



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 07:36 am BST

PDB ID : 6HIF  
Title : Kuenenia stuttgartiensis hydrazine dehydrogenase complex  
Authors : Akram, M.; Dietl, A.; Mersdorf, U.; Prinz, S.; Maalcke, W.; Keltjens, J.; Ferousi, C.; de Almeida, N.M.; Reimann, J.; Kartal, B.; Jetten, M.S.M.; Parey, K.; Barends, T.R.M.  
Deposited on : 2018-08-29  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

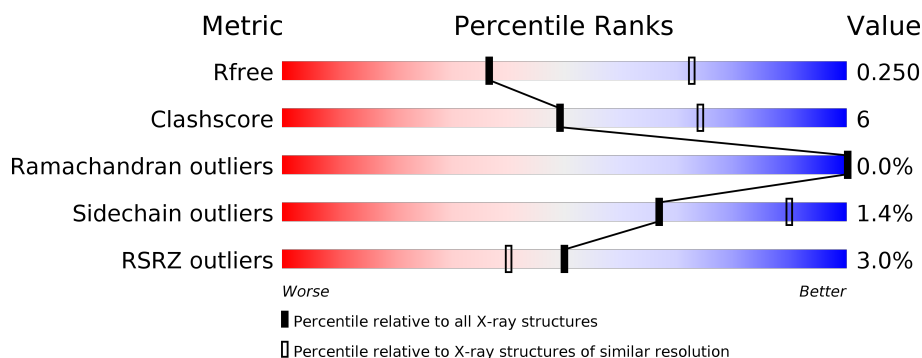
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3140 (2.80-2.80)                                      |
| Clashscore            | 141614                      | 3569 (2.80-2.80)                                      |
| Ramachandran outliers | 138981                      | 3498 (2.80-2.80)                                      |
| Sidechain outliers    | 138945                      | 3500 (2.80-2.80)                                      |
| RSRZ outliers         | 127900                      | 3078 (2.80-2.80)                                      |

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

| Mol | Chain | Length | Quality of chain                                 |
|-----|-------|--------|--|
| 1   | A     | 582    | <div> <div>2%</div> <div>80% 11% 9%</div> </div> |
| 1   | B     | 582    | <div> <div>2%</div> <div>82% 9% 9%</div> </div>  |
| 1   | C     | 582    | <div> <div>82% 10% 9%</div> </div>               |
| 1   | D     | 582    | <div> <div>74% 17% 9%</div> </div>               |
| 1   | E     | 582    | <div> <div>2%</div> <div>81% 10% 9%</div> </div> |
| 1   | F     | 582    | <div> <div>2%</div> <div>80% 11% 9%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 582    |                  |
| 1   | H     | 582    |                  |
| 1   | I     | 582    |                  |
| 1   | J     | 582    |                  |
| 1   | K     | 582    |                  |
| 1   | L     | 582    |                  |
| 1   | M     | 582    |                  |
| 1   | N     | 582    |                  |
| 1   | O     | 582    |                  |
| 1   | P     | 582    |                  |
| 1   | Q     | 582    |                  |
| 1   | R     | 582    |                  |
| 1   | S     | 582    |                  |
| 1   | T     | 582    |                  |
| 1   | U     | 582    |                  |
| 1   | V     | 582    |                  |
| 1   | W     | 582    |                  |
| 1   | X     | 582    |                  |
| 2   | Y     | 114    |                  |
| 2   | Z     | 114    |                  |
| 2   | a     | 114    |                  |
| 2   | b     | 114    |                  |
| 2   | c     | 114    |                  |
| 2   | d     | 114    |                  |
| 2   | e     | 114    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | f     | 114    |                  |
| 2   | g     | 114    |                  |
| 2   | h     | 114    |                  |
| 2   | i     | 114    |                  |
| 2   | j     | 114    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | SO4  | G     | 610 | -         | -        | X       | -                |
| 4   | SO4  | G     | 611 | -         | -        | -       | X                |
| 4   | SO4  | J     | 611 | -         | -        | X       | -                |
| 5   | GOL  | H     | 614 | -         | -        | X       | -                |
| 5   | GOL  | H     | 615 | -         | -        | X       | X                |
| 5   | GOL  | I     | 614 | -         | -        | X       | -                |
| 5   | GOL  | K     | 614 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 118753 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 Hydrazine dehydrogenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | G     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | A     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | B     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | C     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | D     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | E     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | F     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | H     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | I     | 527      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4201  | 2633 | 739 | 793 | 36 |         |         |       |
| 1   | J     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | K     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | L     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | M     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | N     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | O     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | P     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | Q     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | R     | 531      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 4237  | 2653 | 749 | 799 | 36 |         |         |       |
| 1   | S     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | T     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | U     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | V     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | W     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |
| 1   | X     | 531      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4226  | 2647 | 745 | 798 | 36 |         |         |       |

- Molecule 2 is a protein called hdh assembly factor Kustc1130.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | Y     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | Z     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | a     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | b     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | c     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | d     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | e     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | f     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | g     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | h     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |
| 2   | i     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | j     | 86       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 640   | 403 | 110 | 125 | 2 |         |         |       |

- 
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure includes various side chains and a central hydrogen atom (H). The atoms are labeled with green and red text, and the bonds are color-coded (green for C-C, red for C=O, blue for N-Fe).
- Key labels include:
- Central atom: Fe
  - Ring nitrogens: NA, NB, NC, ND
  - Side chain labels: C1A, C1B, C1C, C1D, C2A, C2B, C2C, C2D, C3A, C3B, C3C, C3D, C4A, C4B, C4C, C4D, CAA, CBA, CAD, CBD, CMA, CMB, CMC, CMD, CBB, CAB, CAC, CBC, CHA, CHB, CHC, CHD.
  - Carboxylate groups: O1A, O2A, O1D, O2D (red), CGA, CGA, CGD, CGD (green).

| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | A     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | C     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | J     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | L     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | M     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | N     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | O     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | Q     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | T     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | T     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | V     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | W     | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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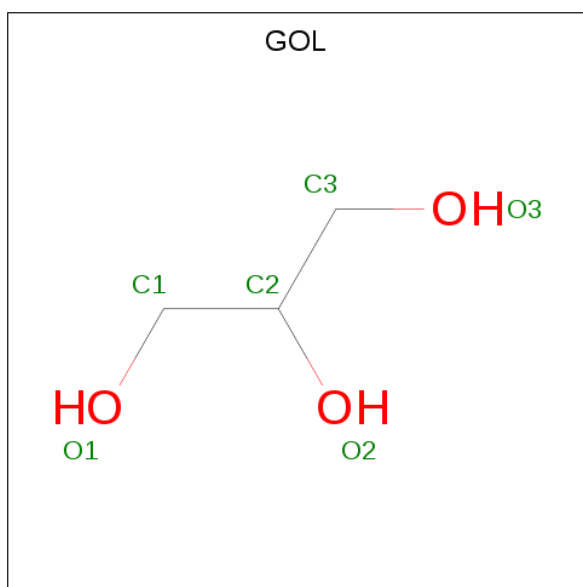
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | N     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | N     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | N     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | P     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | S     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | S     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | T     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | U     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | U     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | U     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | W     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | X     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | X     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | X     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | Y     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | Y     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | a     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 4   | c     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | G     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | H     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | I     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | J     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | K     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |
| 5   | L     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6   | H     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | X     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | Q     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |
| 6   | K     | 1        | Total | K | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | G     | 78       | Total | O  | 0       | 0       |
|     |       |          | 78    | 78 |         |         |
| 7   | A     | 33       | Total | O  | 0       | 0       |
|     |       |          | 33    | 33 |         |         |
| 7   | B     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 7   | C     | 36       | Total | O  | 0       | 0       |
|     |       |          | 36    | 36 |         |         |
| 7   | D     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 7   | E     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 7   | F     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 7   | H     | 70       | Total | O  | 0       | 0       |
|     |       |          | 70    | 70 |         |         |
| 7   | I     | 62       | Total | O  | 0       | 0       |
|     |       |          | 62    | 62 |         |         |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 7   | J     | 78       | Total O<br>78 78 | 0       | 0       |
| 7   | K     | 57       | Total O<br>57 57 | 0       | 0       |
| 7   | L     | 69       | Total O<br>69 69 | 0       | 0       |
| 7   | M     | 27       | Total O<br>27 27 | 0       | 0       |
| 7   | N     | 37       | Total O<br>37 37 | 0       | 0       |
| 7   | O     | 40       | Total O<br>40 40 | 0       | 0       |
| 7   | P     | 50       | Total O<br>50 50 | 0       | 0       |
| 7   | Q     | 48       | Total O<br>48 48 | 0       | 0       |
| 7   | R     | 49       | Total O<br>49 49 | 0       | 0       |
| 7   | S     | 4        | Total O<br>4 4   | 0       | 0       |
| 7   | T     | 15       | Total O<br>15 15 | 0       | 0       |
| 7   | U     | 15       | Total O<br>15 15 | 0       | 0       |
| 7   | V     | 17       | Total O<br>17 17 | 0       | 0       |
| 7   | W     | 12       | Total O<br>12 12 | 0       | 0       |
| 7   | X     | 13       | Total O<br>13 13 | 0       | 0       |
| 7   | Y     | 2        | Total O<br>2 2   | 0       | 0       |
| 7   | Z     | 1        | Total O<br>1 1   | 0       | 0       |
| 7   | a     | 2        | Total O<br>2 2   | 0       | 0       |
| 7   | b     | 2        | Total O<br>2 2   | 0       | 0       |
| 7   | c     | 2        | Total O<br>2 2   | 0       | 0       |
| 7   | d     | 2        | Total O<br>2 2   | 0       | 0       |

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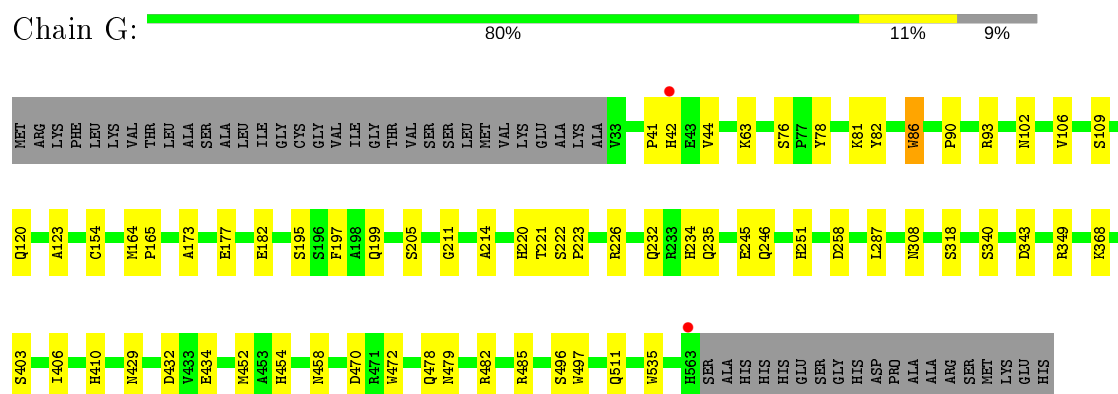
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 7   | e     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 7   | f     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 7   | g     | 1        | Total<br>1 | O<br>1 | 0       | 0       |
| 7   | i     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 7   | j     | 1        | Total<br>1 | O<br>1 | 0       | 0       |

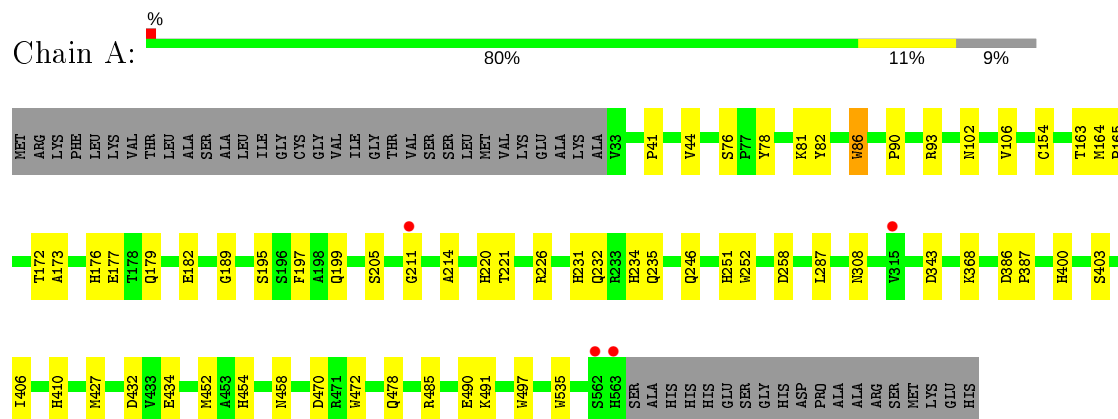
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

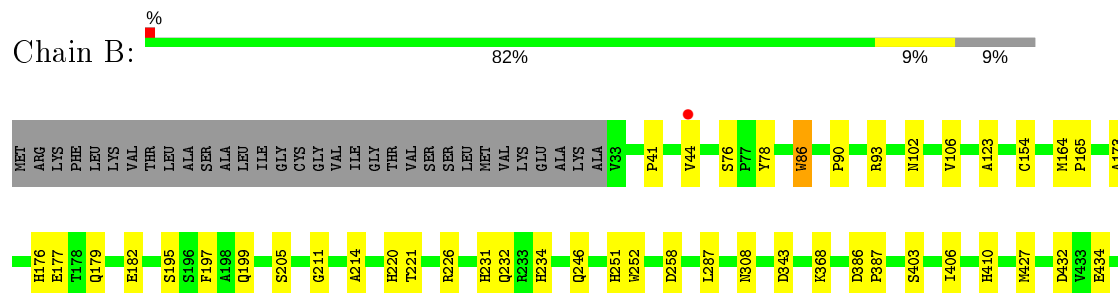
#### • Molecule 1: Hydrazine dehydrogenase

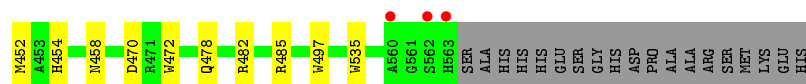


#### • Molecule 1: Hydrazine dehydrogenase



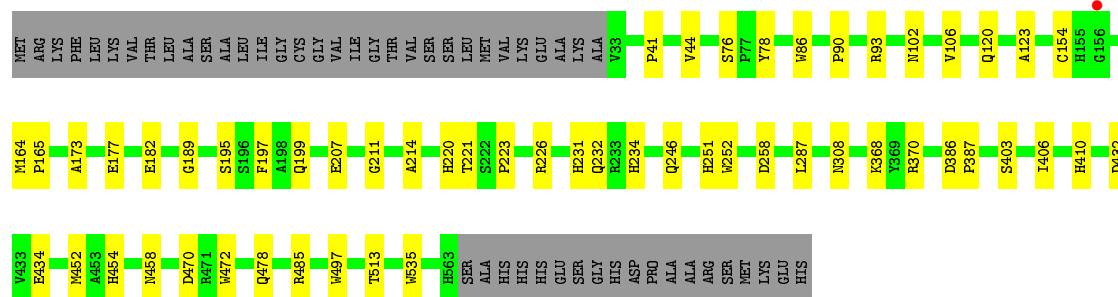
#### • Molecule 1: Hydrazine dehydrogenase





