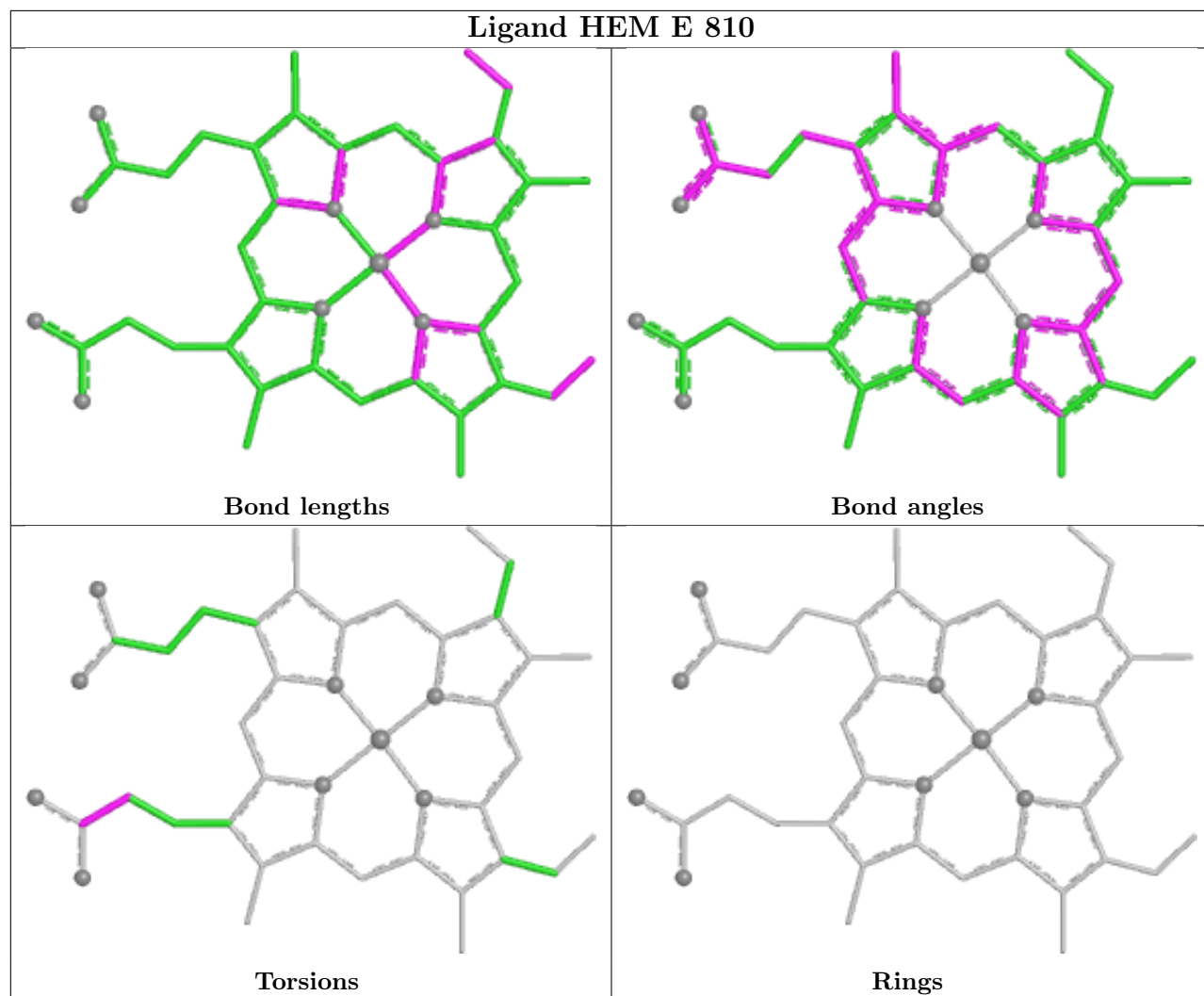


Rings

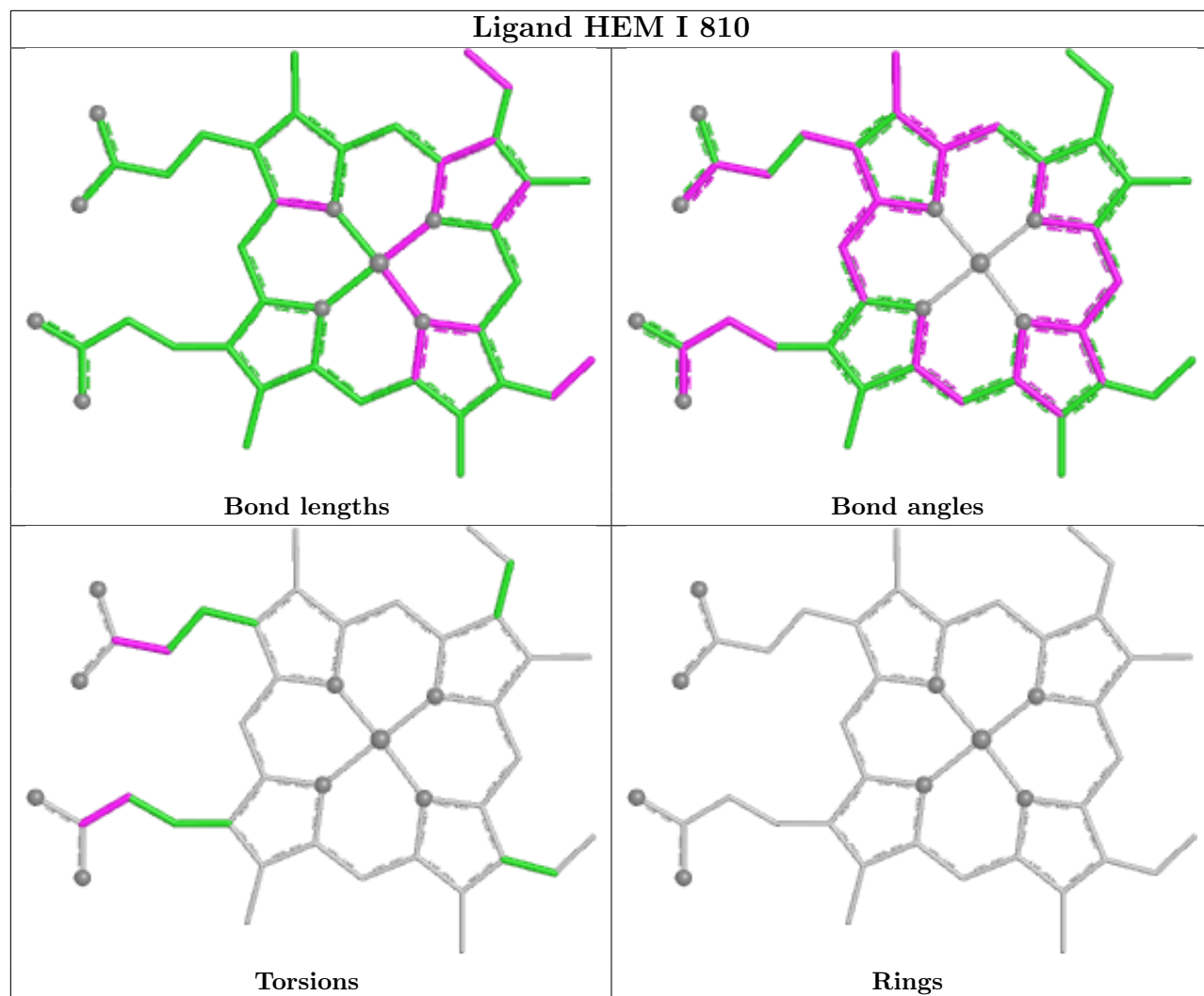


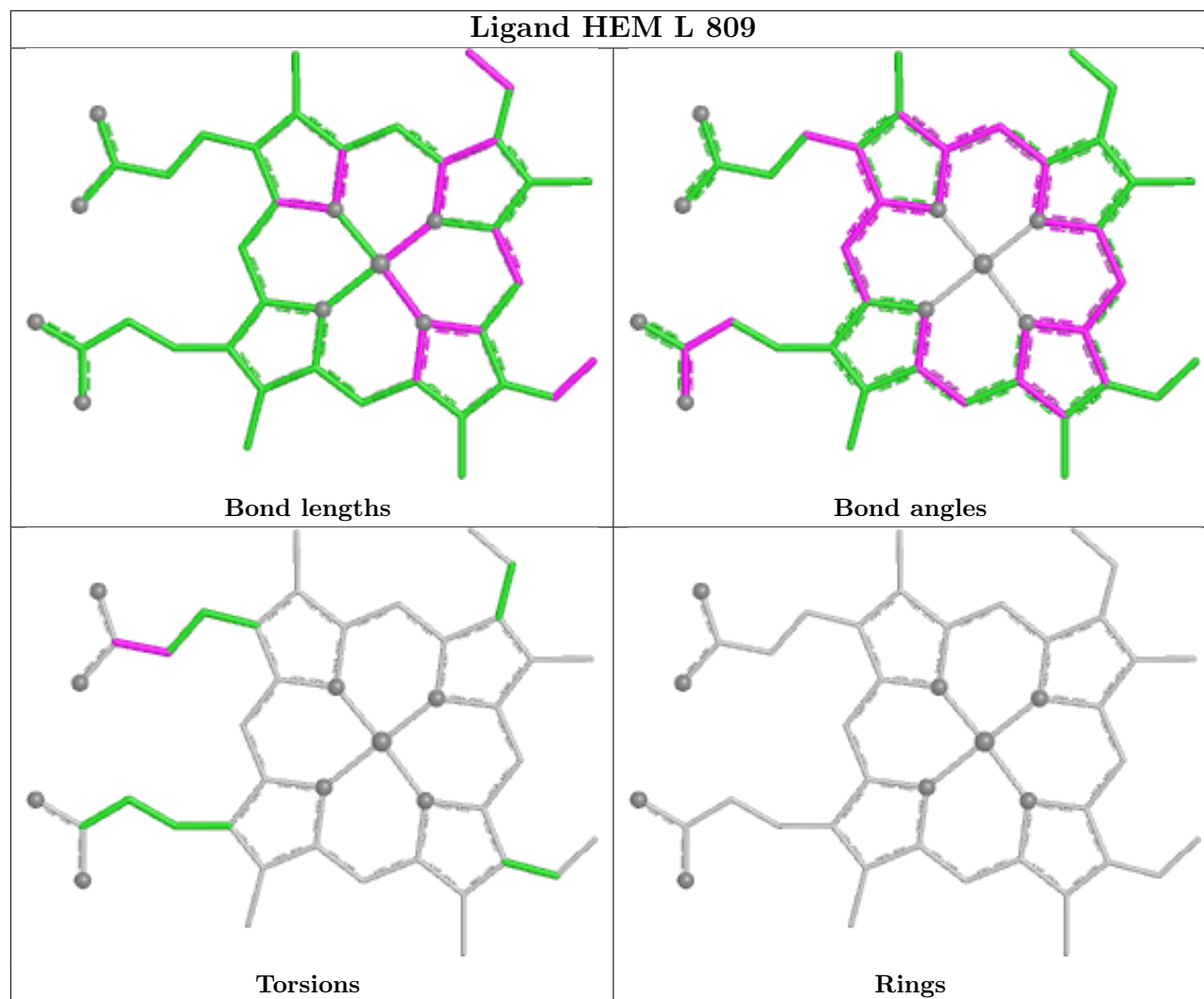




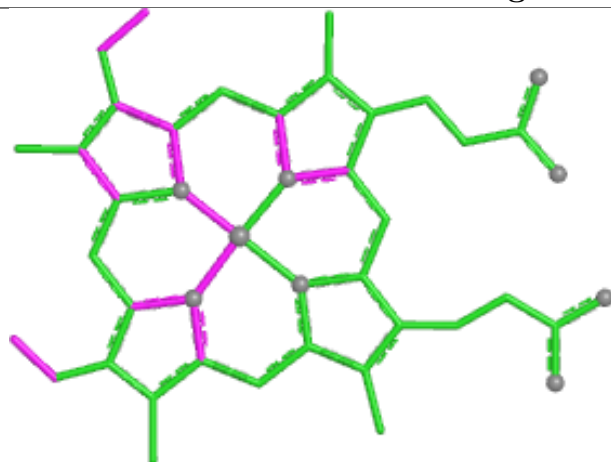


## Ligand HEM I 810

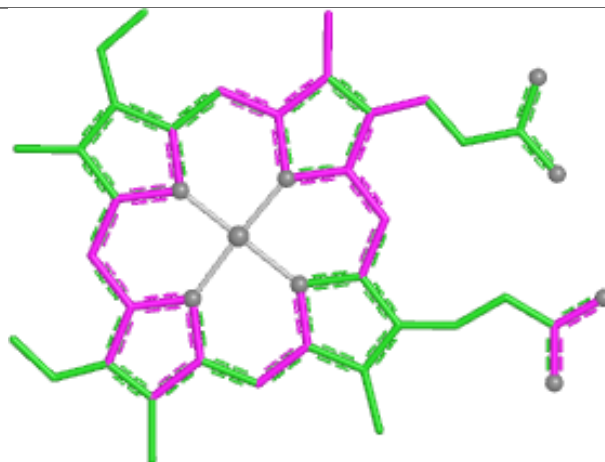




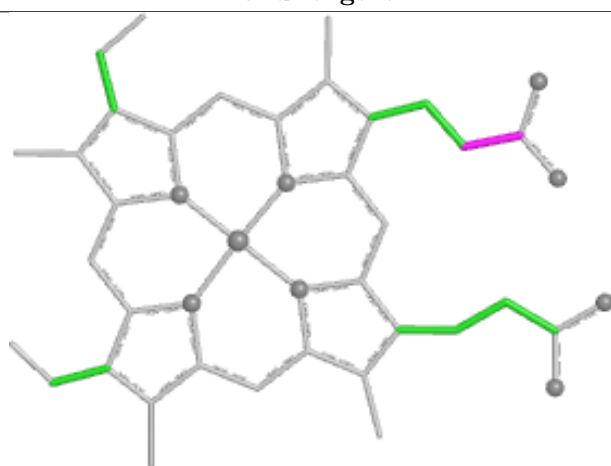
## Ligand HEM D 809



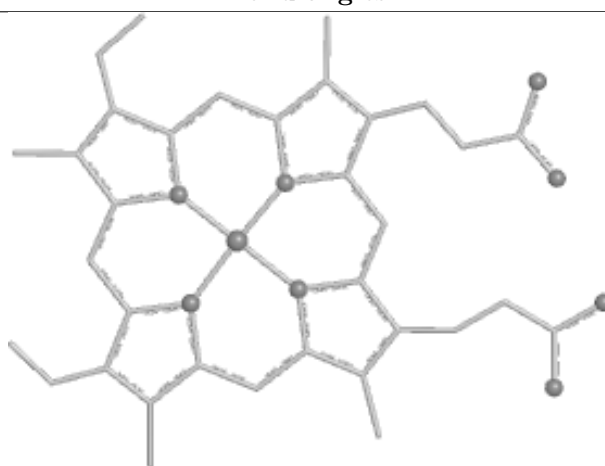
Bond lengths



Bond angles

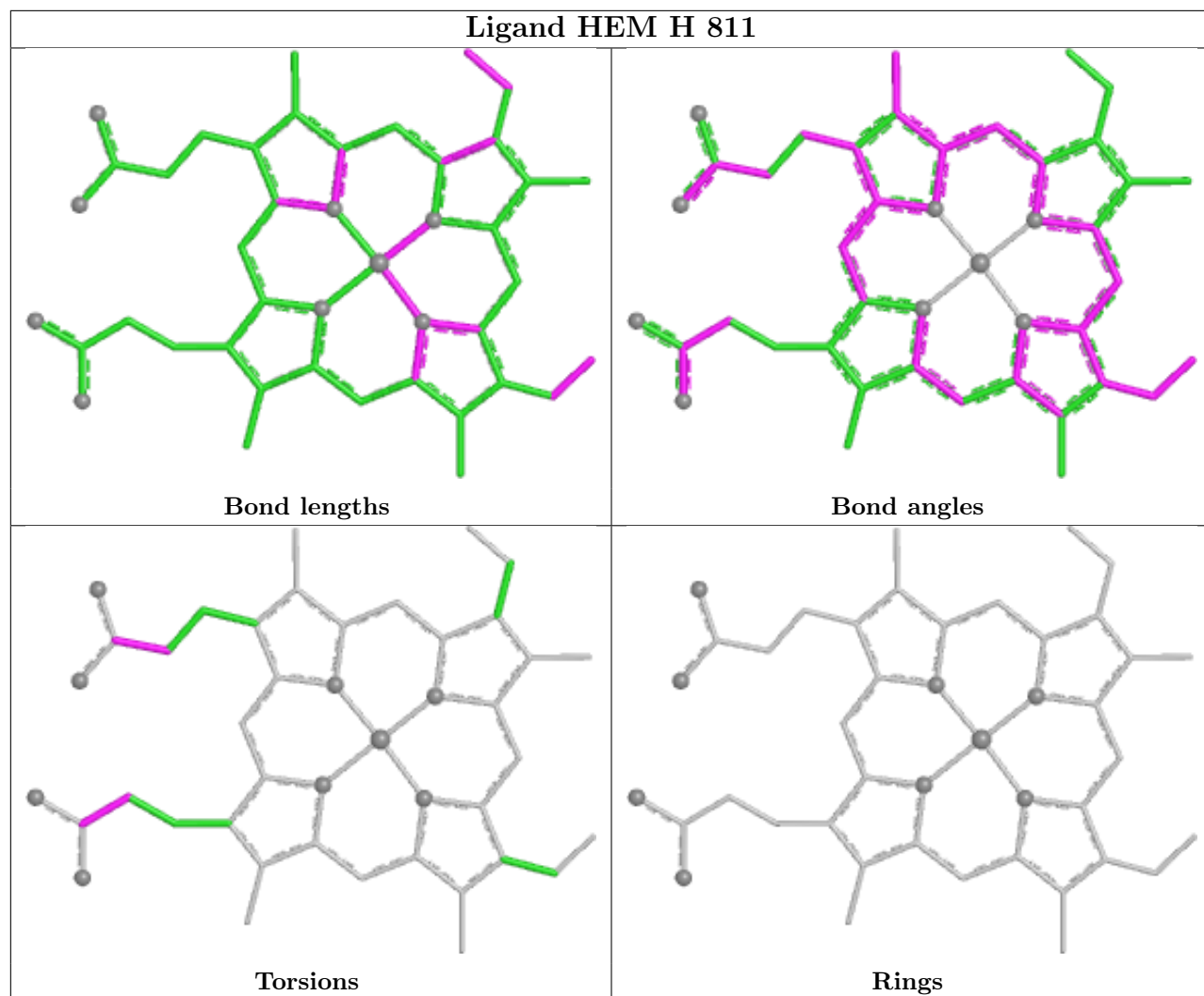


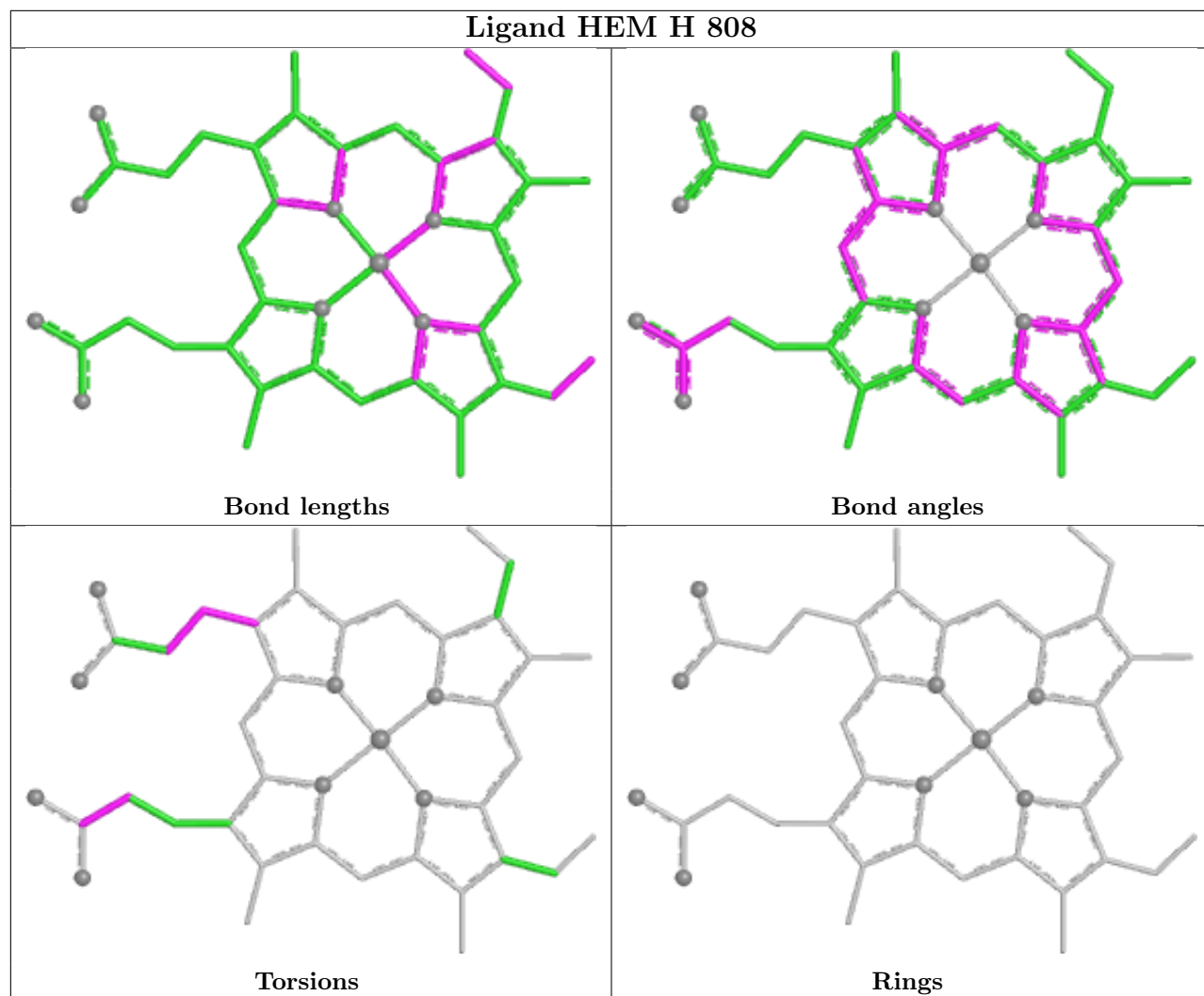
Torsions

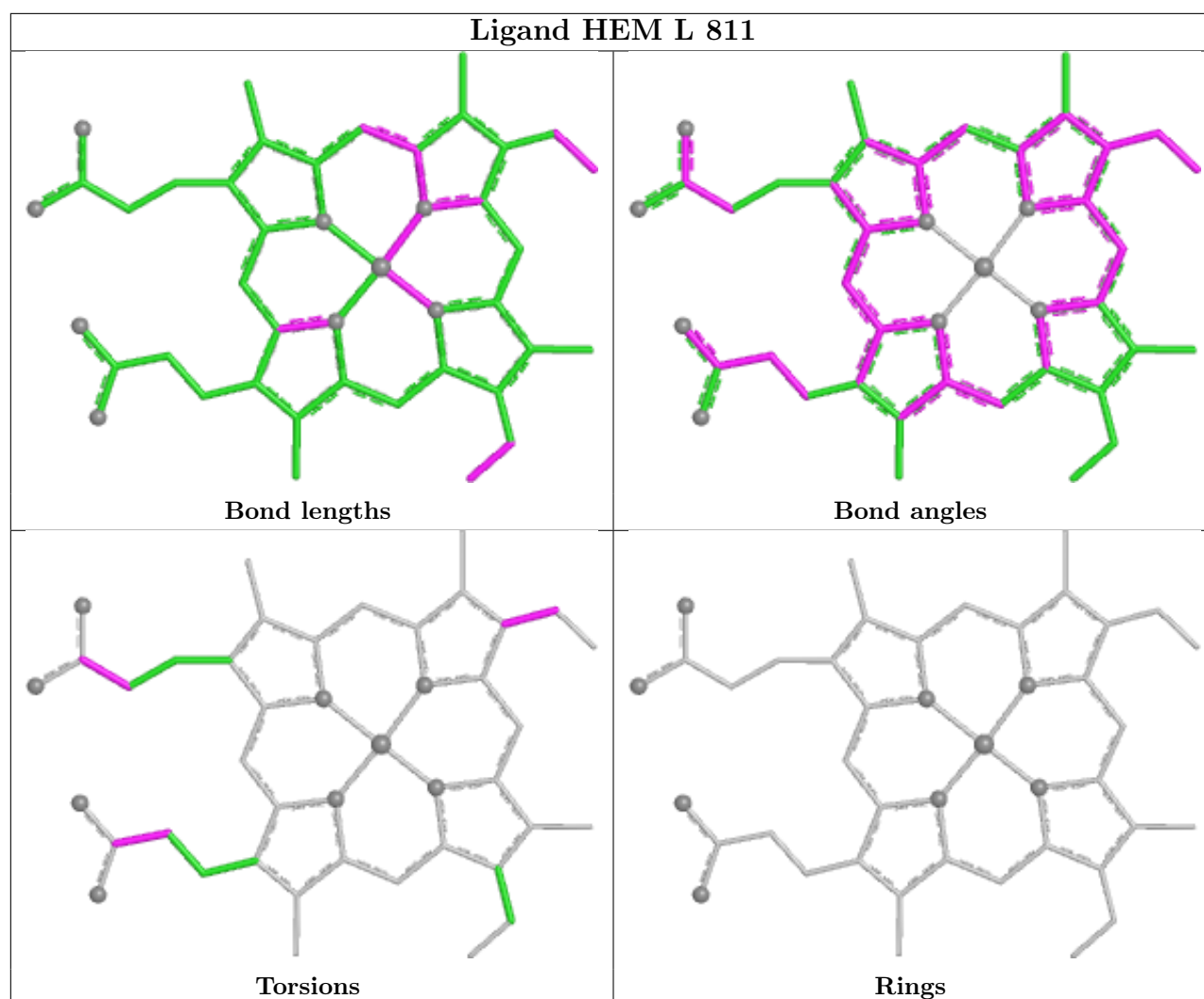


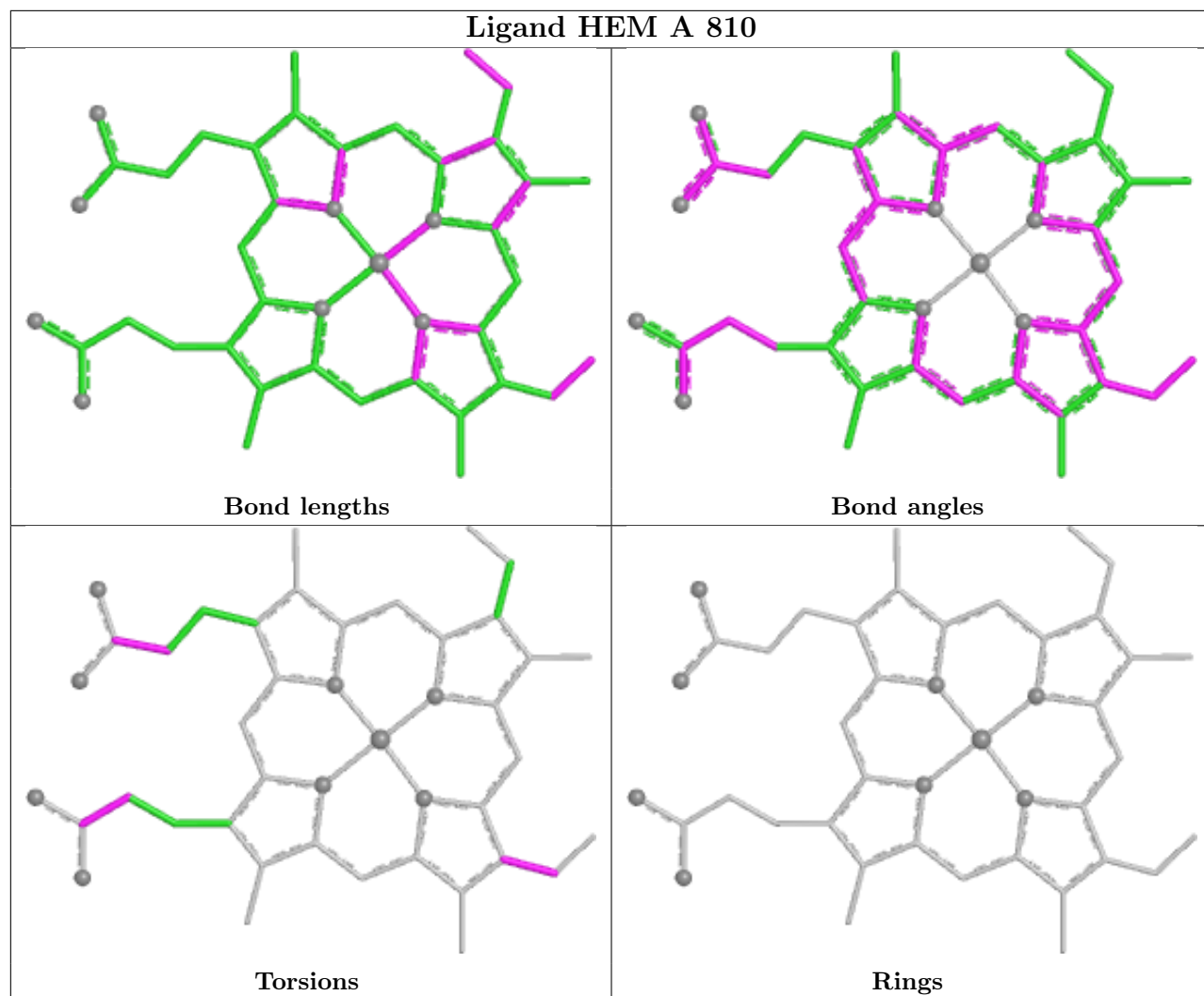
Rings



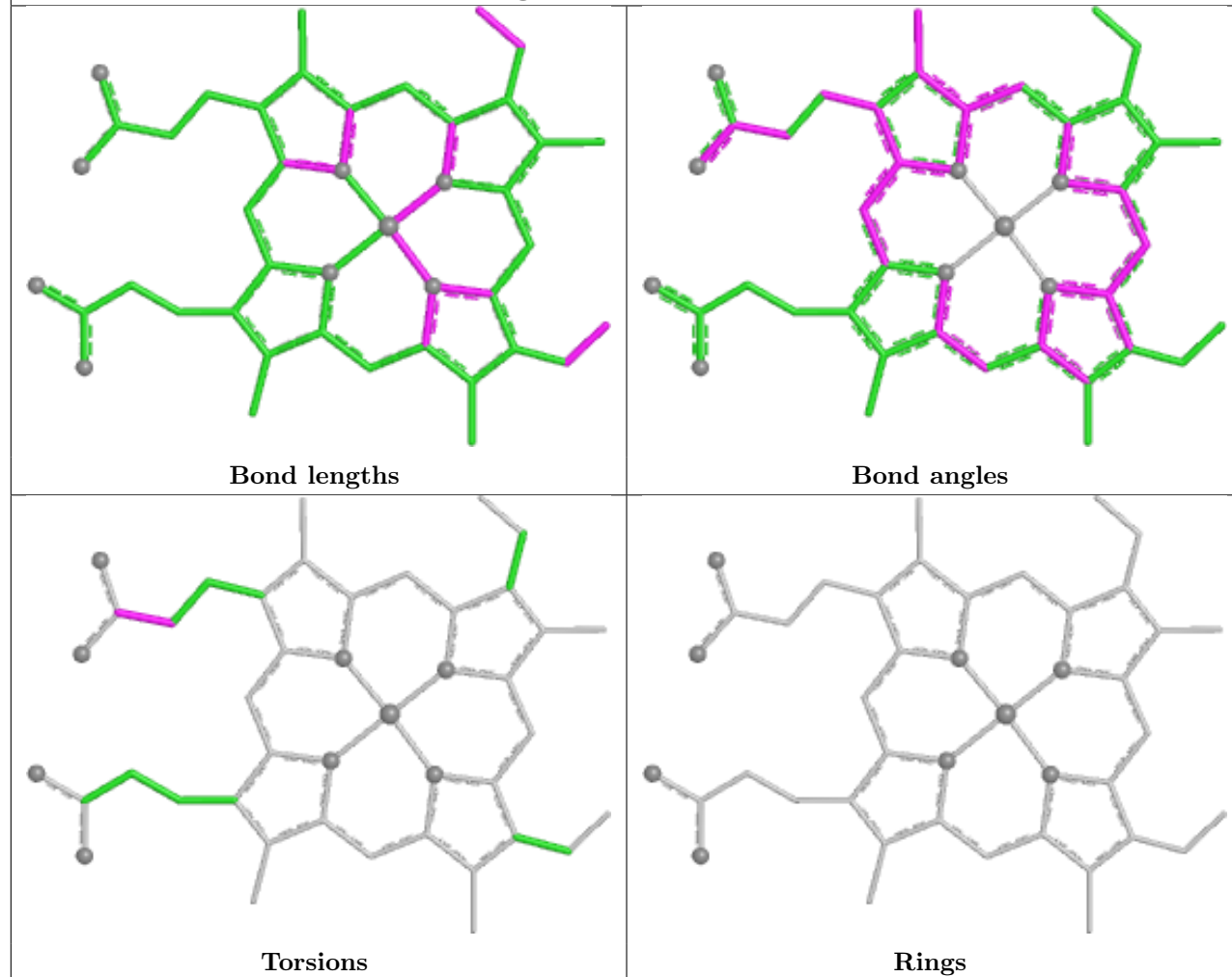


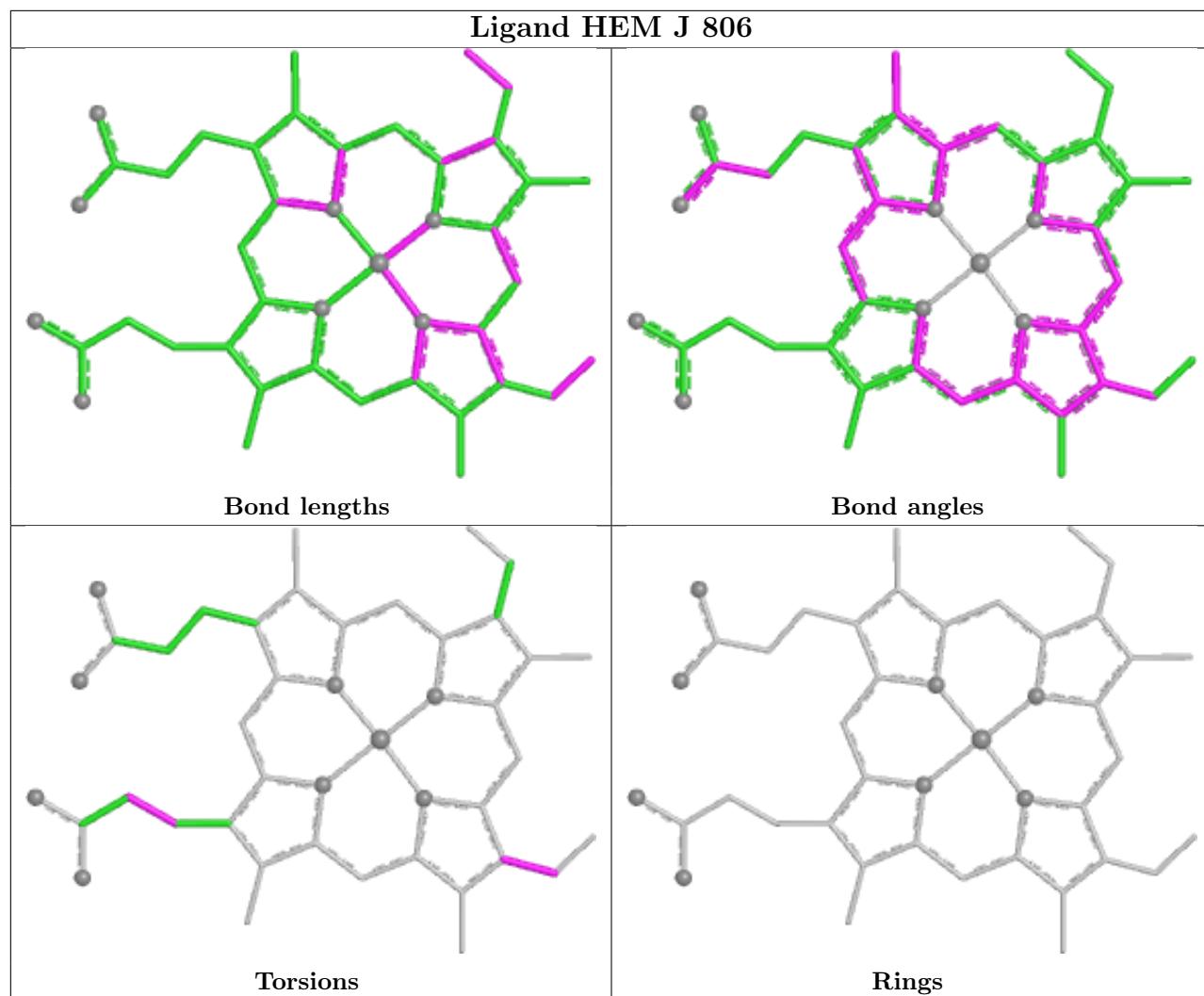


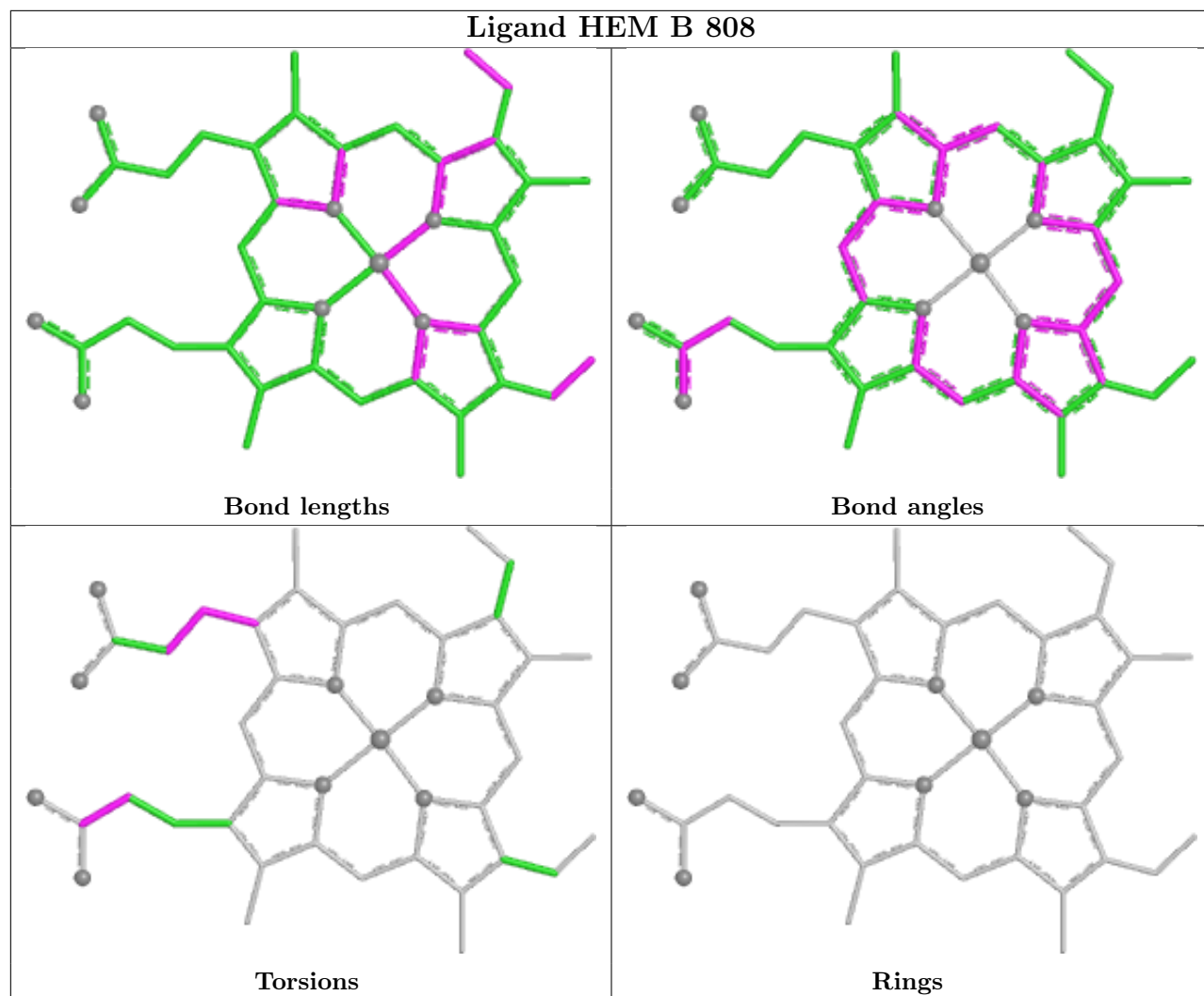


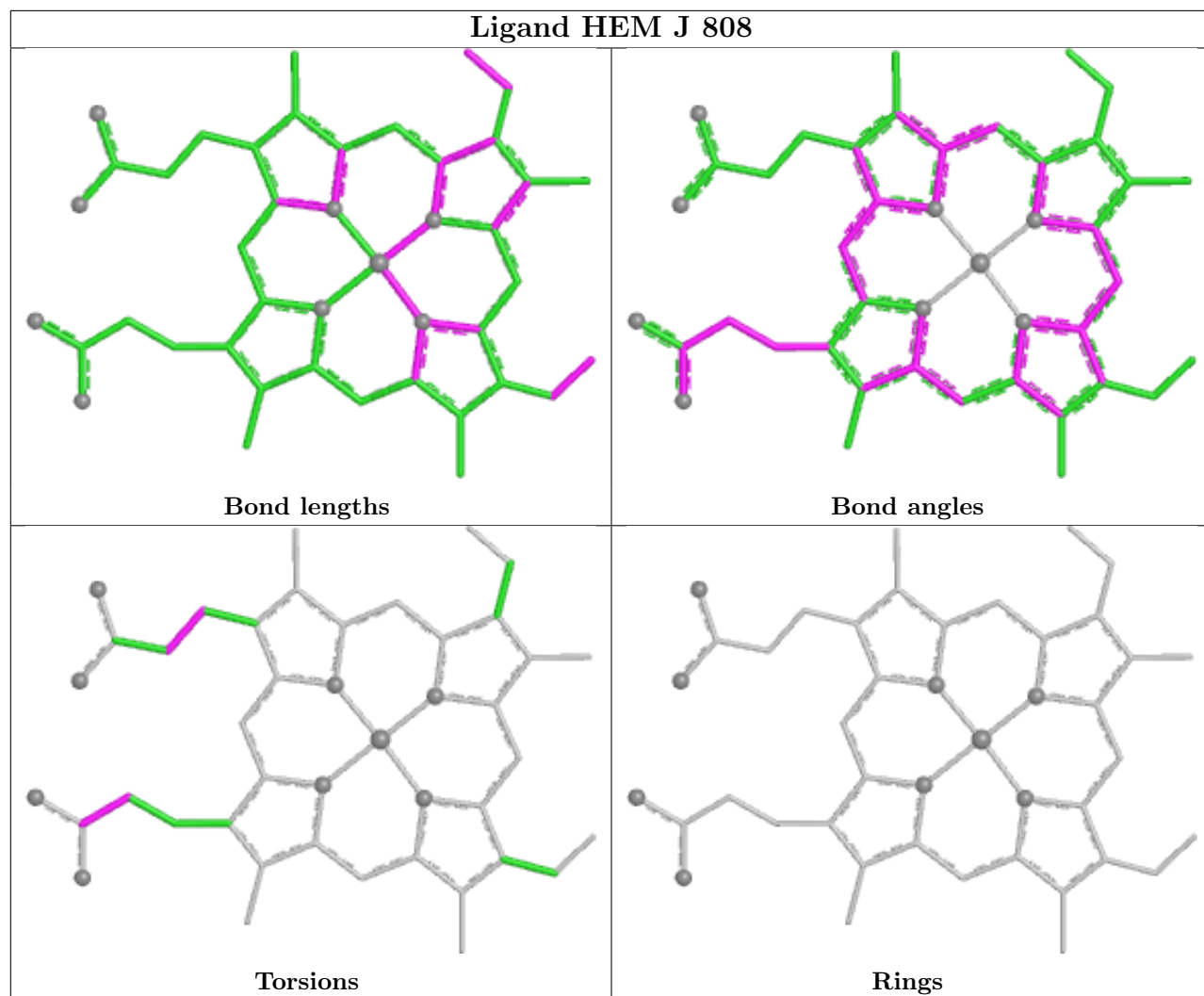


## Ligand HEM I 809

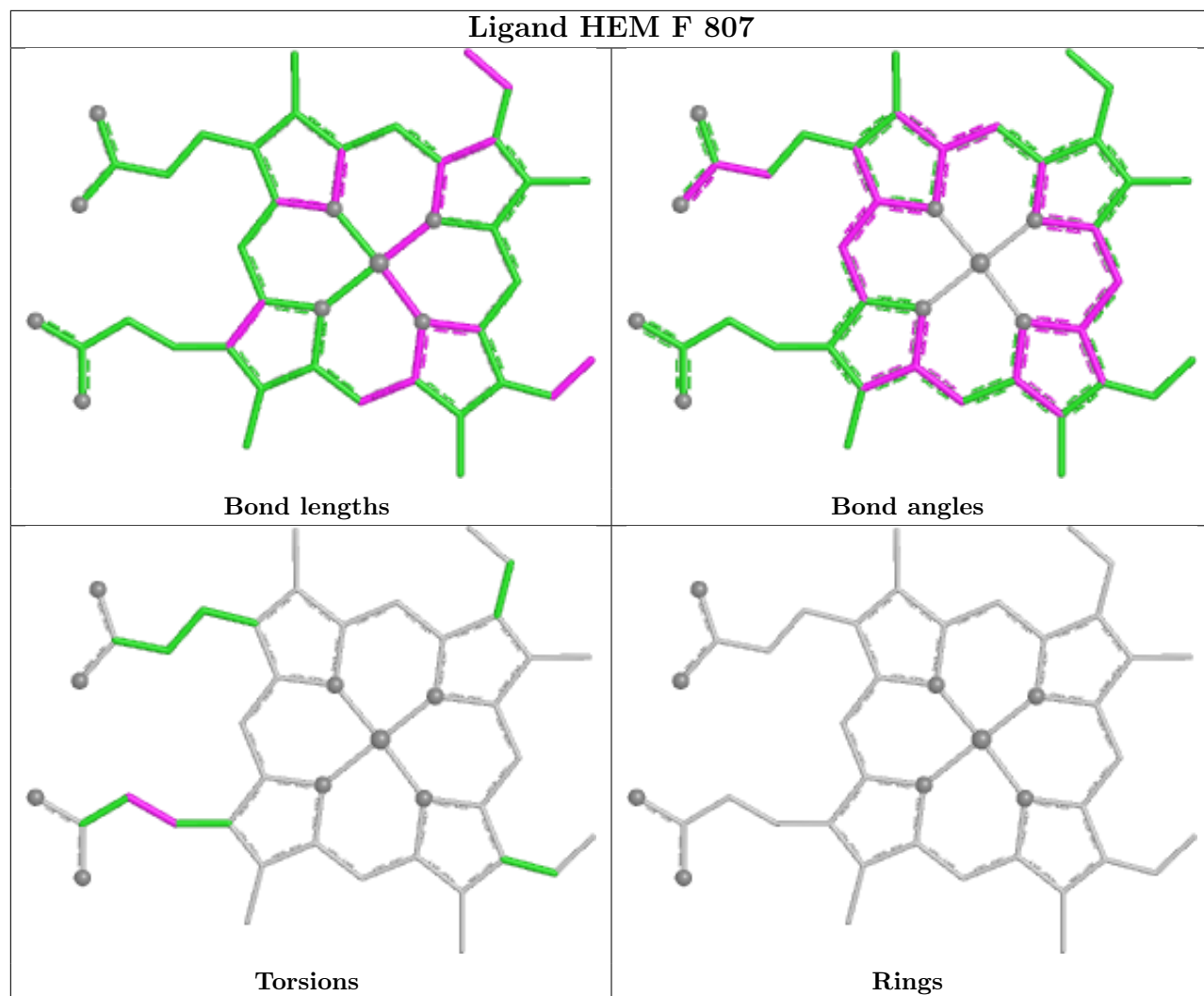


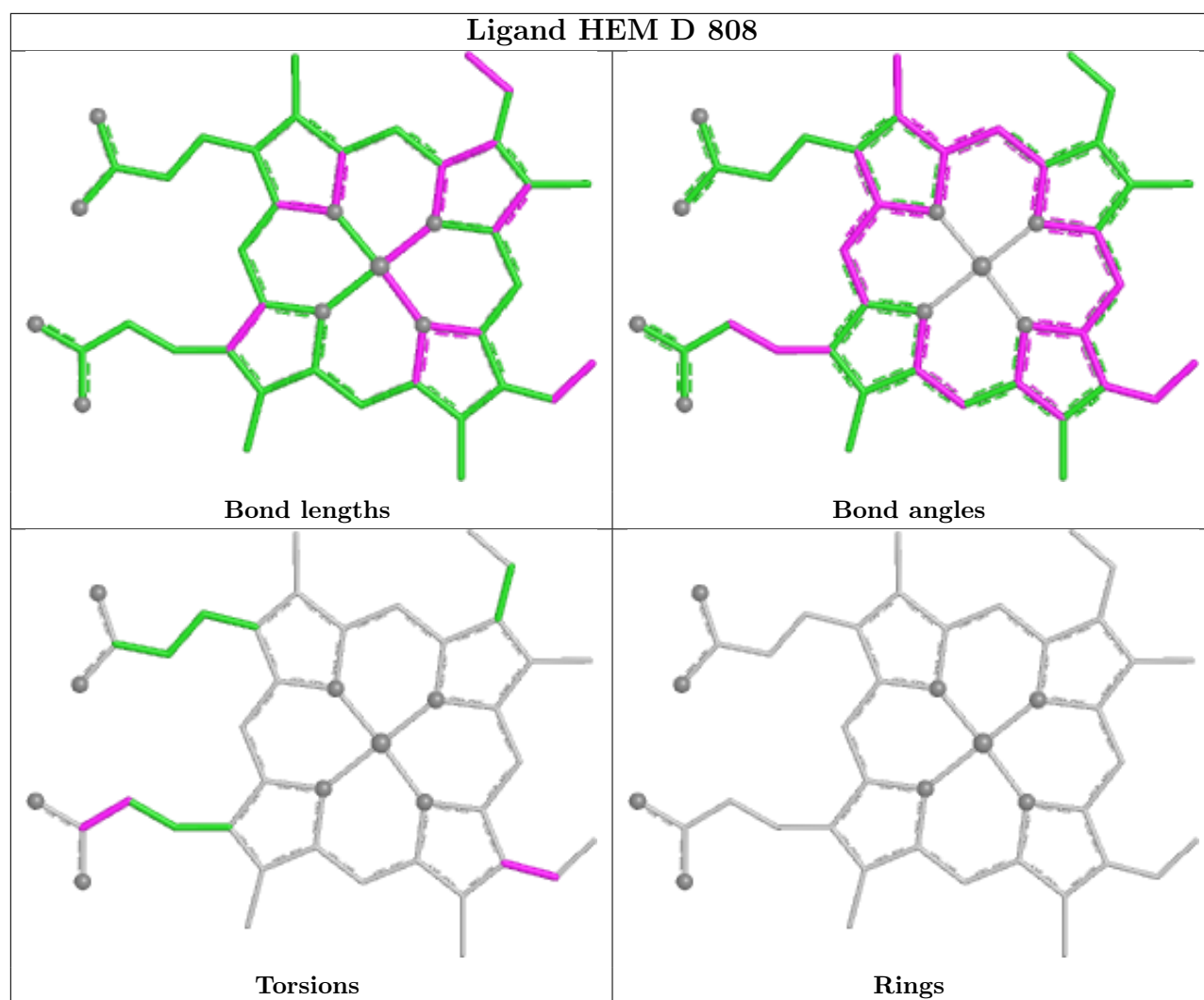


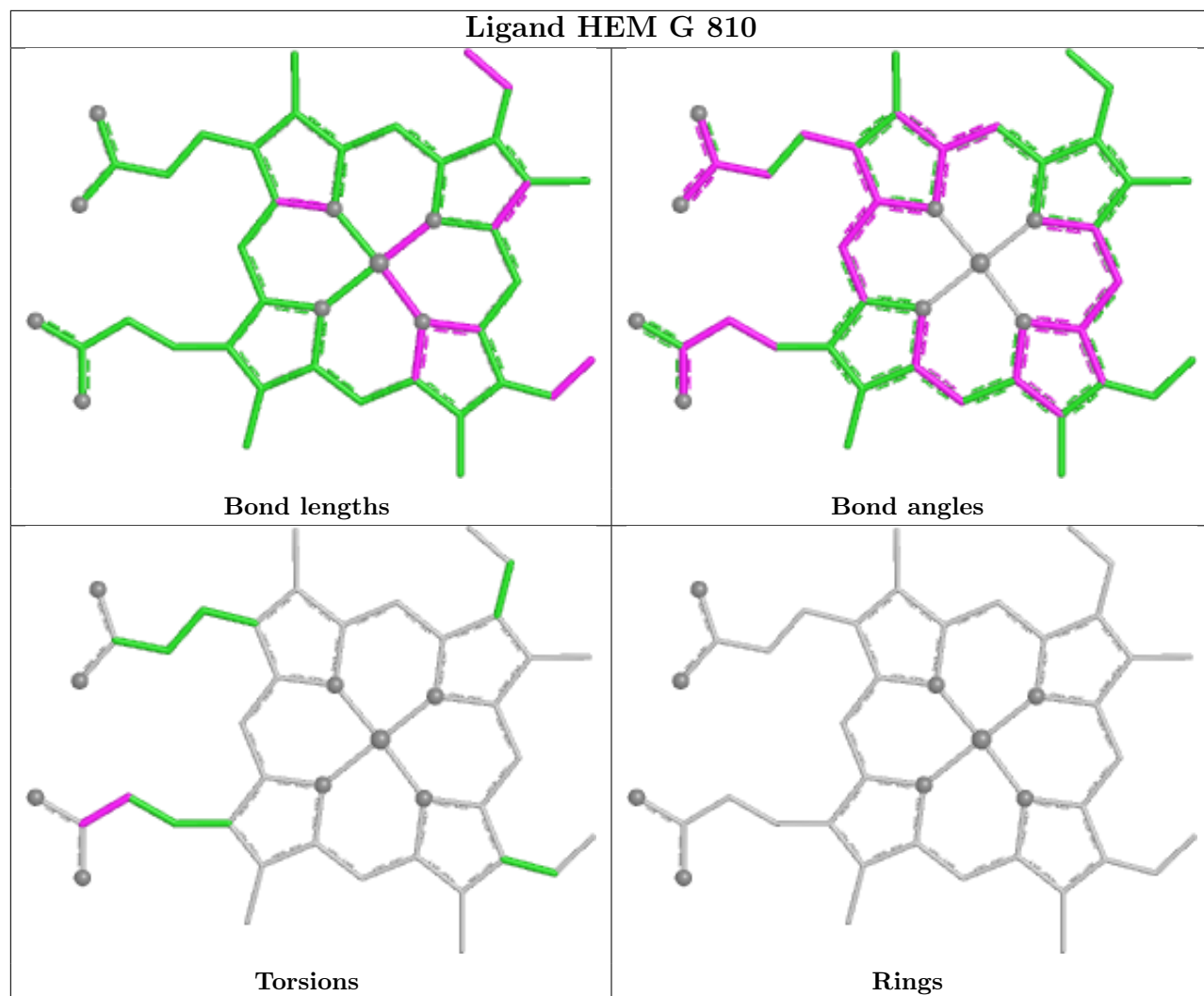




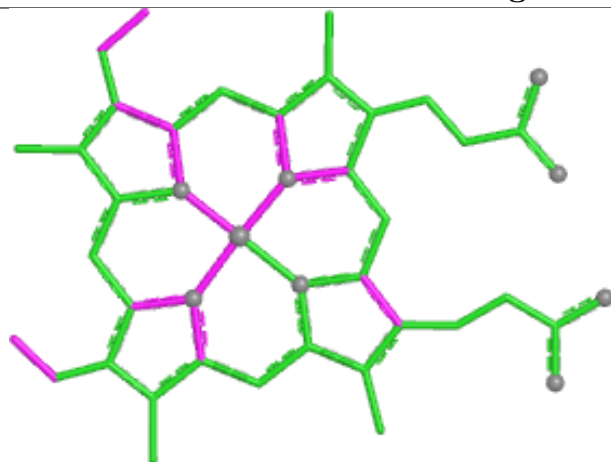




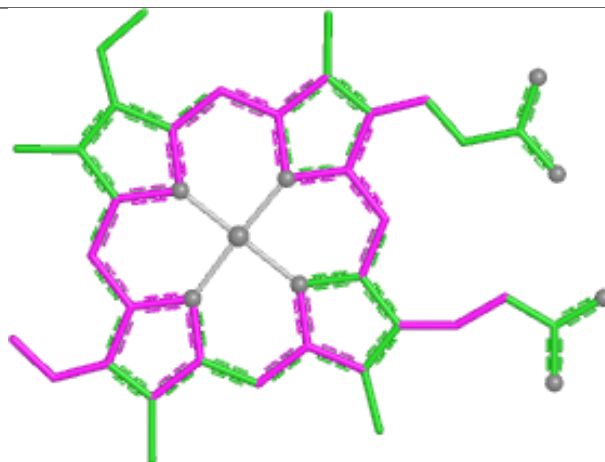




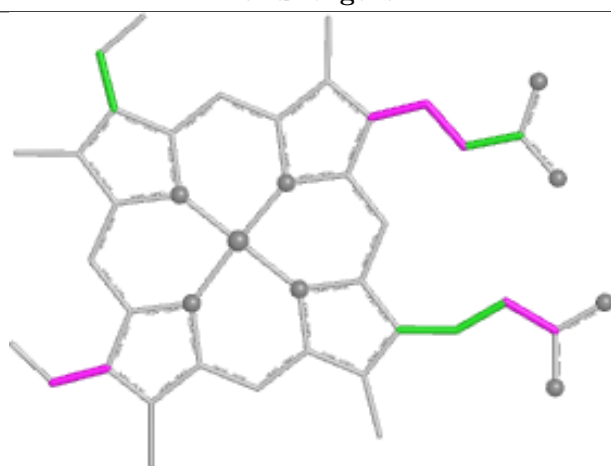
## Ligand HEM C 808



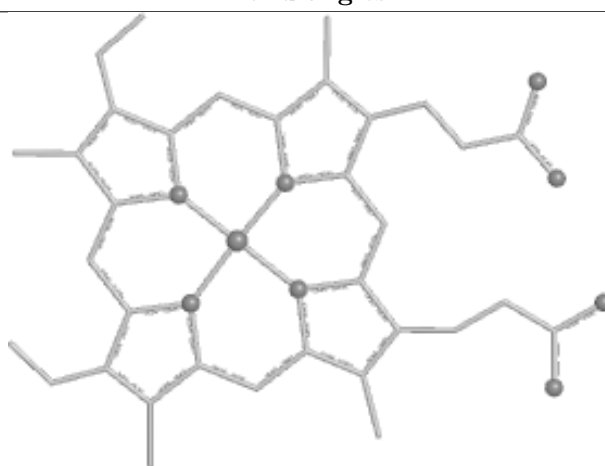
Bond lengths



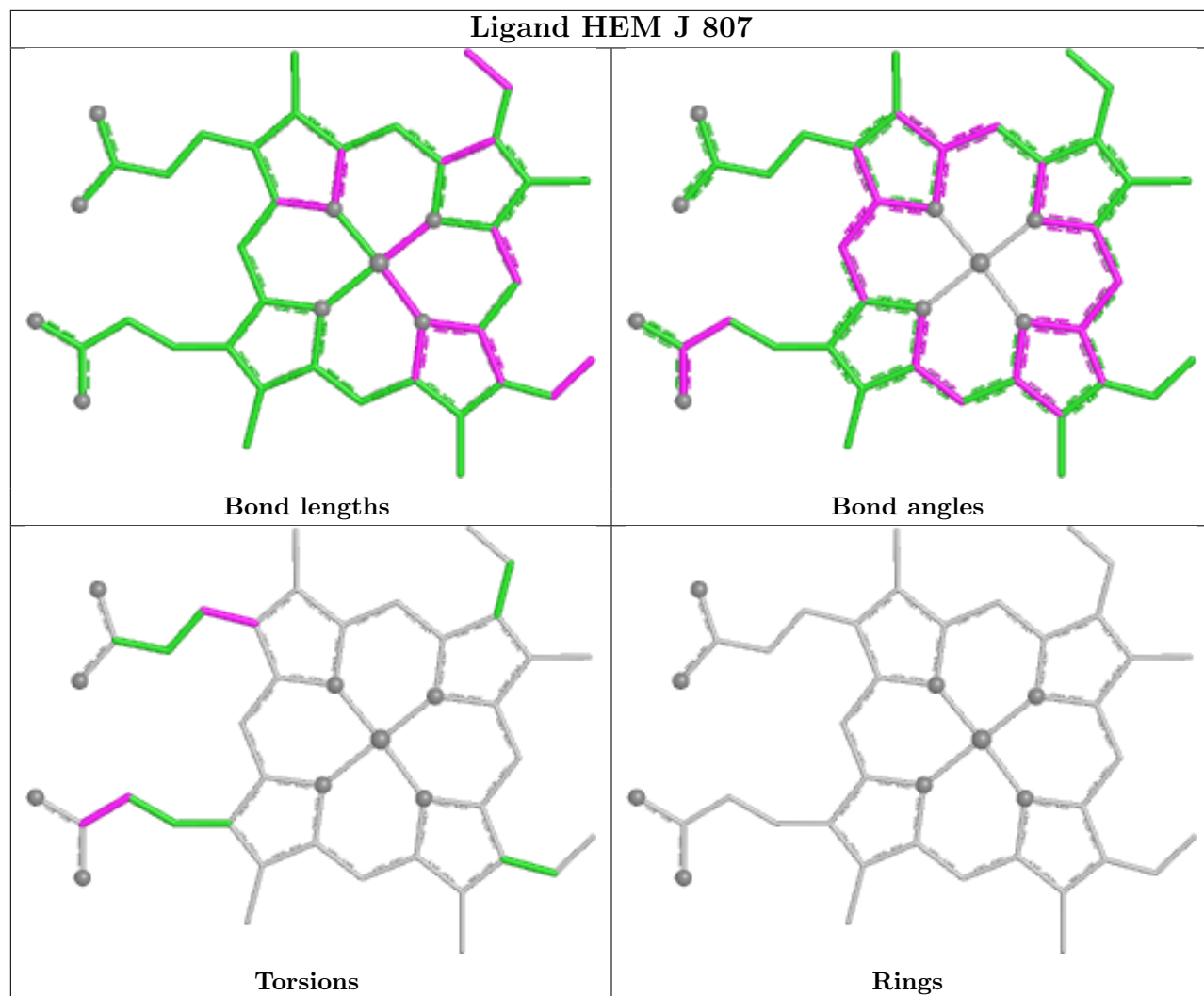
Bond angles

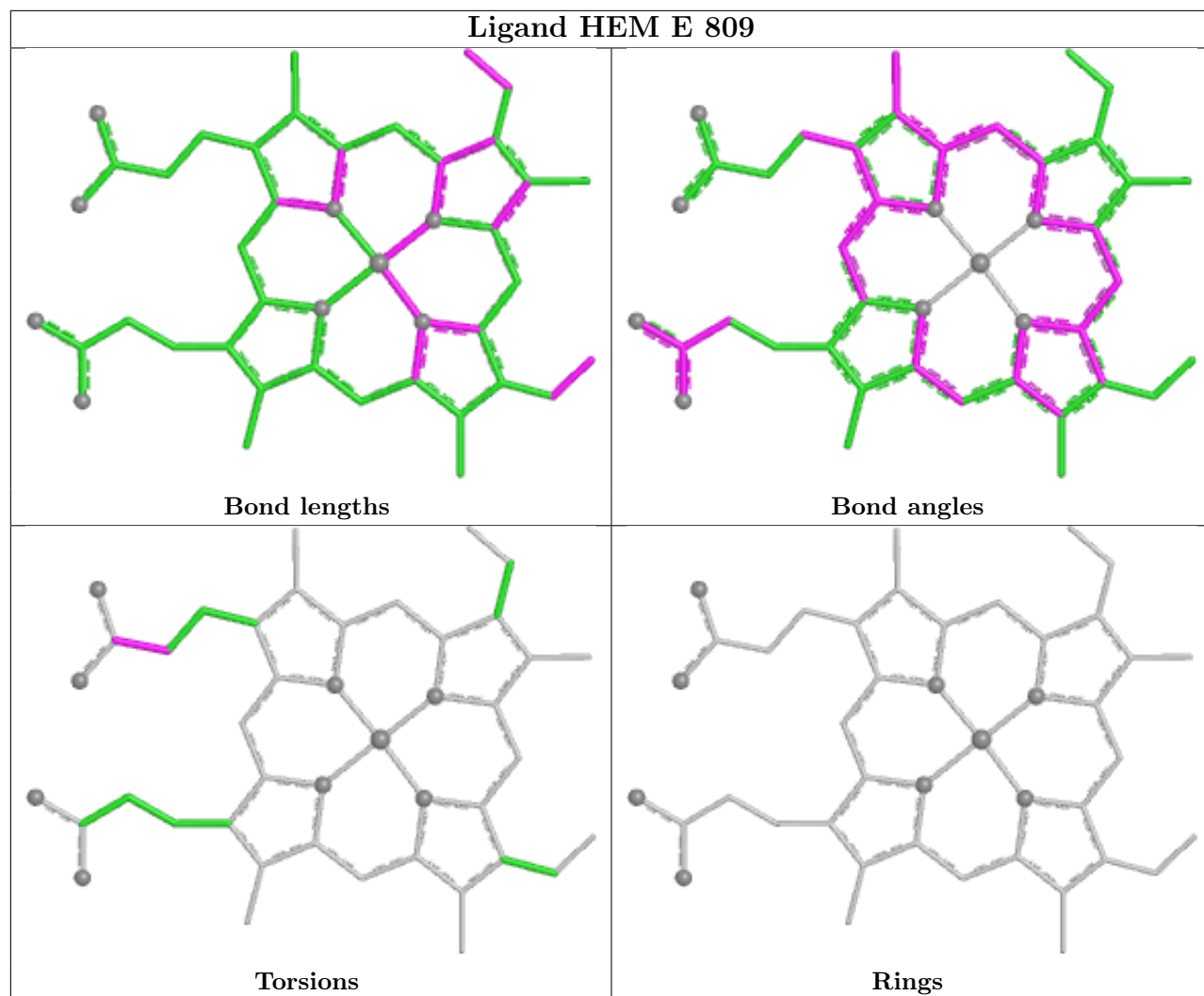


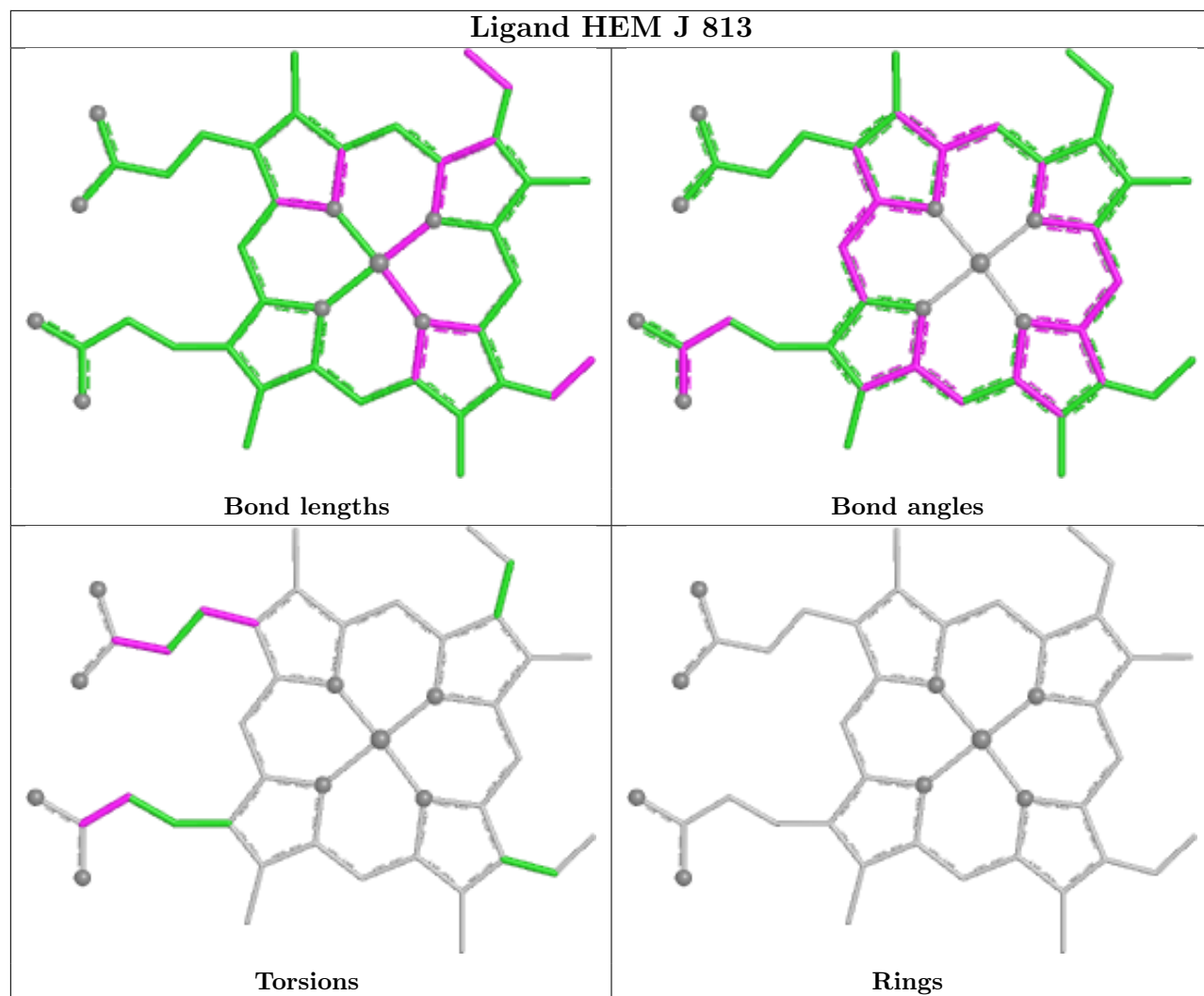
Torsions

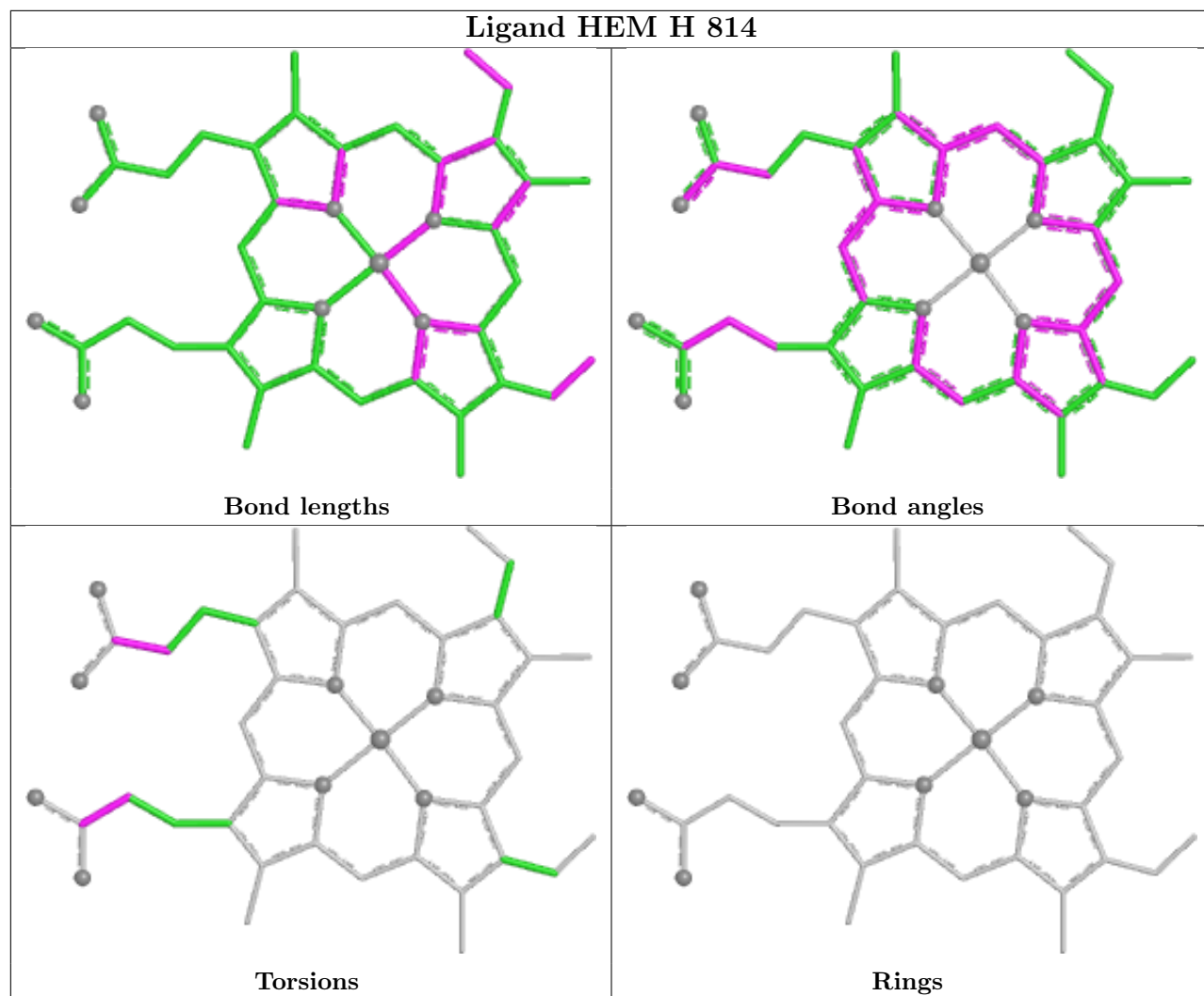


Rings

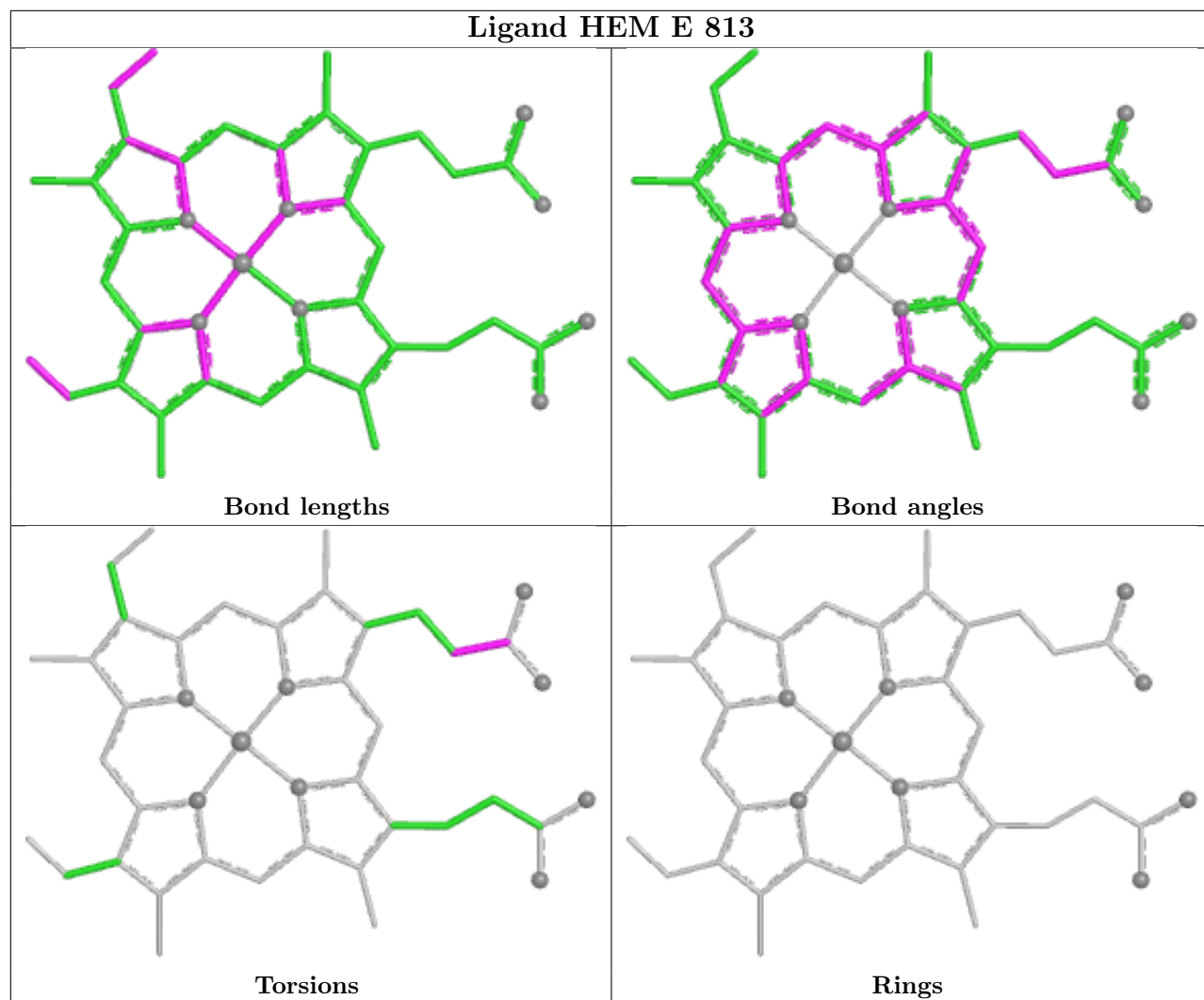




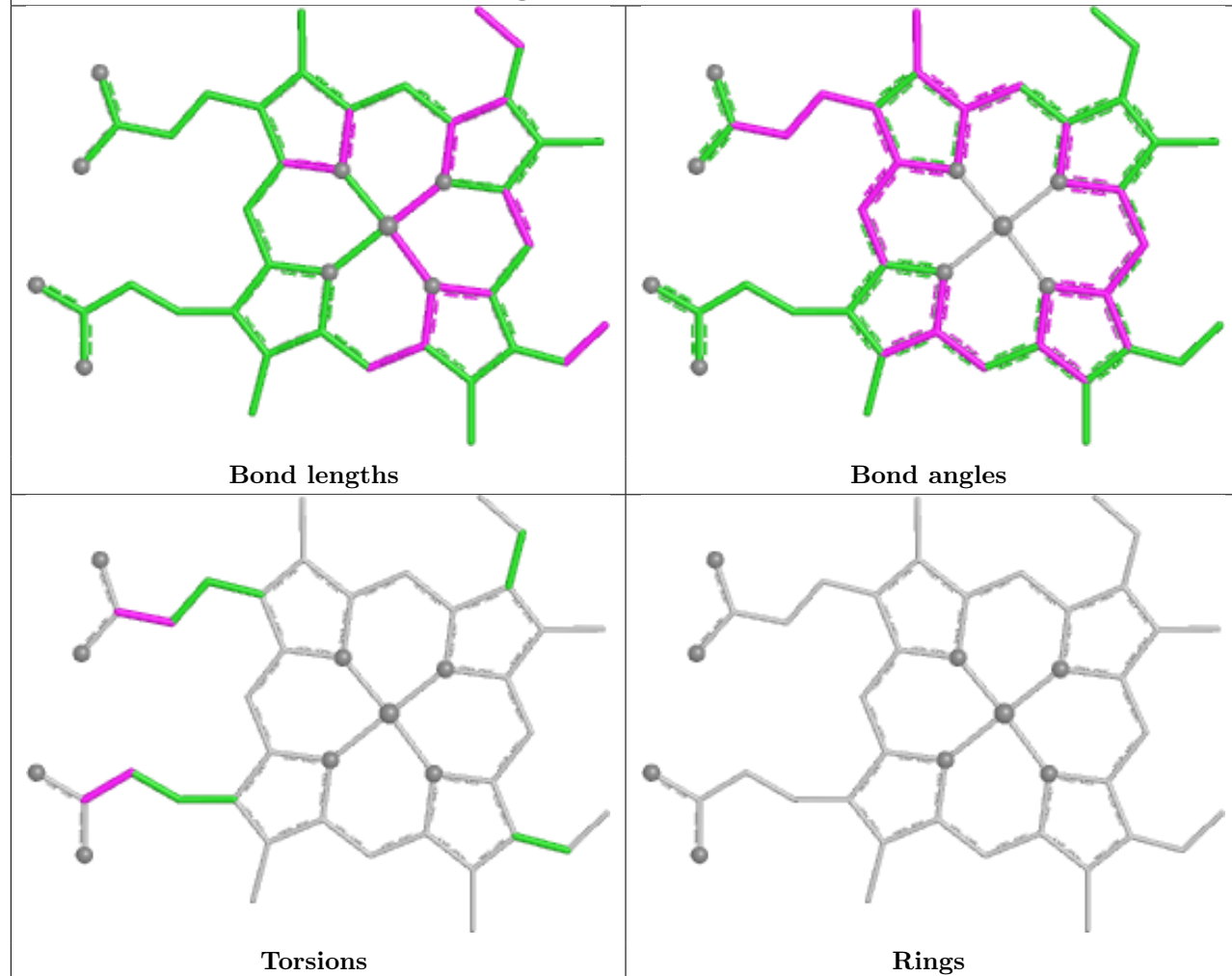




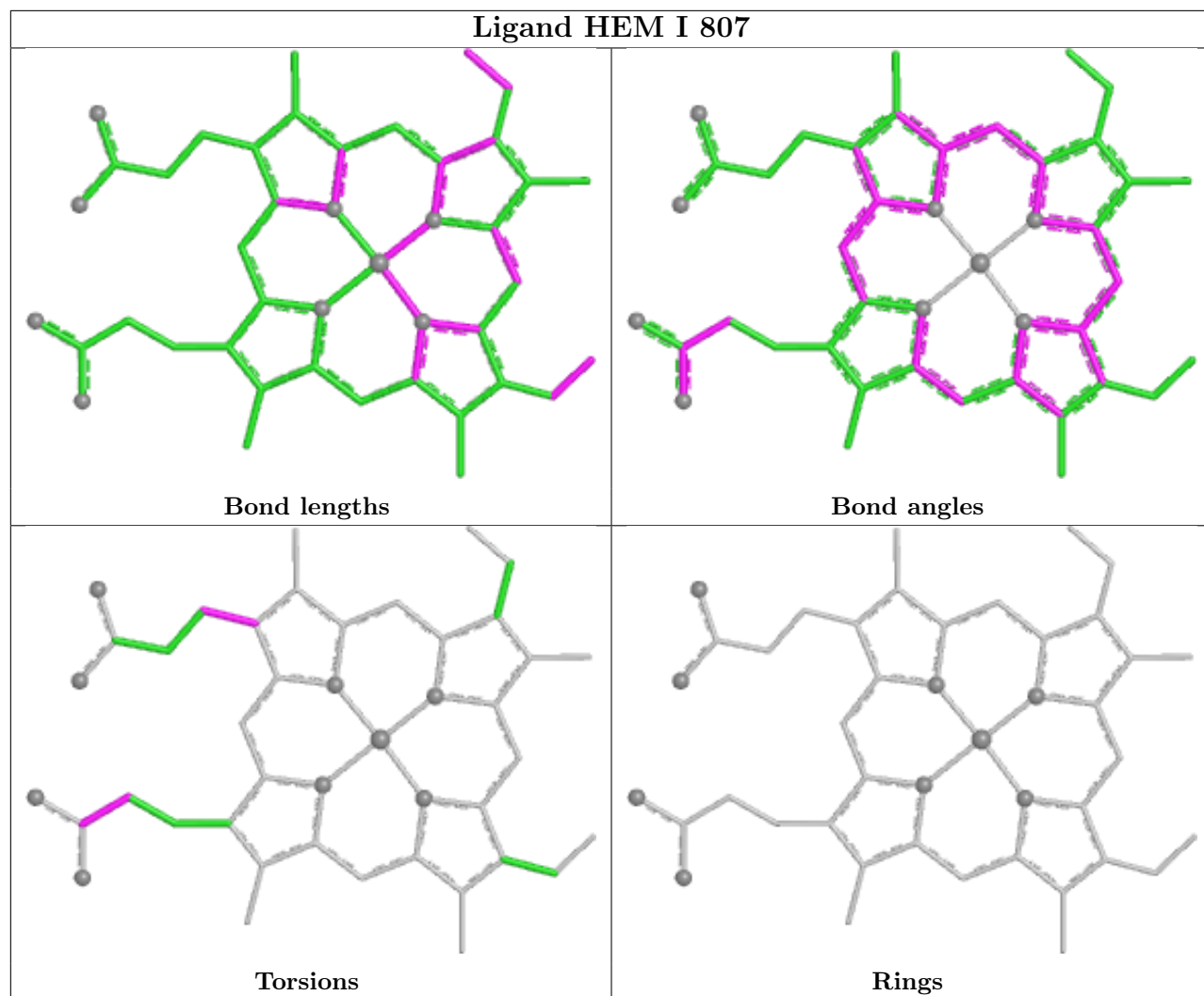


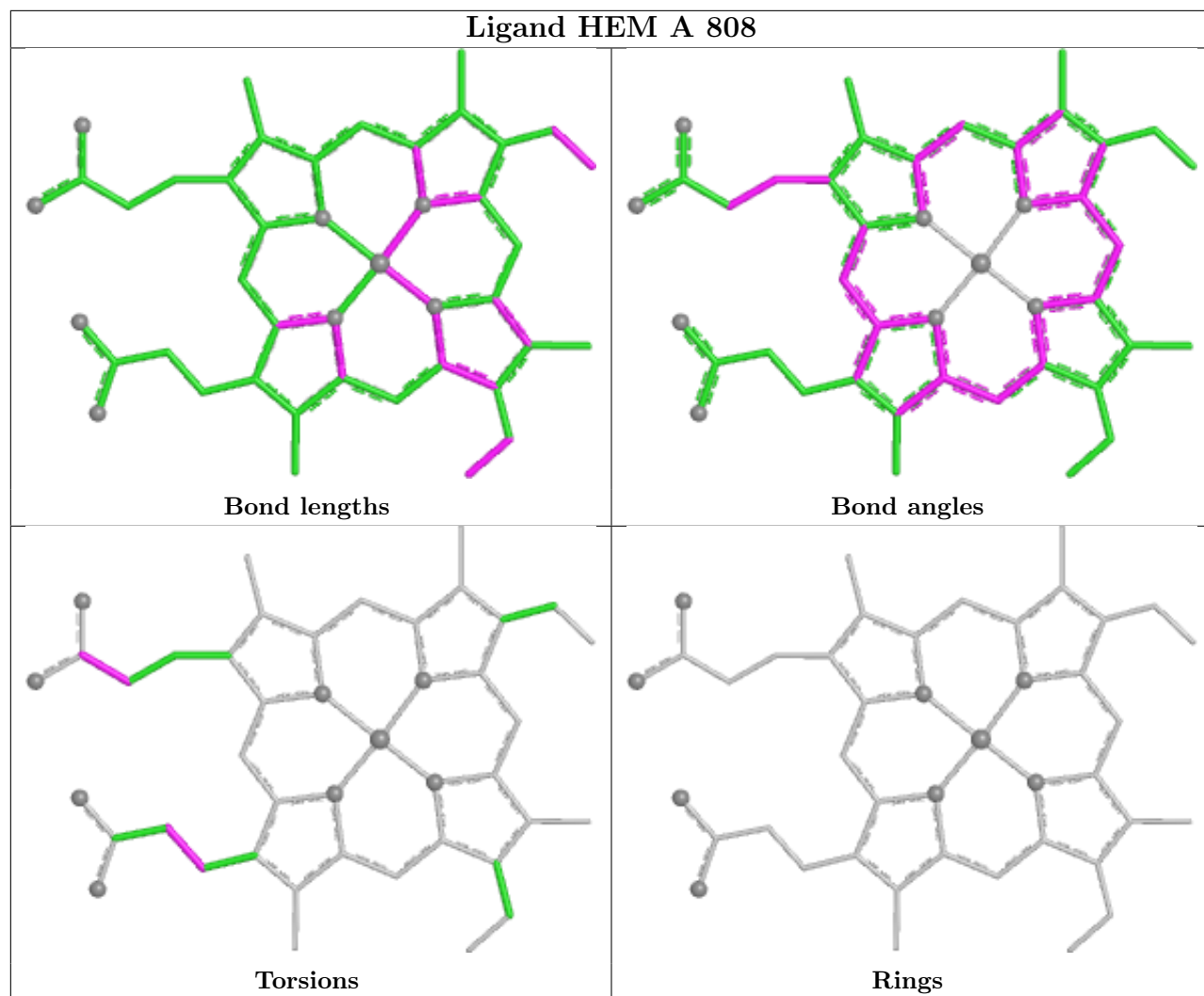


## Ligand HEM I 813

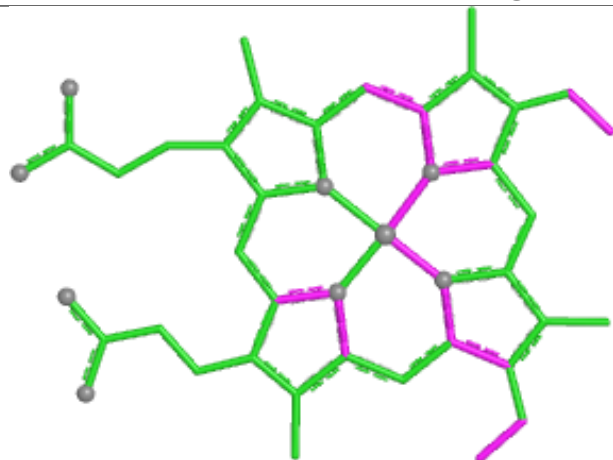


## Ligand HEM I 807

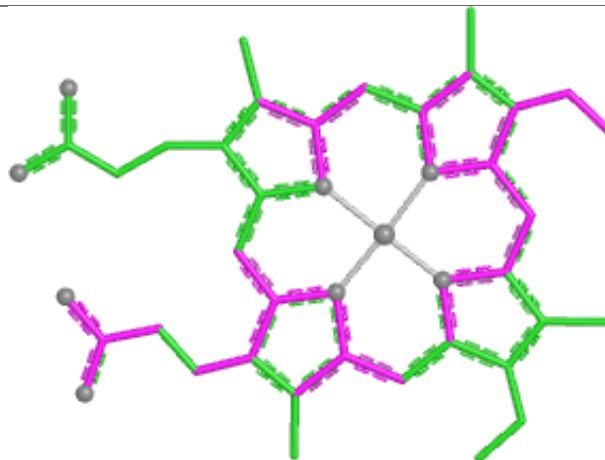




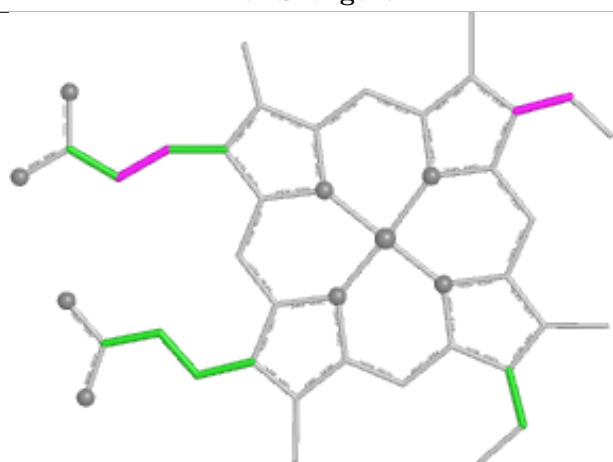
## Ligand HEM A 806



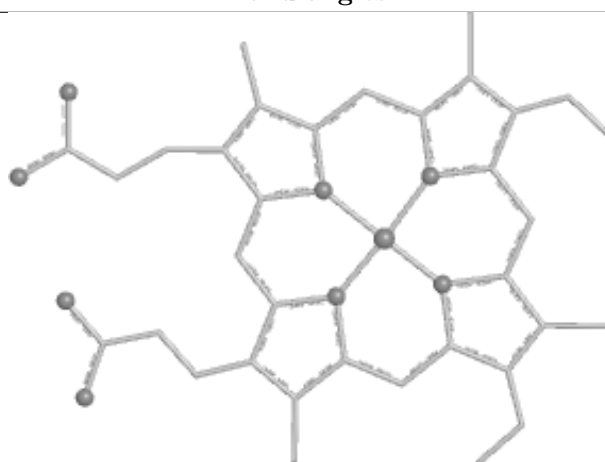
Bond lengths



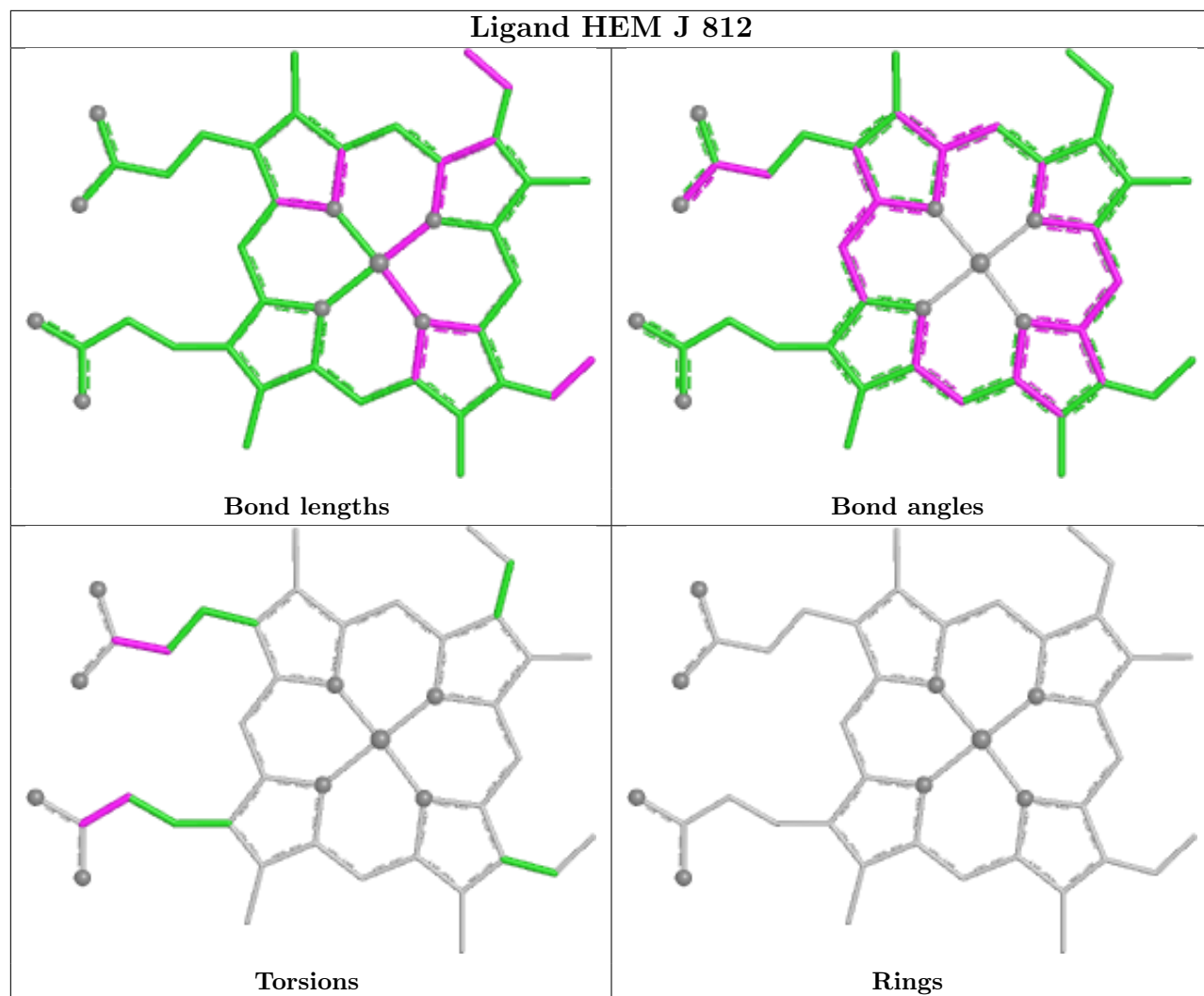
Bond angles

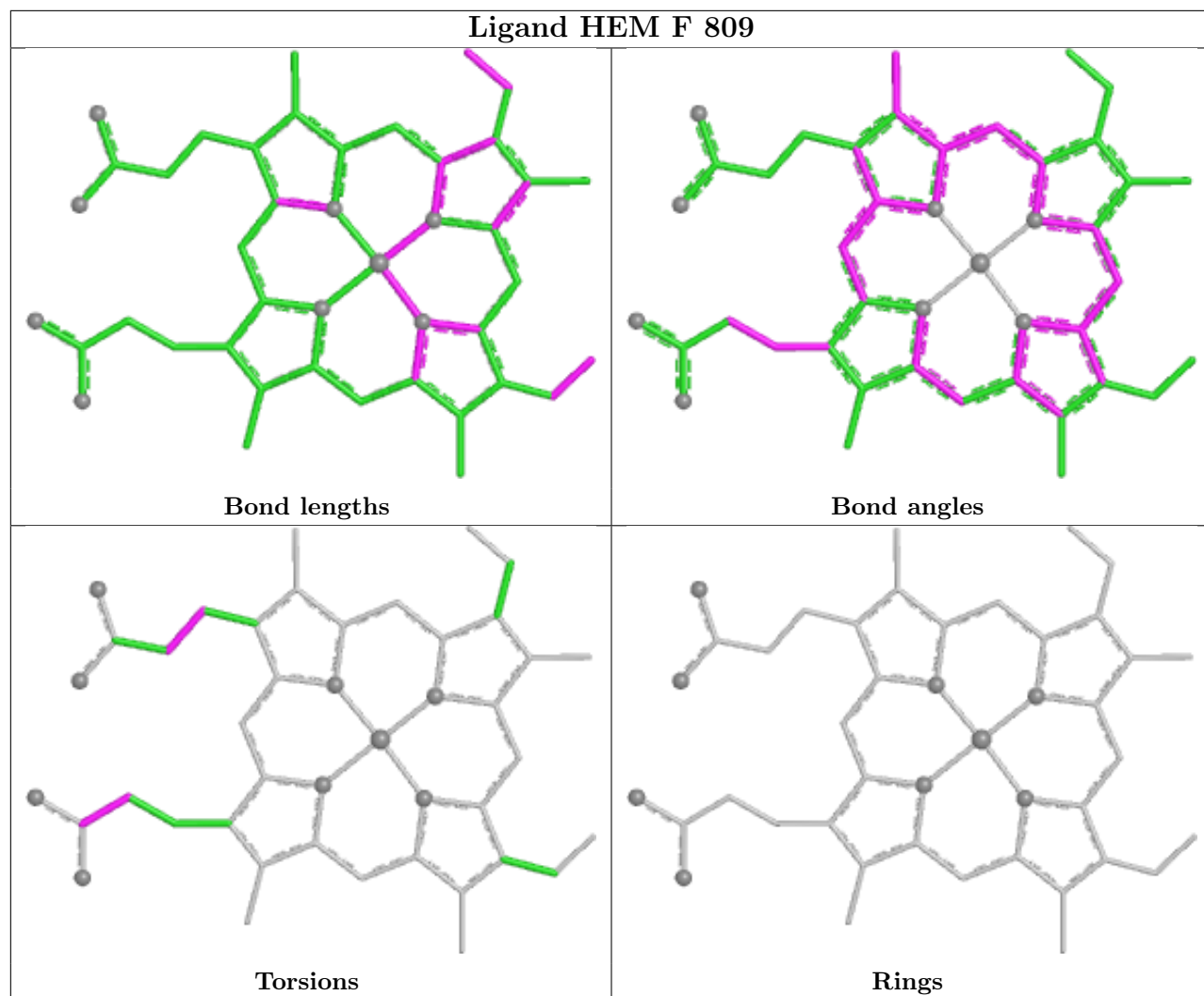


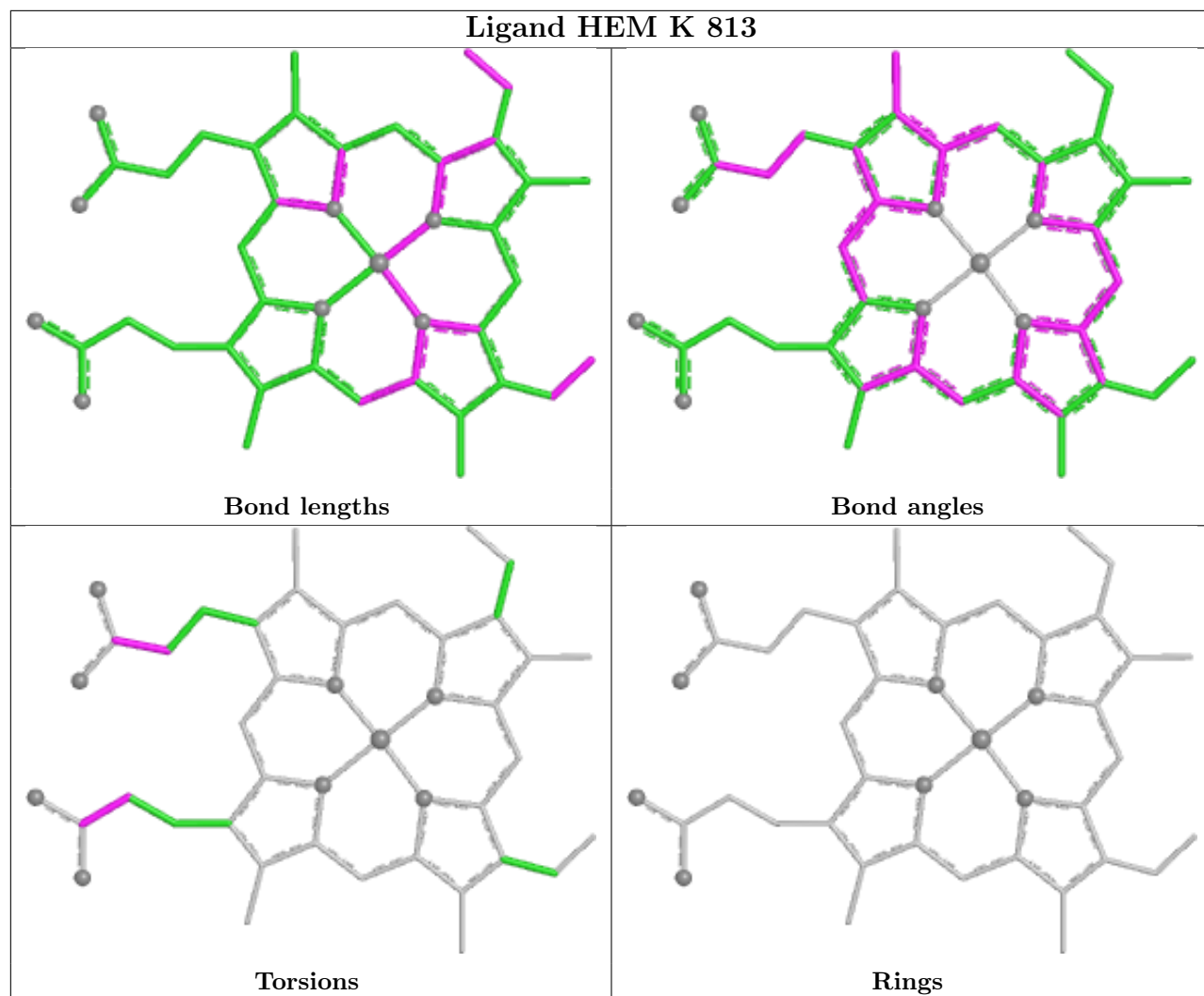
Torsions



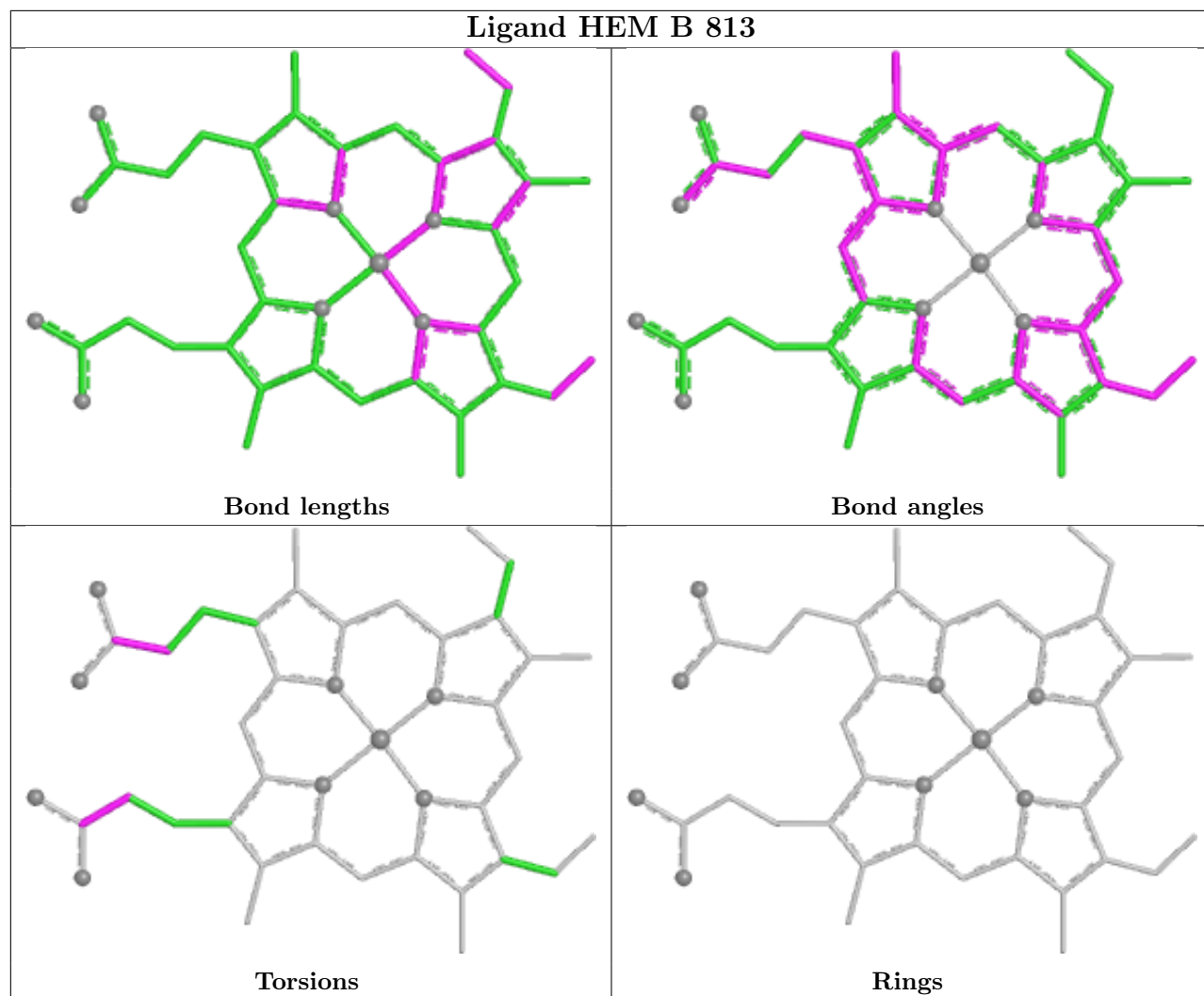
Rings

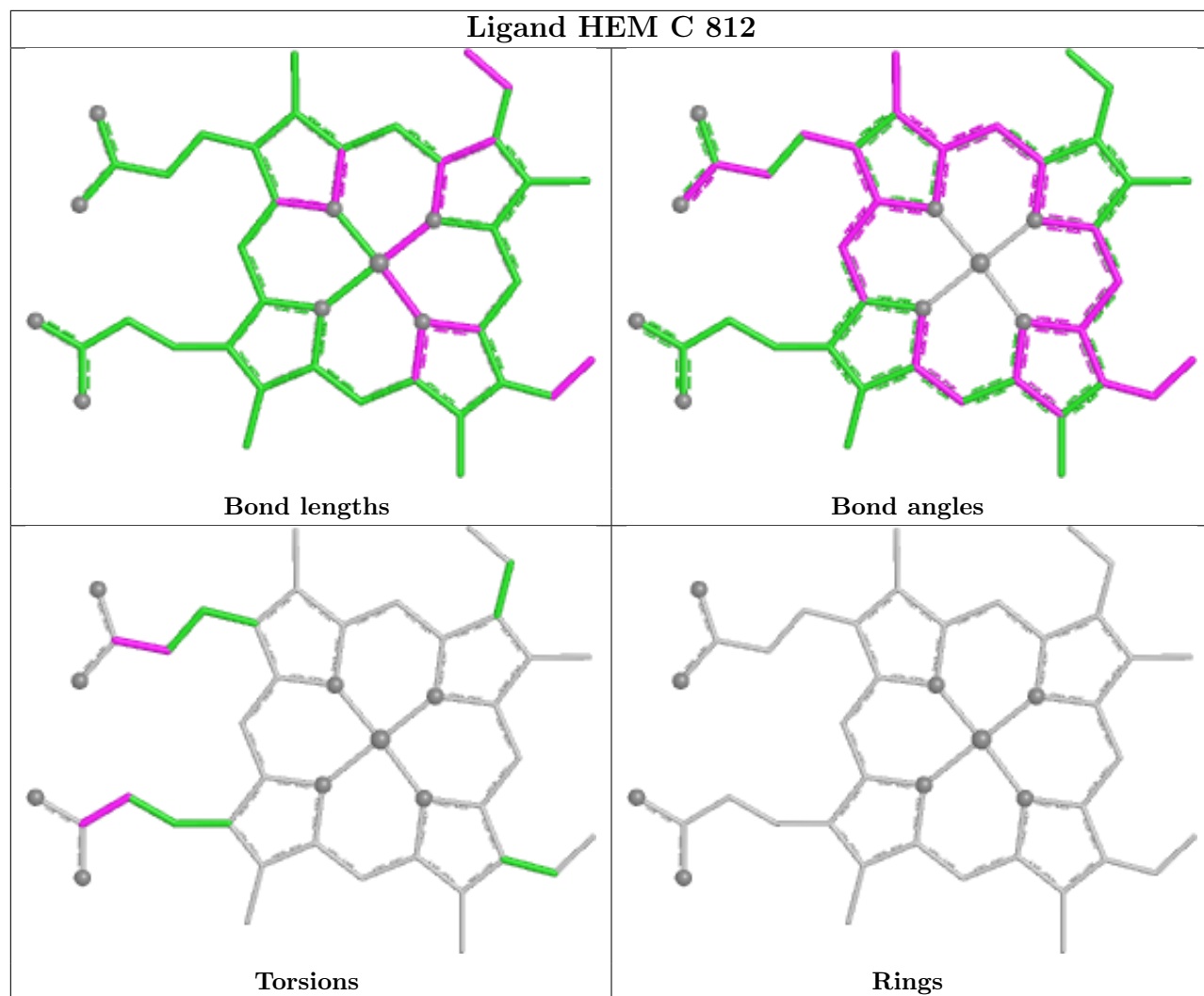




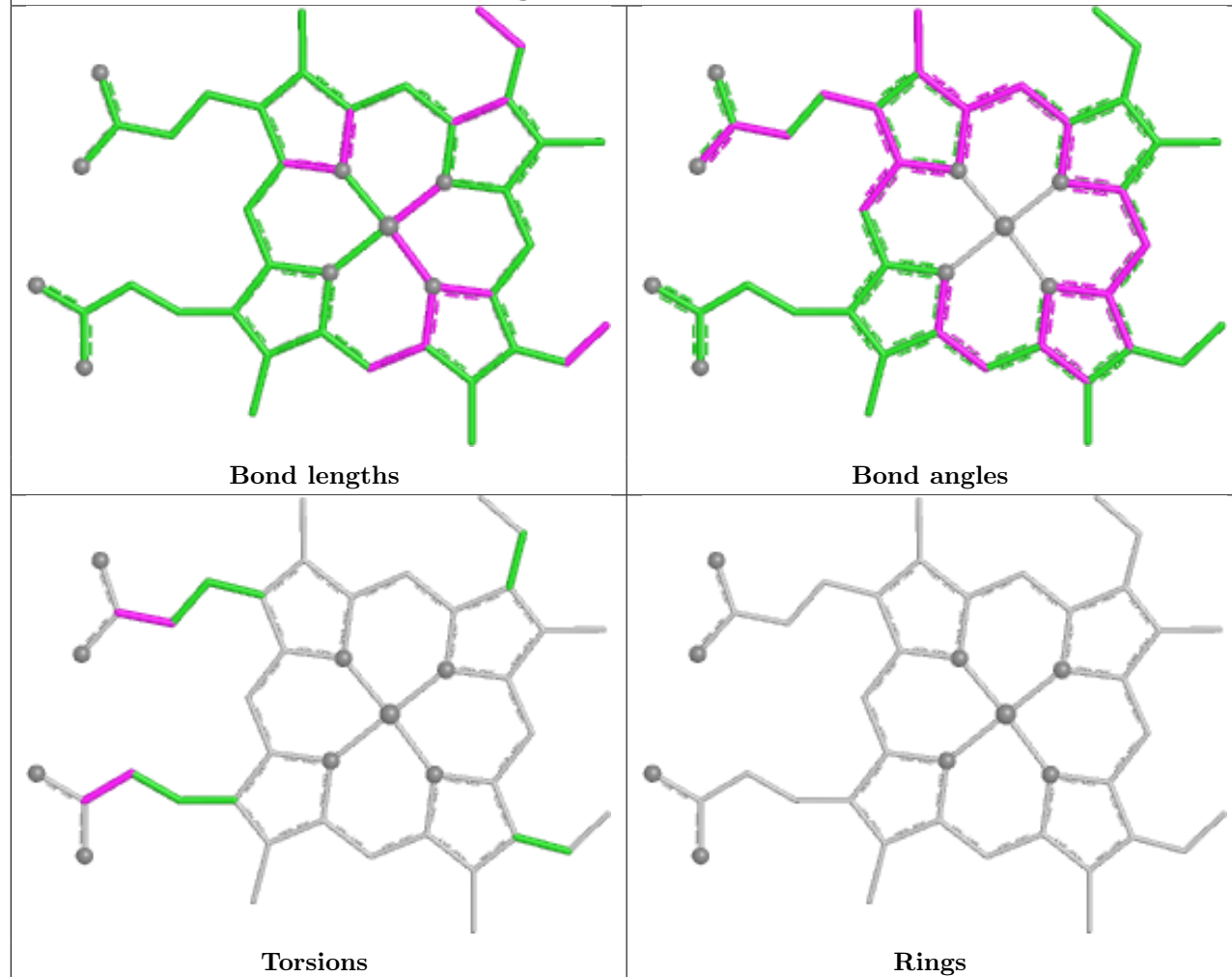


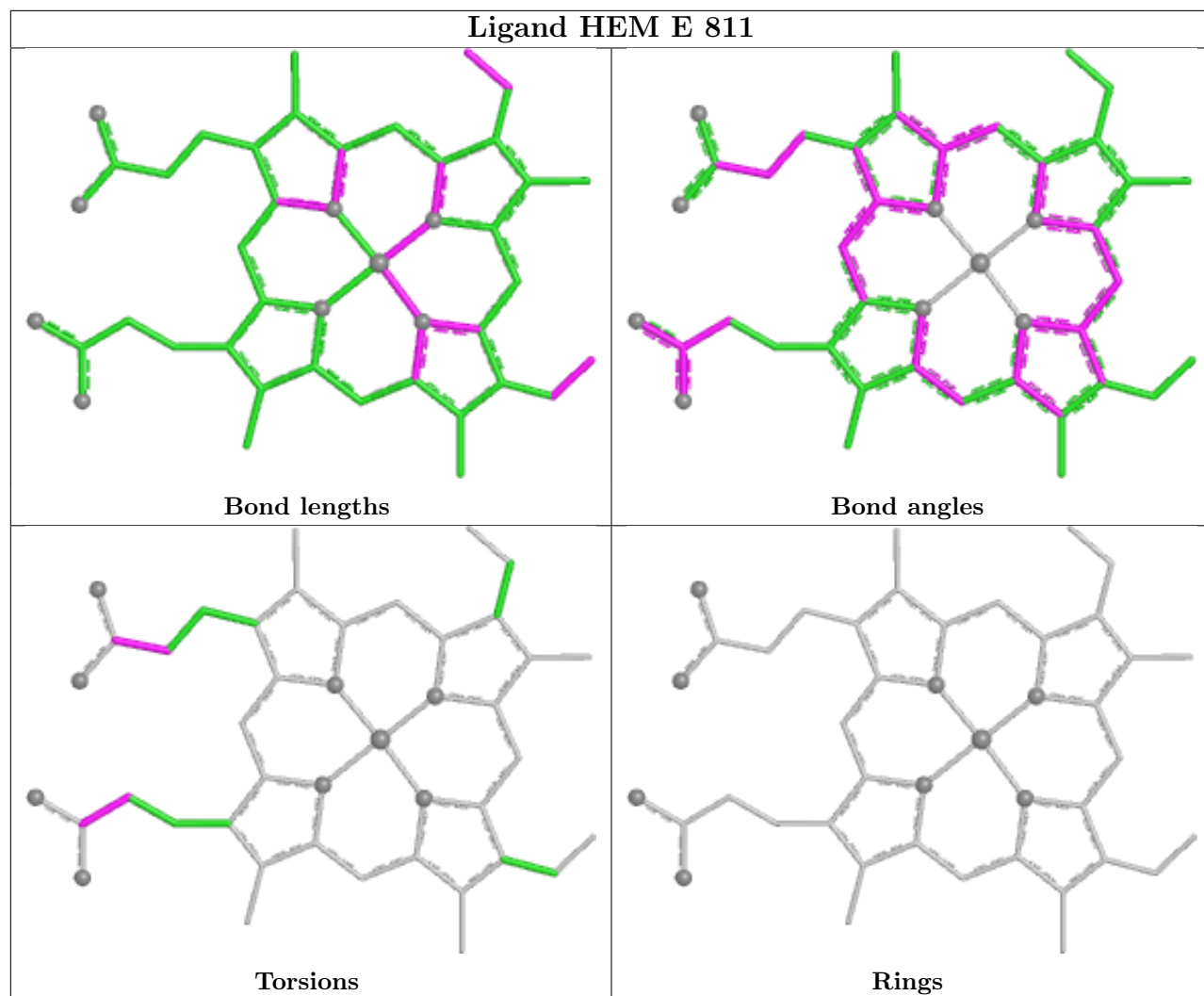


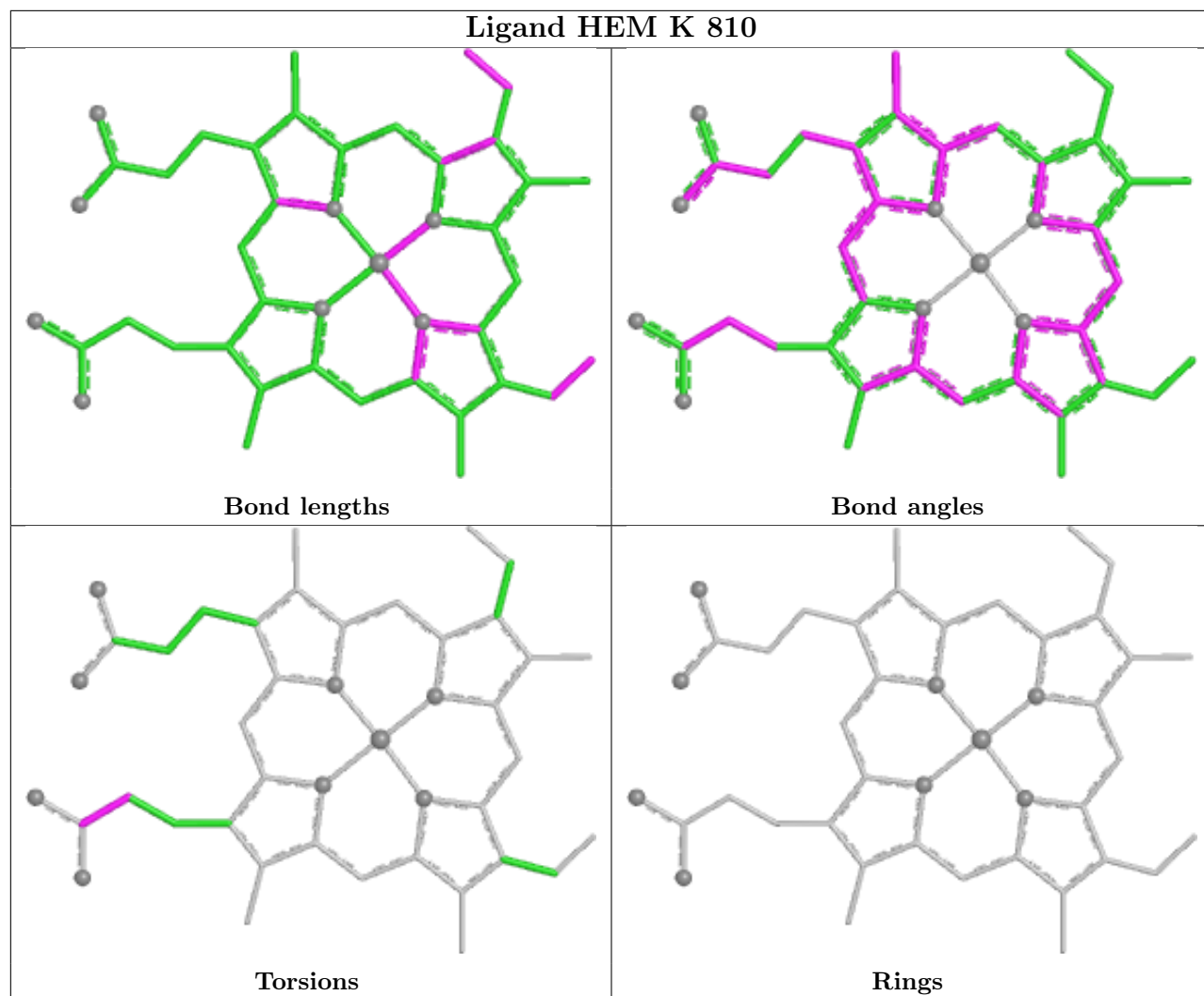


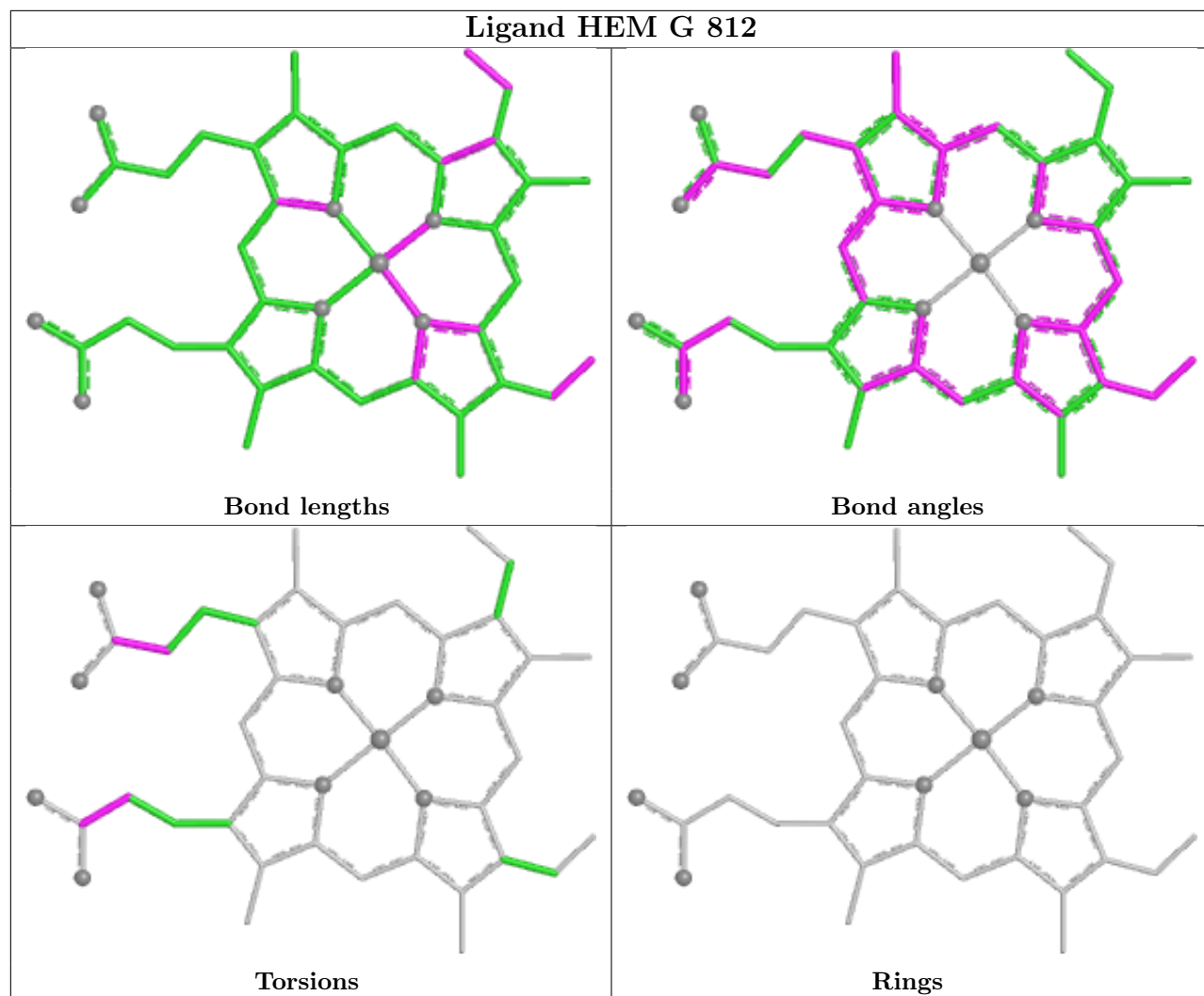


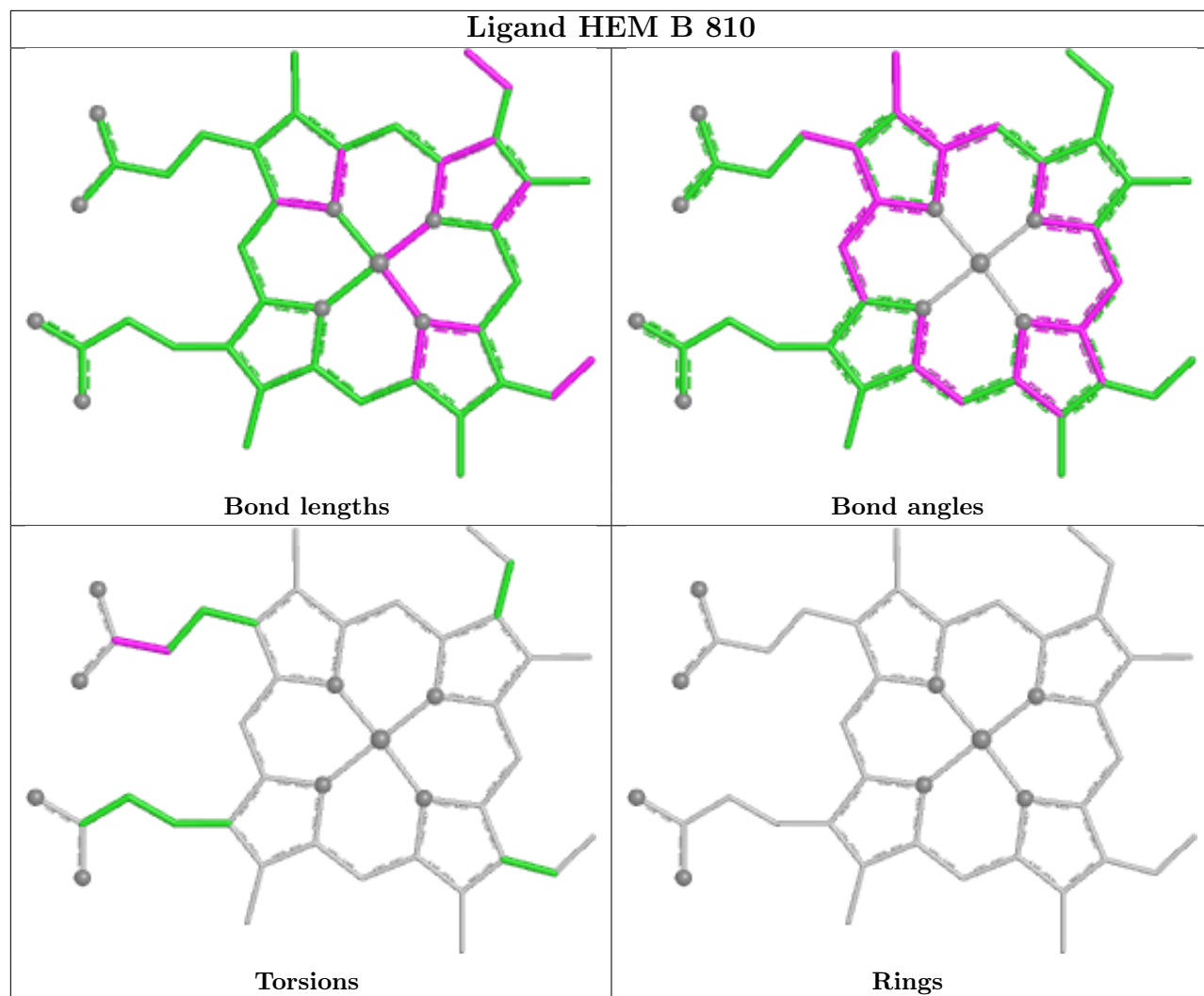
## Ligand HEM I 812

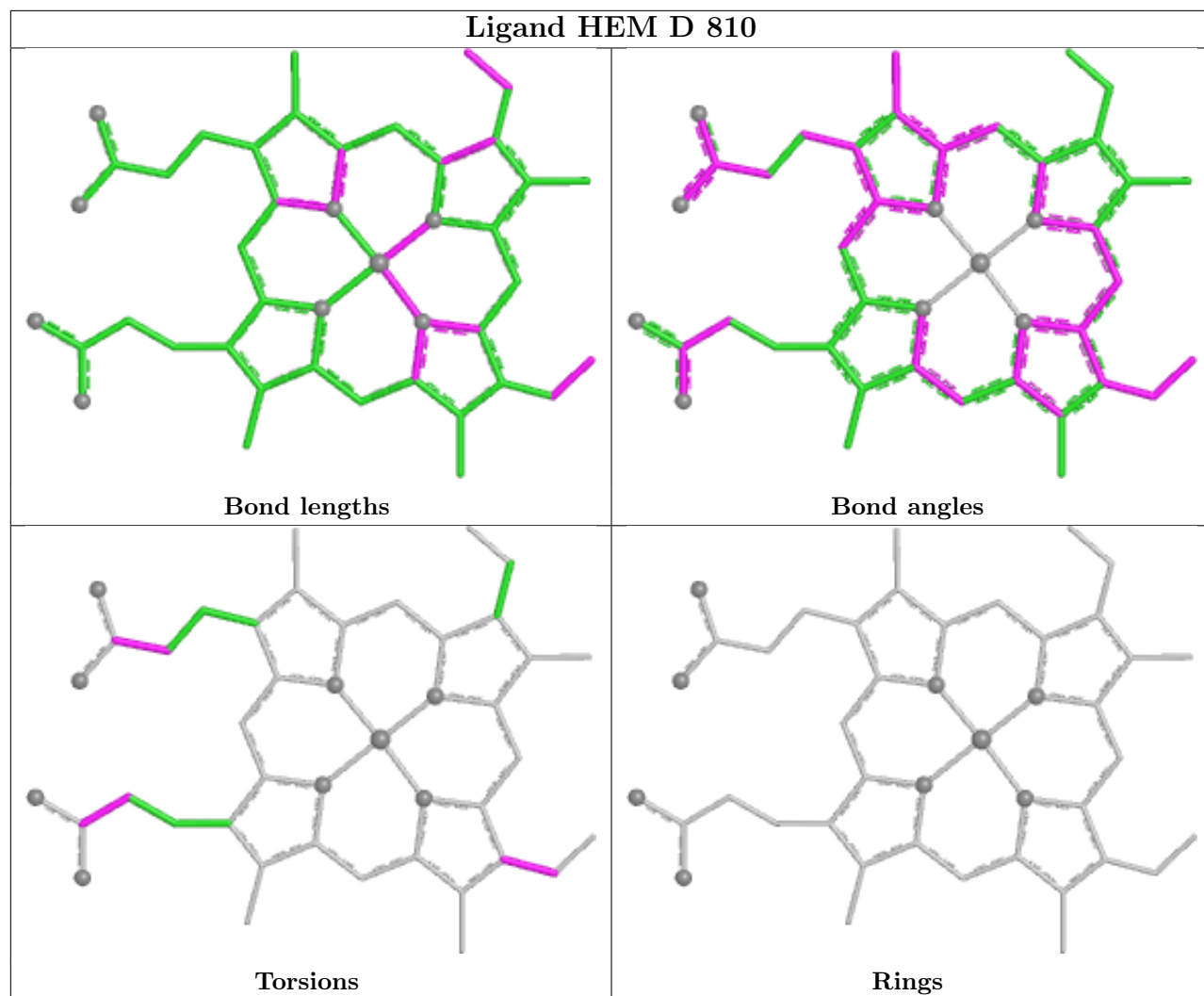




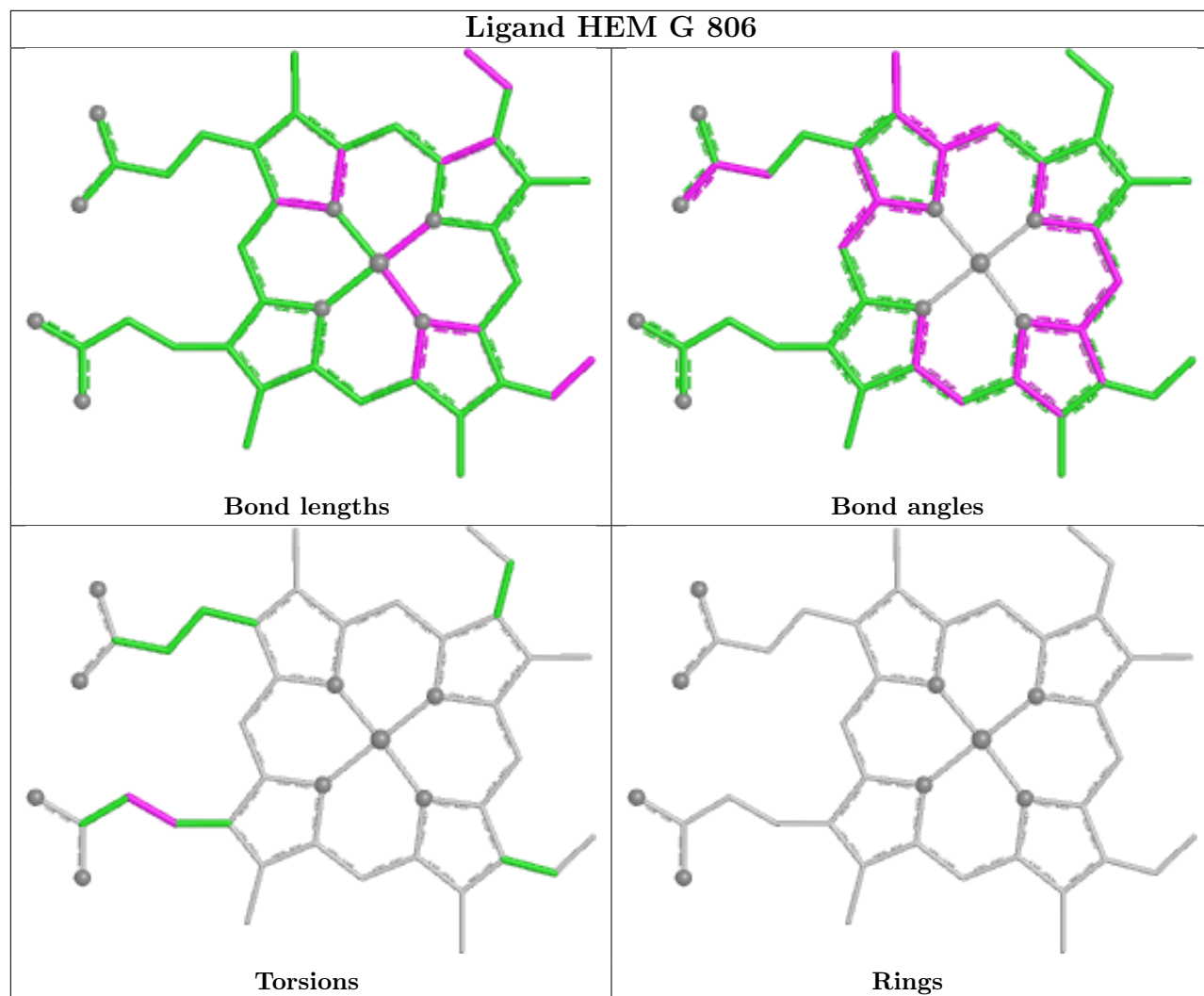


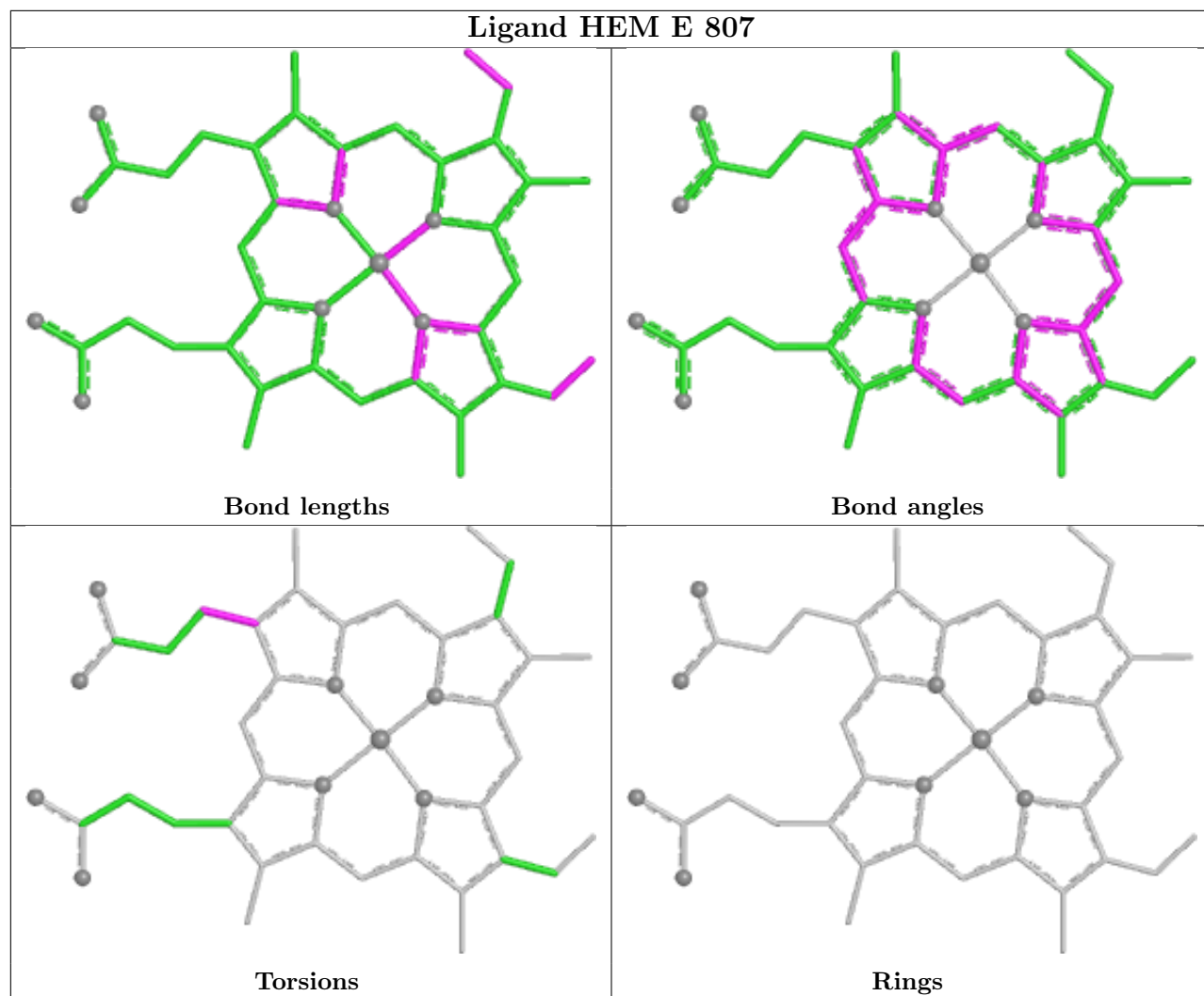


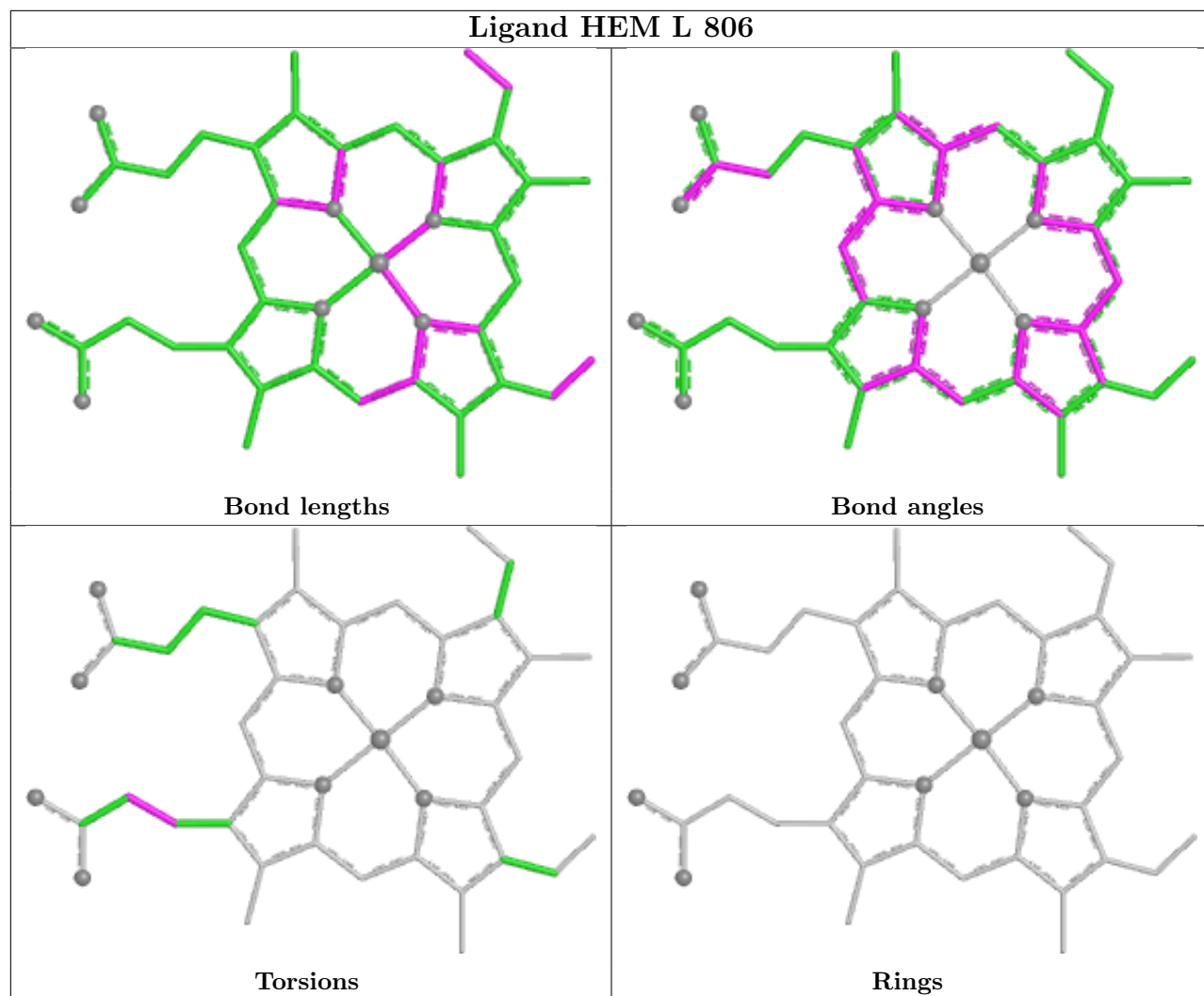


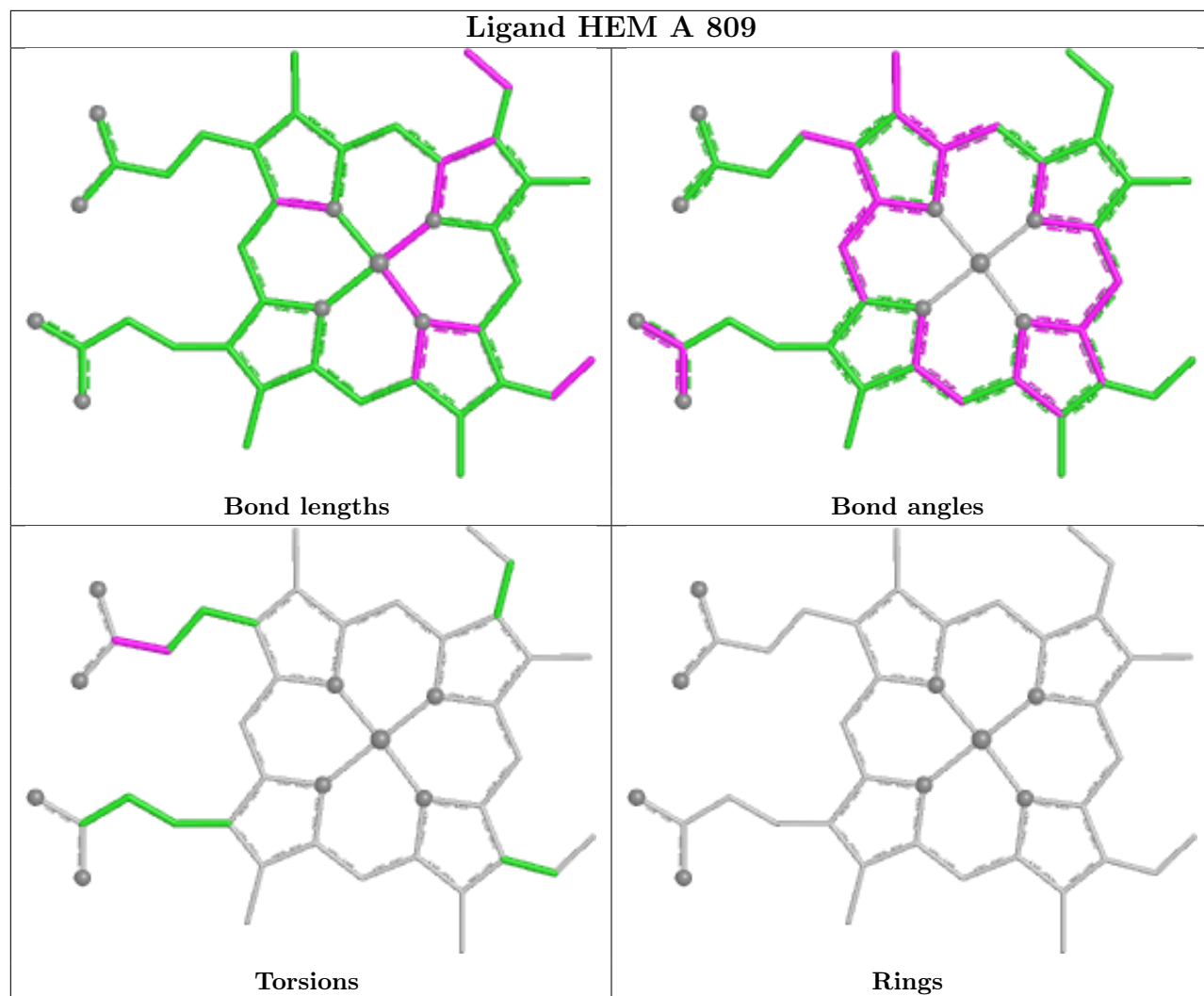


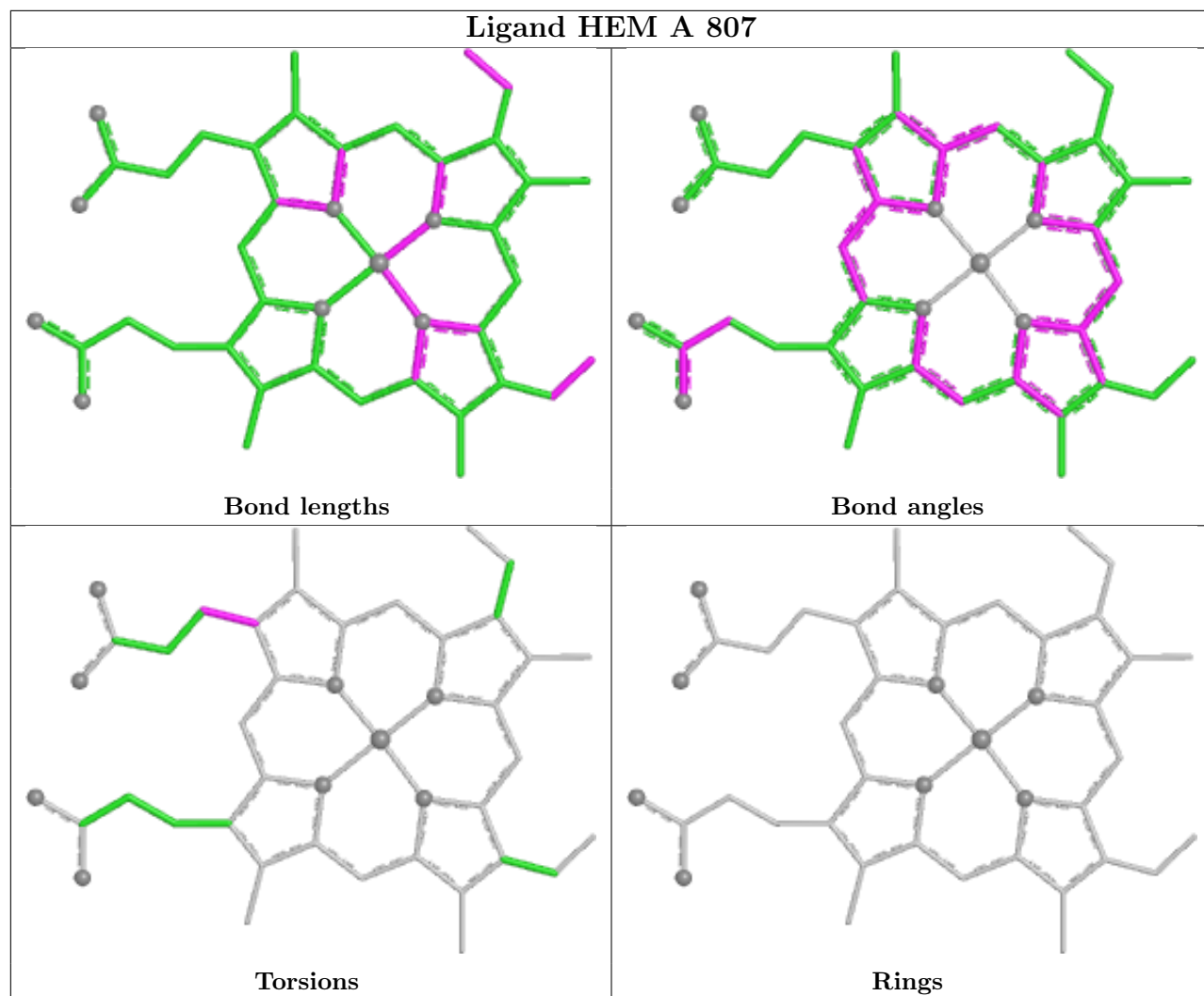


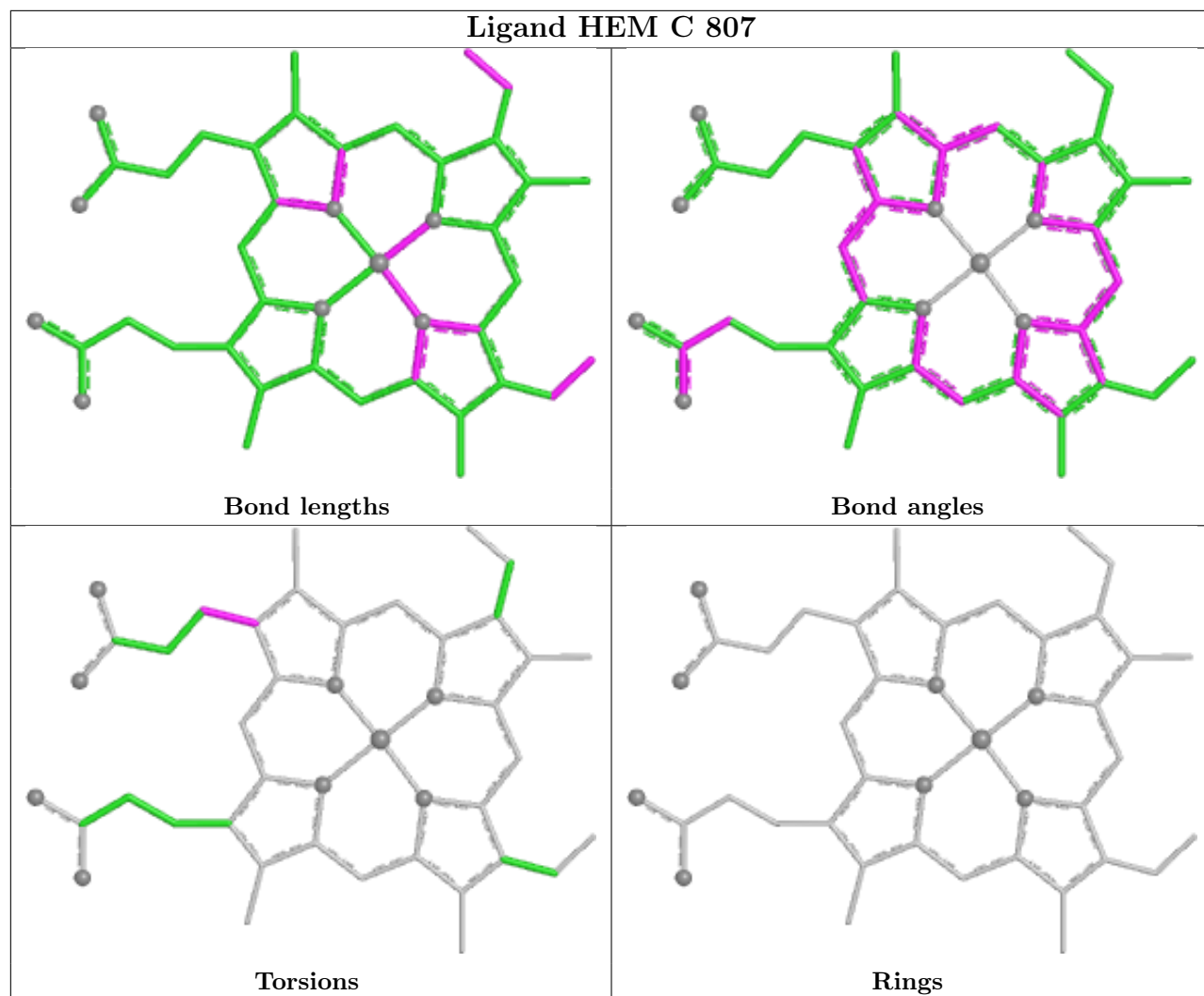


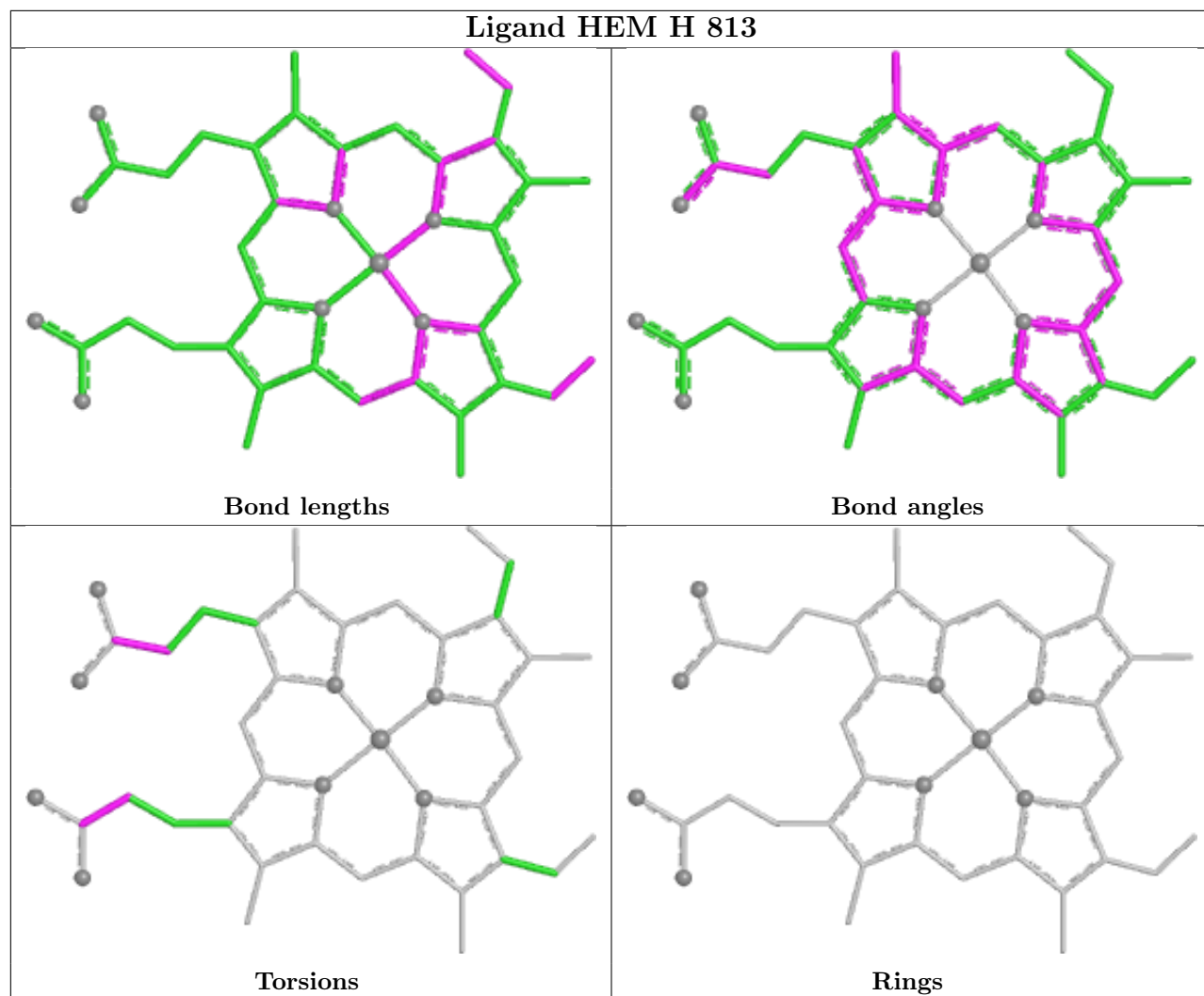


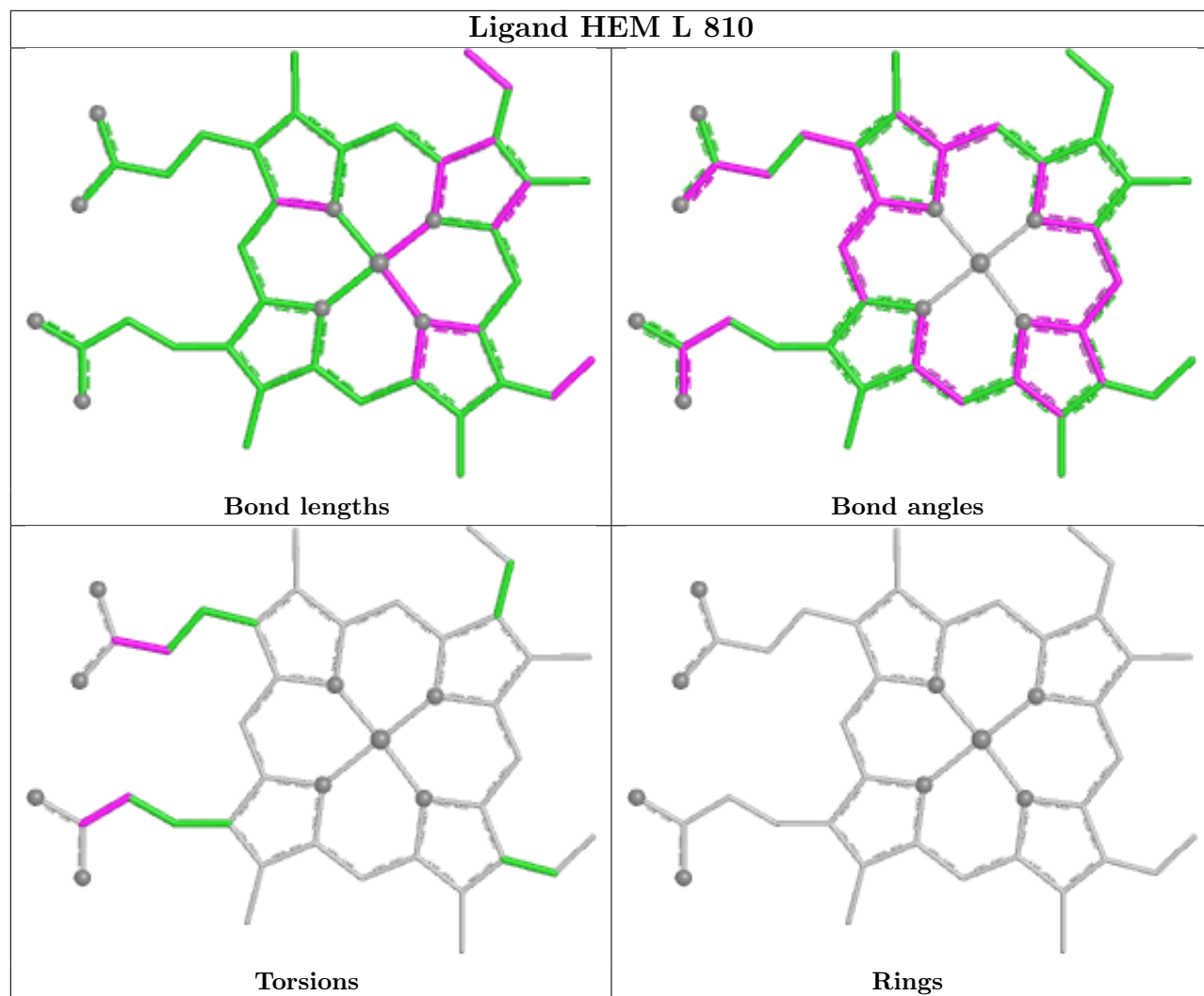




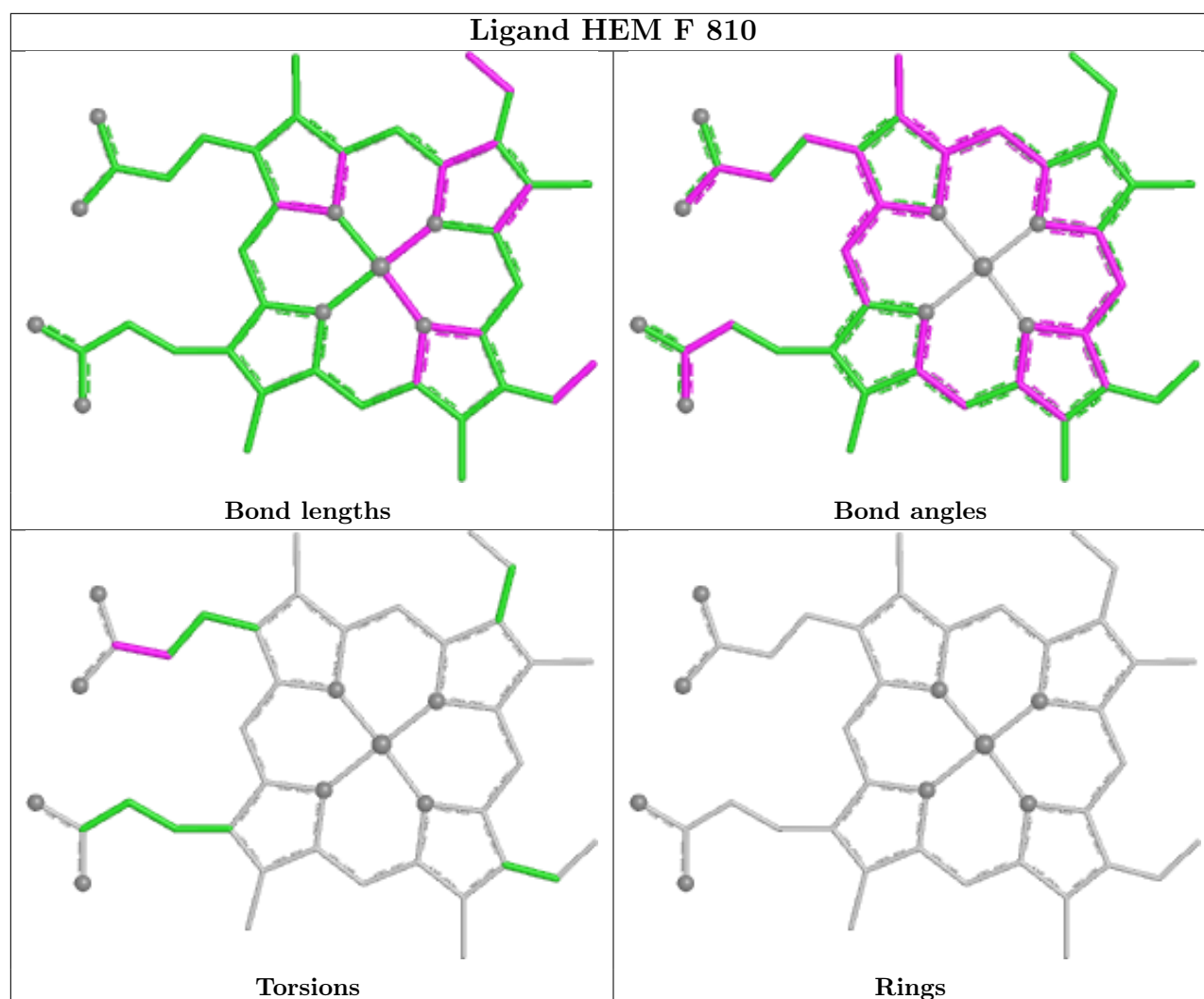












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 659/732 (90%)   | -0.42  | 7 (1%) 78 76   | 16, 24, 45, 95        | 0     |
| 1   | B     | 660/732 (90%)   | -0.23  | 2 (0%) 90 88   | 20, 33, 49, 82        | 0     |
| 1   | C     | 659/732 (90%)   | -0.18  | 8 (1%) 76 74   | 18, 32, 54, 86        | 0     |
| 1   | D     | 659/732 (90%)   | -0.21  | 14 (2%) 63 60  | 21, 32, 56, 102       | 0     |
| 1   | E     | 659/732 (90%)   | 0.02   | 11 (1%) 69 66  | 23, 38, 59, 104       | 0     |
| 1   | F     | 659/732 (90%)   | 0.12   | 7 (1%) 78 76   | 21, 38, 63, 107       | 0     |
| 1   | G     | 658/732 (89%)   | -0.02  | 10 (1%) 72 69  | 25, 37, 57, 93        | 0     |
| 1   | H     | 660/732 (90%)   | 0.01   | 5 (0%) 82 80   | 25, 37, 61, 95        | 0     |
| 1   | I     | 659/732 (90%)   | 0.04   | 3 (0%) 87 85   | 26, 39, 58, 76        | 0     |
| 1   | J     | 659/732 (90%)   | 0.34   | 13 (1%) 65 62  | 27, 46, 69, 96        | 0     |
| 1   | K     | 659/732 (90%)   | 0.35   | 6 (0%) 81 79   | 25, 46, 68, 85        | 0     |
| 1   | L     | 659/732 (90%)   | 0.49   | 18 (2%) 56 53  | 30, 51, 76, 89        | 0     |
| All | All   | 7909/8784 (90%) | 0.03   | 104 (1%) 75 73 | 16, 37, 65, 107       | 0     |

All (104) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 690 | LEU  | 5.9  |
| 1   | F     | 629 | VAL  | 4.9  |
| 1   | H     | 690 | LEU  | 4.5  |
| 1   | J     | 629 | VAL  | 4.4  |
| 1   | E     | 629 | VAL  | 4.2  |
| 1   | A     | 629 | VAL  | 4.1  |
| 1   | G     | 379 | LEU  | 4.0  |
| 1   | E     | 632 | LEU  | 3.8  |
| 1   | D     | 632 | LEU  | 3.7  |
| 1   | D     | 641 | TYR  | 3.7  |
| 1   | E     | 633 | ALA  | 3.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 689 | SER  | 3.7  |
| 1   | E     | 637 | LYS  | 3.7  |
| 1   | H     | 629 | VAL  | 3.6  |
| 1   | D     | 634 | PRO  | 3.6  |
| 1   | D     | 624 | TYR  | 3.6  |
| 1   | E     | 641 | TYR  | 3.5  |
| 1   | E     | 634 | PRO  | 3.4  |
| 1   | K     | 689 | SER  | 3.4  |
| 1   | E     | 689 | SER  | 3.4  |
| 1   | D     | 640 | VAL  | 3.3  |
| 1   | E     | 638 | THR  | 3.2  |
| 1   | D     | 629 | VAL  | 3.1  |
| 1   | J     | 476 | ALA  | 3.0  |
| 1   | B     | 476 | ALA  | 3.0  |
| 1   | A     | 624 | TYR  | 3.0  |
| 1   | D     | 637 | LYS  | 2.8  |
| 1   | D     | 627 | LEU  | 2.8  |
| 1   | E     | 631 | LYS  | 2.8  |
| 1   | L     | 379 | LEU  | 2.8  |
| 1   | G     | 629 | VAL  | 2.8  |