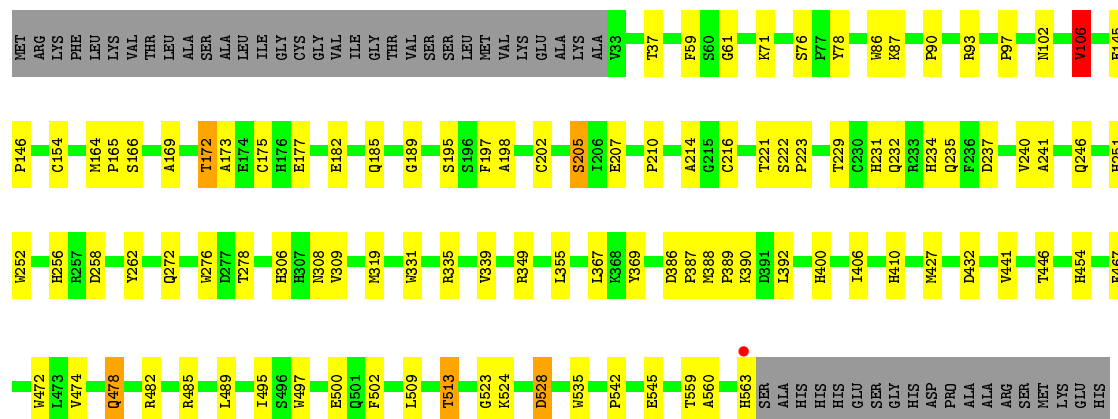
• Molecule 1: Hydrazine dehydrogenase

Chain C: 82% 10% 9%



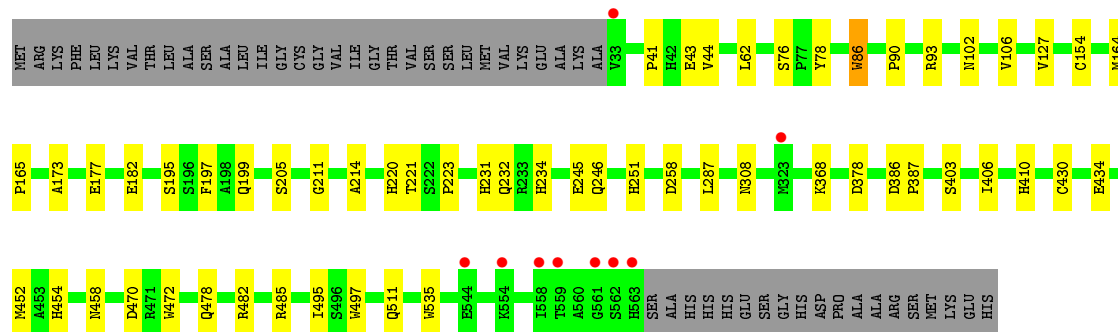
• Molecule 1: Hydrazine dehydrogenase

Chain D: 74% 17% 9%



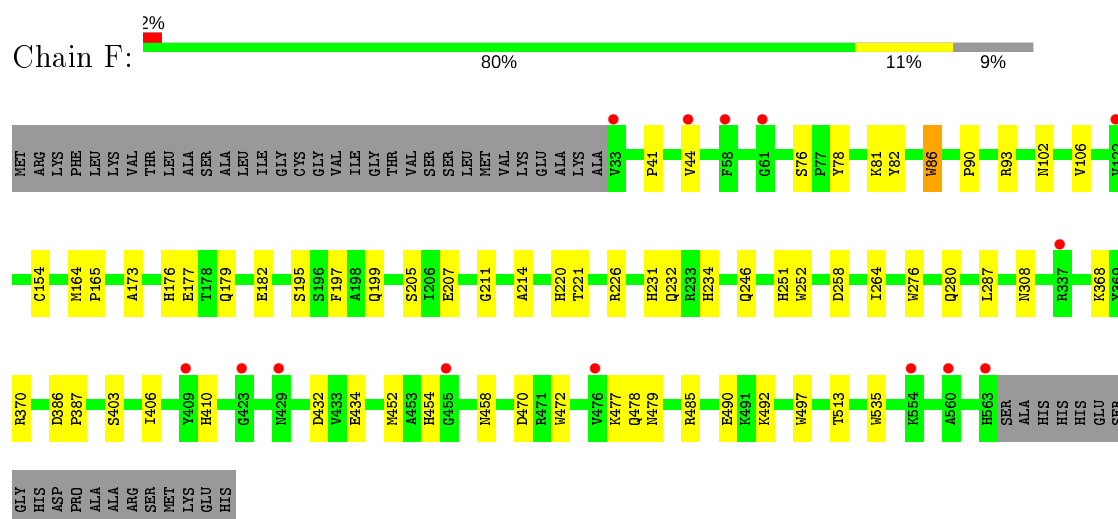
• Molecule 1: Hydrazine dehydrogenase

Chain E: 2% 81% 10% 9%

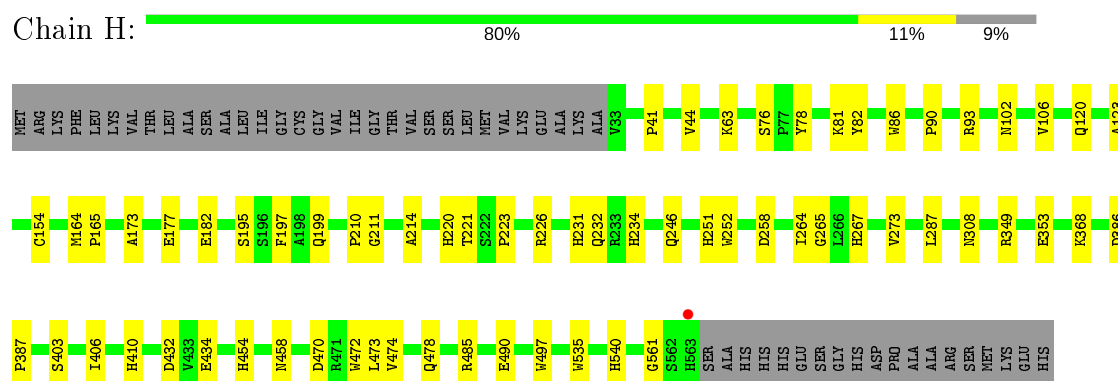


• Molecule 1: Hydrazine dehydrogenase

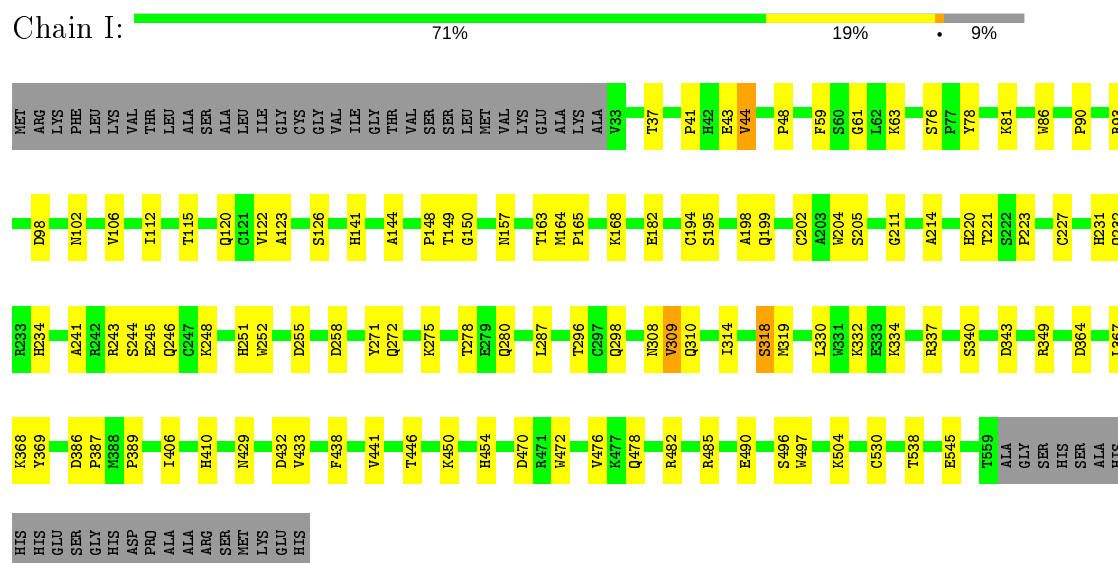




- Molecule 1: Hydrazine dehydrogenase

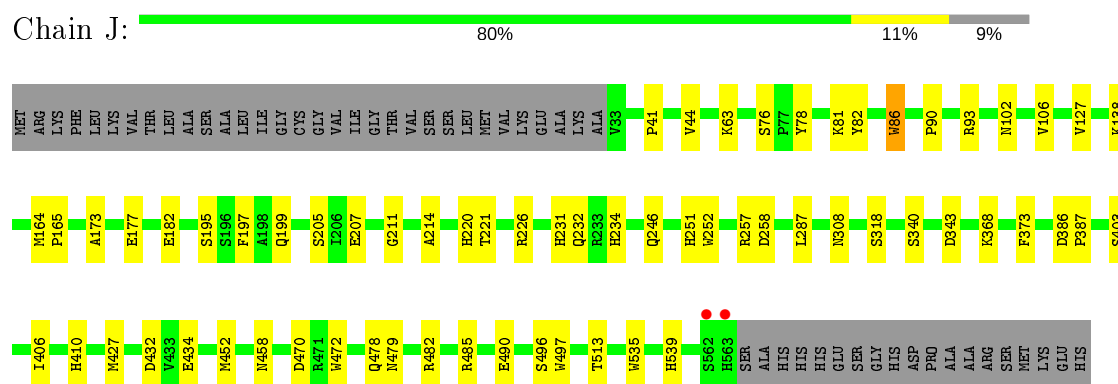


- Molecule 1: Hydrazine dehydrogenase



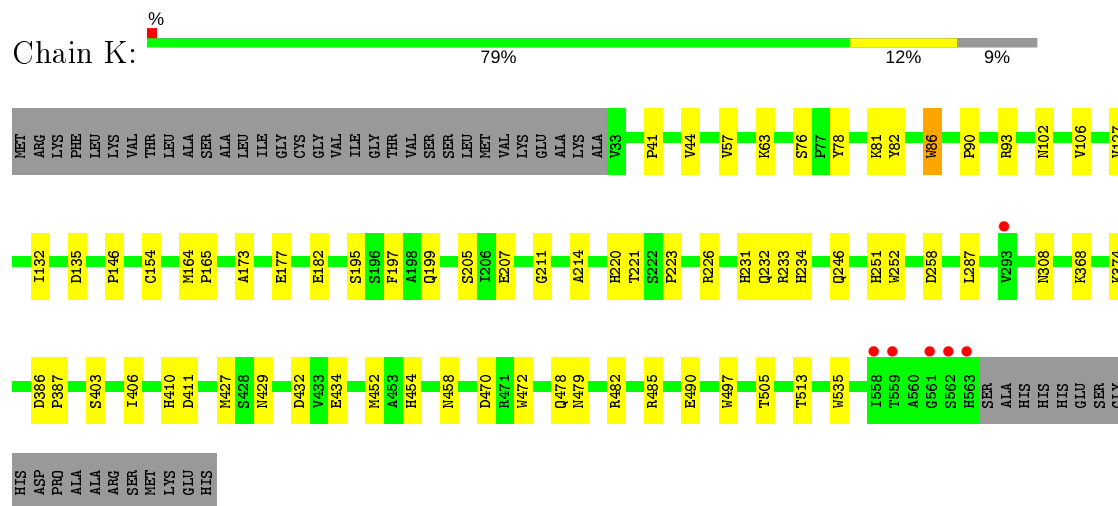
- Molecule 1: Hydrazine dehydrogenase

## Chain J:



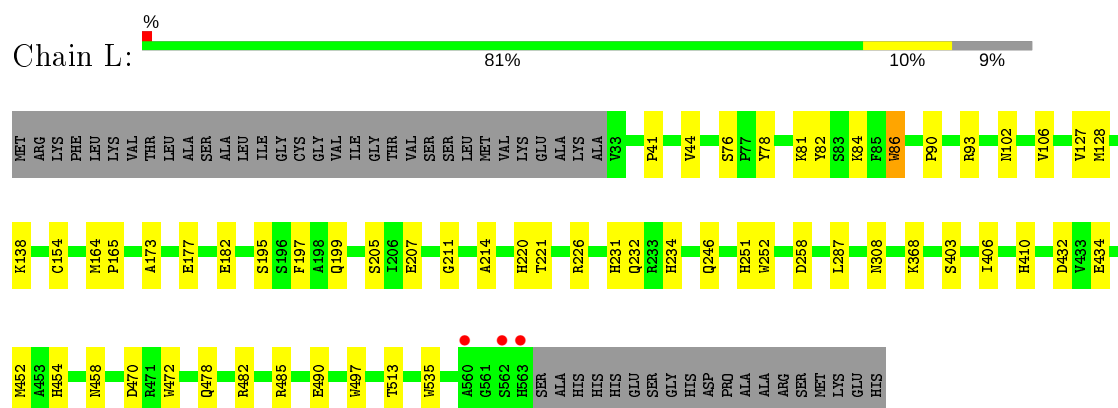
## • Molecule 1: Hydrazine dehydrogenase

## Chain K:



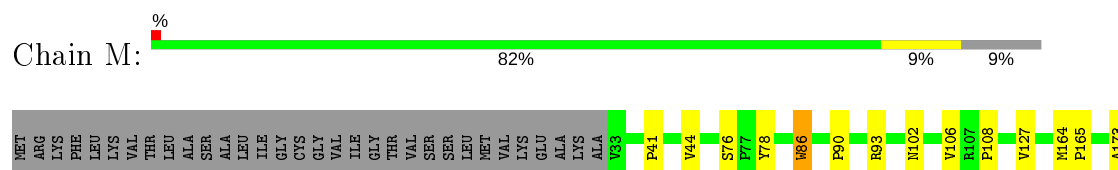
## • Molecule 1: Hydrazine dehydrogenase