| 1   | J     | 183 | LYS  | 2.7  |
| 1   | L     | 76  | ILE  | 2.7  |
| 1   | A     | 641 | TYR  | 2.6  |
| 1   | J     | 688 | LYS  | 2.6  |
| 1   | J     | 627 | LEU  | 2.6  |
| 1   | L     | 216 | LEU  | 2.6  |
| 1   | E     | 536 | LYS  | 2.6  |
| 1   | L     | 88  | LEU  | 2.5  |
| 1   | C     | 379 | LEU  | 2.5  |
| 1   | L     | 252 | PRO  | 2.5  |
| 1   | D     | 630 | LYS  | 2.5  |
| 1   | C     | 641 | TYR  | 2.5  |
| 1   | D     | 631 | LYS  | 2.5  |
| 1   | K     | 438 | LYS  | 2.5  |
| 1   | F     | 43  | HIS  | 2.5  |
| 1   | I     | 539 | ARG  | 2.4  |
| 1   | C     | 624 | TYR  | 2.4  |
| 1   | I     | 379 | LEU  | 2.4  |
| 1   | C     | 438 | LYS  | 2.4  |
| 1   | J     | 196 | ASP  | 2.4  |
| 1   | D     | 633 | ALA  | 2.4  |
| 1   | L     | 78  | THR  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 228 | LEU  | 2.4  |
| 1   | C     | 689 | SER  | 2.4  |
| 1   | F     | 628 | GLU  | 2.4  |
| 1   | I     | 689 | SER  | 2.3  |
| 1   | G     | 627 | LEU  | 2.3  |
| 1   | H     | 628 | GLU  | 2.3  |
| 1   | D     | 635 | SER  | 2.3  |
| 1   | F     | 379 | LEU  | 2.3  |
| 1   | A     | 634 | PRO  | 2.2  |
| 1   | L     | 81  | GLY  | 2.2  |
| 1   | L     | 297 | ALA  | 2.2  |
| 1   | D     | 638 | THR  | 2.2  |
| 1   | L     | 435 | LYS  | 2.2  |
| 1   | C     | 629 | VAL  | 2.2  |
| 1   | G     | 626 | LEU  | 2.2  |
| 1   | J     | 31  | MET  | 2.2  |
| 1   | C     | 630 | LYS  | 2.2  |
| 1   | J     | 689 | SER  | 2.2  |
| 1   | L     | 437 | ILE  | 2.2  |
| 1   | H     | 632 | LEU  | 2.2  |
| 1   | F     | 631 | LYS  | 2.2  |
| 1   | K     | 670 | GLN  | 2.2  |
| 1   | E     | 379 | LEU  | 2.2  |
| 1   | J     | 269 | LEU  | 2.2  |
| 1   | J     | 681 | GLU  | 2.2  |
| 1   | K     | 589 | THR  | 2.2  |
| 1   | J     | 272 | TYR  | 2.1  |
| 1   | G     | 623 | LEU  | 2.1  |
| 1   | G     | 476 | ALA  | 2.1  |
| 1   | C     | 627 | LEU  | 2.1  |
| 1   | L     | 35  | LYS  | 2.1  |
| 1   | D     | 628 | GLU  | 2.1  |
| 1   | G     | 378 | PRO  | 2.1  |
| 1   | F     | 237 | ALA  | 2.1  |
| 1   | G     | 688 | LYS  | 2.1  |
| 1   | J     | 626 | LEU  | 2.1  |
| 1   | L     | 227 | LEU  | 2.1  |
| 1   | J     | 624 | TYR  | 2.1  |
| 1   | G     | 624 | TYR  | 2.1  |
| 1   | L     | 236 | VAL  | 2.1  |
| 1   | L     | 629 | VAL  | 2.1  |
| 1   | A     | 686 | MET  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 31  | MET  | 2.1  |
| 1   | H     | 39  | GLU  | 2.1  |
| 1   | A     | 627 | LEU  | 2.1  |
| 1   | L     | 235 | ILE  | 2.1  |
| 1   | G     | 253 | GLU  | 2.0  |
| 1   | K     | 76  | ILE  | 2.0  |
| 1   | A     | 632 | LEU  | 2.0  |
| 1   | K     | 88  | LEU  | 2.0  |
| 1   | F     | 630 | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | BU3  | K     | 804 | 6/6   | 0.77 | 0.22 | 74,77,78,79                | 0     |
| 5   | ACT  | H     | 806 | 4/4   | 0.79 | 0.27 | 59,63,64,64                | 0     |
| 4   | BU3  | E     | 804 | 6/6   | 0.80 | 0.25 | 77,79,79,79                | 0     |
| 4   | BU3  | L     | 804 | 6/6   | 0.80 | 0.19 | 69,70,70,72                | 0     |
| 4   | BU3  | H     | 805 | 6/6   | 0.80 | 0.20 | 49,50,51,53                | 0     |
| 5   | ACT  | K     | 805 | 4/4   | 0.80 | 0.22 | 58,58,58,59                | 0     |
| 5   | ACT  | A     | 805 | 4/4   | 0.81 | 0.21 | 47,50,50,51                | 0     |
| 5   | ACT  | B     | 806 | 4/4   | 0.81 | 0.20 | 46,47,48,49                | 0     |
| 5   | ACT  | D     | 805 | 4/4   | 0.83 | 0.25 | 59,62,62,63                | 0     |
| 4   | BU3  | I     | 804 | 6/6   | 0.83 | 0.20 | 60,61,62,62                | 0     |
| 4   | BU3  | J     | 804 | 6/6   | 0.83 | 0.20 | 64,65,66,66                | 0     |
| 4   | BU3  | K     | 803 | 6/6   | 0.84 | 0.23 | 56,58,59,60                | 0     |
| 4   | BU3  | L     | 803 | 6/6   | 0.84 | 0.20 | 57,58,58,60                | 0     |
| 4   | BU3  | C     | 804 | 6/6   | 0.85 | 0.16 | 48,49,49,50                | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | BU3  | A     | 803 | 6/6   | 0.85 | 0.19 | 47,47,48,48                 | 0     |
| 4   | BU3  | F     | 805 | 6/6   | 0.85 | 0.21 | 58,60,61,62                 | 0     |
| 4   | BU3  | A     | 804 | 6/6   | 0.85 | 0.17 | 40,41,42,43                 | 0     |
| 4   | BU3  | C     | 803 | 6/6   | 0.85 | 0.20 | 52,53,54,55                 | 0     |
| 5   | ACT  | C     | 805 | 4/4   | 0.86 | 0.23 | 58,59,61,61                 | 0     |
| 5   | ACT  | F     | 806 | 4/4   | 0.86 | 0.18 | 54,56,56,56                 | 0     |
| 5   | ACT  | G     | 805 | 4/4   | 0.86 | 0.20 | 51,51,52,52                 | 0     |
| 7   | SO2  | I     | 802 | 3/3   | 0.86 | 0.16 | 63,63,64,71                 | 0     |
| 4   | BU3  | F     | 804 | 6/6   | 0.87 | 0.16 | 62,63,64,65                 | 0     |
| 4   | BU3  | D     | 804 | 6/6   | 0.87 | 0.14 | 45,46,47,47                 | 0     |
| 4   | BU3  | B     | 803 | 6/6   | 0.87 | 0.19 | 50,51,52,52                 | 0     |
| 4   | BU3  | D     | 803 | 6/6   | 0.88 | 0.18 | 50,54,54,55                 | 0     |
| 5   | ACT  | L     | 805 | 4/4   | 0.88 | 0.22 | 61,63,63,64                 | 0     |