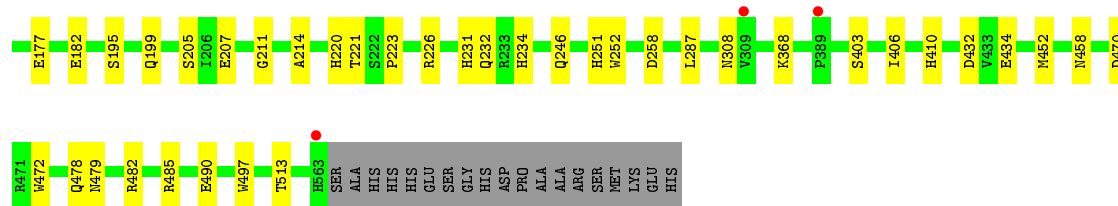
## Chain L:



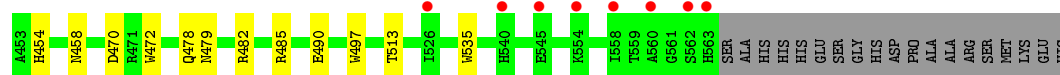
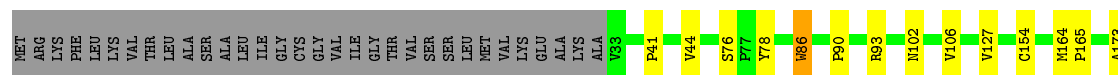
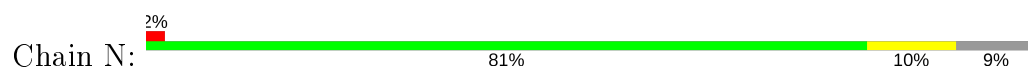
## • Molecule 1: Hydrazine dehydrogenase

## Chain M:

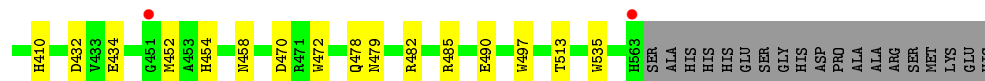
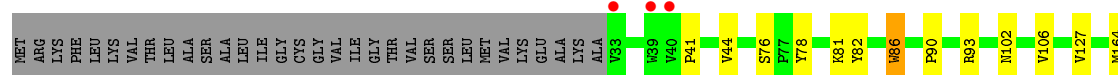
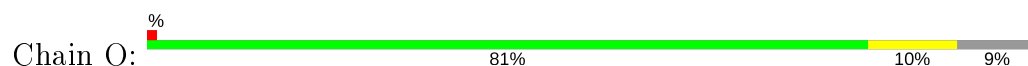




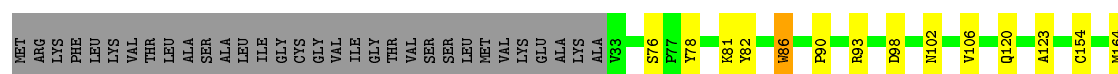
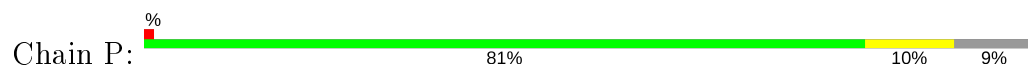
• Molecule 1: Hydrazine dehydrogenase



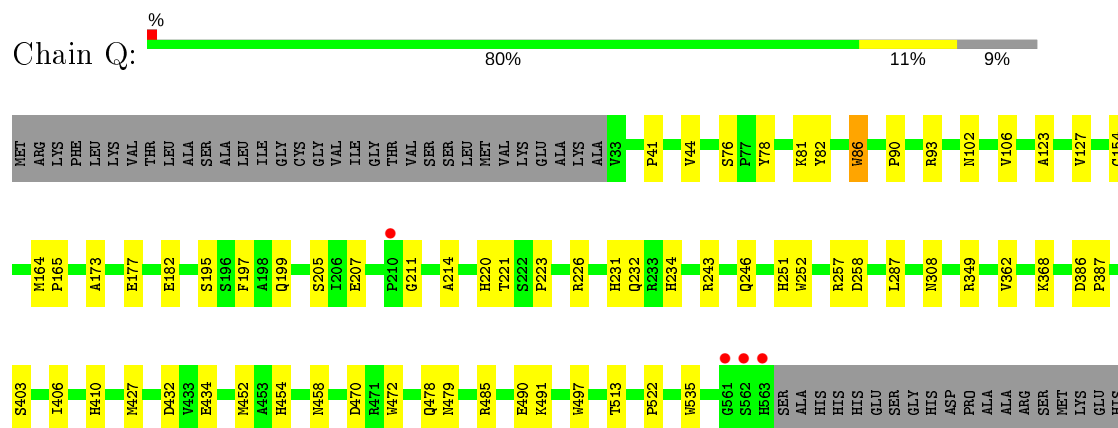
• Molecule 1: Hydrazine dehydrogenase



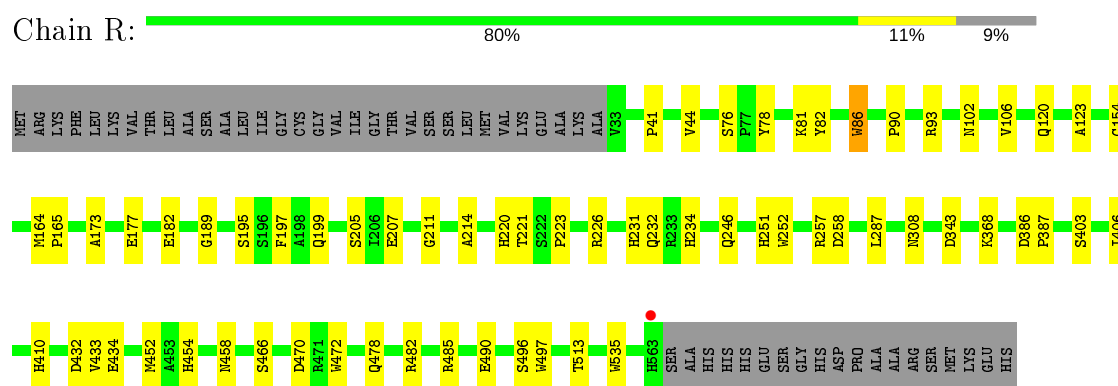
• Molecule 1: Hydrazine dehydrogenase



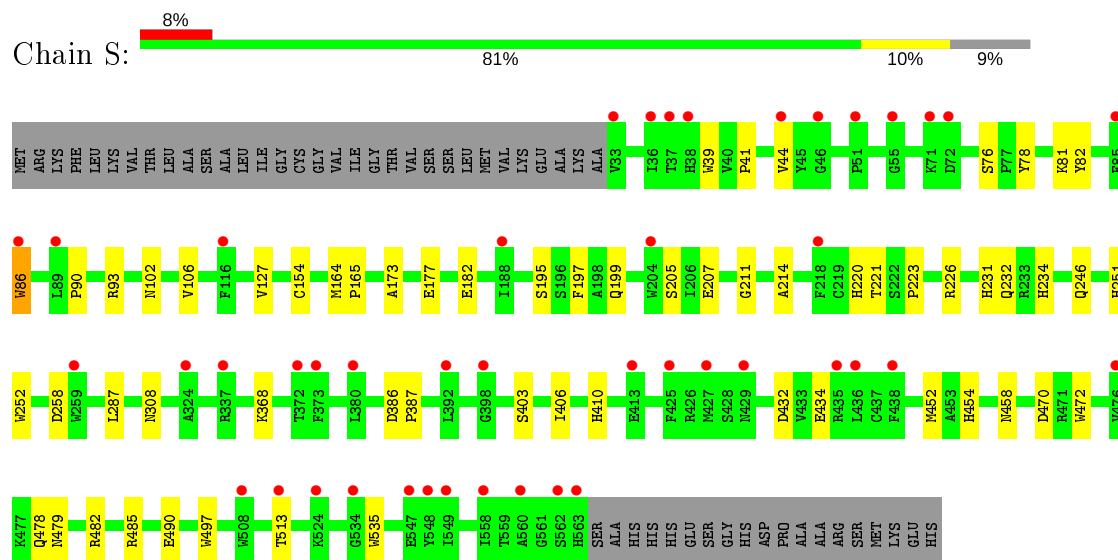
• Molecule 1: Hydrazine dehydrogenase



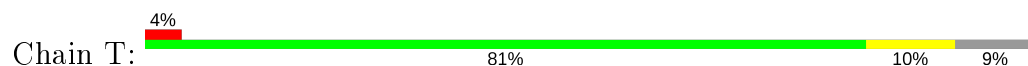
• Molecule 1: Hydrazine dehydrogenase

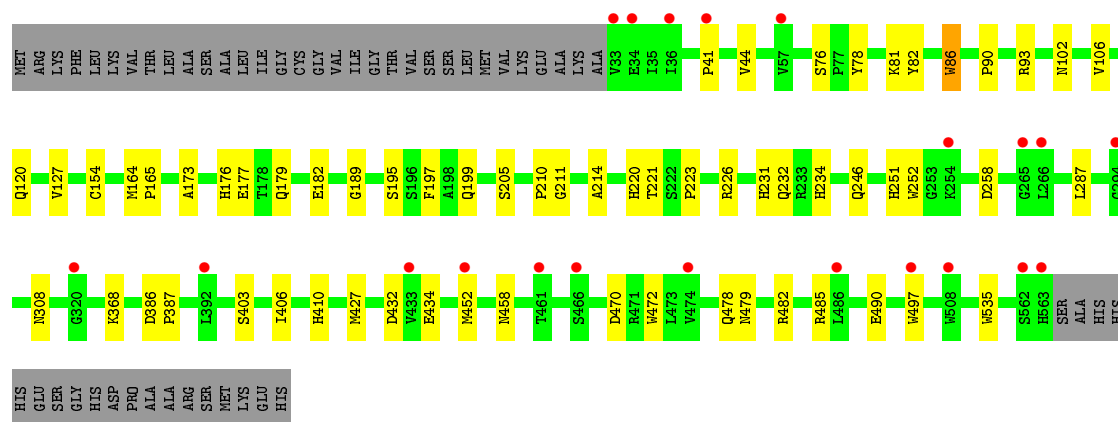


• Molecule 1: Hydrazine dehydrogenase

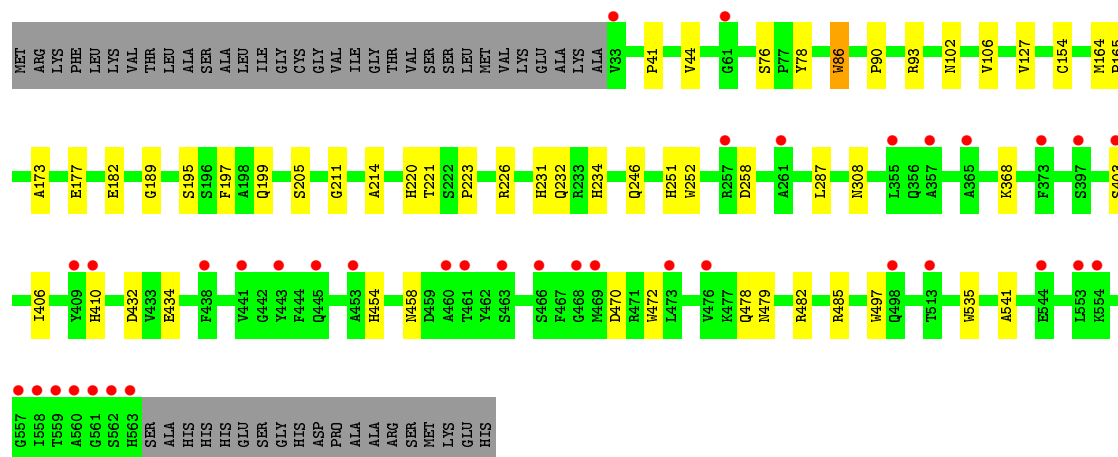
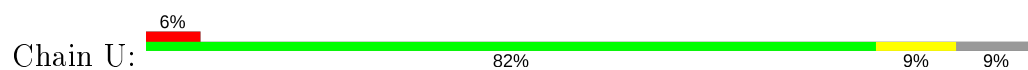


• Molecule 1: Hydrazine dehydrogenase

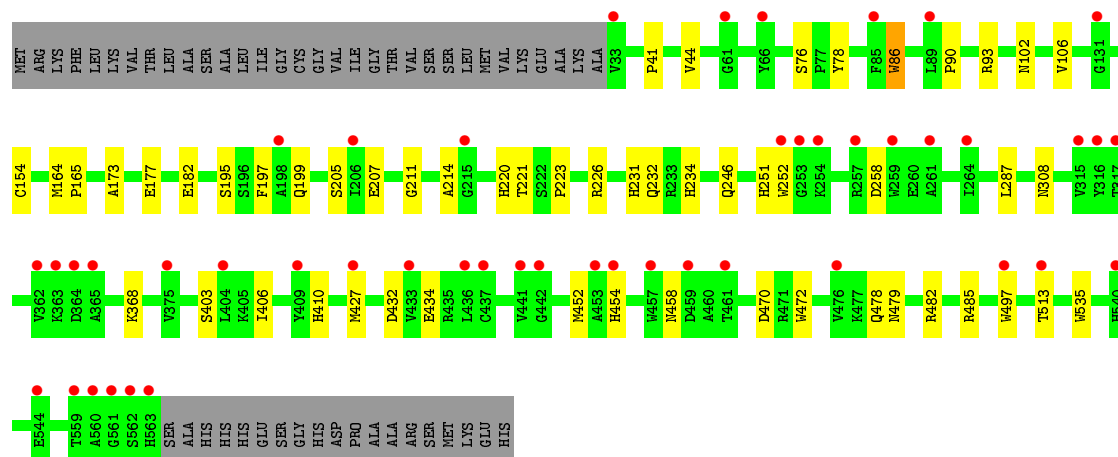
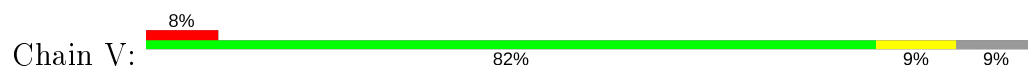