| 4   | BU3  | H     | 803 | 6/6   | 0.88 | 0.21 | 62,63,64,65                 | 0     |
| 3   | SX   | B     | 802 | 2/2   | 0.88 | 0.17 | 51,51,51,52                 | 0     |
| 4   | BU3  | F     | 803 | 6/6   | 0.89 | 0.16 | 49,50,50,50                 | 0     |
| 5   | ACT  | J     | 805 | 4/4   | 0.89 | 0.23 | 62,62,62,63                 | 0     |
| 4   | BU3  | I     | 803 | 6/6   | 0.89 | 0.16 | 48,50,51,51                 | 0     |
| 4   | BU3  | E     | 803 | 6/6   | 0.89 | 0.18 | 50,51,54,55                 | 0     |
| 4   | BU3  | H     | 804 | 6/6   | 0.89 | 0.16 | 61,62,62,64                 | 0     |
| 4   | BU3  | G     | 803 | 6/6   | 0.89 | 0.14 | 49,50,51,52                 | 0     |
| 4   | BU3  | B     | 804 | 6/6   | 0.90 | 0.14 | 50,52,53,53                 | 0     |
| 4   | BU3  | G     | 804 | 6/6   | 0.90 | 0.16 | 58,59,61,61                 | 0     |
| 5   | ACT  | E     | 805 | 4/4   | 0.90 | 0.19 | 58,60,61,61                 | 0     |
| 4   | BU3  | B     | 805 | 6/6   | 0.90 | 0.16 | 55,59,59,60                 | 0     |
| 3   | SX   | A     | 802 | 2/2   | 0.90 | 0.17 | 45,45,45,50                 | 2     |
| 4   | BU3  | J     | 803 | 6/6   | 0.91 | 0.18 | 55,57,58,58                 | 0     |
| 3   | SX   | F     | 802 | 2/2   | 0.91 | 0.21 | 69,69,69,73                 | 0     |
| 3   | SX   | K     | 802 | 2/2   | 0.92 | 0.12 | 67,67,67,71                 | 0     |
| 3   | SX   | E     | 802 | 2/2   | 0.92 | 0.16 | 66,66,66,68                 | 0     |
| 5   | ACT  | I     | 805 | 4/4   | 0.92 | 0.16 | 50,50,52,52                 | 0     |
| 3   | SX   | H     | 802 | 2/2   | 0.92 | 0.13 | 58,58,58,61                 | 0     |
| 3   | SX   | C     | 802 | 2/2   | 0.93 | 0.19 | 55,55,55,56                 | 0     |
| 3   | SX   | G     | 802 | 2/2   | 0.94 | 0.16 | 31,31,31,32                 | 2     |
| 7   | SO2  | G     | 814 | 3/3   | 0.94 | 0.21 | 74,74,74,76                 | 3     |
| 3   | SX   | J     | 802 | 2/2   | 0.95 | 0.09 | 57,57,57,62                 | 0     |
| 6   | HEM  | L     | 813 | 43/43 | 0.95 | 0.10 | 46,48,58,65                 | 0     |
| 7   | SO2  | A     | 814 | 3/3   | 0.95 | 0.12 | 16,16,16,16                 | 3     |
| 2   | CU1  | H     | 801 | 1/1   | 0.95 | 0.07 | 45,45,45,45                 | 0     |
| 3   | SX   | L     | 802 | 2/2   | 0.95 | 0.10 | 65,65,65,68                 | 0     |
| 6   | HEM  | J     | 807 | 43/43 | 0.96 | 0.08 | 34,36,38,39                 | 0     |
| 6   | HEM  | J     | 811 | 43/43 | 0.96 | 0.09 | 29,31,41,51                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6   | HEM  | K     | 813 | 43/43 | 0.96 | 0.09 | 39,41,52,55                 | 0     |
| 6   | HEM  | L     | 807 | 43/43 | 0.96 | 0.09 | 37,39,42,44                 | 0     |
| 6   | HEM  | L     | 810 | 43/43 | 0.96 | 0.09 | 31,32,39,43                 | 0     |
| 6   | HEM  | L     | 811 | 43/43 | 0.96 | 0.09 | 34,37,45,49                 | 0     |
| 6   | HEM  | L     | 812 | 43/43 | 0.96 | 0.09 | 37,39,41,42                 | 0     |
| 6   | HEM  | C     | 813 | 43/43 | 0.96 | 0.08 | 30,32,45,50                 | 0     |
| 6   | HEM  | H     | 807 | 43/43 | 0.96 | 0.08 | 32,33,35,36                 | 0     |
| 7   | SO2  | D     | 802 | 3/3   | 0.96 | 0.13 | 51,51,53,54                 | 0     |
| 6   | HEM  | I     | 809 | 43/43 | 0.96 | 0.09 | 26,27,30,32                 | 0     |
| 6   | HEM  | I     | 813 | 43/43 | 0.96 | 0.09 | 33,35,46,49                 | 0     |
| 6   | HEM  | D     | 810 | 43/43 | 0.97 | 0.07 | 21,22,25,28                 | 0     |
| 6   | HEM  | E     | 807 | 43/43 | 0.97 | 0.07 | 28,29,31,33                 | 0     |
| 6   | HEM  | E     | 808 | 43/43 | 0.97 | 0.07 | 23,24,25,27                 | 0     |
| 6   | HEM  | E     | 809 | 43/43 | 0.97 | 0.07 | 24,25,26,26                 | 0     |
| 6   | HEM  | E     | 810 | 43/43 | 0.97 | 0.07 | 24,25,29,34                 | 0     |
| 6   | HEM  | E     | 811 | 43/43 | 0.97 | 0.08 | 27,29,36,43                 | 0     |
| 6   | HEM  | E     | 812 | 43/43 | 0.97 | 0.07 | 26,28,31,32                 | 0     |
| 6   | HEM  | E     | 813 | 43/43 | 0.97 | 0.08 | 30,32,44,55                 | 0     |
| 6   | HEM  | F     | 807 | 43/43 | 0.97 | 0.07 | 25,29,32,33                 | 0     |
| 6   | HEM  | F     | 808 | 43/43 | 0.97 | 0.08 | 25,28,32,35                 | 0     |
| 6   | HEM  | F     | 809 | 43/43 | 0.97 | 0.08 | 28,29,30,31                 | 0     |
| 6   | HEM  | F     | 811 | 43/43 | 0.97 | 0.07 | 21,22,26,31                 | 0     |
| 6   | HEM  | F     | 812 | 43/43 | 0.97 | 0.08 | 21,23,32,42                 | 0     |
| 6   | HEM  | F     | 813 | 43/43 | 0.97 | 0.07 | 21,23,24,26                 | 0     |
| 6   | HEM  | F     | 814 | 43/43 | 0.97 | 0.08 | 24,26,34,39                 | 0     |
| 2   | CU1  | L     | 801 | 1/1   | 0.97 | 0.05 | 55,55,55,55                 | 0     |
| 6   | HEM  | H     | 808 | 43/43 | 0.97 | 0.07 | 24,29,31,33                 | 0     |
| 6   | HEM  | H     | 809 | 43/43 | 0.97 | 0.08 | 29,31,34,39                 | 0     |
| 6   | HEM  | H     | 810 | 43/43 | 0.97 | 0.07 | 28,30,31,32                 | 0     |
| 6   | HEM  | H     | 811 | 43/43 | 0.97 | 0.08 | 25,27,30,33                 | 0     |
| 6   | HEM  | H     | 812 | 43/43 | 0.97 | 0.08 | 23,26,35,43                 | 0     |
| 6   | HEM  | H     | 813 | 43/43 | 0.97 | 0.07 | 26,27,28,29                 | 0     |
| 6   | HEM  | H     | 814 | 43/43 | 0.97 | 0.08 | 25,26,36,40                 | 0     |
| 6   | HEM  | I     | 806 | 43/43 | 0.97 | 0.07 | 27,30,32,32                 | 0     |
| 6   | HEM  | I     | 807 | 43/43 | 0.97 | 0.07 | 29,32,33,34                 | 0     |
| 6   | HEM  | I     | 808 | 43/43 | 0.97 | 0.09 | 27,28,30,30                 | 0     |
| 2   | CU1  | J     | 801 | 1/1   | 0.97 | 0.05 | 51,51,51,51                 | 0     |
| 6   | HEM  | I     | 810 | 43/43 | 0.97 | 0.07 | 24,26,30,35                 | 0     |
| 6   | HEM  | I     | 811 | 43/43 | 0.97 | 0.08 | 25,26,35,43                 | 0     |
| 6   | HEM  | I     | 812 | 43/43 | 0.97 | 0.08 | 27,28,31,33                 | 0     |
| 6   | HEM  | A     | 811 | 43/43 | 0.97 | 0.07 | 19,20,28,33                 | 0     |
| 6   | HEM  | J     | 806 | 43/43 | 0.97 | 0.07 | 28,30,32,34                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6   | HEM  | A     | 812 | 43/43 | 0.97 | 0.07 | 18,19,22,25                 | 0     |
| 6   | HEM  | J     | 808 | 43/43 | 0.97 | 0.07 | 27,28,29,30                 | 0     |
| 6   | HEM  | J     | 809 | 43/43 | 0.97 | 0.07 | 29,31,33,35                 | 0     |
| 6   | HEM  | A     | 813 | 43/43 | 0.97 | 0.07 | 21,23,31,34                 | 0     |
| 6   | HEM  | J     | 812 | 43/43 | 0.97 | 0.08 | 34,36,37,39                 | 0     |
| 6   | HEM  | J     | 813 | 43/43 | 0.97 | 0.09 | 37,40,53,62                 | 0     |
| 6   | HEM  | K     | 806 | 43/43 | 0.97 | 0.08 | 26,28,31,32                 | 0     |
| 6   | HEM  | K     | 807 | 43/43 | 0.97 | 0.09 | 38,41,45,49                 | 0     |
| 6   | HEM  | K     | 808 | 43/43 | 0.97 | 0.07 | 27,27,29,31                 | 0     |
| 6   | HEM  | K     | 809 | 43/43 | 0.97 | 0.08 | 28,31,34,35                 | 0     |
| 6   | HEM  | K     | 810 | 43/43 | 0.97 | 0.08 | 27,29,33,37                 | 0     |
| 6   | HEM  | K     | 811 | 43/43 | 0.97 | 0.08 | 27,30,39,47                 | 0     |
| 6   | HEM  | K     | 812 | 43/43 | 0.97 | 0.08 | 31,34,36,37                 | 0     |
| 6   | HEM  | B     | 807 | 43/43 | 0.97 | 0.07 | 21,22,23,24                 | 0     |
| 6   | HEM  | L     | 806 | 43/43 | 0.97 | 0.07 | 24,30,33,34                 | 0     |
| 6   | HEM  | B     | 811 | 43/43 | 0.97 | 0.07 | 21,22,28,34                 | 0     |
| 6   | HEM  | L     | 808 | 43/43 | 0.97 | 0.08 | 31,33,35,38                 | 0     |
| 6   | HEM  | L     | 809 | 43/43 | 0.97 | 0.09 | 32,34,38,40                 | 0     |
| 6   | HEM  | B     | 812 | 43/43 | 0.97 | 0.07 | 23,24,33,43                 | 0     |
| 6   | HEM  | B     | 813 | 43/43 | 0.97 | 0.08 | 24,26,29,30                 | 0     |
| 6   | HEM  | B     | 814 | 43/43 | 0.97 | 0.08 | 29,31,43,46                 | 0     |
| 6   | HEM  | C     | 811 | 43/43 | 0.97 | 0.07 | 24,26,36,46                 | 0     |
| 6   | HEM  | G     | 806 | 43/43 | 0.97 | 0.07 | 27,28,29,29                 | 0     |
| 6   | HEM  | G     | 808 | 43/43 | 0.97 | 0.07 | 25,26,28,30                 | 0     |
| 6   | HEM  | G     | 809 | 43/43 | 0.97 | 0.07 | 24,27,28,28                 | 0     |
| 6   | HEM  | G     | 810 | 43/43 | 0.97 | 0.07 | 24,24,29,31                 | 0     |
| 6   | HEM  | G     | 811 | 43/43 | 0.97 | 0.09 | 28,31,43,49                 | 0     |
| 6   | HEM  | G     | 812 | 43/43 | 0.97 | 0.07 | 26,28,32,33                 | 0     |
| 6   | HEM  | G     | 813 | 43/43 | 0.97 | 0.08 | 28,31,38,45                 | 0     |
| 2   | CU1  | K     | 801 | 1/1   | 0.97 | 0.07 | 53,53,53,53                 | 0     |
| 6   | HEM  | D     | 806 | 43/43 | 0.97 | 0.08 | 28,30,32,33                 | 0     |
| 6   | HEM  | D     | 807 | 43/43 | 0.97 | 0.07 | 21,22,24,25                 | 0     |
| 6   | HEM  | D     | 808 | 43/43 | 0.97 | 0.07 | 25,27,31,35                 | 0     |
| 6   | HEM  | C     | 808 | 43/43 | 0.98 | 0.07 | 18,19,21,23                 | 0     |
| 6   | HEM  | C     | 809 | 43/43 | 0.98 | 0.07 | 18,20,21,21                 | 0     |
| 6   | HEM  | C     | 810 | 43/43 | 0.98 | 0.06 | 20,21,24,28                 | 0     |
| 6   | HEM  | A     | 809 | 43/43 | 0.98 | 0.06 | 14,15,17,19                 | 0     |
| 6   | HEM  | C     | 812 | 43/43 | 0.98 | 0.06 | 23,25,28,31                 | 0     |
| 6   | HEM  | B     | 808 | 43/43 | 0.98 | 0.06 | 24,25,26,28                 | 0     |
| 6   | HEM  | F     | 810 | 43/43 | 0.98 | 0.07 | 25,27,27,27                 | 0     |
| 6   | HEM  | B     | 809 | 43/43 | 0.98 | 0.07 | 20,22,23,27                 | 0     |
| 6   | HEM  | B     | 810 | 43/43 | 0.98 | 0.06 | 20,23,25,27                 | 0     |