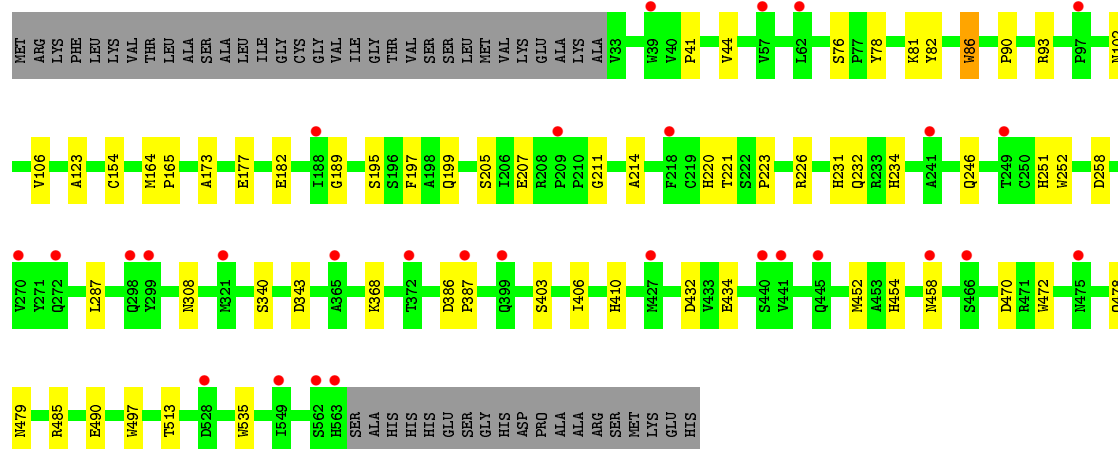
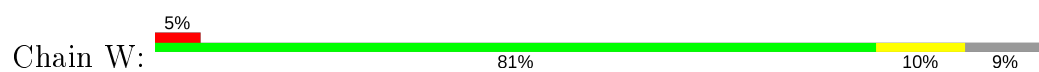
• Molecule 1: Hydrazine dehydrogenase



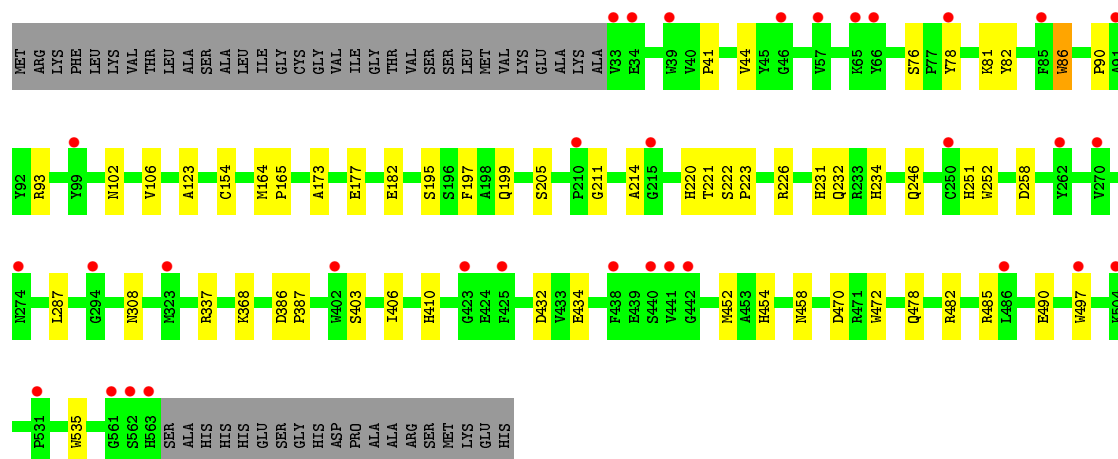
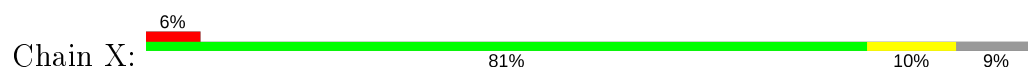
• Molecule 1: Hydrazine dehydrogenase



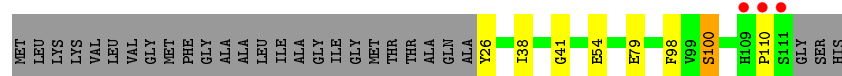
• Molecule 1: Hydrazine dehydrogenase



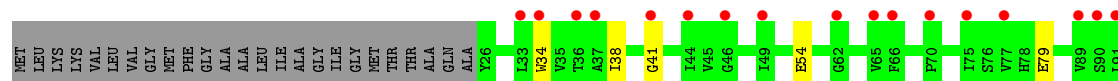
• Molecule 1: Hydrazine dehydrogenase

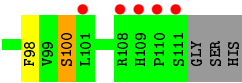


• Molecule 2: hdh assembly factor Kustc1130



• Molecule 2: hdh assembly factor Kustc1130

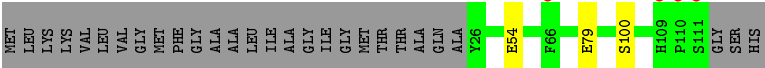




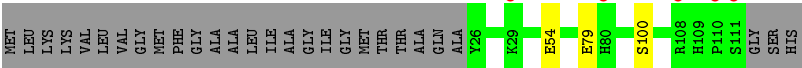
• Molecule 2: hdh assembly factor Kustc1130



• Molecule 2: hdh assembly factor Kustc1130



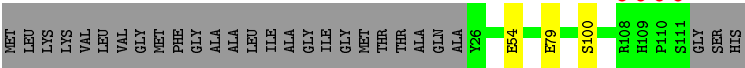
• Molecule 2: hdh assembly factor Kustc1130



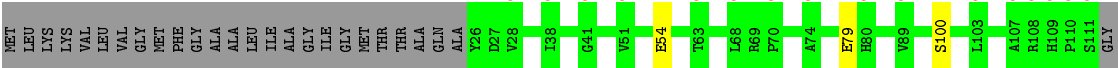
• Molecule 2: hdh assembly factor Kustc1130



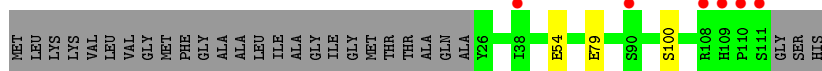
• Molecule 2: hdh assembly factor Kustc1130



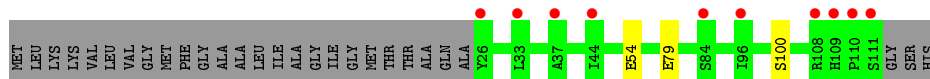
• Molecule 2: hdh assembly factor Kustc1130



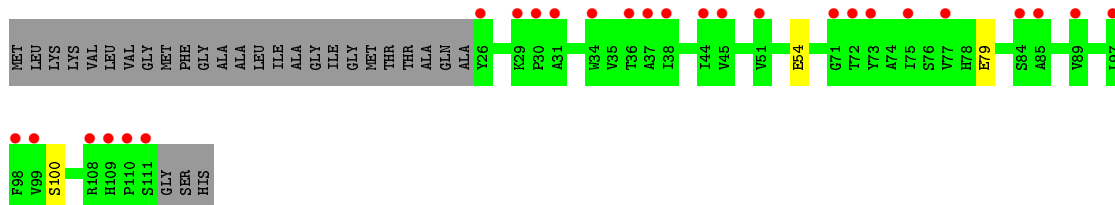
- Molecule 2: hdh assembly factor Kustc1130



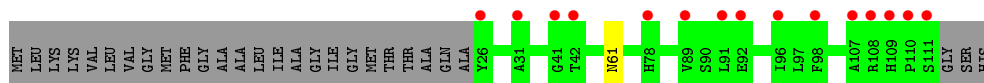
- Molecule 2: hdh assembly factor Kustc1130