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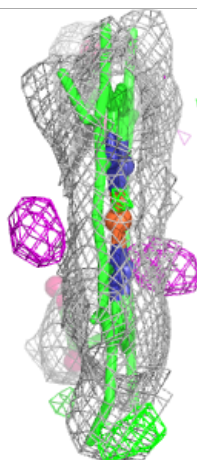
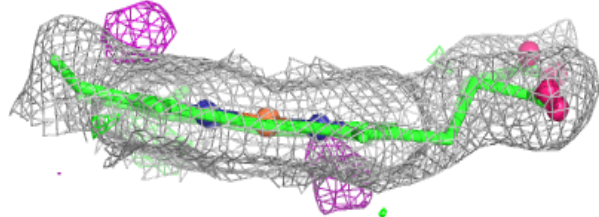
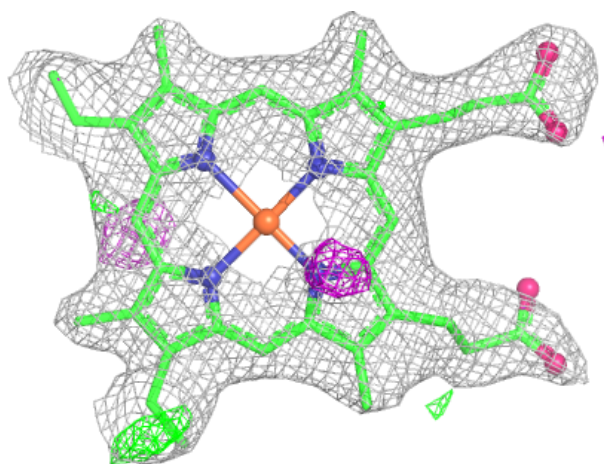
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6   | HEM  | A     | 810 | 43/43 | 0.98 | 0.07 | 16,17,21,24                 | 0     |
| 6   | HEM  | D     | 809 | 43/43 | 0.98 | 0.06 | 21,22,23,25                 | 0     |
| 6   | HEM  | G     | 807 | 43/43 | 0.98 | 0.06 | 25,26,28,29                 | 0     |
| 6   | HEM  | J     | 810 | 43/43 | 0.98 | 0.07 | 26,28,33,37                 | 0     |
| 6   | HEM  | A     | 806 | 43/43 | 0.98 | 0.07 | 19,20,21,21                 | 0     |
| 6   | HEM  | D     | 811 | 43/43 | 0.98 | 0.07 | 21,23,33,42                 | 0     |
| 6   | HEM  | D     | 812 | 43/43 | 0.98 | 0.07 | 20,22,24,27                 | 0     |
| 6   | HEM  | D     | 813 | 43/43 | 0.98 | 0.07 | 25,26,34,36                 | 0     |
| 6   | HEM  | E     | 806 | 43/43 | 0.98 | 0.07 | 23,24,26,26                 | 0     |
| 6   | HEM  | A     | 807 | 43/43 | 0.98 | 0.07 | 16,16,17,17                 | 0     |
| 6   | HEM  | A     | 808 | 43/43 | 0.98 | 0.06 | 17,18,20,23                 | 0     |
| 6   | HEM  | C     | 806 | 43/43 | 0.98 | 0.05 | 16,17,18,19                 | 0     |
| 6   | HEM  | C     | 807 | 43/43 | 0.98 | 0.07 | 21,23,23,24                 | 0     |
| 2   | CU1  | C     | 801 | 1/1   | 0.99 | 0.02 | 31,31,31,31                 | 0     |
| 2   | CU1  | D     | 801 | 1/1   | 0.99 | 0.03 | 33,33,33,33                 | 0     |
| 2   | CU1  | G     | 801 | 1/1   | 0.99 | 0.03 | 34,34,34,34                 | 0     |
| 2   | CU1  | E     | 801 | 1/1   | 0.99 | 0.03 | 37,37,37,37                 | 0     |
| 2   | CU1  | F     | 801 | 1/1   | 0.99 | 0.03 | 38,38,38,38                 | 0     |
| 2   | CU1  | A     | 801 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 2   | CU1  | I     | 801 | 1/1   | 0.99 | 0.03 | 39,39,39,39                 | 0     |
| 2   | CU1  | B     | 801 | 1/1   | 0.99 | 0.02 | 35,35,35,35                 | 0     |

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

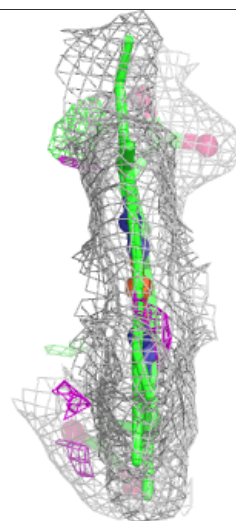
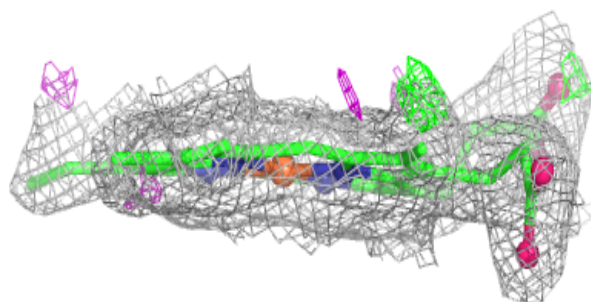
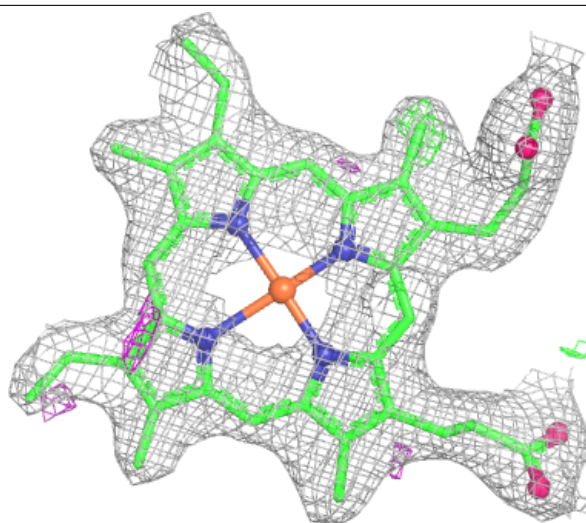
**Electron density around HEM L 813:**

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



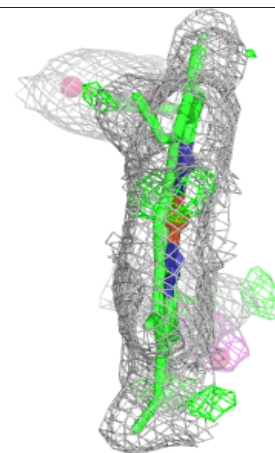
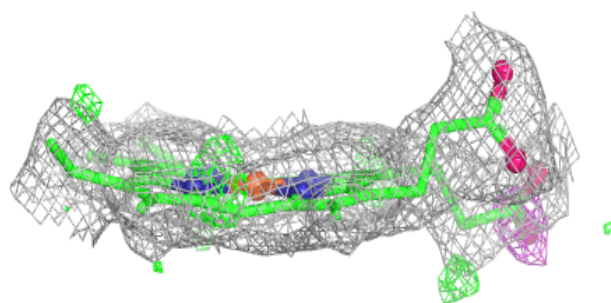
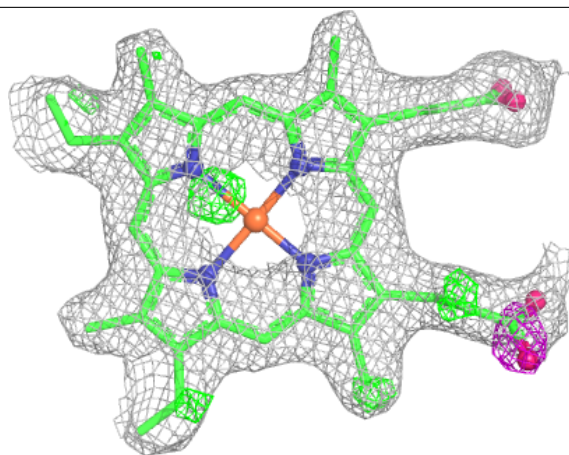
**Electron density around HEM J 807:**

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



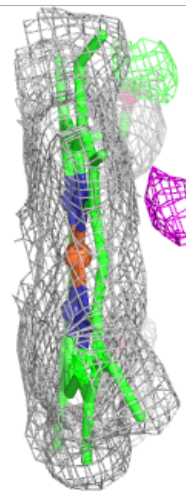
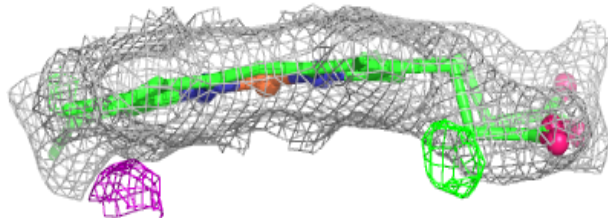
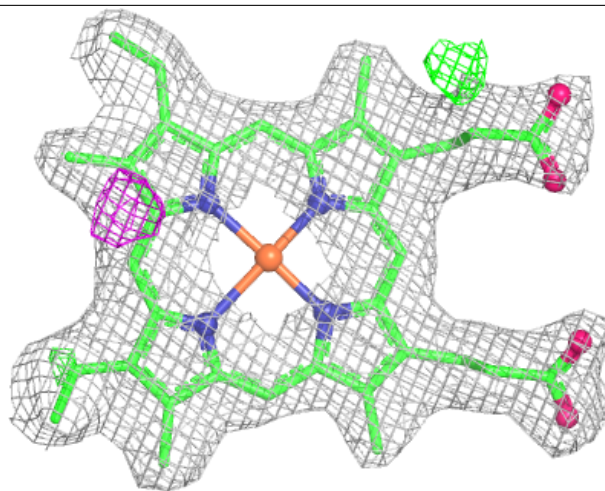
**Electron density around HEM J 811:**

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



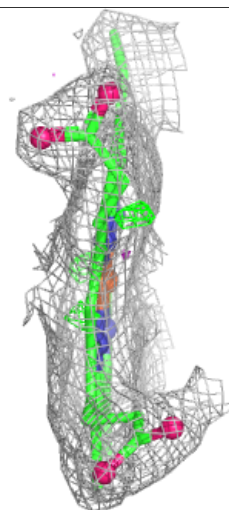
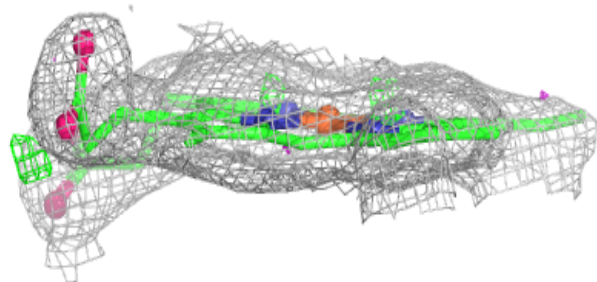
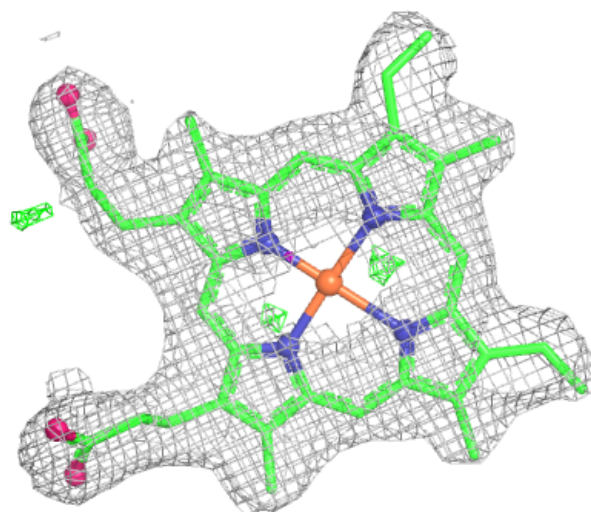
**Electron density around HEM K 813:**

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



**Electron density around HEM L 807:**

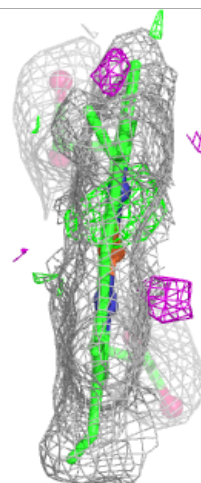
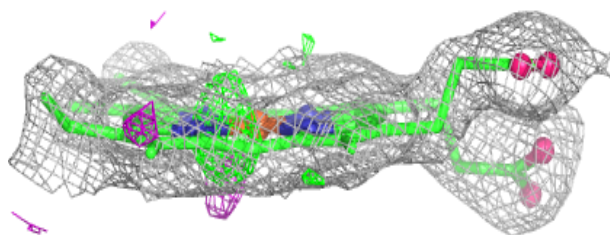
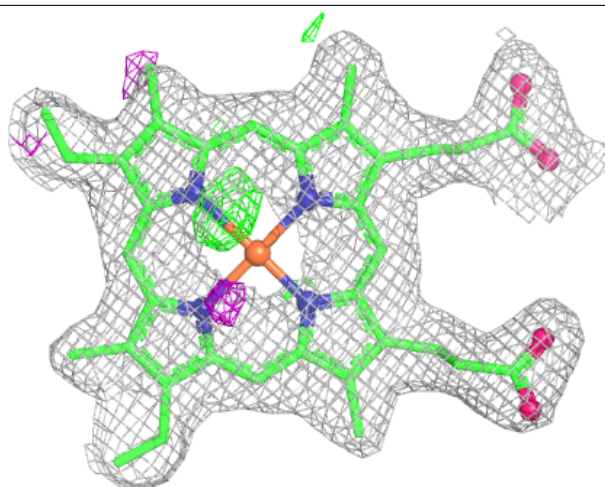
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





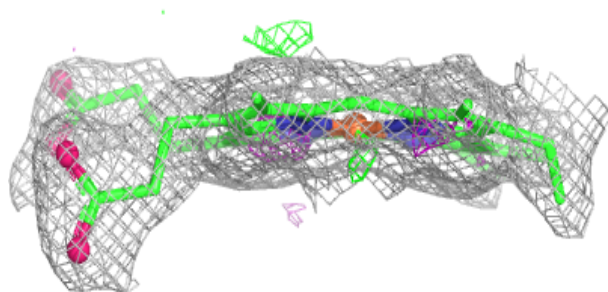
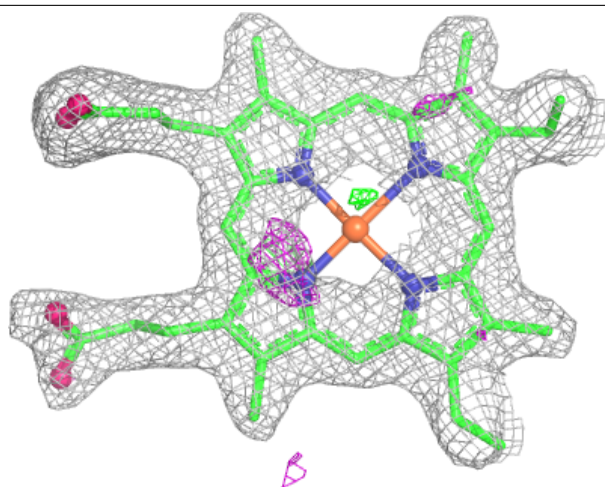
**Electron density around HEM L 810:**

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



**Electron density around HEM L 811:**

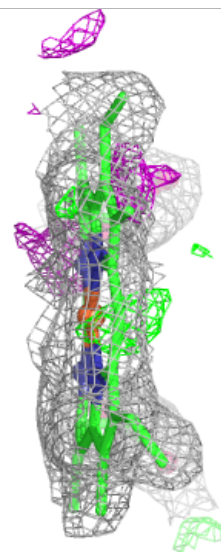
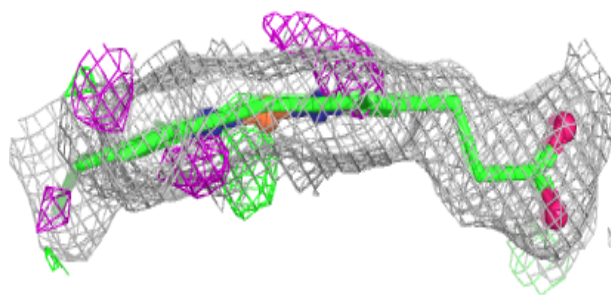
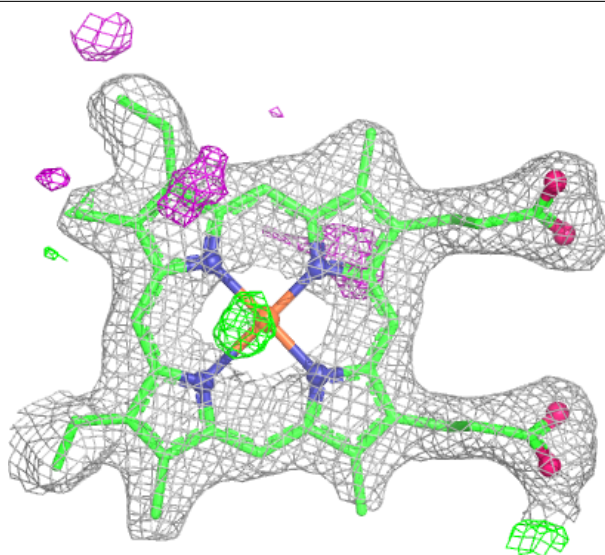
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





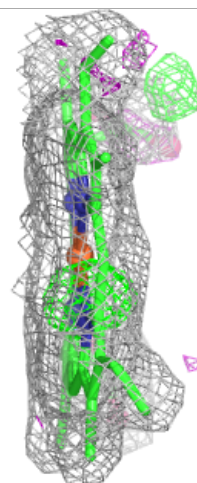
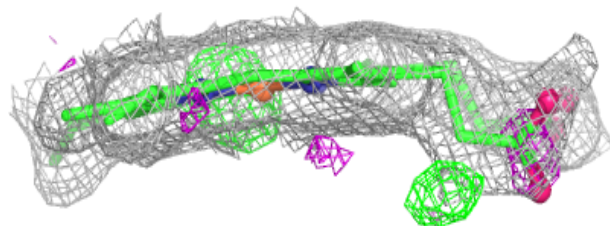
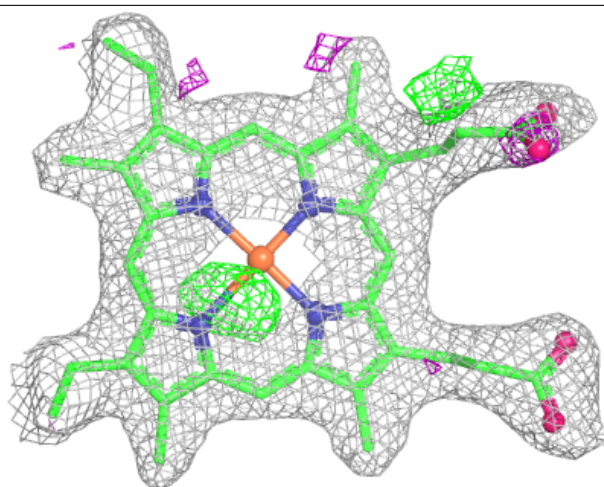
**Electron density around HEM L 812:**

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



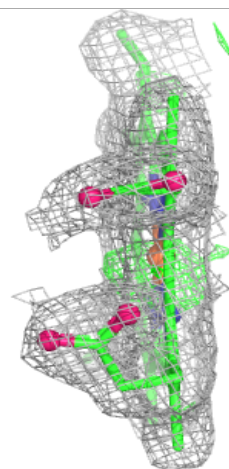
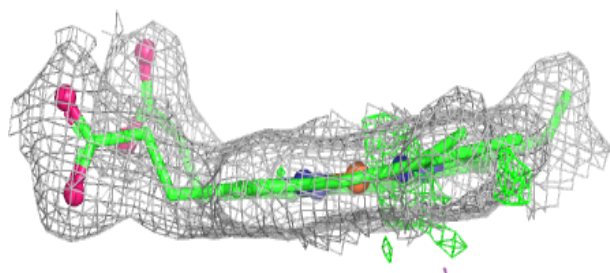
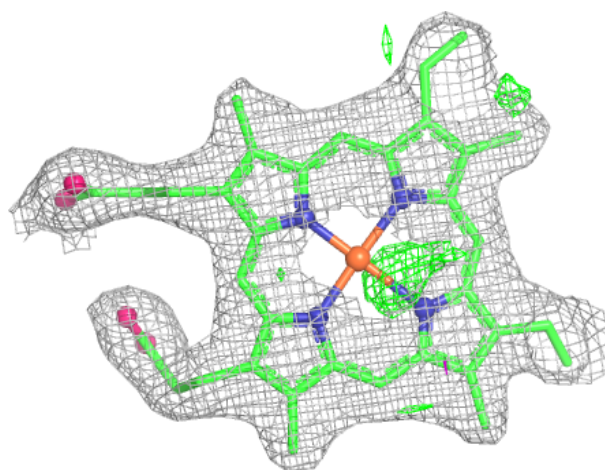
**Electron density around HEM C 813:**

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



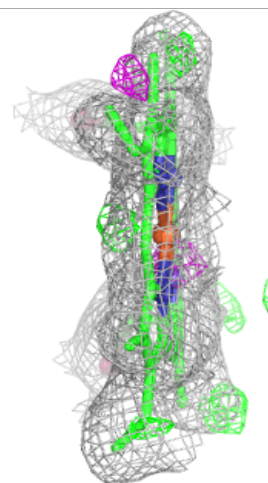
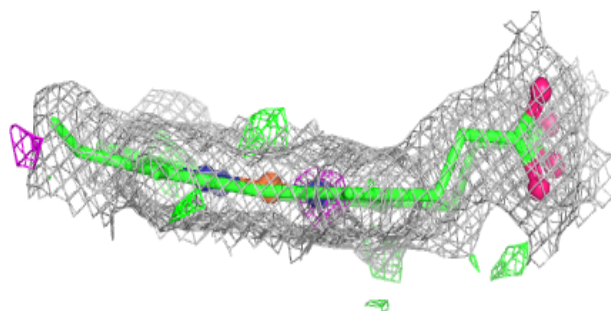
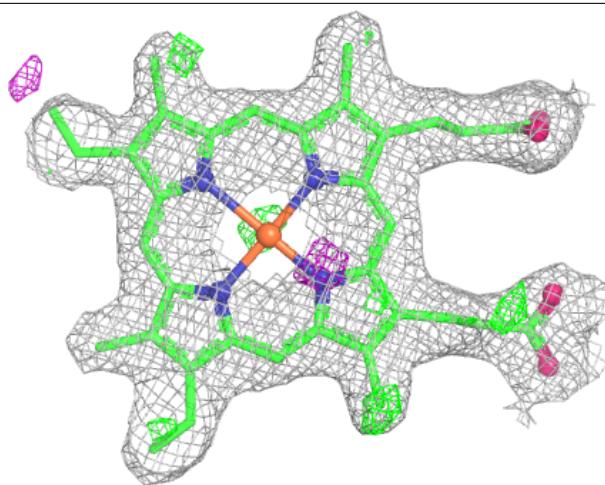
**Electron density around HEM H 807:**

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



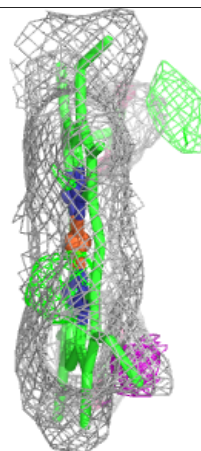
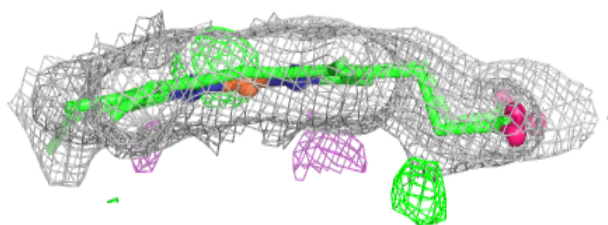
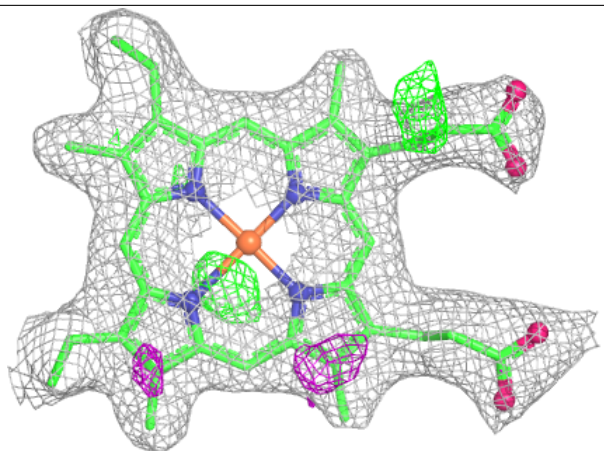
**Electron density around HEM I 809:**

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



**Electron density around HEM I 813:**

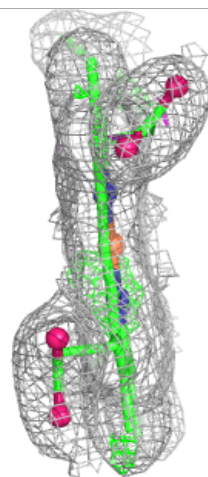
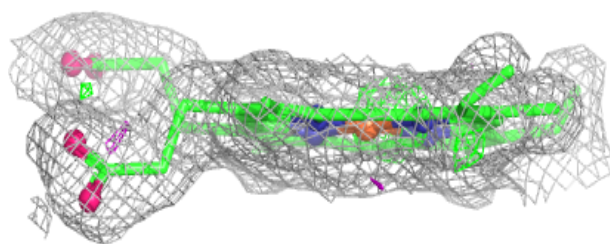
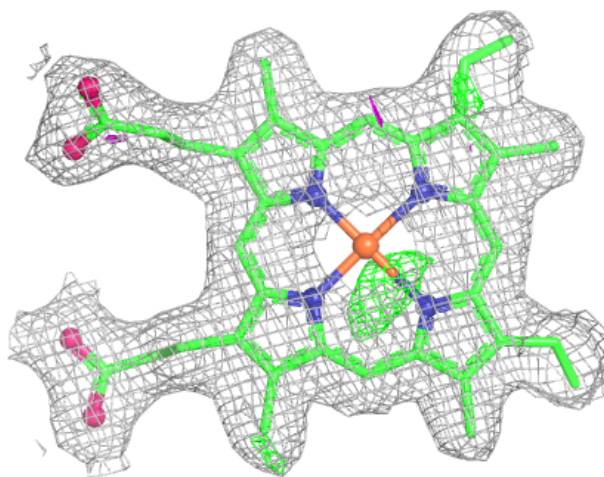
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





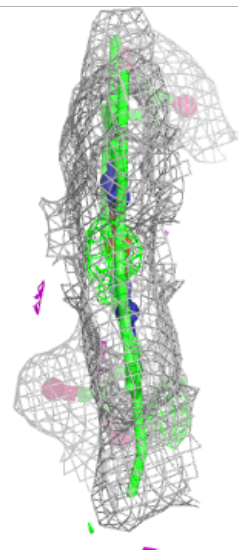
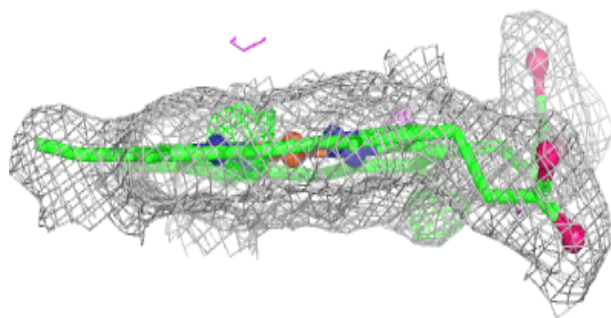
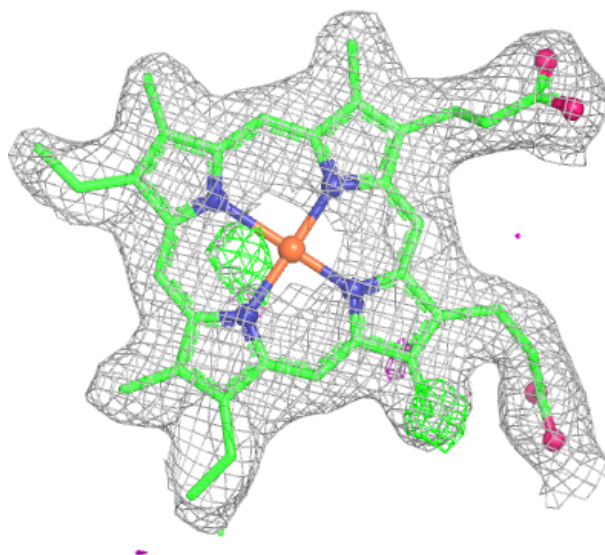
**Electron density around HEM D 810:**

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



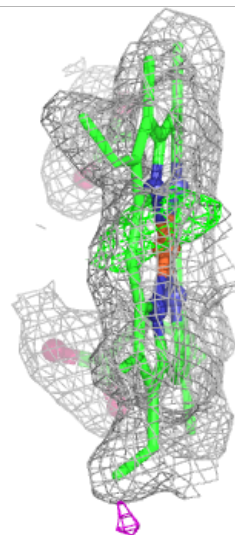
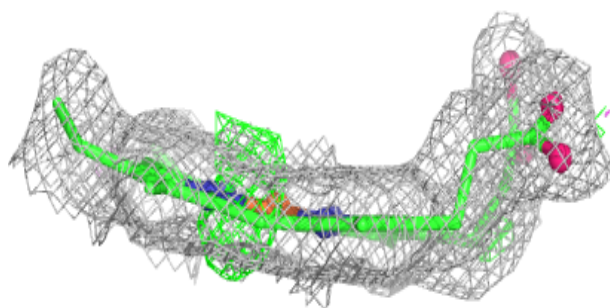
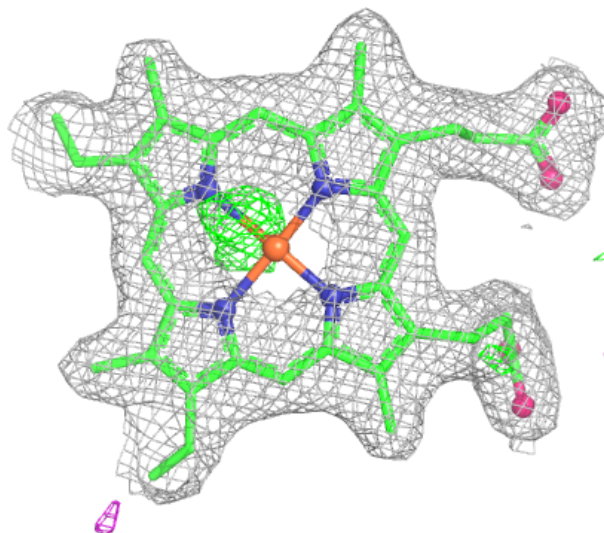
**Electron density around HEM E 807:**

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



**Electron density around HEM E 808:**

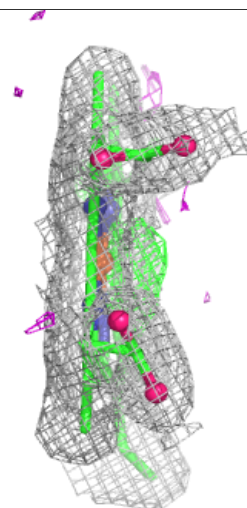
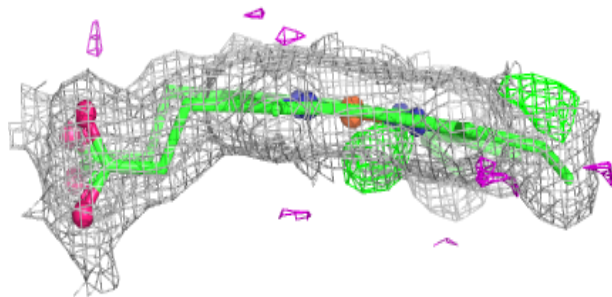
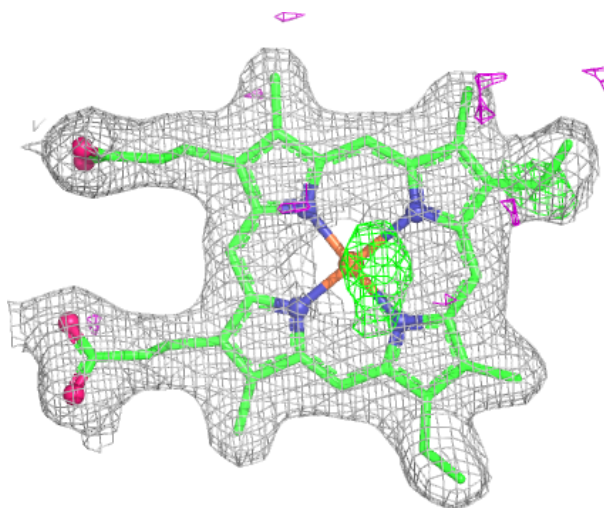
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





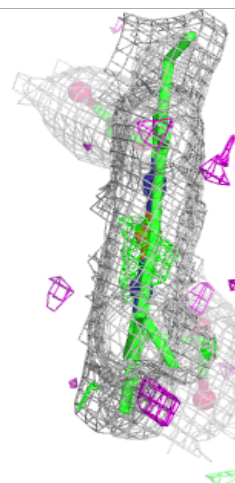
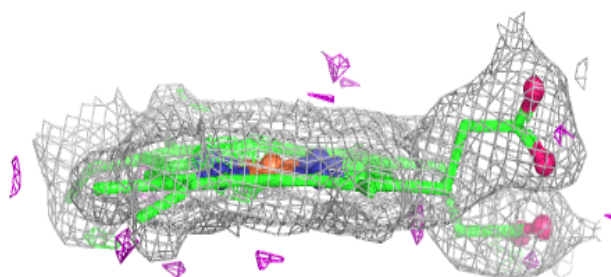
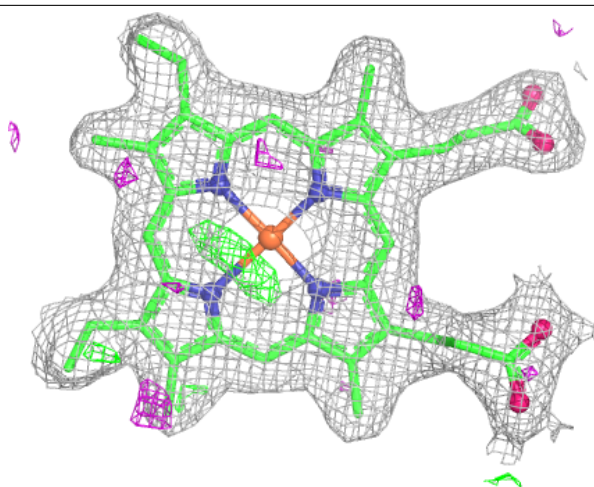
**Electron density around HEM E 809:**

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



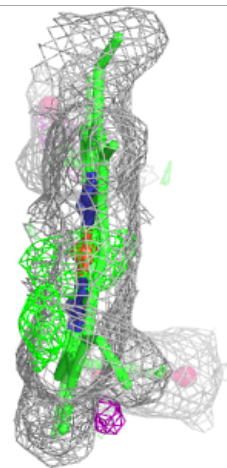
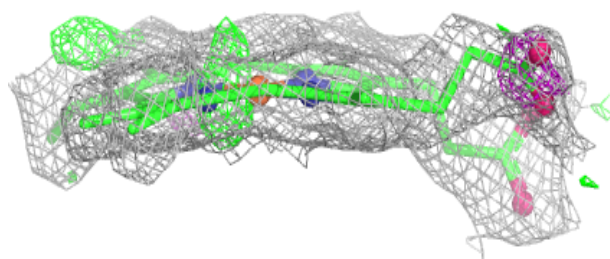
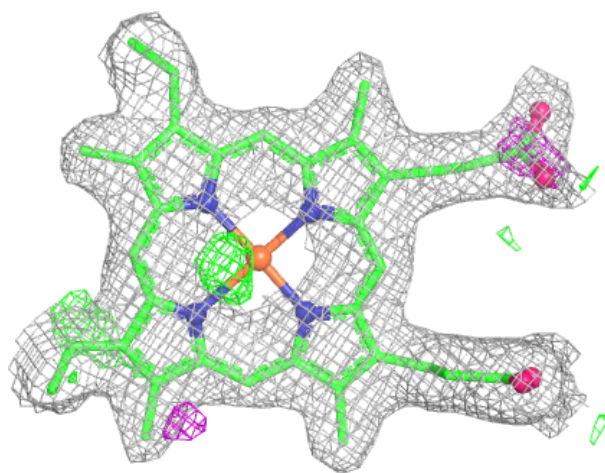
**Electron density around HEM E 810:**

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and green (positive)



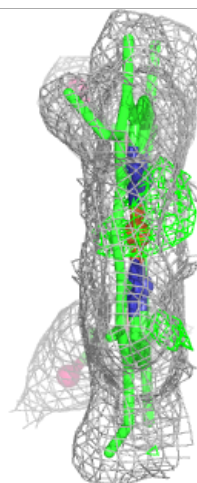
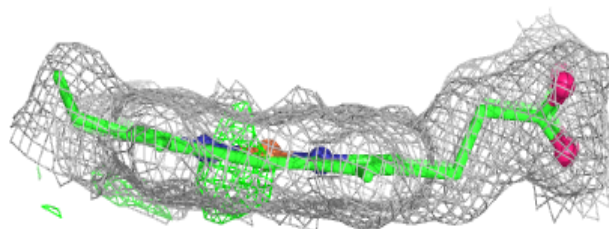
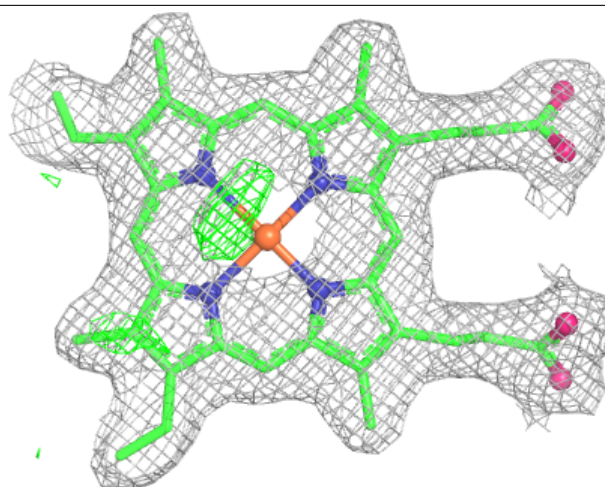
**Electron density around HEM E 811:**

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and green (positive)



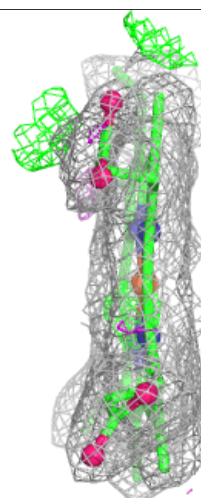
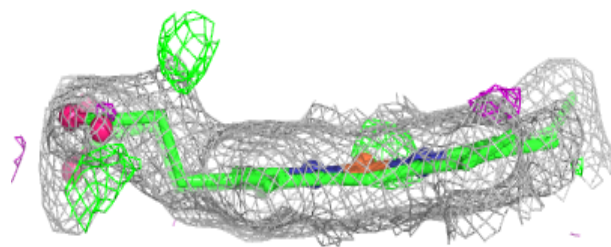
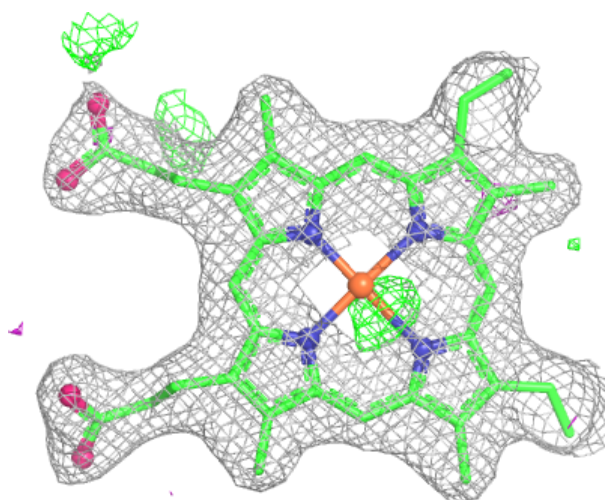
**Electron density around HEM E 812:**

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and green (positive)



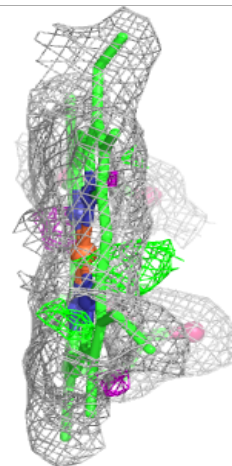
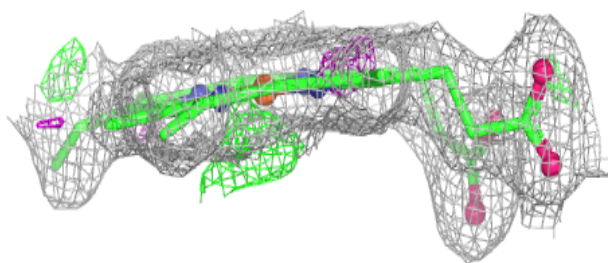
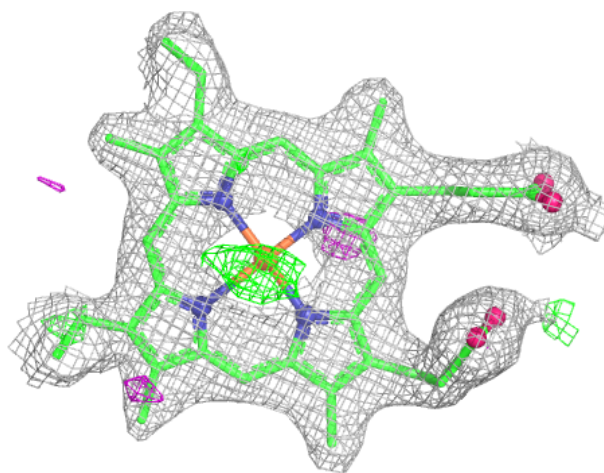
**Electron density around HEM E 813:**

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



**Electron density around HEM F 807:**

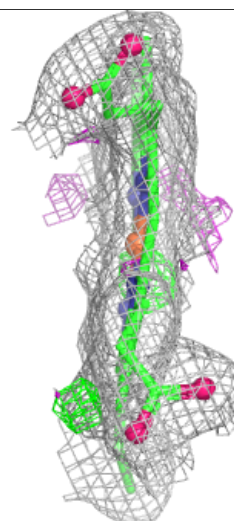
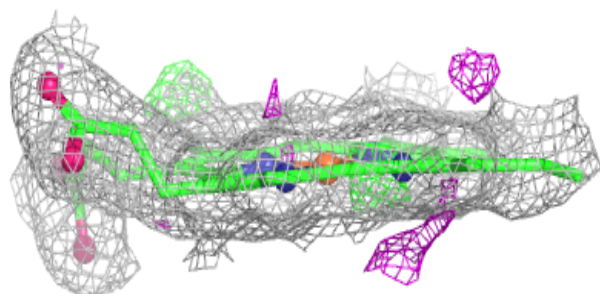
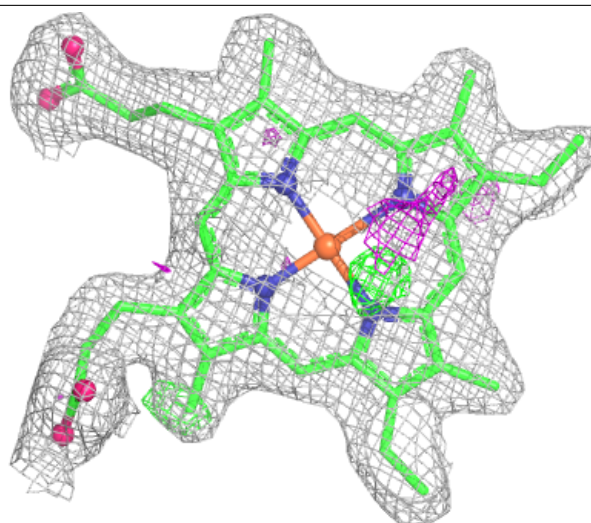
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





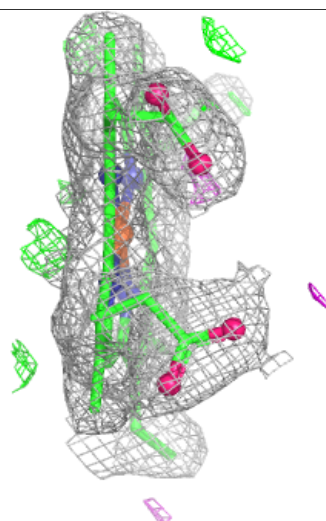
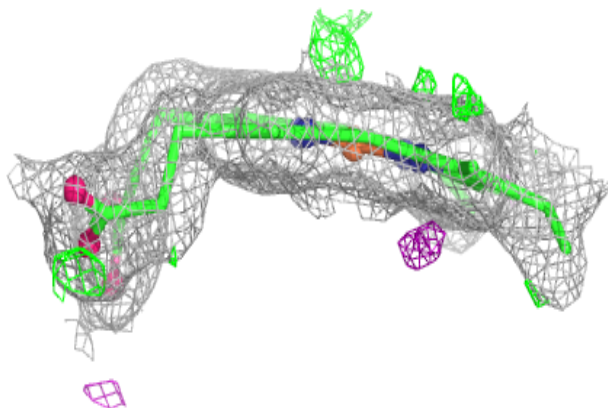
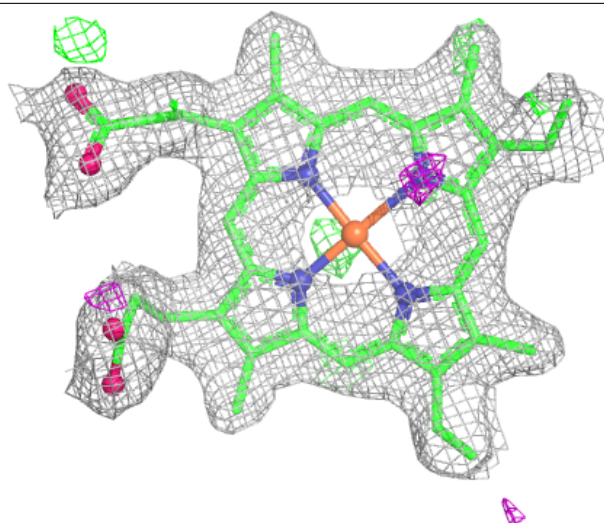
**Electron density around HEM F 808:**

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



**Electron density around HEM F 809:**

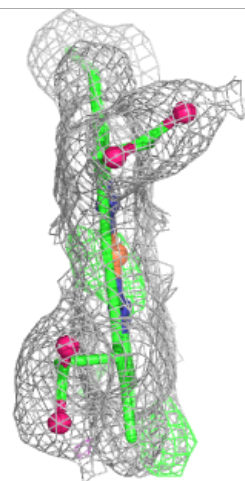
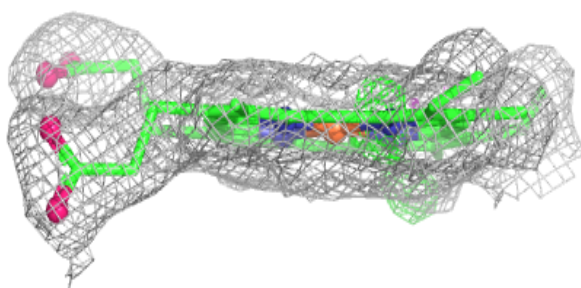
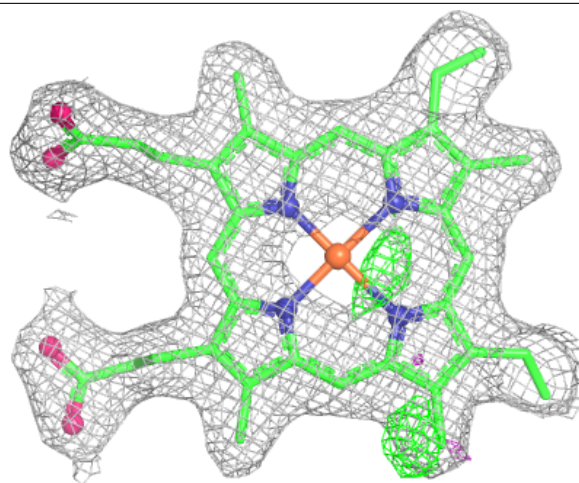
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





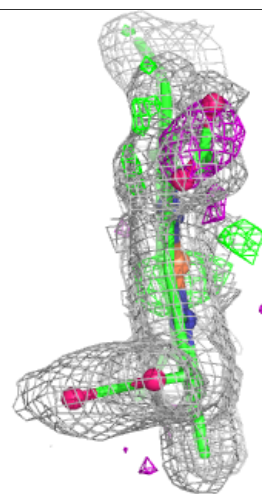
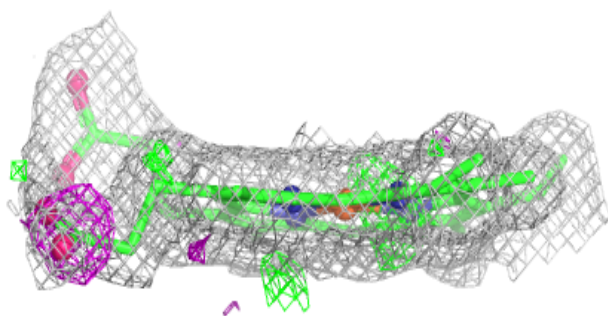
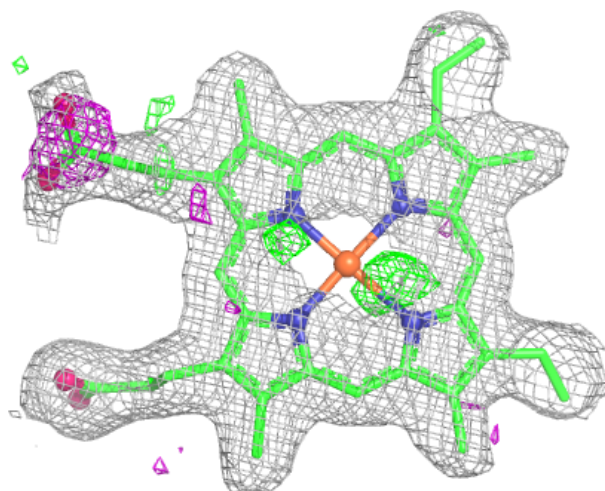
**Electron density around HEM F 811:**

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



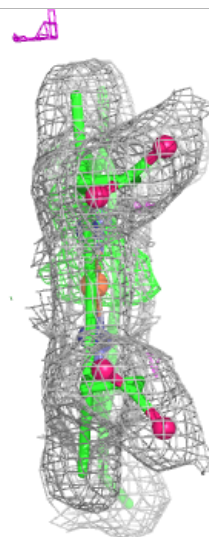
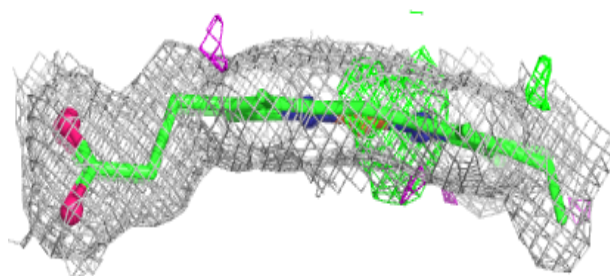
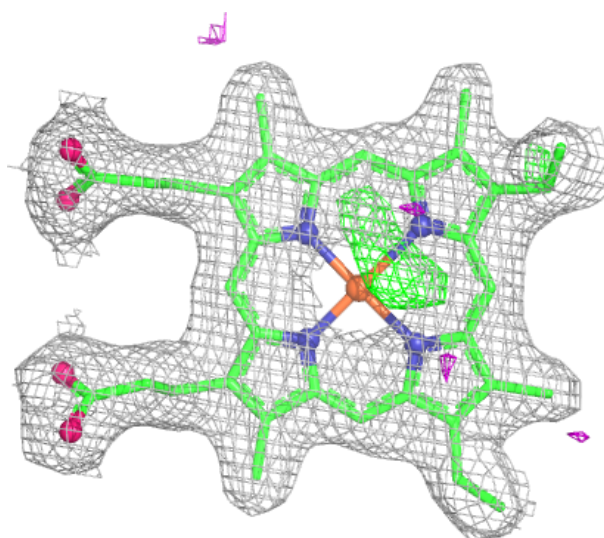
**Electron density around HEM F 812:**

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



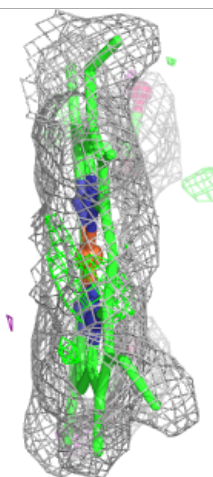
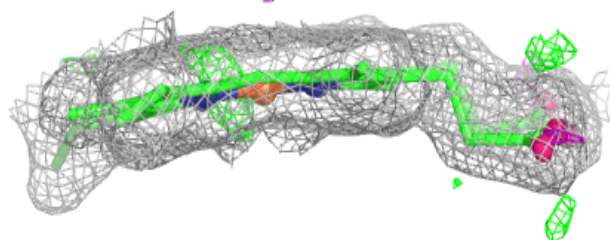
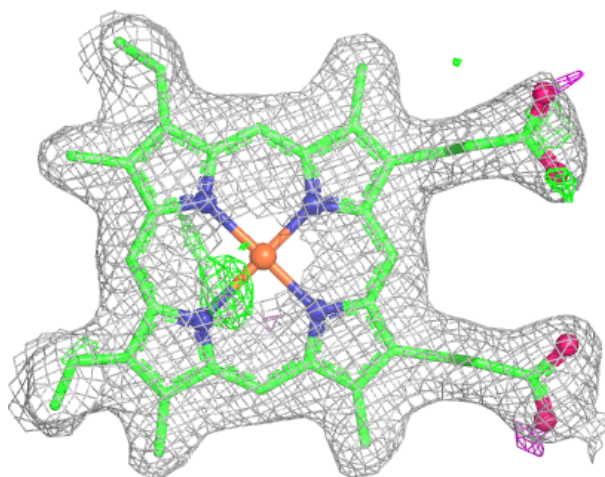
**Electron density around HEM F 813:**

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



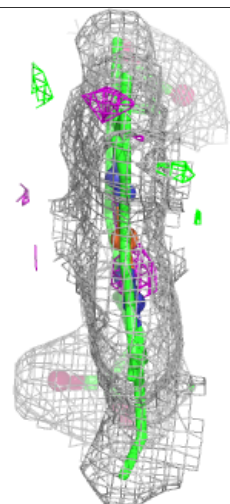
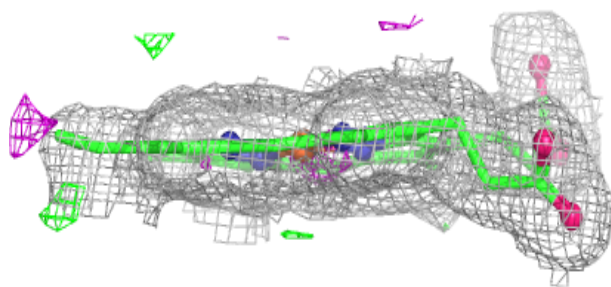
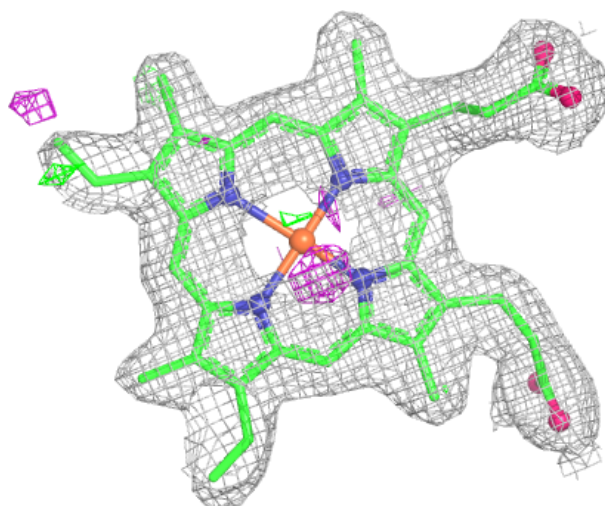
**Electron density around HEM F 814:**

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



**Electron density around HEM H 808:**

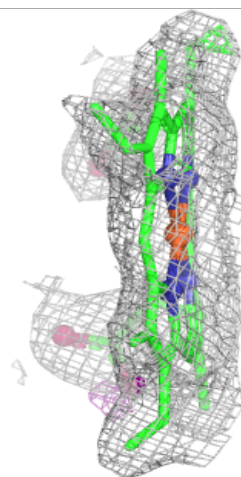
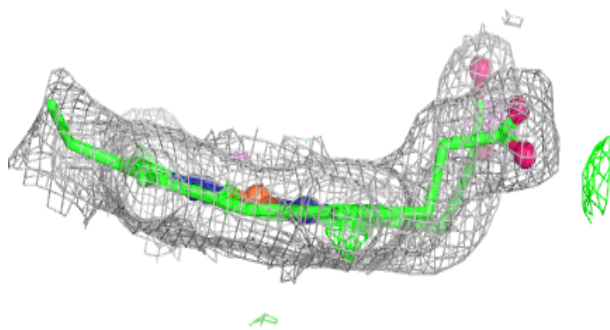
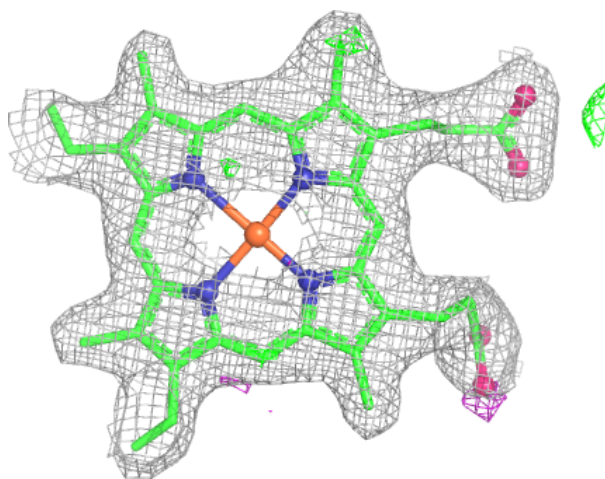
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





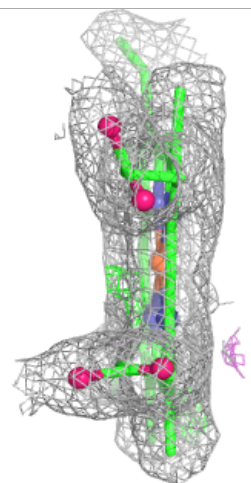
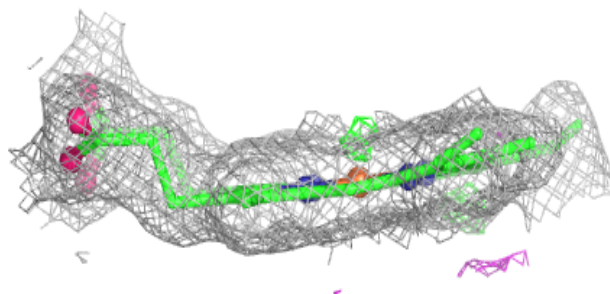
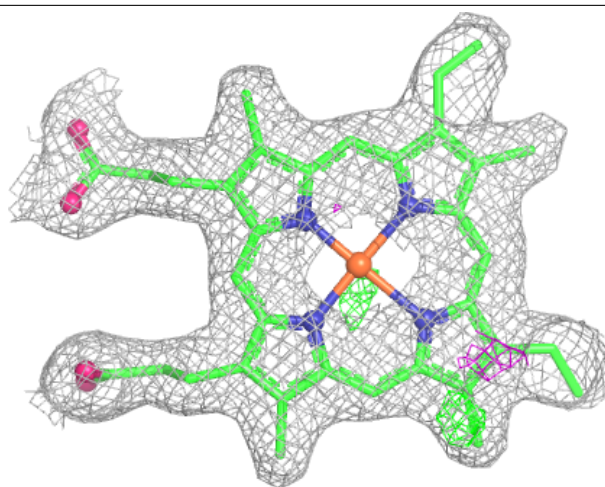
**Electron density around HEM H 809:**

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



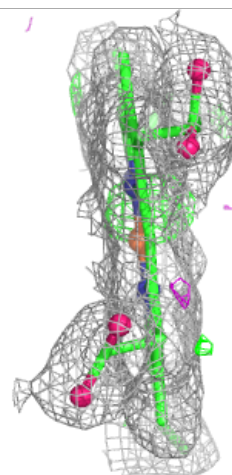
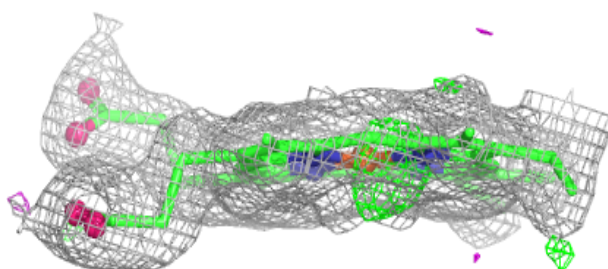
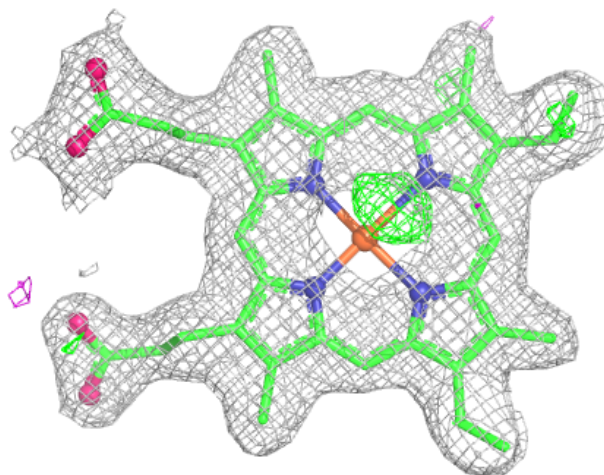
**Electron density around HEM H 810:**

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



**Electron density around HEM H 811:**

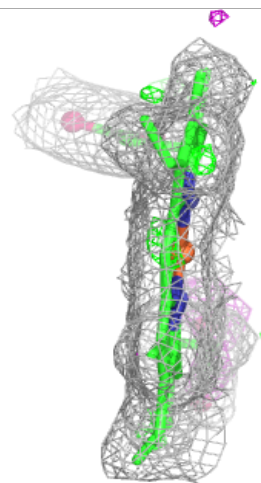
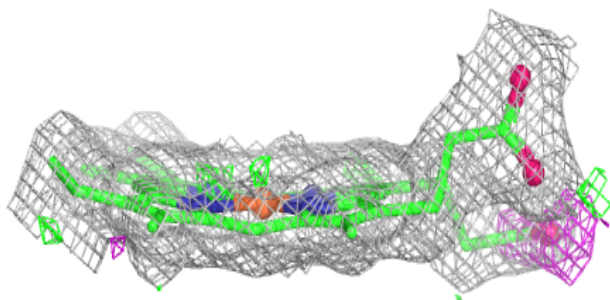
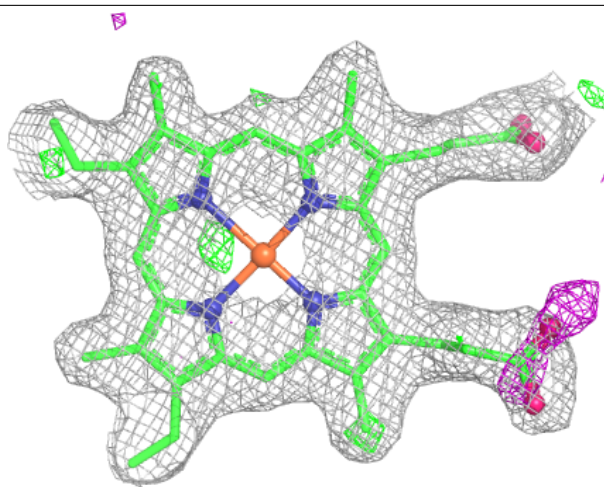
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





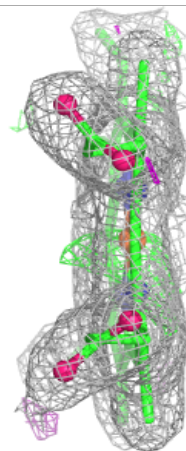
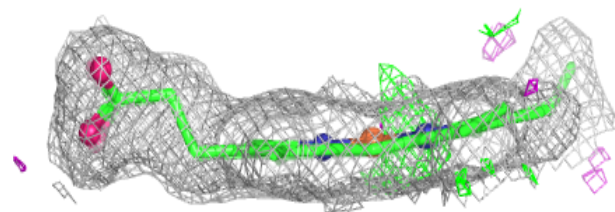
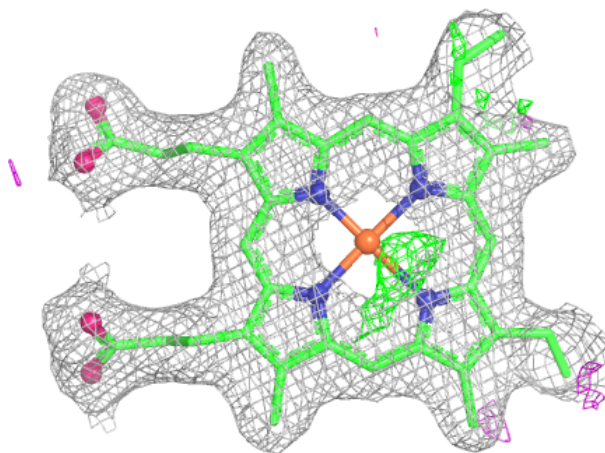
**Electron density around HEM H 812:**

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



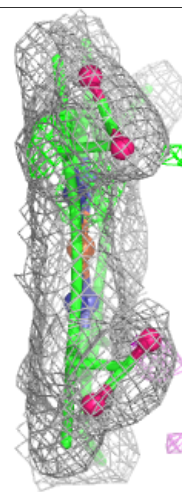
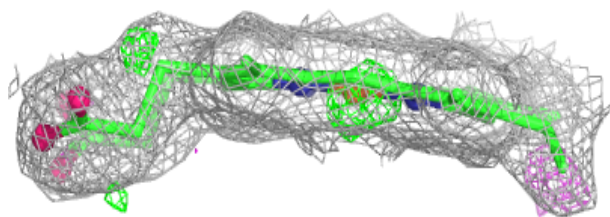
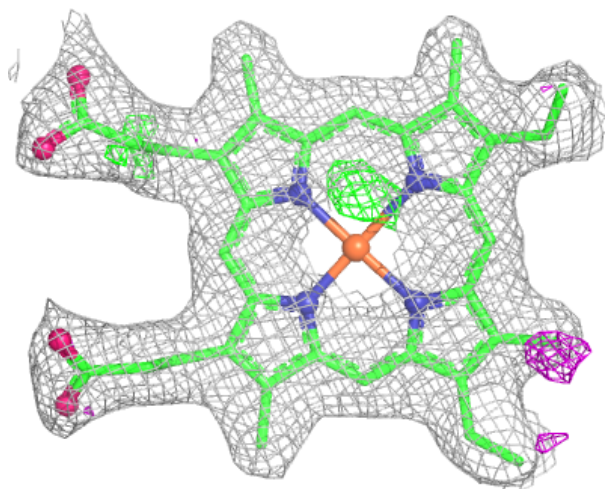
**Electron density around HEM H 813:**

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



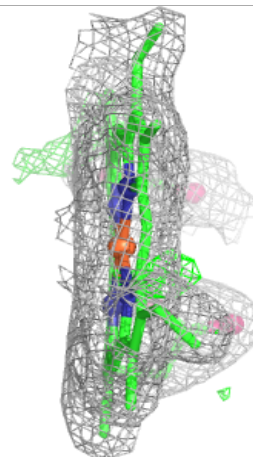
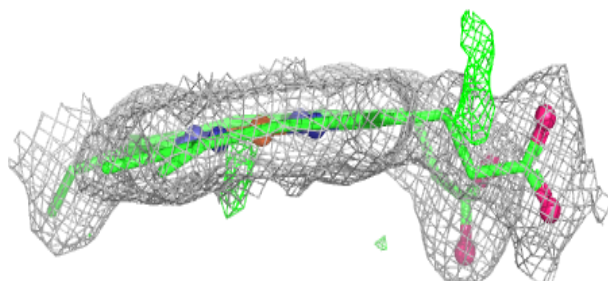
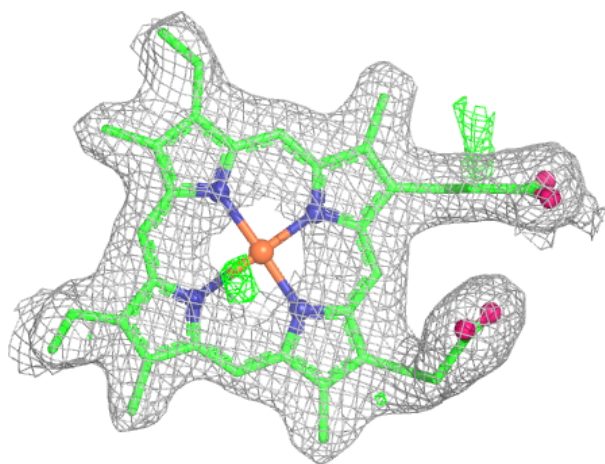
**Electron density around HEM H 814:**

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



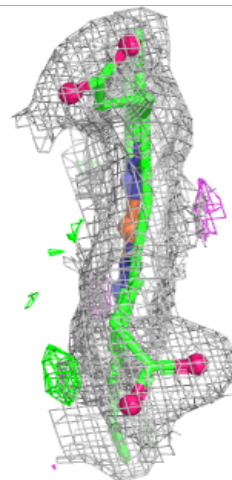
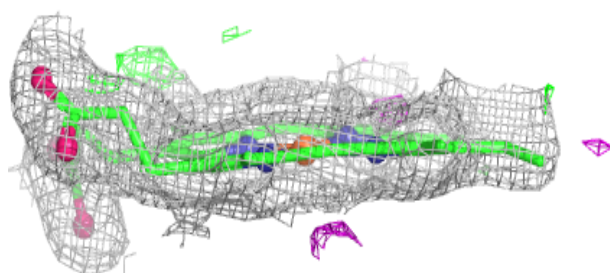
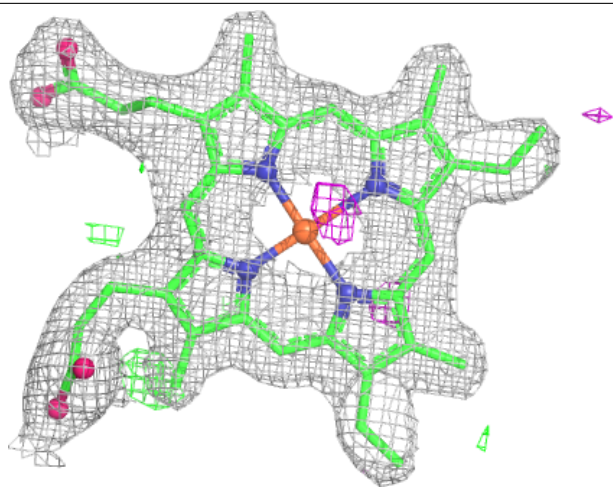
**Electron density around HEM I 806:**

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



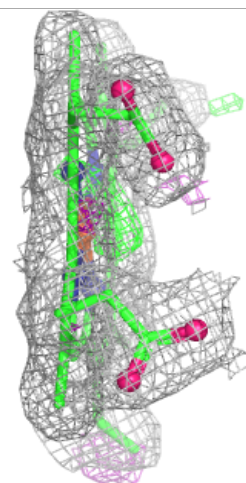
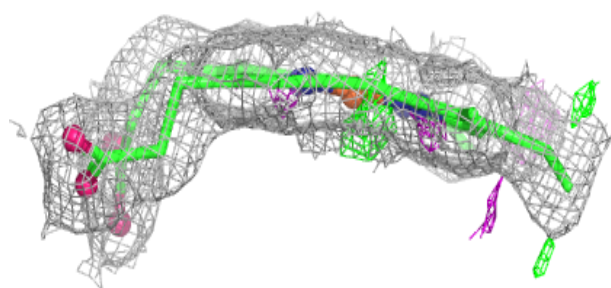
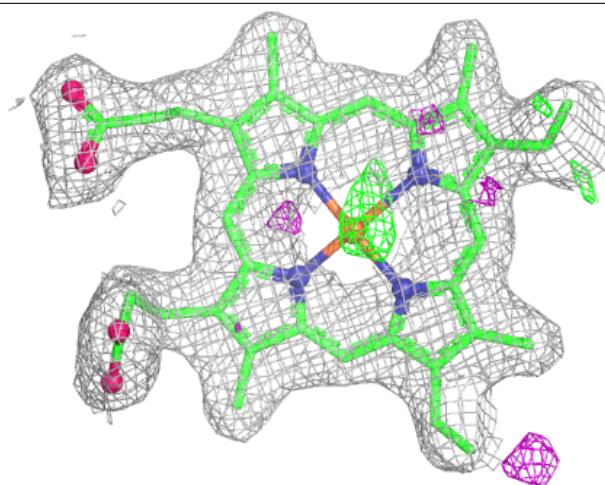
**Electron density around HEM I 807:**

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



**Electron density around HEM I 808:**

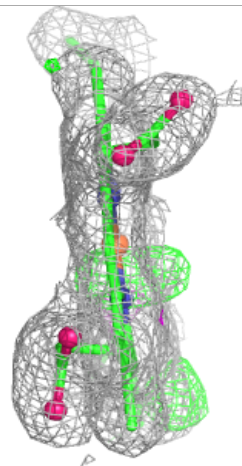
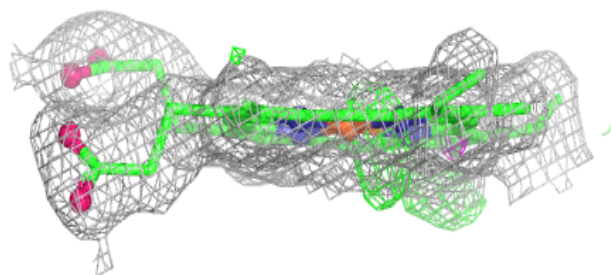
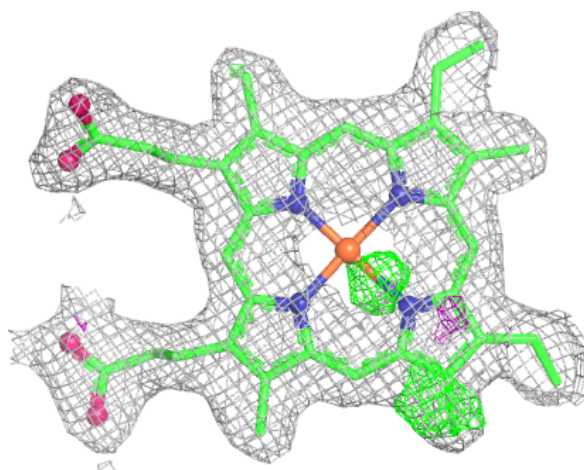
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





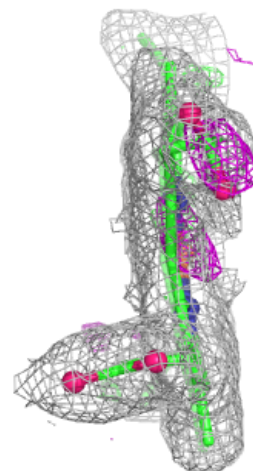
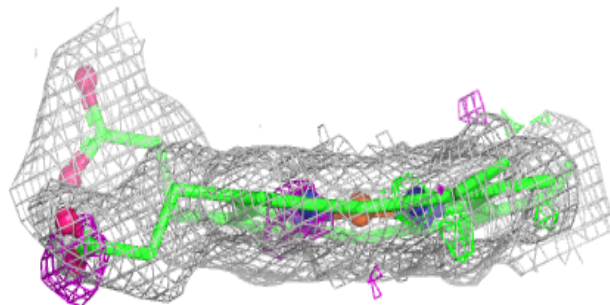
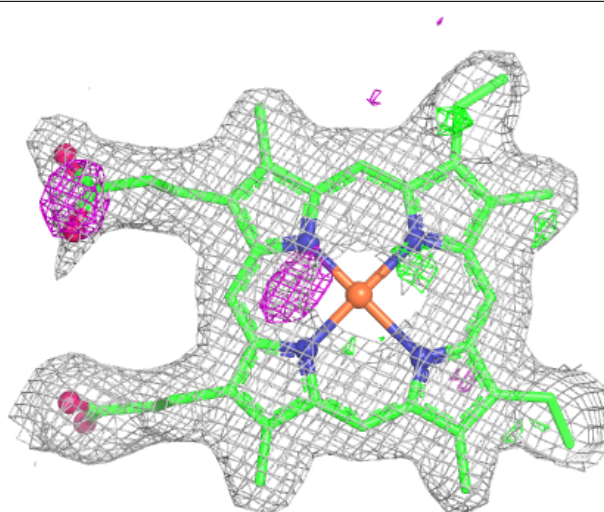
**Electron density around HEM I 810:**

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



**Electron density around HEM I 811:**

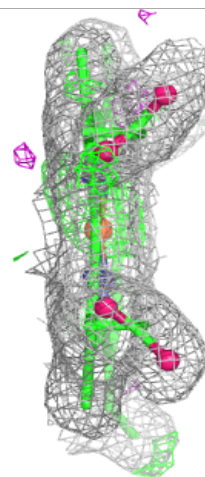
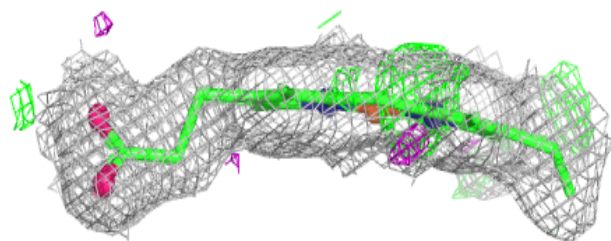
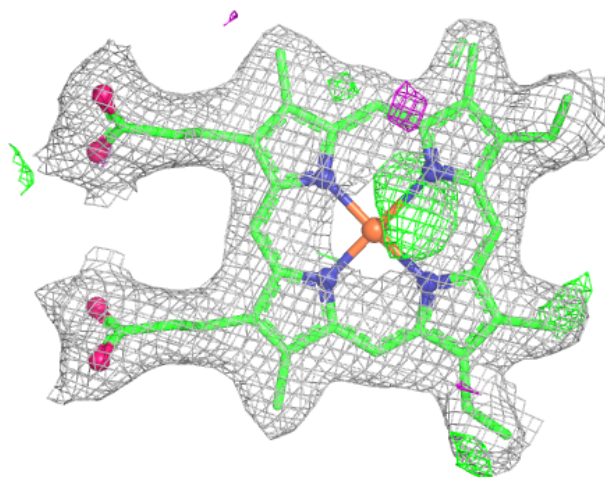
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





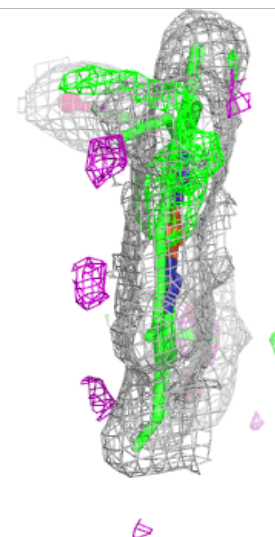
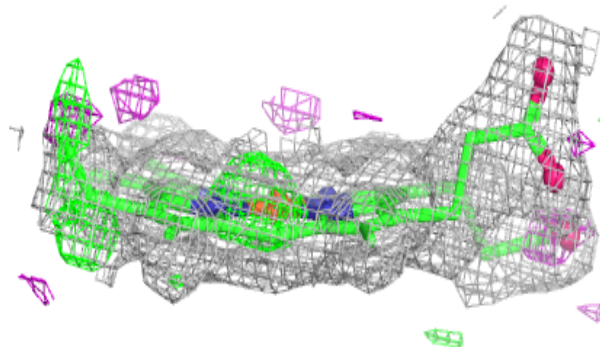
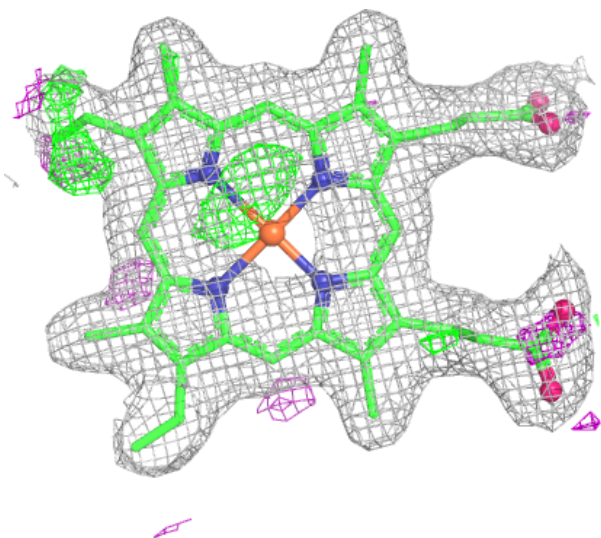
**Electron density around HEM I 812:**

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



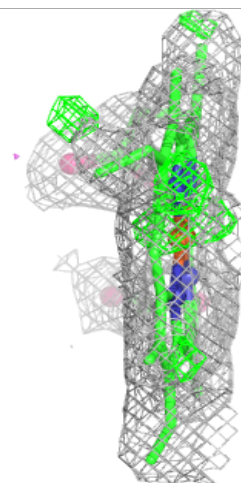
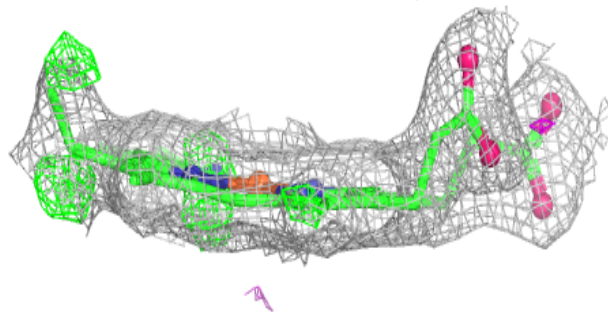
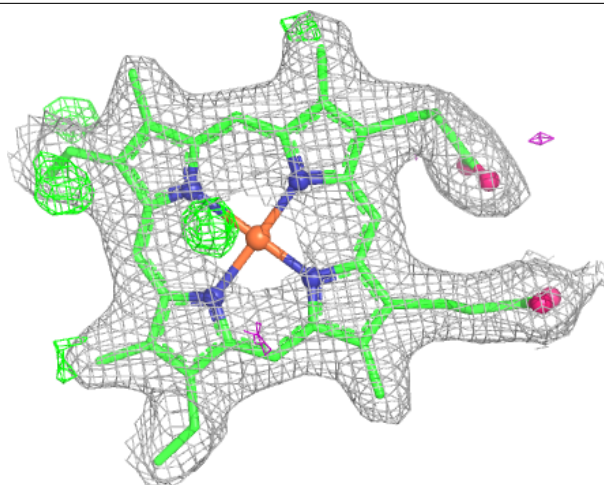
**Electron density around HEM A 811:**

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



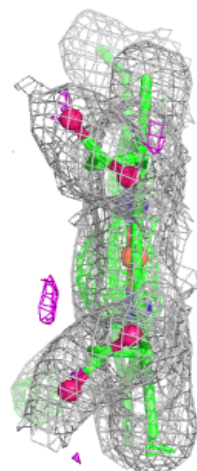
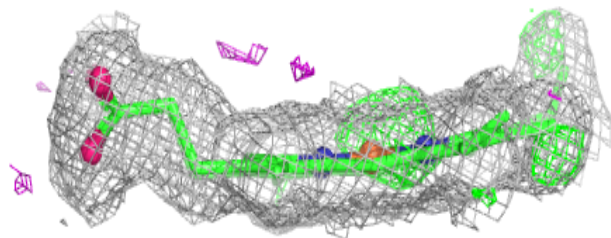
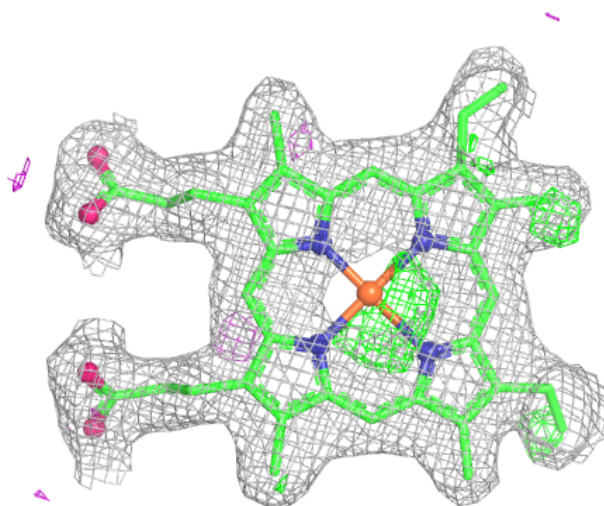
**Electron density around HEM J 806:**

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



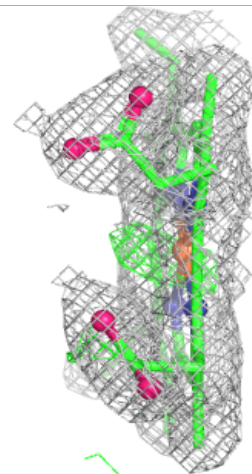
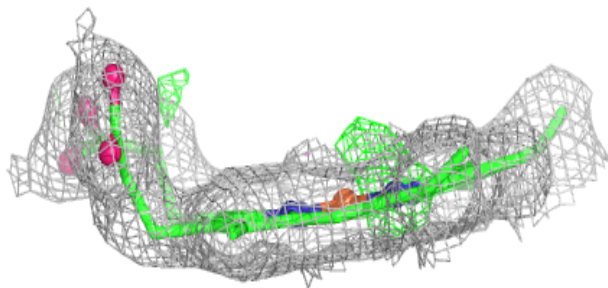
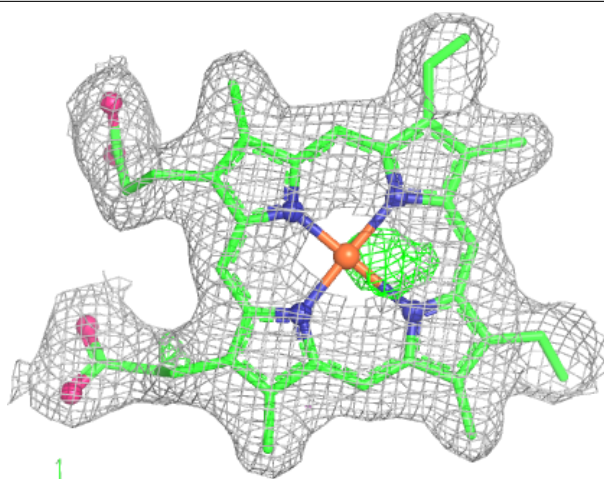
**Electron density around HEM A 812:**

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



**Electron density around HEM J 808:**

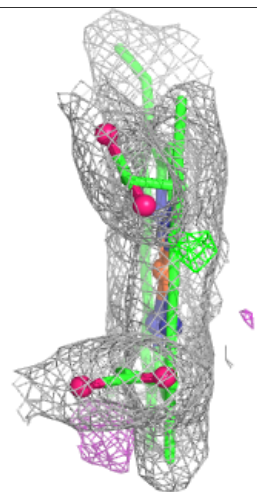
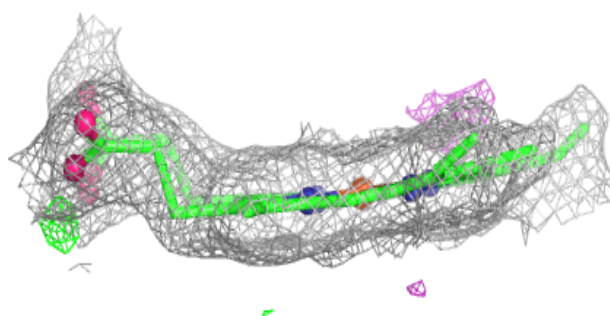
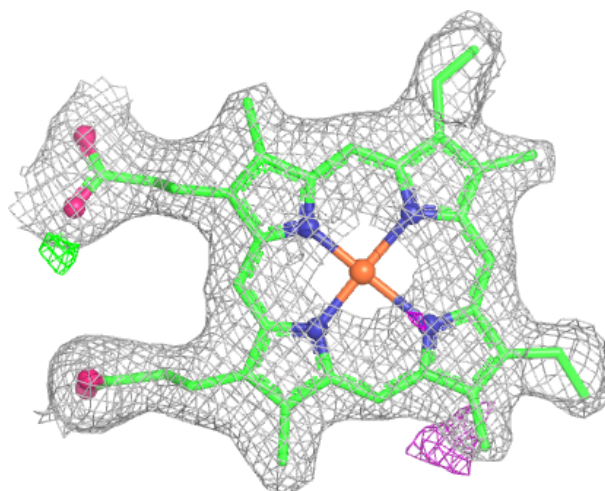
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





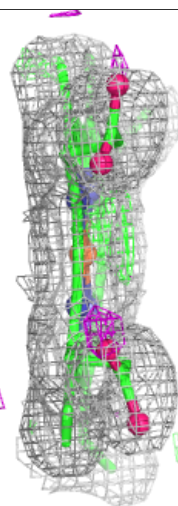
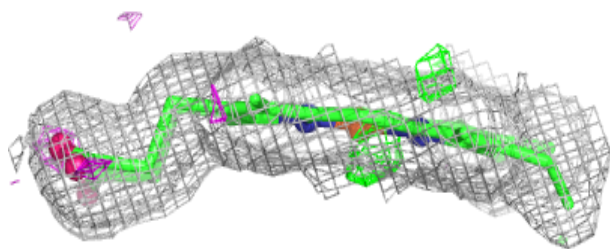
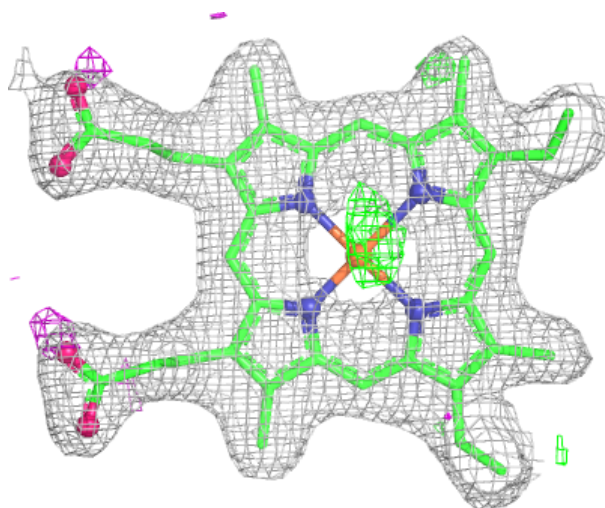
**Electron density around HEM J 809:**

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



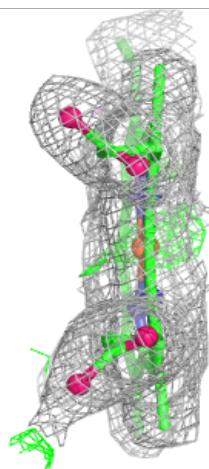
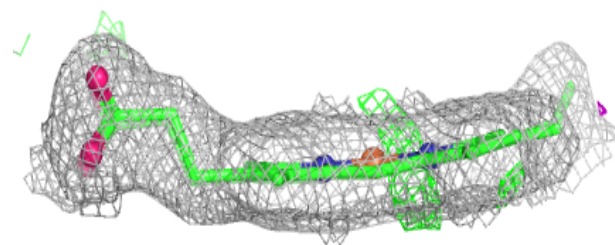
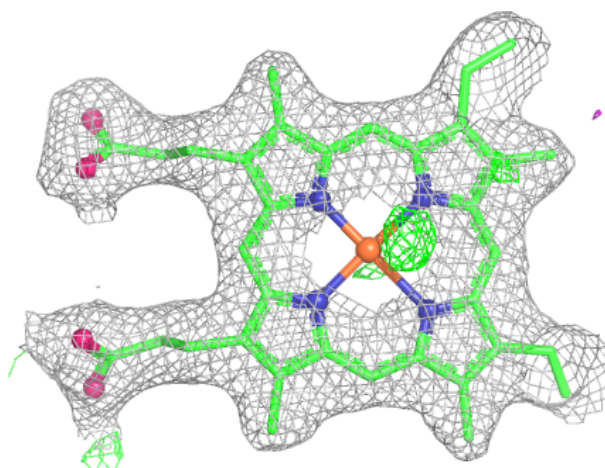
**Electron density around HEM A 813:**

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



**Electron density around HEM J 812:**

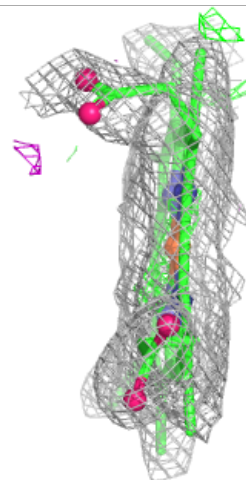
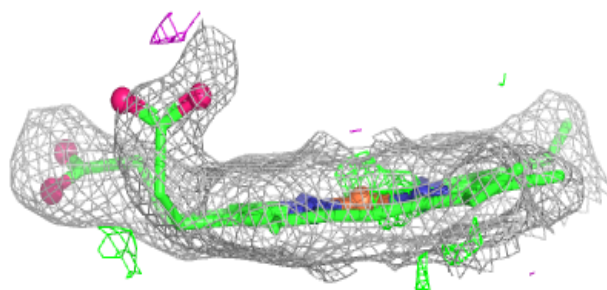
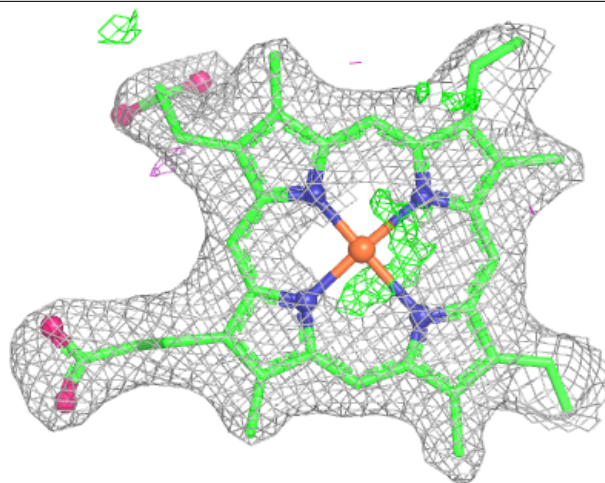
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





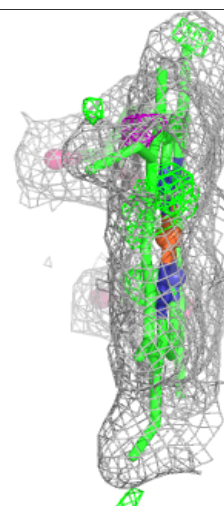
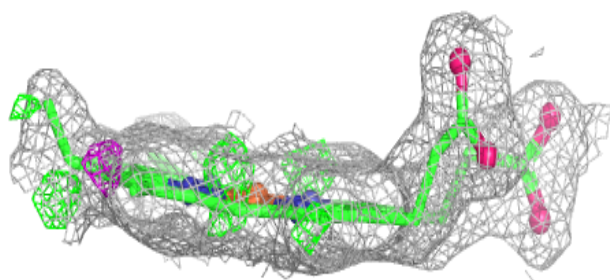
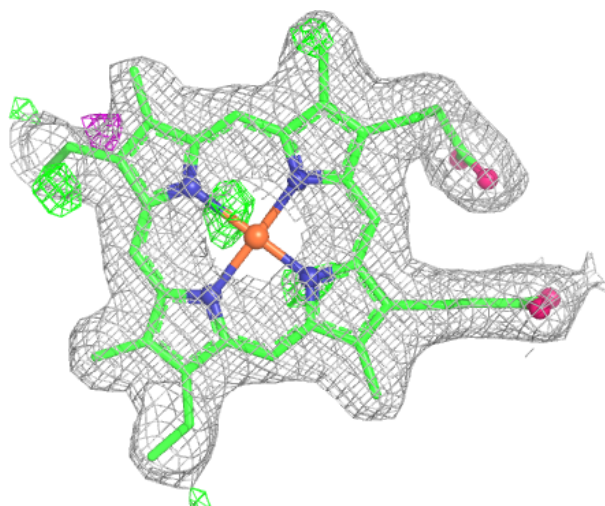
**Electron density around HEM J 813:**

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



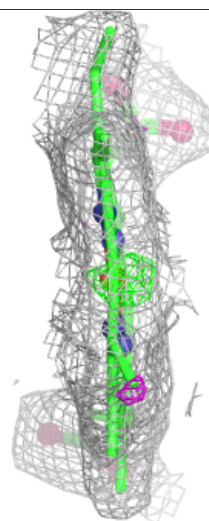
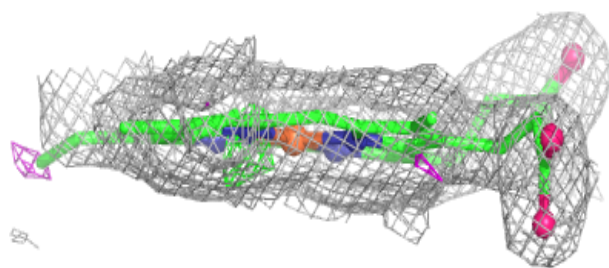
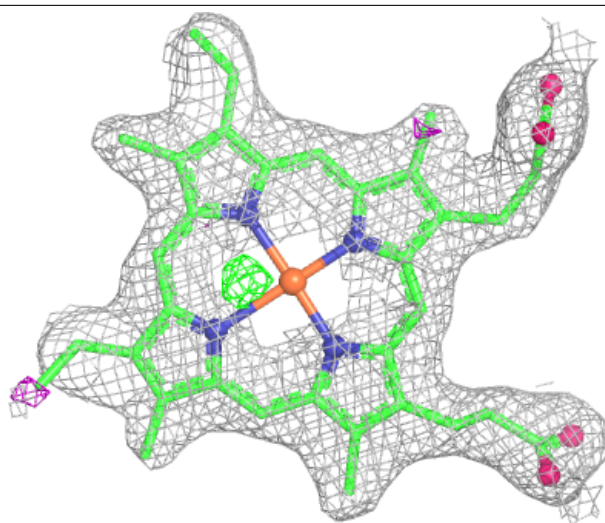
**Electron density around HEM K 806:**

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



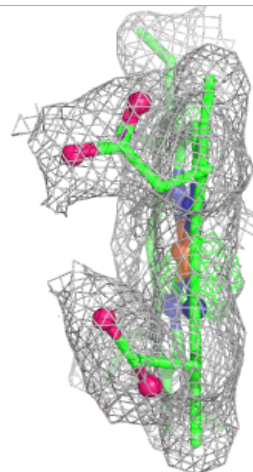
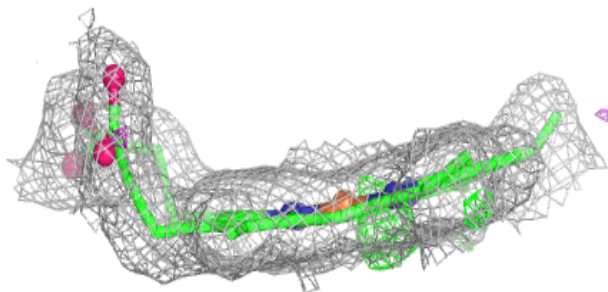
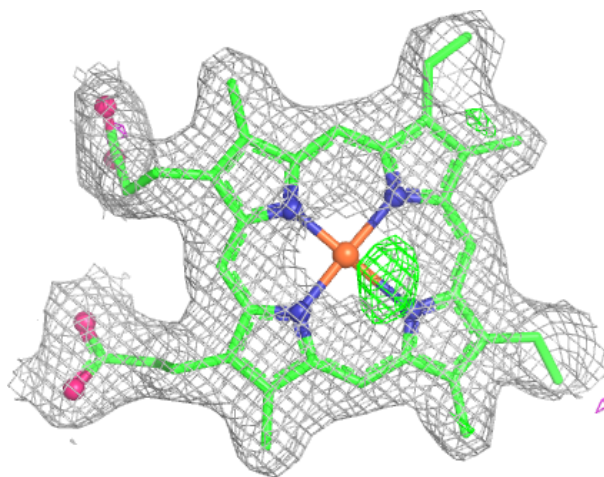
**Electron density around HEM K 807:**

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



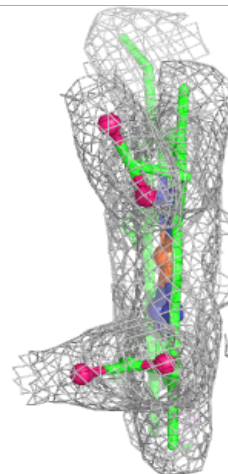
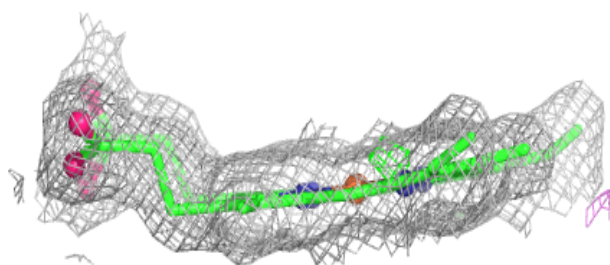
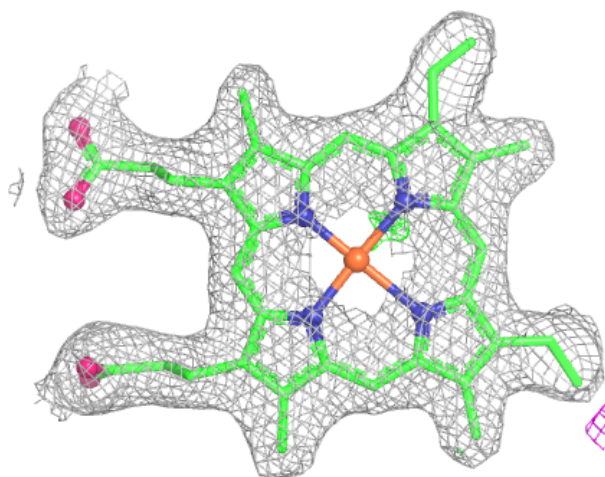
**Electron density around HEM K 808:**

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



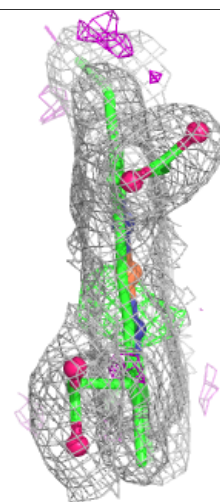
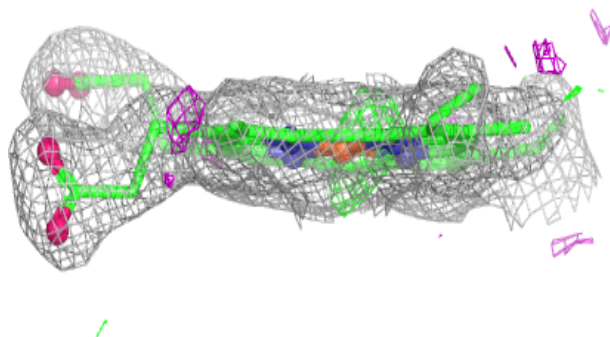
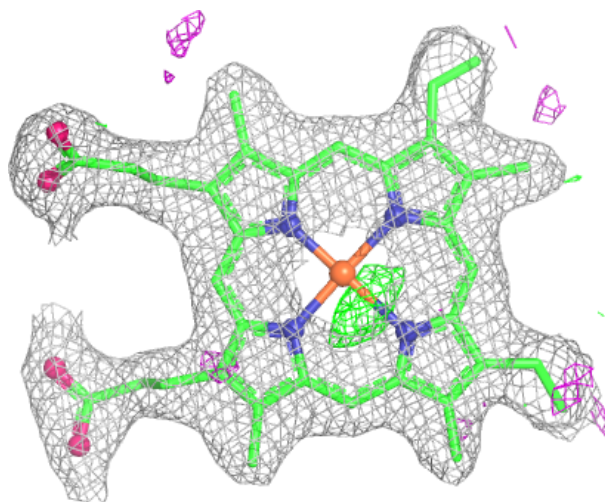
**Electron density around HEM K 809:**

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



**Electron density around HEM K 810:**

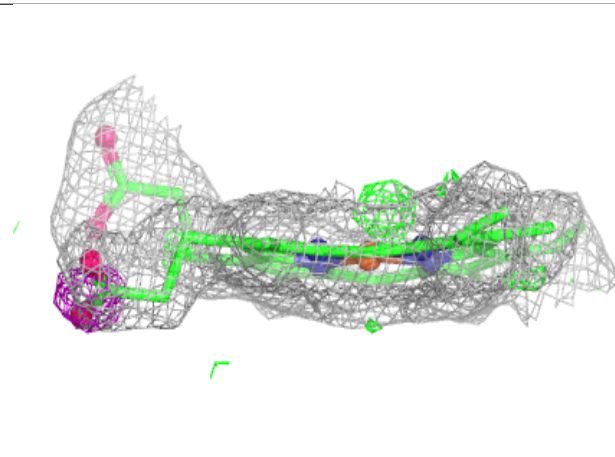
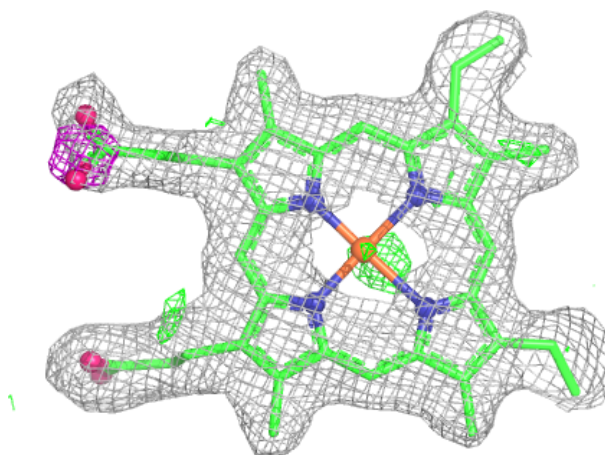
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





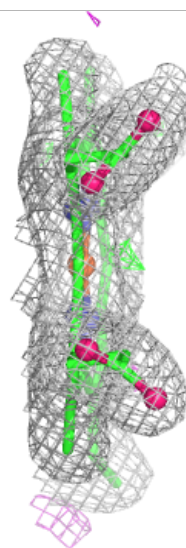
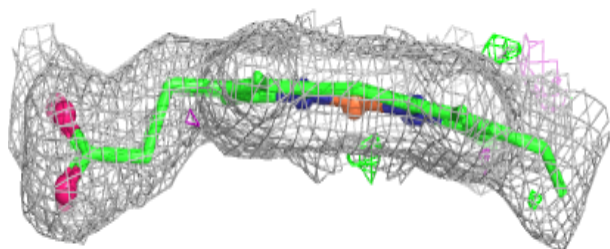
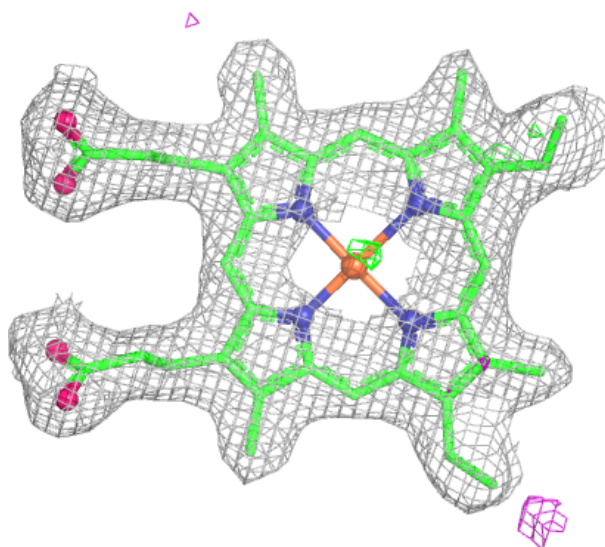
**Electron density around HEM K 811:**

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



**Electron density around HEM K 812:**

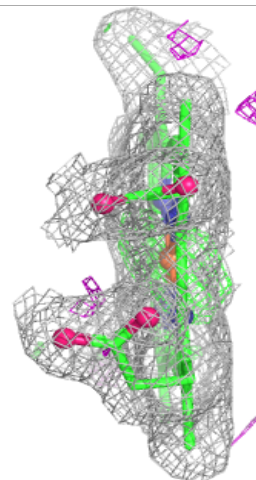
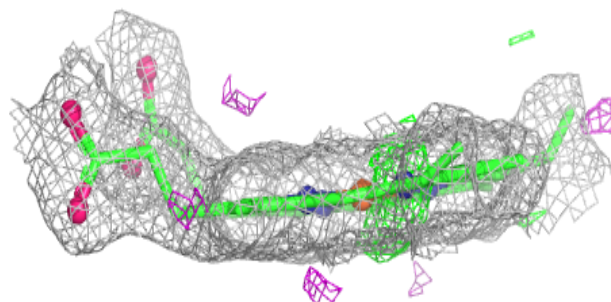
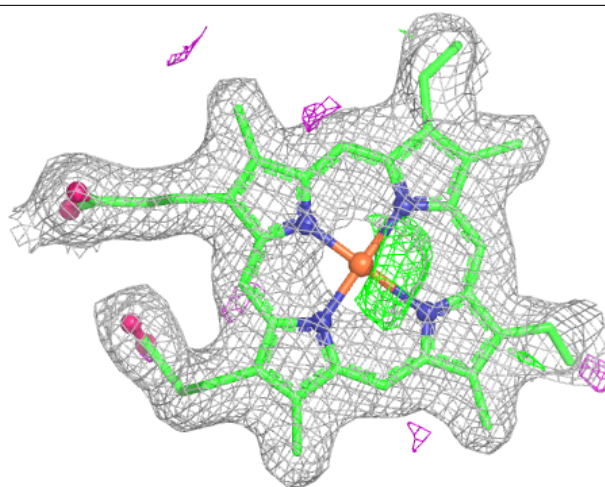
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





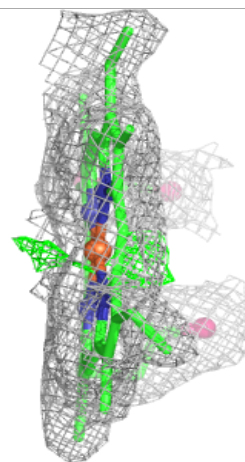
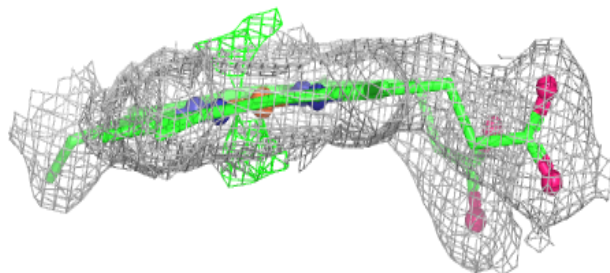
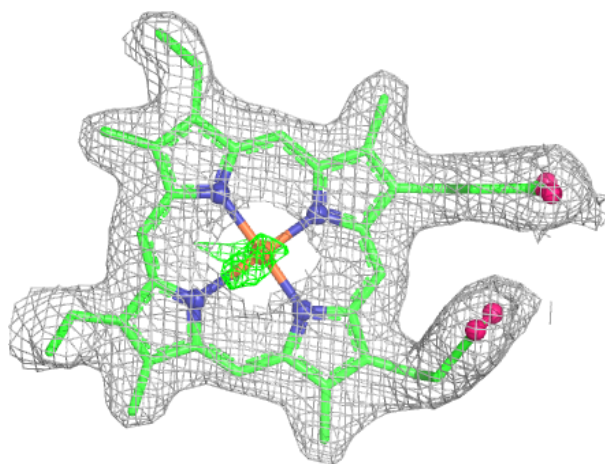
**Electron density around HEM B 807:**

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



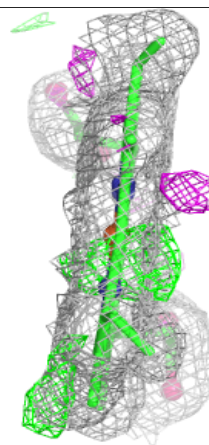
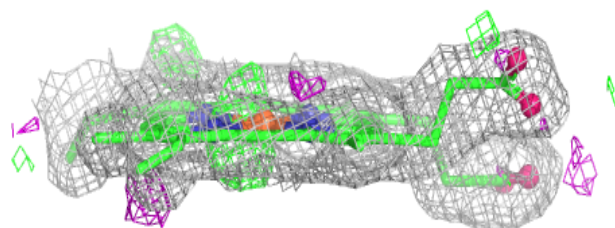
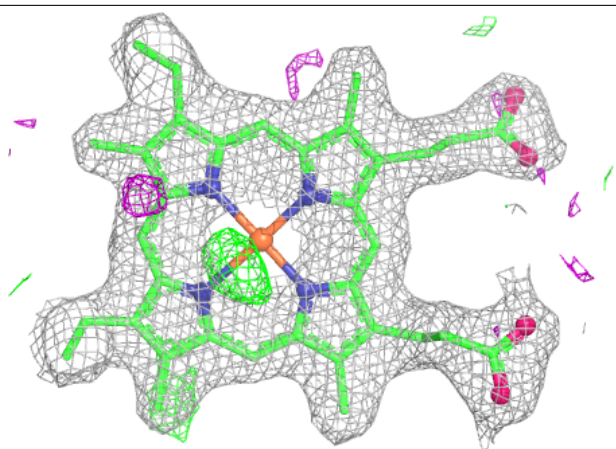
**Electron density around HEM L 806:**

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



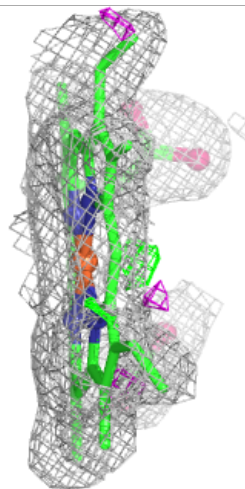
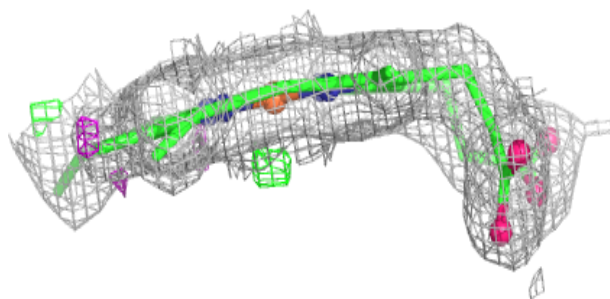
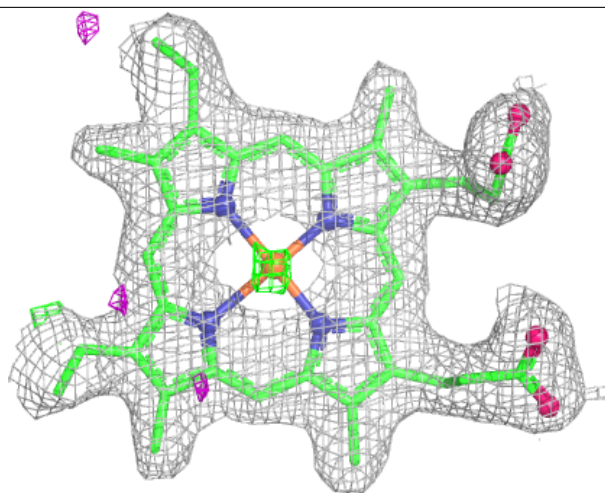
**Electron density around HEM B 811:**

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



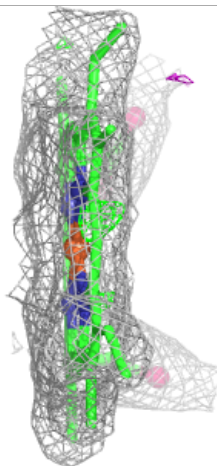
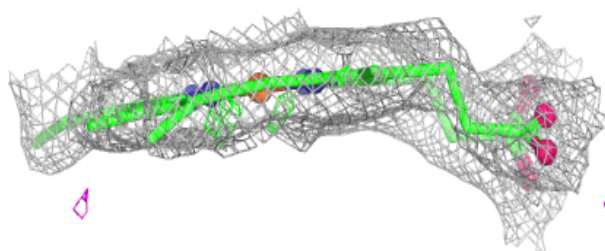
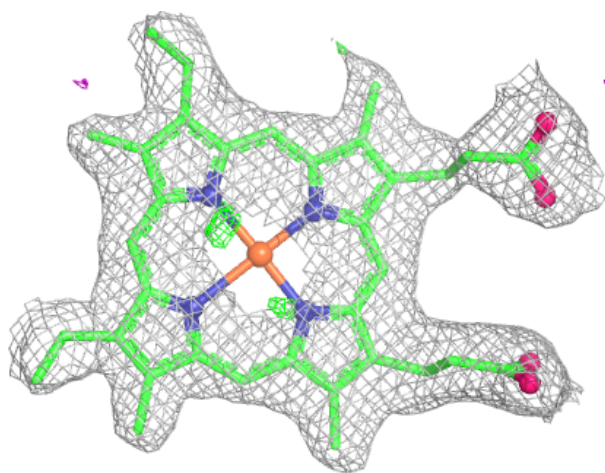
**Electron density around HEM L 808:**

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



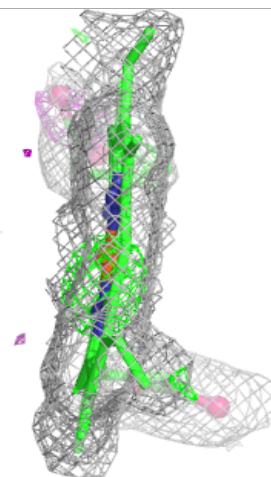
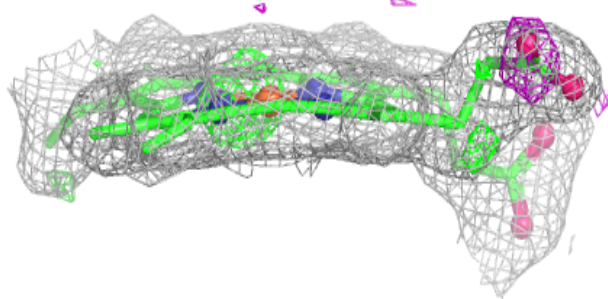
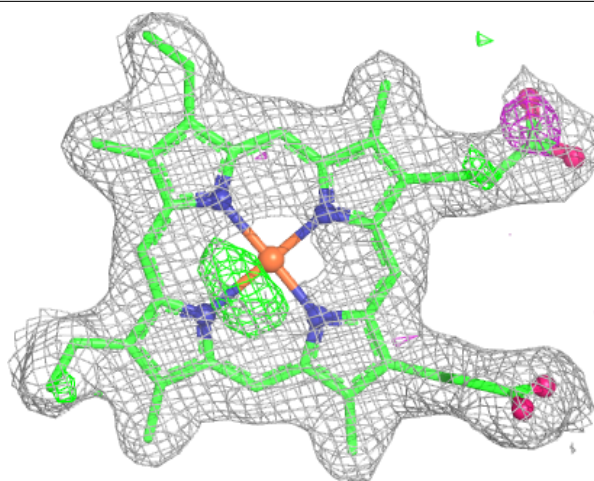
**Electron density around HEM L 809:**

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



**Electron density around HEM B 812:**

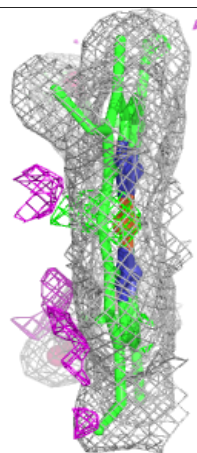
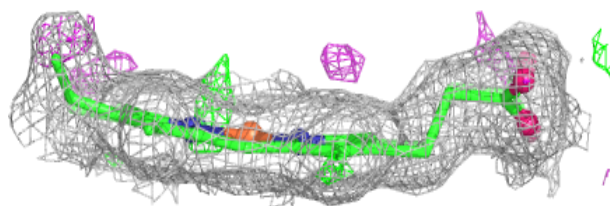
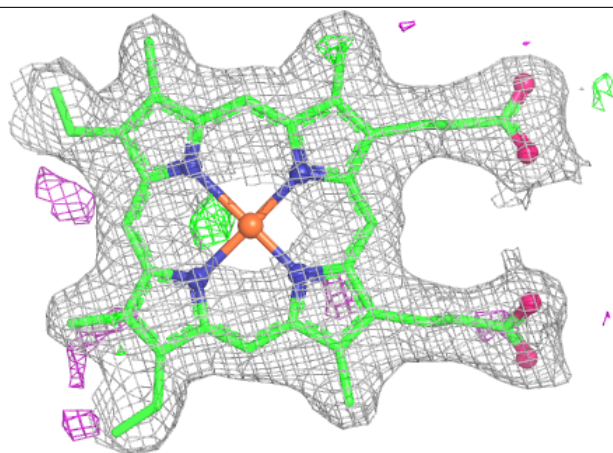
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





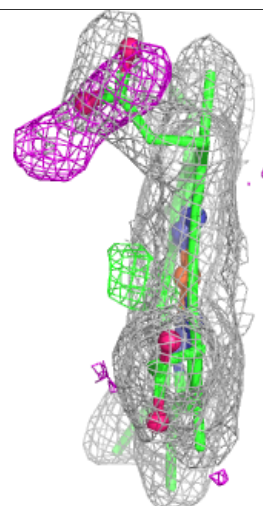
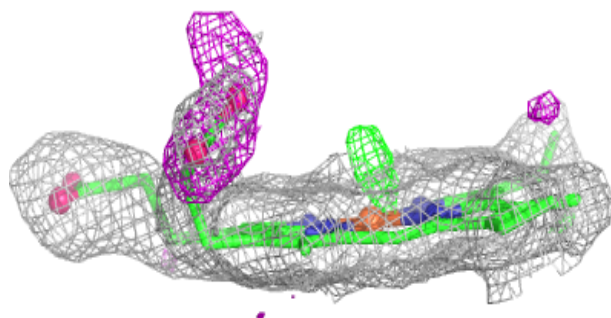
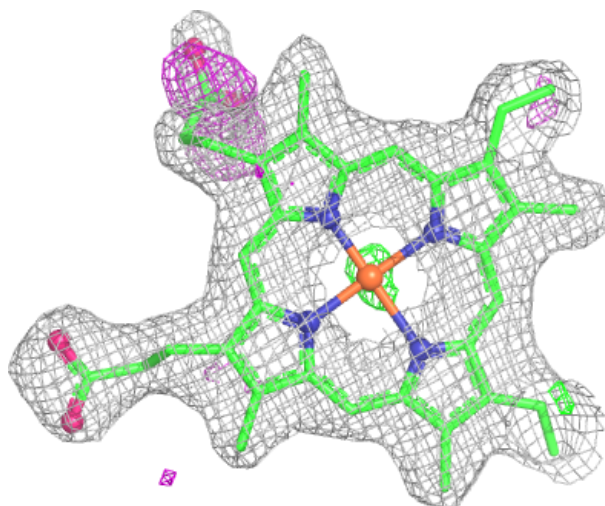
**Electron density around HEM B 813:**

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



**Electron density around HEM B 814:**

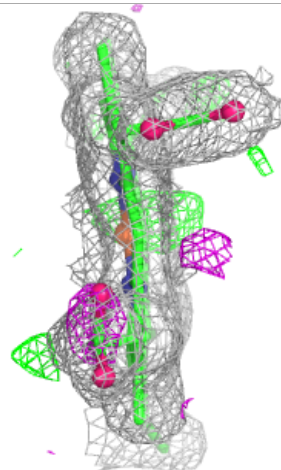
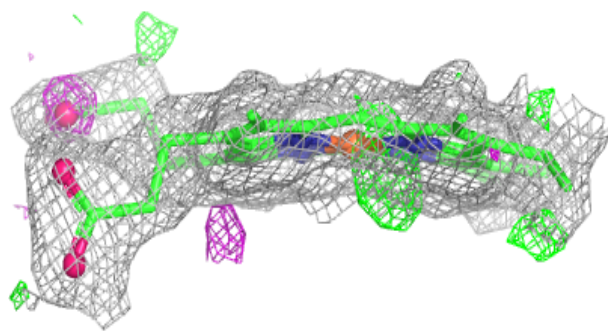
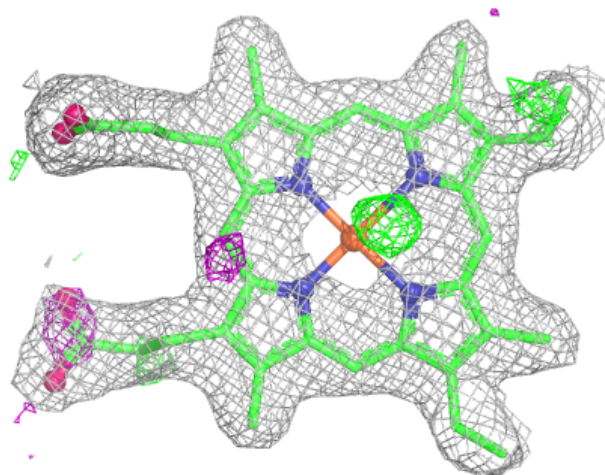
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





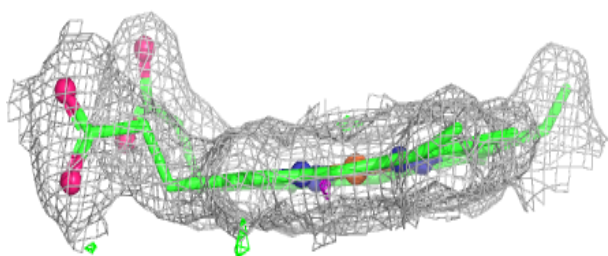
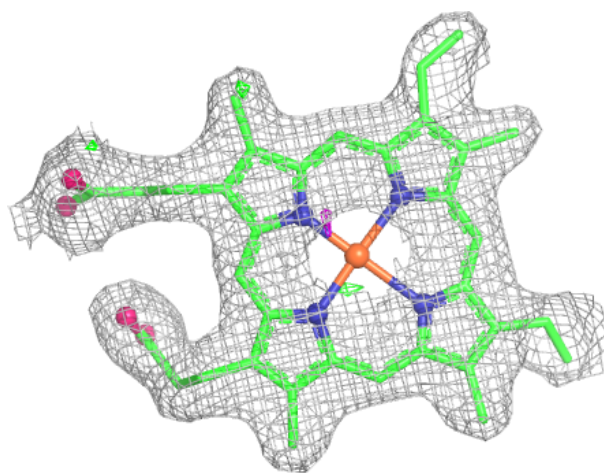
**Electron density around HEM C 811:**

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



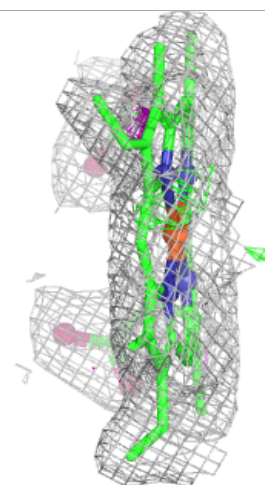
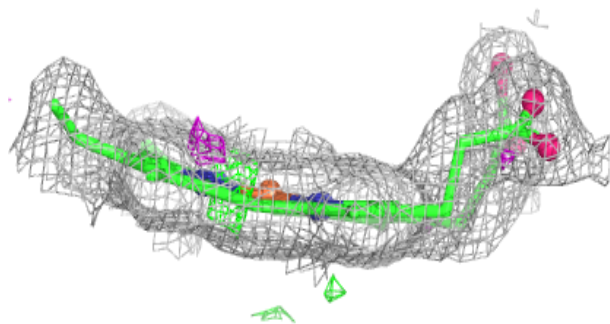
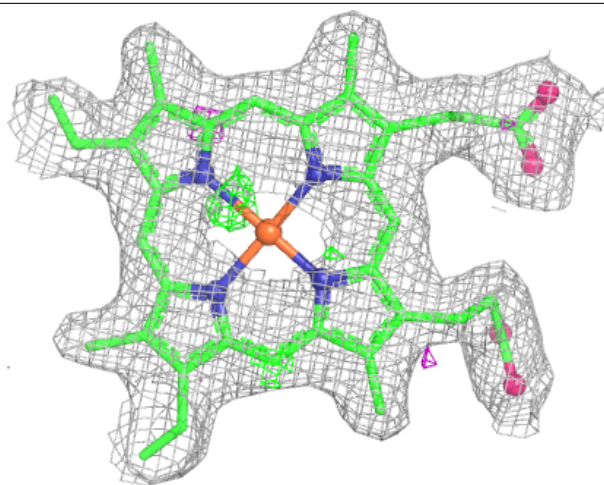
**Electron density around HEM G 806:**

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



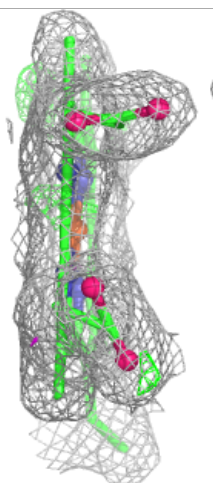
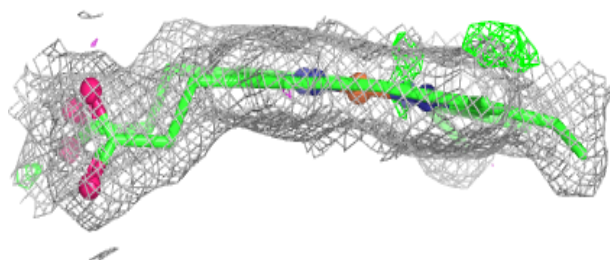
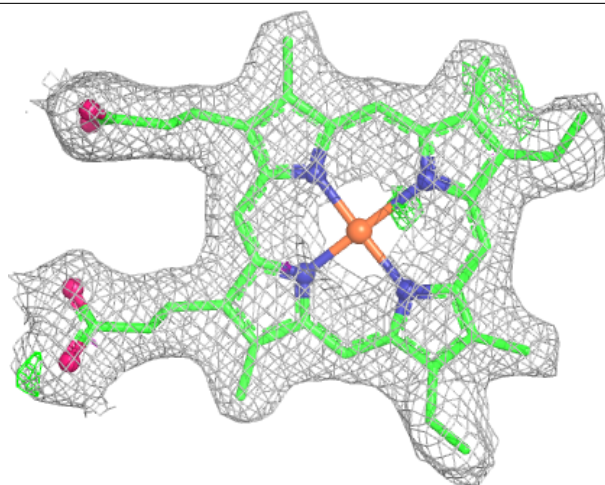
**Electron density around HEM G 808:**

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



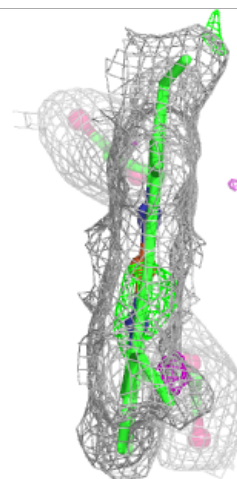
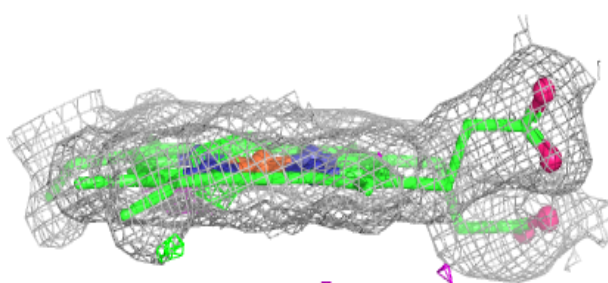
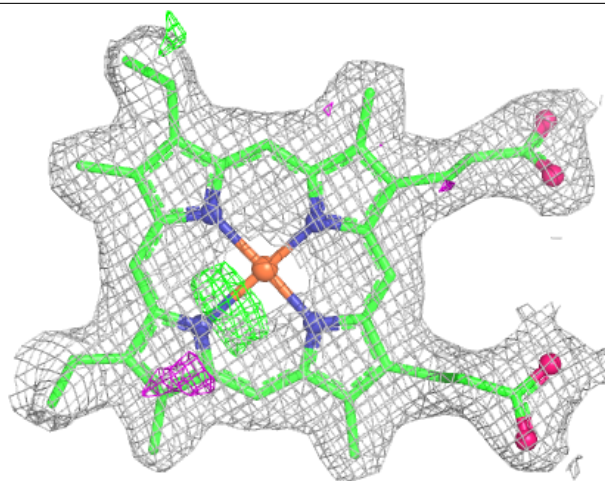
**Electron density around HEM G 809:**

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



**Electron density around HEM G 810:**

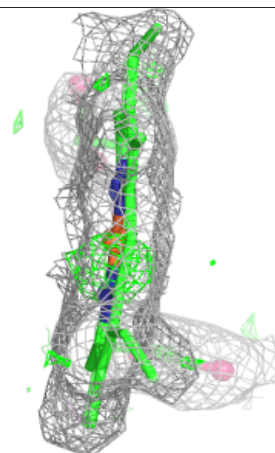
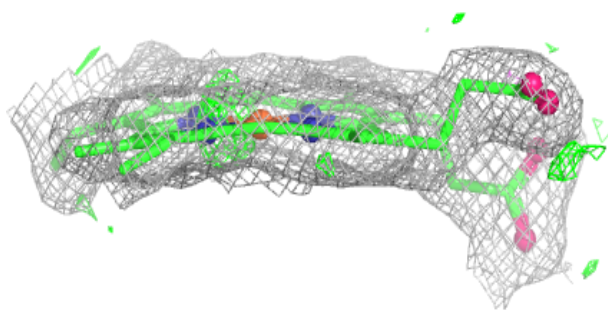
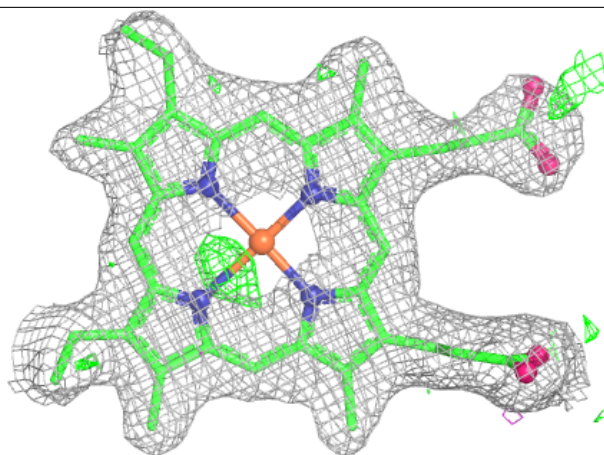
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





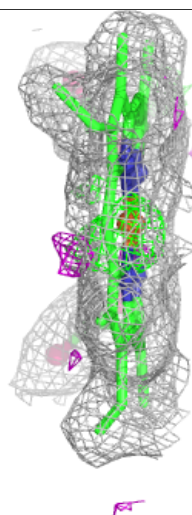
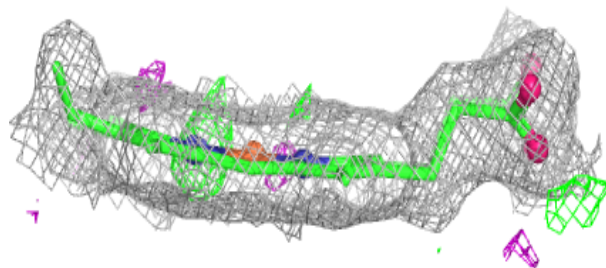
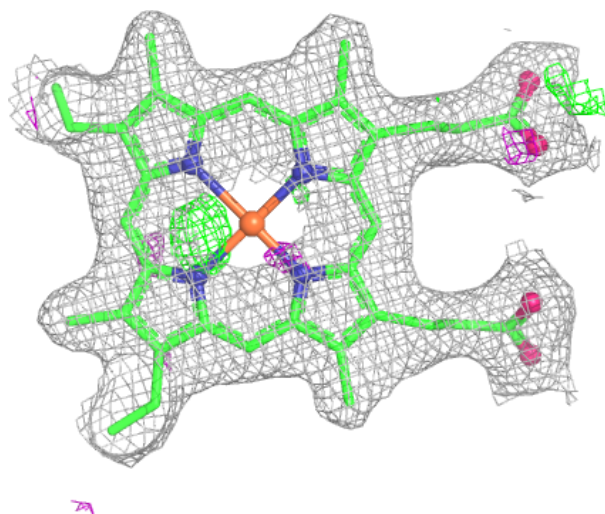
**Electron density around HEM G 811:**

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



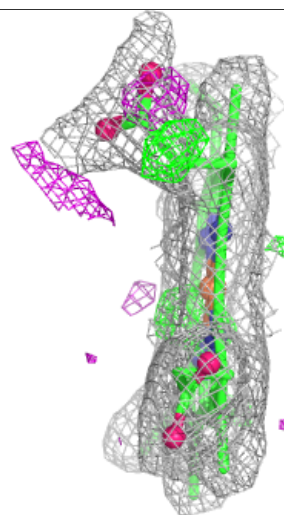
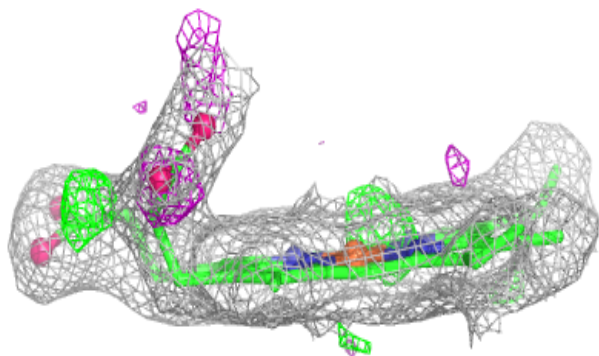
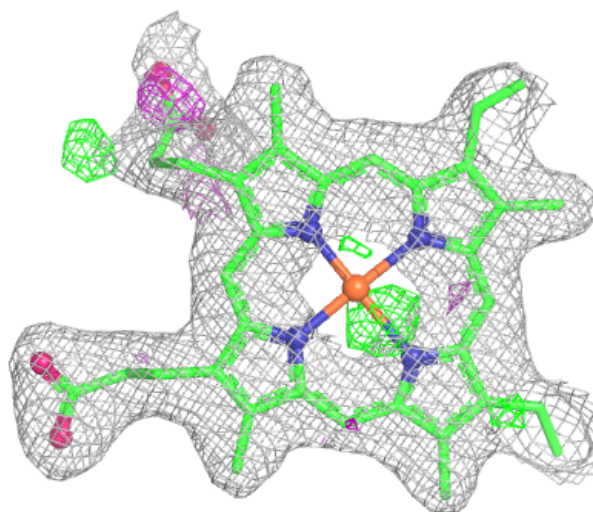
**Electron density around HEM G 812:**

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



**Electron density around HEM G 813:**

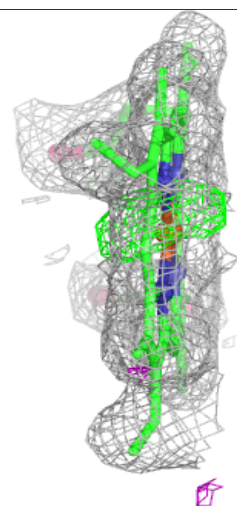
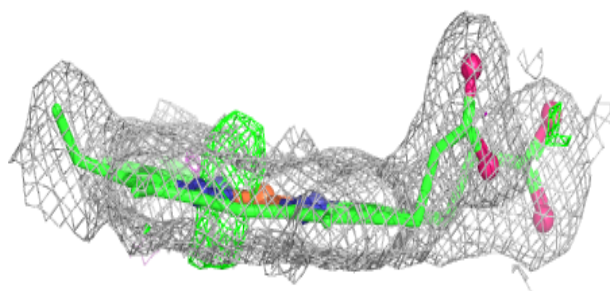
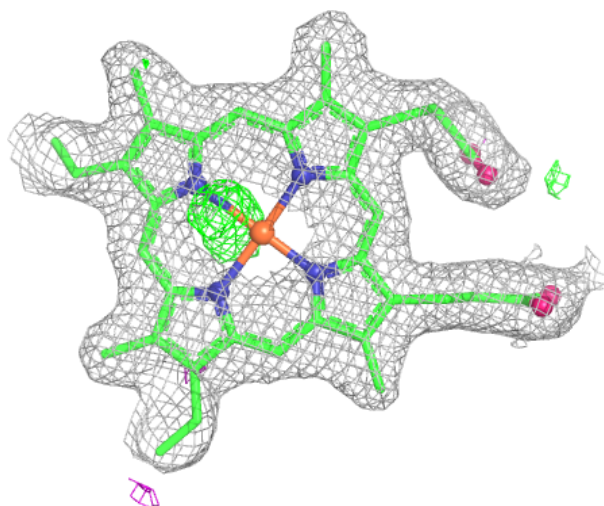
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





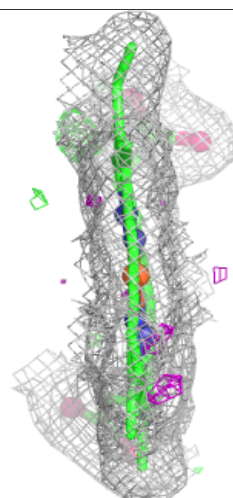
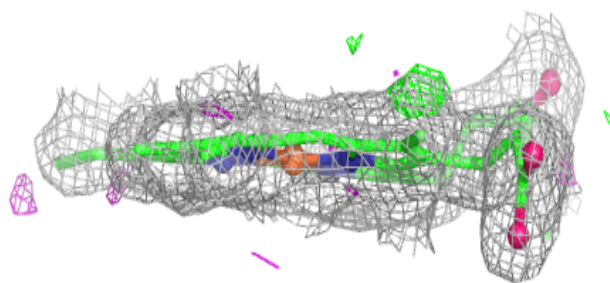
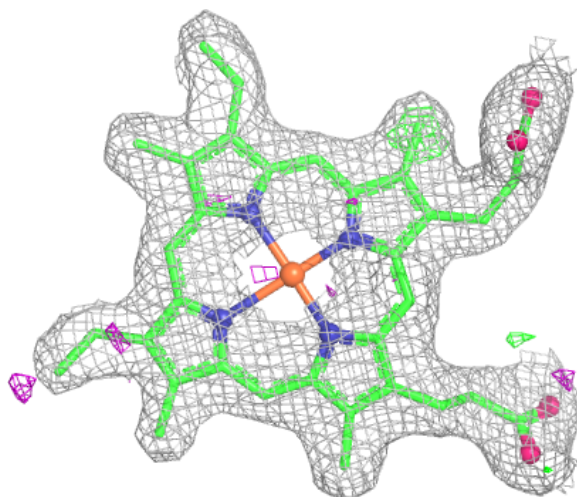
**Electron density around HEM D 806:**

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



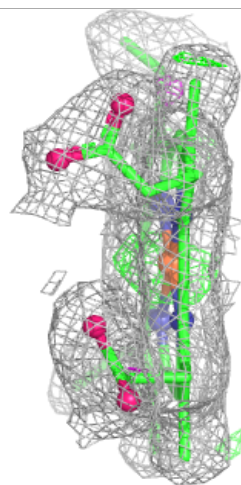
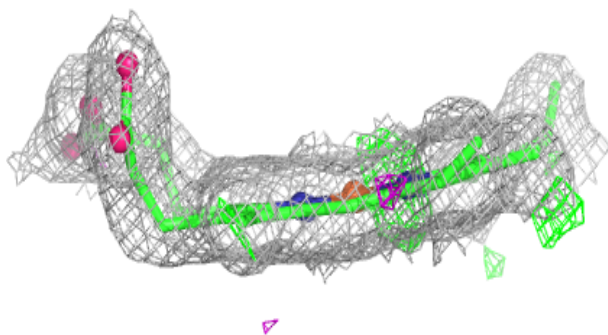
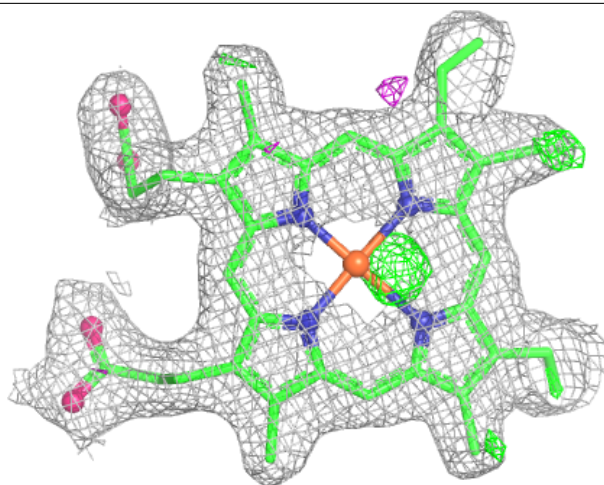
**Electron density around HEM D 807:**

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



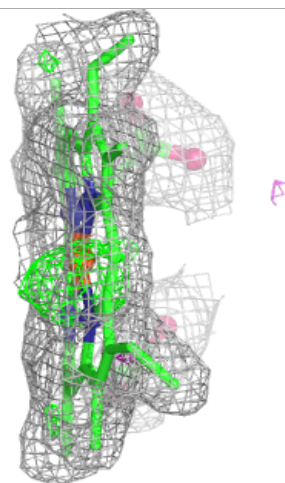
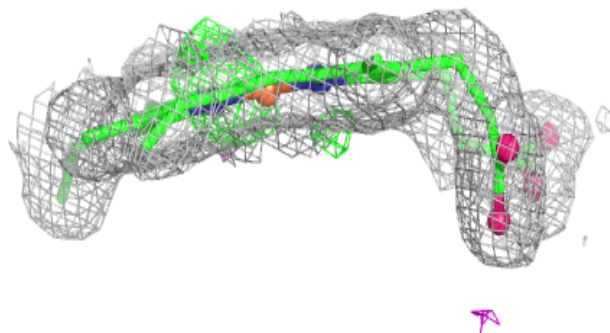
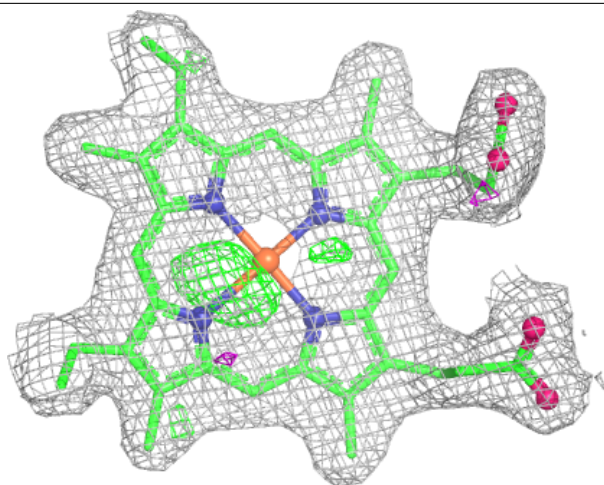
**Electron density around HEM D 808:**

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



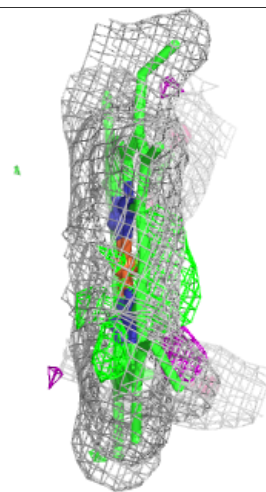
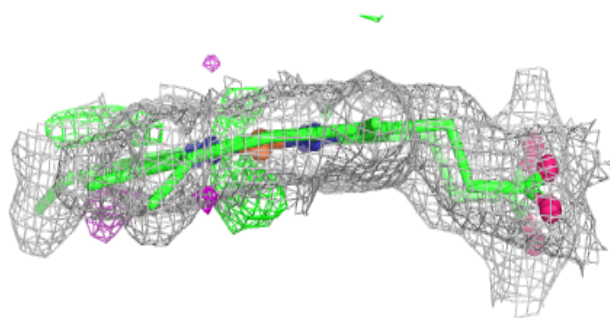
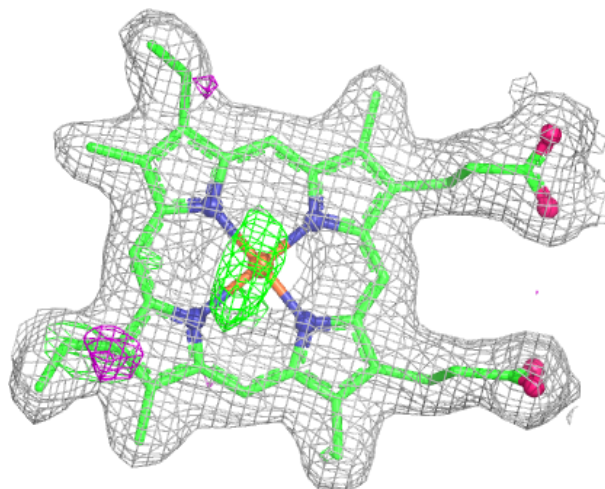
**Electron density around HEM C 808:**

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



**Electron density around HEM C 809:**

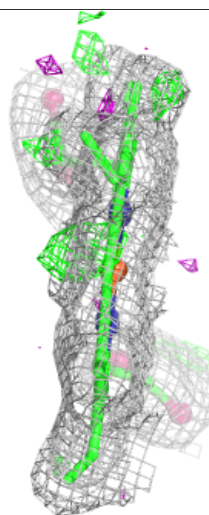
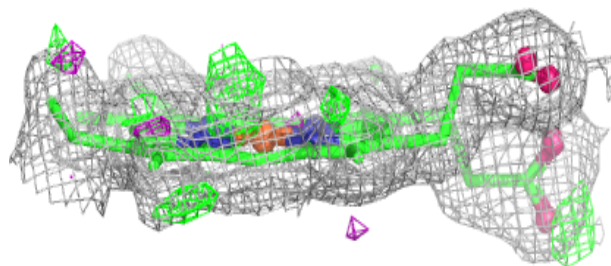
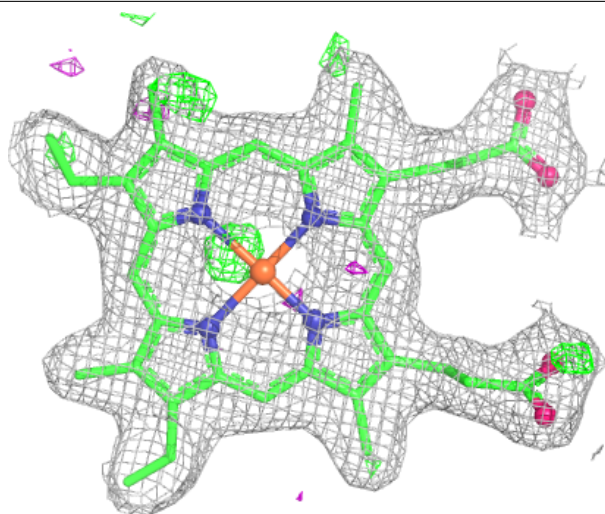
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





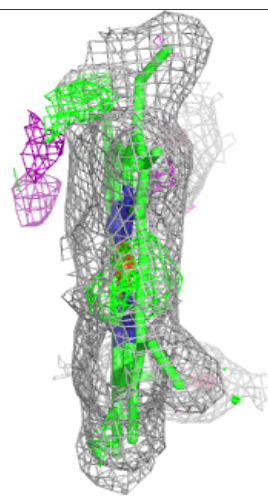
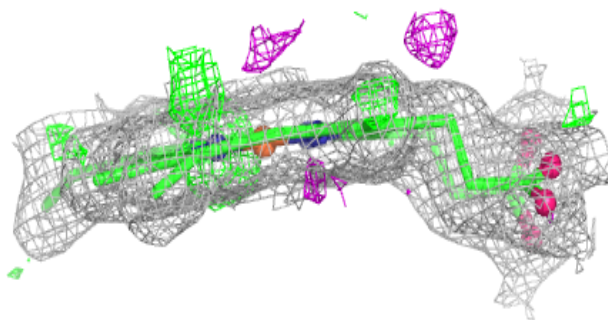
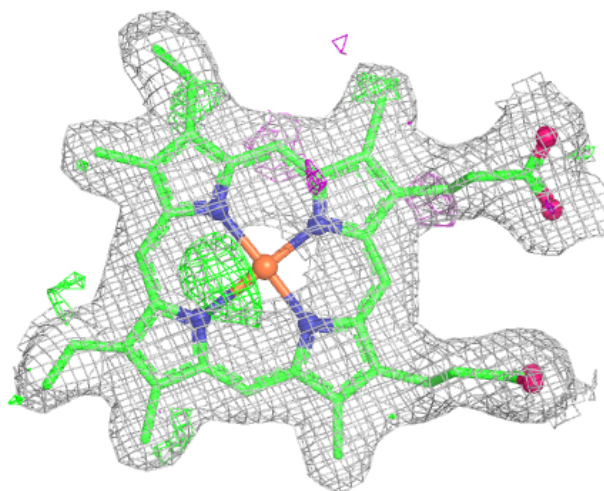
**Electron density around HEM C 810:**

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



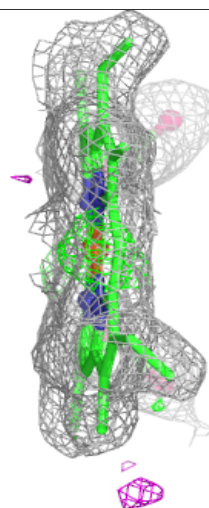
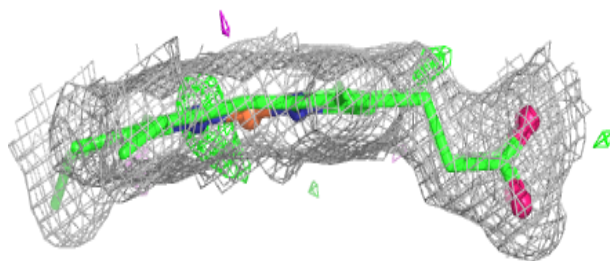
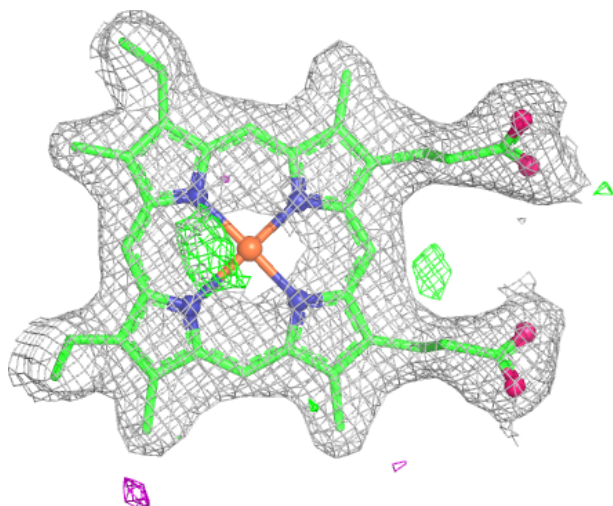
**Electron density around HEM A 809:**

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



**Electron density around HEM C 812:**

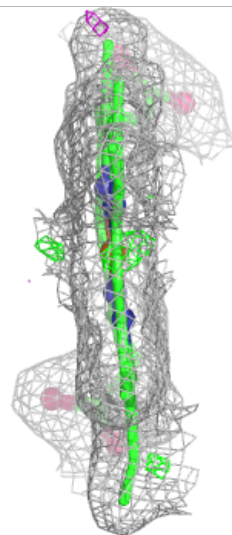
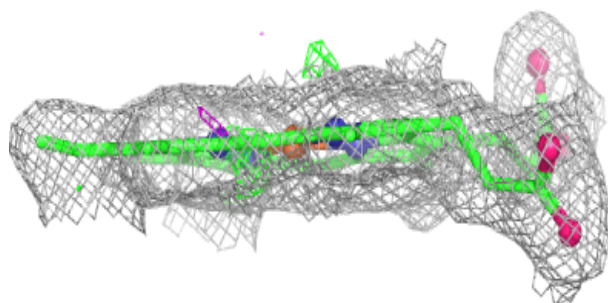
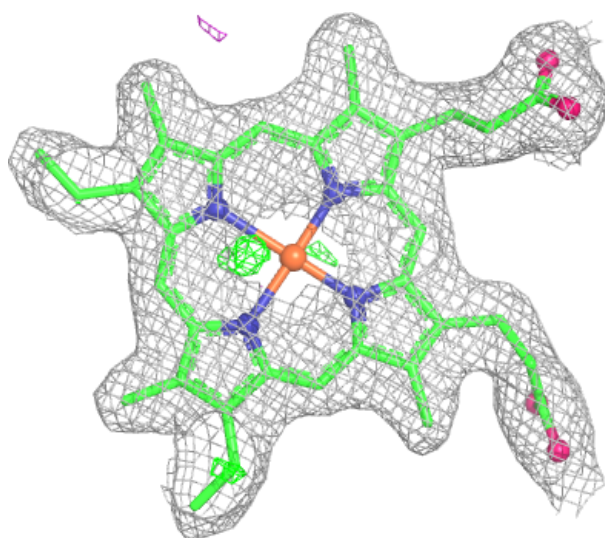
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





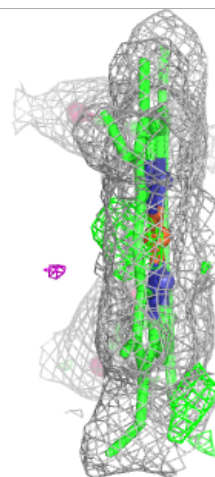
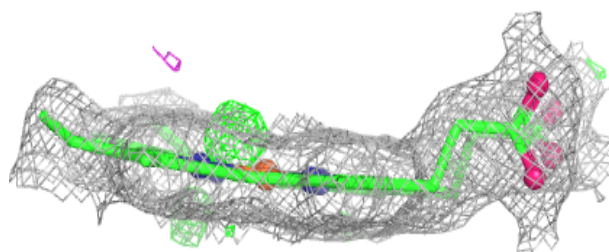
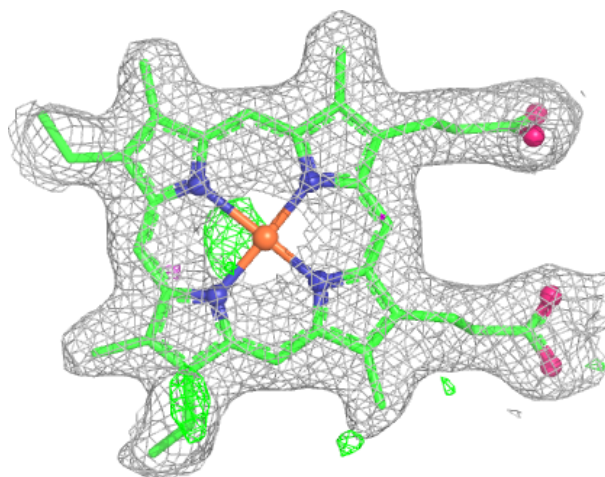
**Electron density around HEM B 808:**

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



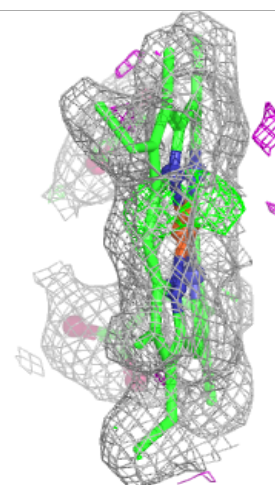
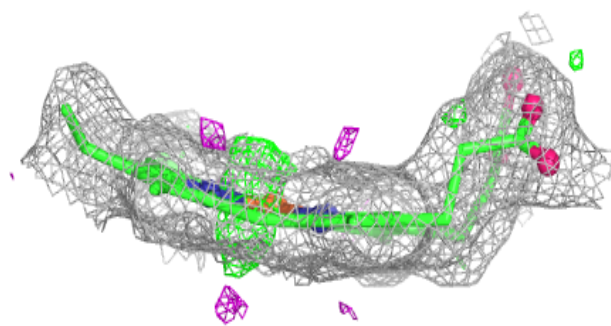
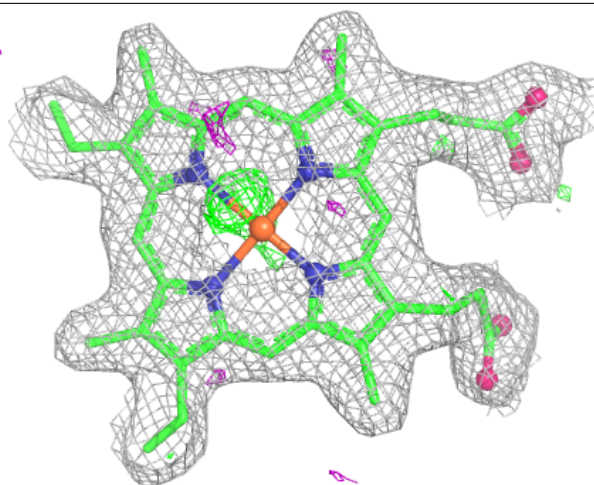
**Electron density around HEM F 810:**

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



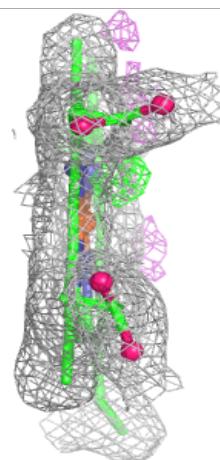
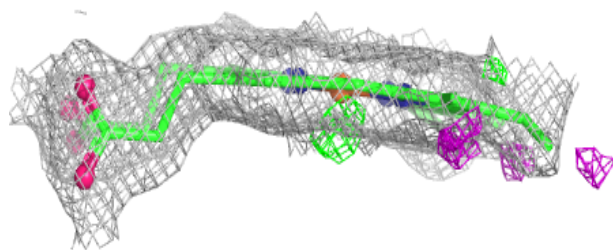
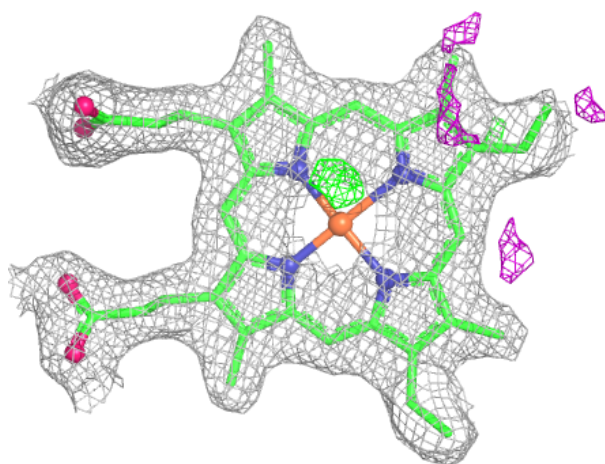
**Electron density around HEM B 809:**

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



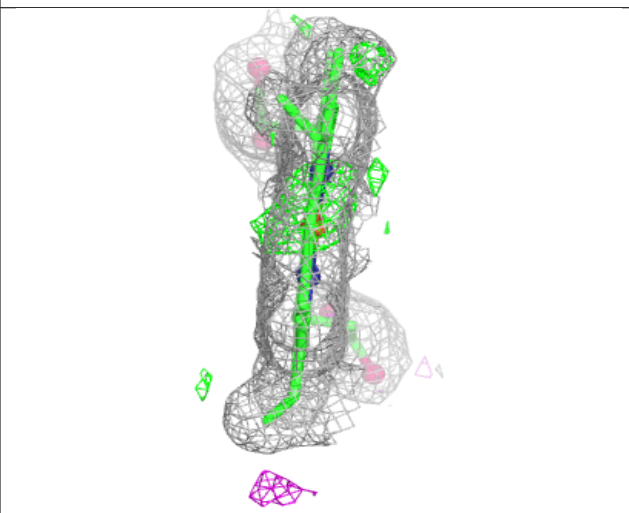
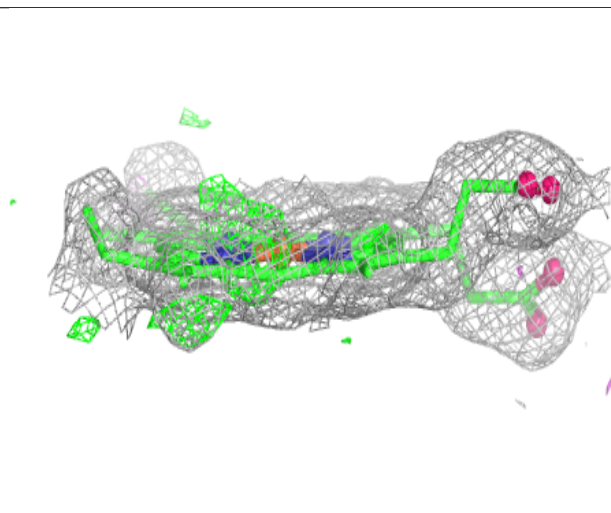
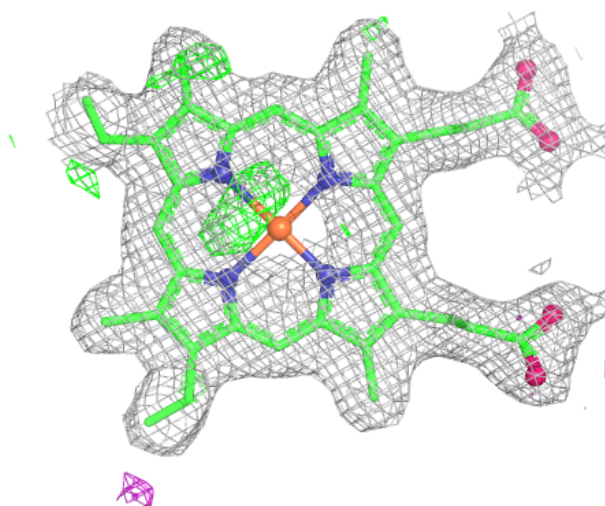
**Electron density around HEM B 810:**

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



**Electron density around HEM A 810:**

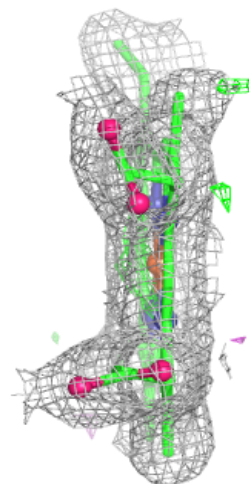
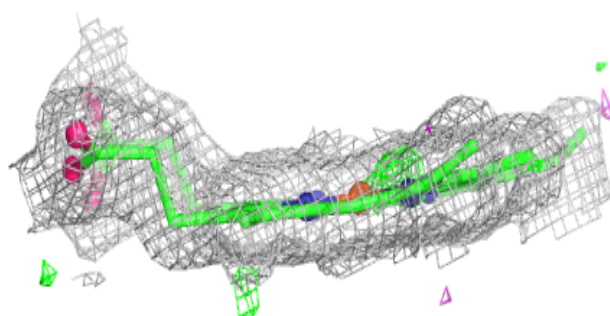
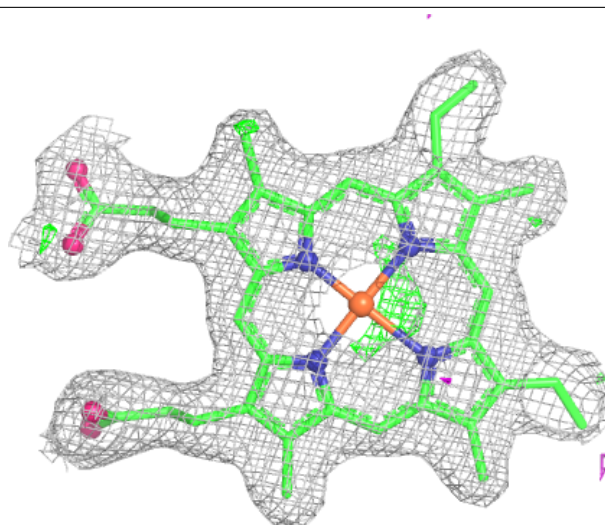
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





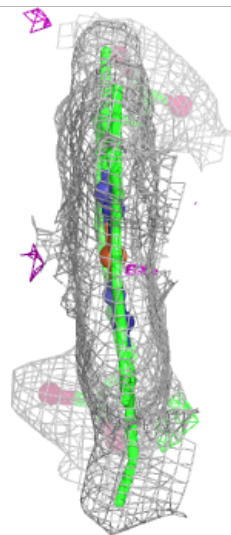
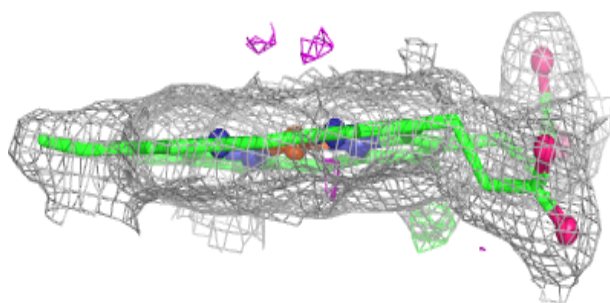
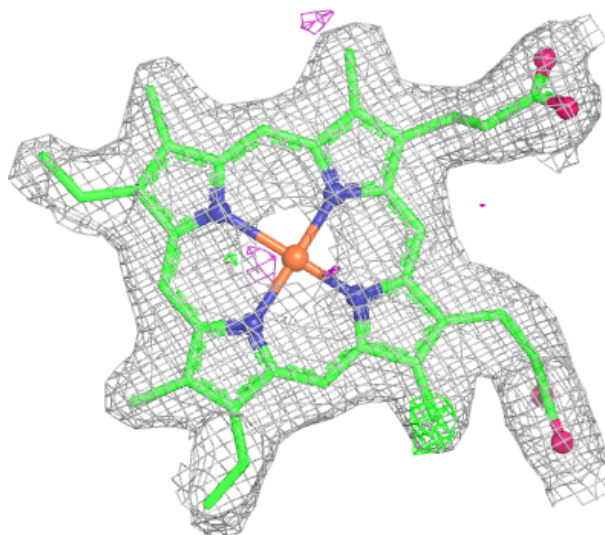
**Electron density around HEM D 809:**

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



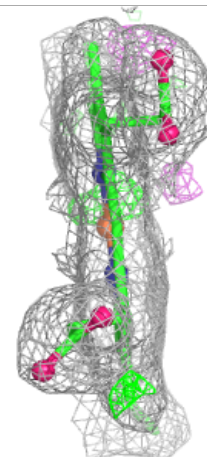
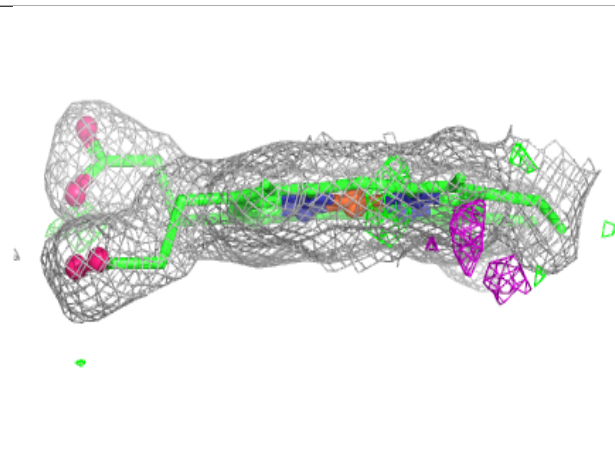
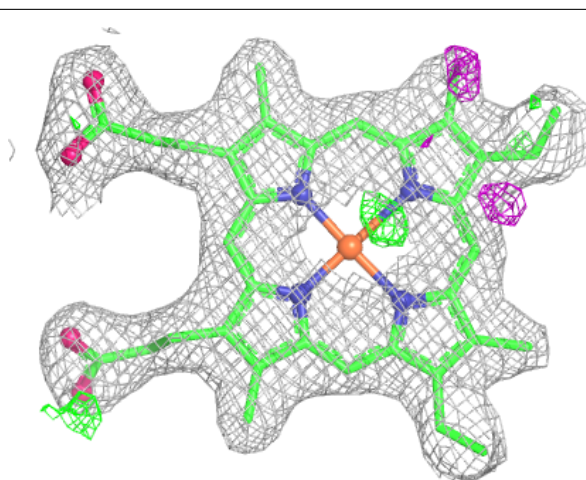
**Electron density around HEM G 807:**

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



**Electron density around HEM J 810:**

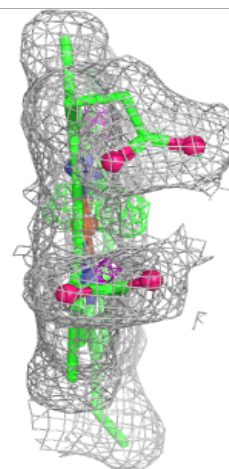
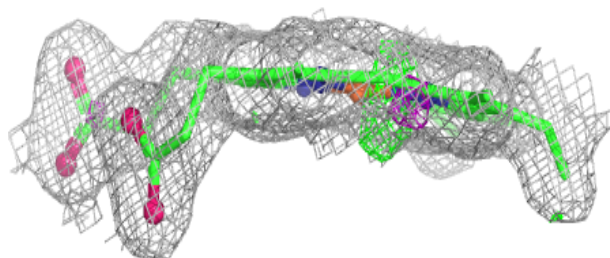
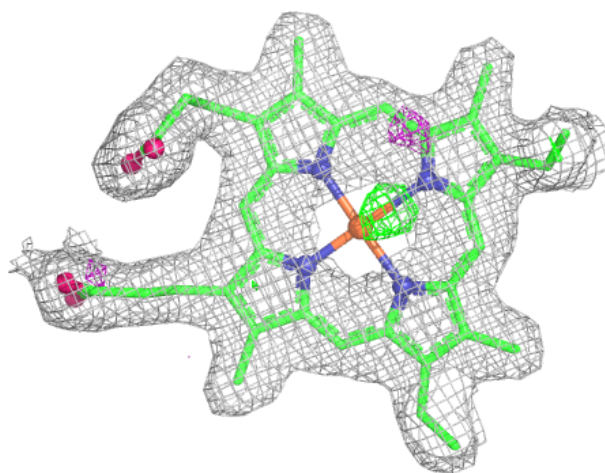
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





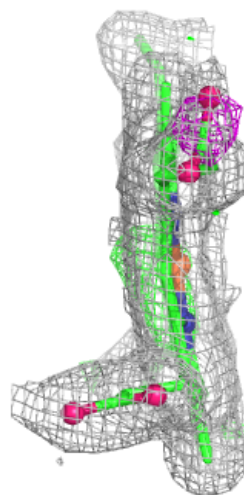
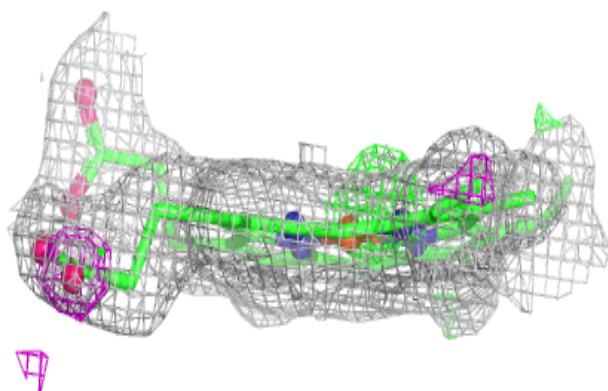
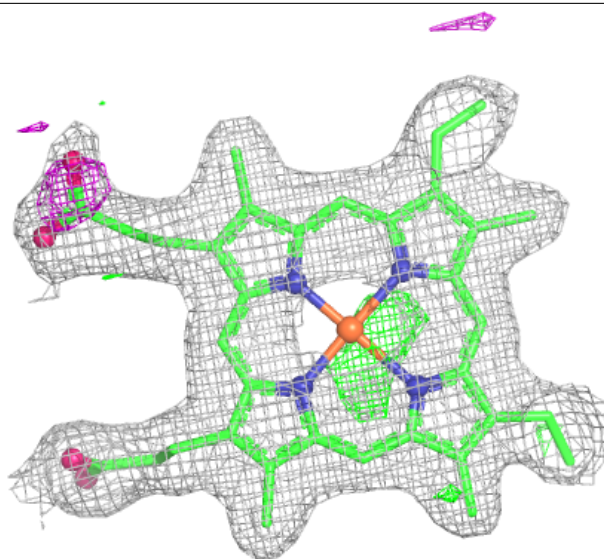
**Electron density around HEM A 806:**

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



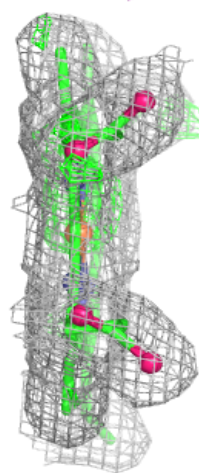
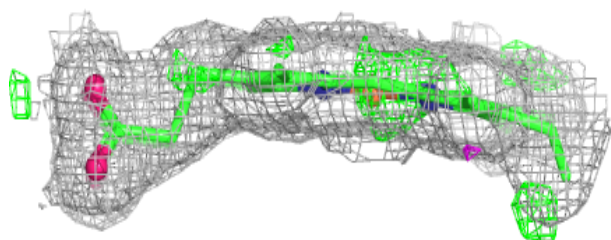
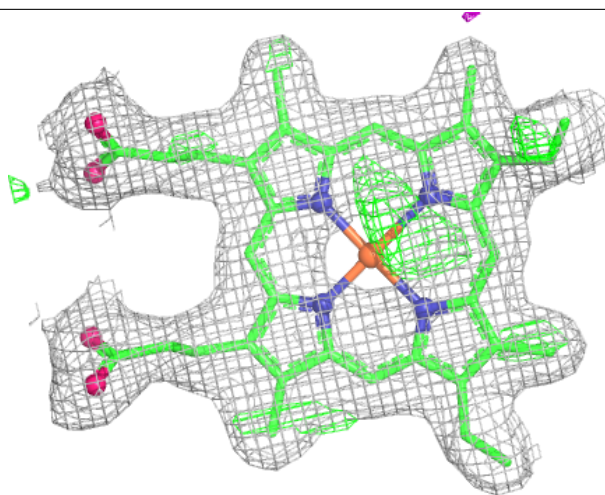
**Electron density around HEM D 811:**

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



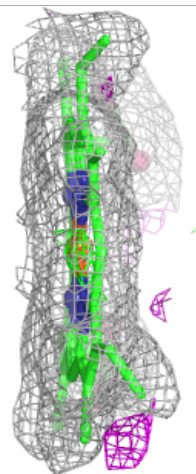
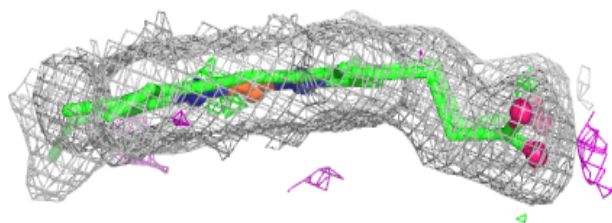
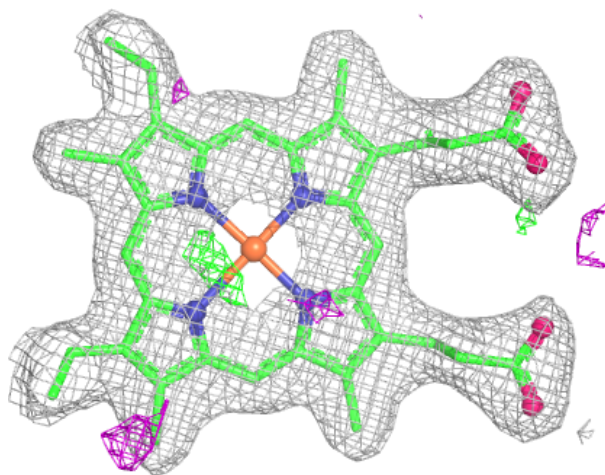
**Electron density around HEM D 812:**

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



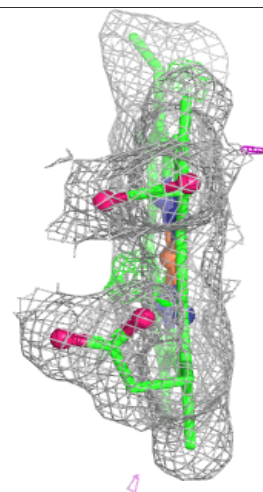
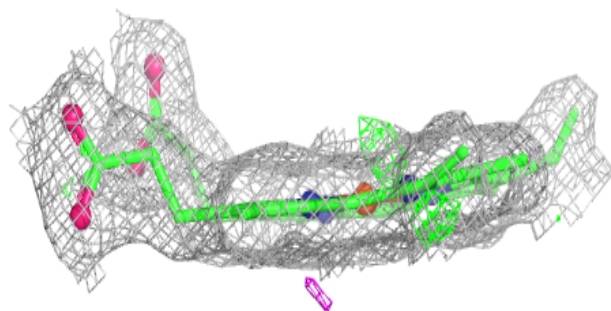
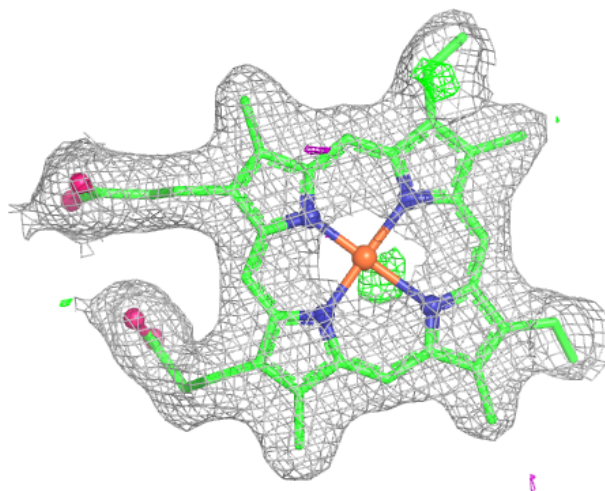
**Electron density around HEM D 813:**

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



**Electron density around HEM E 806:**

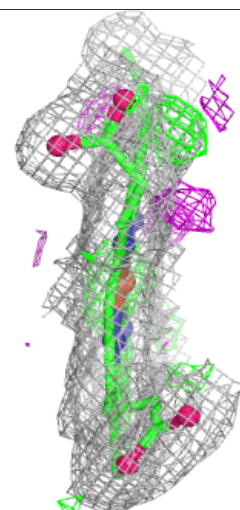
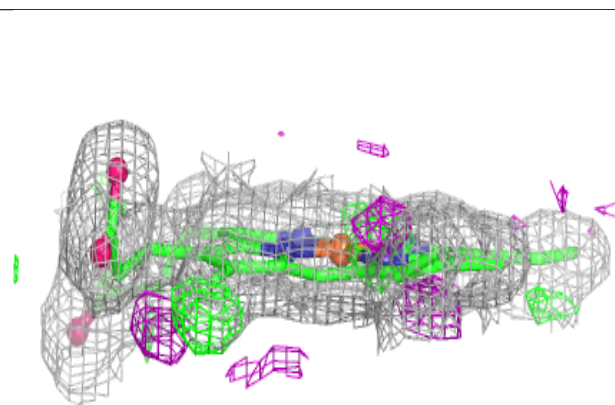
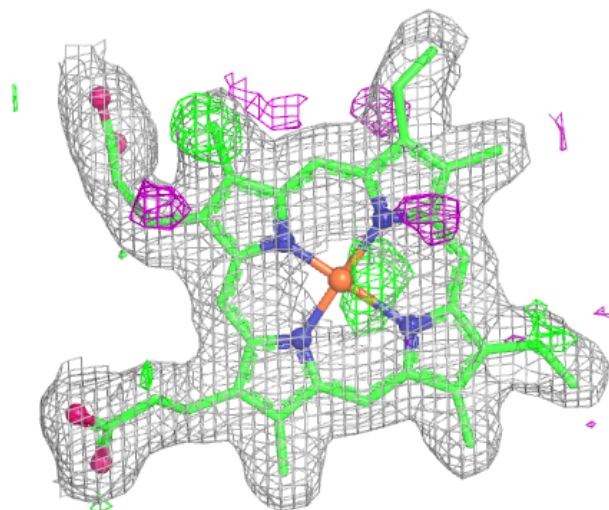
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





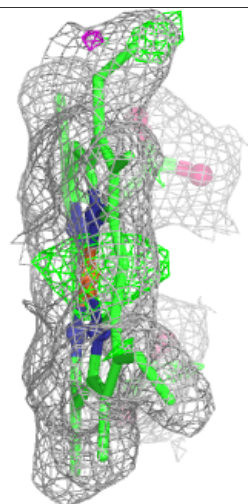
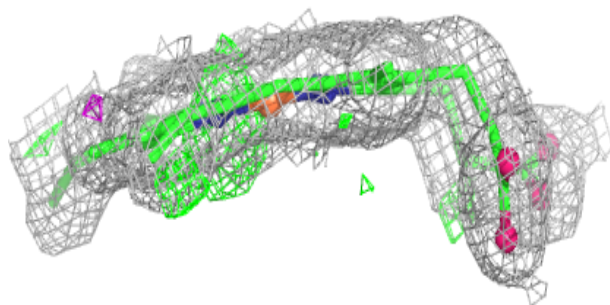
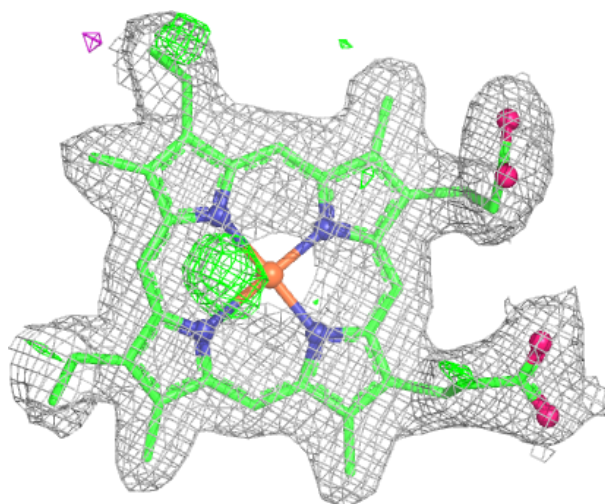
**Electron density around HEM A 807:**

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



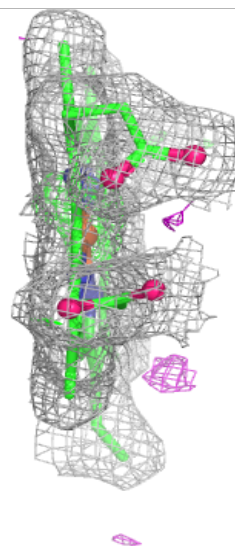
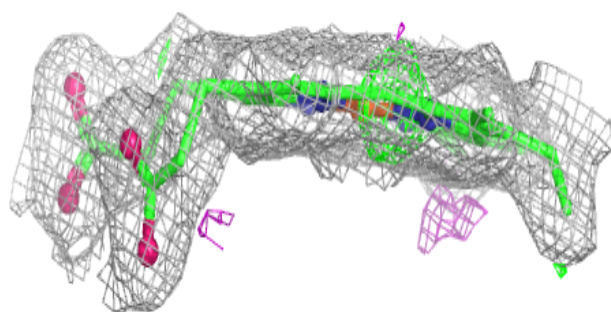
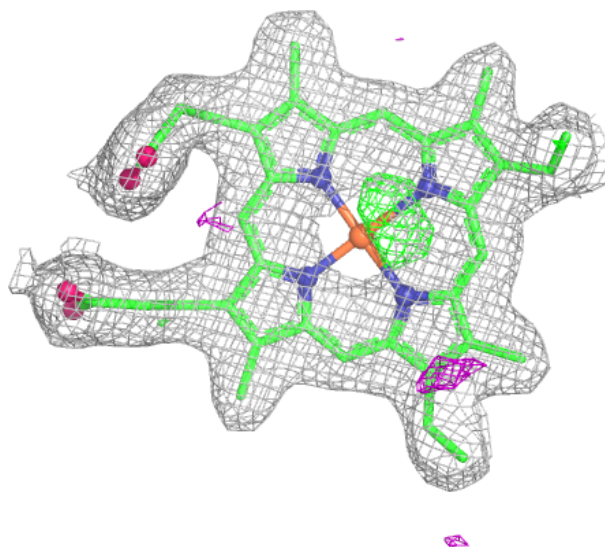
**Electron density around HEM A 808:**

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



**Electron density around HEM C 806:**

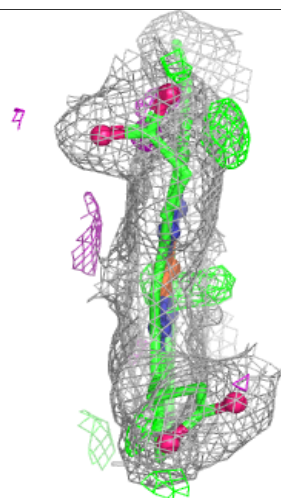
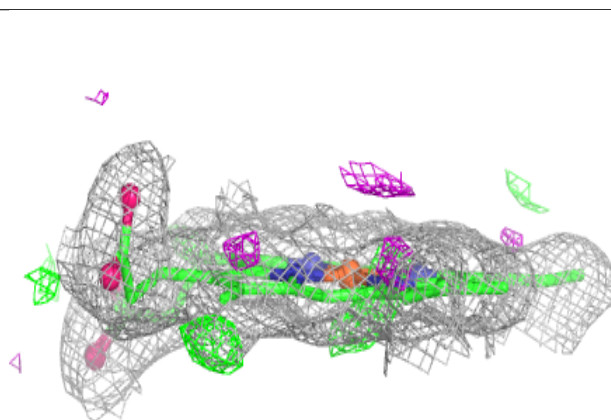
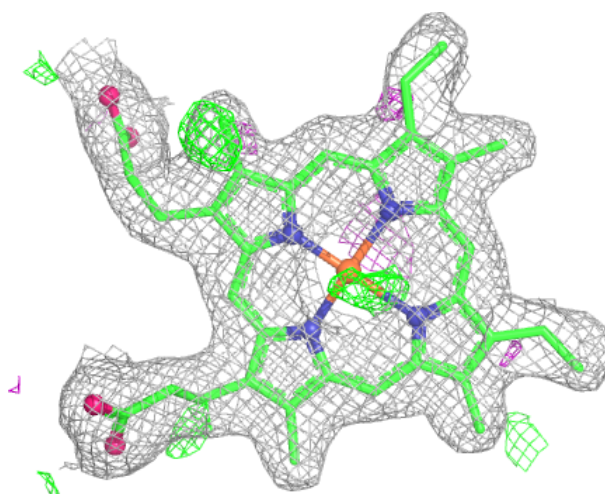
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM C 807:**

$2mF_o-DF_c$  (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.