- Molecule 2: hdh assembly factor Kustc1130



- Molecule 2: hdh assembly factor Kustc1130





## 4 Data and refinement statistics

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | P 31   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 211.86Å 211.86Å 398.57Å<br>90.00° 90.00° 120.00°               | Depositor        |
| Resolution (Å)  | 93.71 – 2.80<br>93.54 – 2.80                                   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.6 (93.71-2.80)<br>96.6 (93.54-2.80)                         | Depositor<br>EDS |
| $R_{merge}$   | 0.11   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.44 (at 2.82Å)  | Xtriage          |
| Refinement program  | REFMAC 5.8.0222  | Depositor        |
| R, $R_{free}$   | 0.221 , 0.238<br>0.220 , 0.250                                 | Depositor<br>DCC |
| $R_{free}$ test set   | 30022 reflections (6.31%)                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 58.7   | Xtriage          |
| Anisotropy  | 0.123  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 42.6  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$    | Xtriage          |
| Estimated twinning fraction   | 0.000 for -h,-k,l<br>0.000 for h,-h-k,-l<br>0.000 for -k,-h,-l | Xtriage          |
| $F_o, F_c$ correlation  | 0.92   | EDS              |
| Total number of atoms   | 118753   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 63.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, K, SO4, HEC

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     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | B     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | C     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | D     | 0.26         | 0/4355      | 0.52        | 0/5901      |
| 1   | E     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | F     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | G     | 0.27         | 0/4355      | 0.50        | 0/5901      |
| 1   | H     | 0.27         | 0/4355      | 0.49        | 0/5901      |
| 1   | I     | 0.28         | 0/4329      | 0.55        | 0/5866      |
| 1   | J     | 0.28         | 0/4355      | 0.49        | 0/5901      |
| 1   | K     | 0.27         | 0/4355      | 0.49        | 0/5901      |
| 1   | L     | 0.27         | 0/4355      | 0.49        | 0/5901      |
| 1   | M     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | N     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | O     | 0.27         | 0/4355      | 0.49        | 0/5901      |
| 1   | P     | 0.27         | 0/4355      | 0.49        | 0/5901      |
| 1   | Q     | 0.27         | 0/4355      | 0.49        | 0/5901      |
| 1   | R     | 0.27         | 0/4366      | 0.49        | 0/5915      |
| 1   | S     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | T     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | U     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | V     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | W     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 1   | X     | 0.26         | 0/4355      | 0.49        | 0/5901      |
| 2   | Y     | 0.27         | 0/653       | 0.54        | 0/887       |
| 2   | Z     | 0.27         | 0/653       | 0.54        | 0/887       |
| 2   | a     | 0.27         | 0/653       | 0.53        | 0/887       |
| 2   | b     | 0.27         | 0/653       | 0.54        | 0/887       |
| 2   | c     | 0.27         | 0/653       | 0.54        | 0/887       |
| 2   | d     | 0.27         | 0/653       | 0.54        | 0/887       |
| 2   | e     | 0.27         | 0/653       | 0.54        | 0/887       |
| 2   | f     | 0.27         | 0/653       | 0.54        | 0/887       |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 2   | g     | 0.27         | 0/653    | 0.54        | 0/887    |
| 2   | h     | 0.27         | 0/653    | 0.54        | 0/887    |
| 2   | i     | 0.27         | 0/653    | 0.54        | 0/887    |
| 2   | j     | 0.27         | 0/653    | 0.53        | 0/887    |
| All | All   | 0.27         | 0/112341 | 0.50        | 0/152247 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4226  | 0        | 3941     | 48      | 1            |
| 1   | B     | 4226  | 0        | 3941     | 44      | 0            |
| 1   | C     | 4226  | 0        | 3941     | 46      | 0            |
| 1   | D     | 4226  | 0        | 3941     | 69      | 0            |
| 1   | E     | 4226  | 0        | 3941     | 46      | 0            |
| 1   | F     | 4226  | 0        | 3941     | 45      | 0            |
| 1   | G     | 4226  | 0        | 3941     | 63      | 2            |
| 1   | H     | 4226  | 0        | 3941     | 71      | 0            |
| 1   | I     | 4201  | 0        | 3921     | 92      | 0            |
| 1   | J     | 4226  | 0        | 3941     | 58      | 1            |
| 1   | K     | 4226  | 0        | 3941     | 67      | 0            |
| 1   | L     | 4226  | 0        | 3941     | 49      | 0            |
| 1   | M     | 4226  | 0        | 3941     | 42      | 0            |
| 1   | N     | 4226  | 0        | 3941     | 47      | 0            |
| 1   | O     | 4226  | 0        | 3941     | 49      | 0            |
| 1   | P     | 4226  | 0        | 3941     | 49      | 0            |
| 1   | Q     | 4226  | 0        | 3941     | 50      | 1            |
| 1   | R     | 4237  | 0        | 3953     | 52      | 1            |
| 1   | S     | 4226  | 0        | 3941     | 41      | 0            |
| 1   | T     | 4226  | 0        | 3941     | 44      | 0            |
| 1   | U     | 4226  | 0        | 3941     | 39      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | V     | 4226  | 0        | 3941     | 38      | 0            |
| 1   | W     | 4226  | 0        | 3941     | 45      | 0            |
| 1   | X     | 4226  | 0        | 3941     | 43      | 0            |
| 2   | Y     | 640   | 0        | 627      | 5       | 0            |
| 2   | Z     | 640   | 0        | 627      | 4       | 0            |
| 2   | a     | 640   | 0        | 627      | 0       | 0            |
| 2   | b     | 640   | 0        | 627      | 0       | 0            |
| 2   | c     | 640   | 0        | 627      | 0       | 0            |
| 2   | d     | 640   | 0        | 627      | 0       | 0            |
| 2   | e     | 640   | 0        | 627      | 0       | 0            |
| 2   | f     | 640   | 0        | 627      | 0       | 0            |
| 2   | g     | 640   | 0        | 627      | 0       | 0            |
| 2   | h     | 640   | 0        | 627      | 0       | 0            |
| 2   | i     | 640   | 0        | 627      | 0       | 0            |
| 2   | j     | 640   | 0        | 627      | 0       | 0            |
| 3   | A     | 344   | 0        | 236      | 15      | 0            |
| 3   | B     | 344   | 0        | 236      | 15      | 0            |
| 3   | C     | 344   | 0        | 236      | 18      | 0            |
| 3   | D     | 344   | 0        | 237      | 20      | 0            |
| 3   | E     | 344   | 0        | 236      | 15      | 0            |
| 3   | F     | 344   | 0        | 236      | 14      | 0            |
| 3   | G     | 344   | 0        | 236      | 15      | 0            |
| 3   | H     | 344   | 0        | 236      | 16      | 0            |
| 3   | I     | 344   | 0        | 237      | 27      | 0            |
| 3   | J     | 344   | 0        | 236      | 14      | 0            |
| 3   | K     | 344   | 0        | 236      | 19      | 0            |
| 3   | L     | 344   | 0        | 236      | 15      | 0            |
| 3   | M     | 344   | 0        | 236      | 14      | 0            |
| 3   | N     | 344   | 0        | 236      | 16      | 0            |
| 3   | O     | 344   | 0        | 236      | 17      | 0            |
| 3   | P     | 344   | 0        | 236      | 16      | 0            |
| 3   | Q     | 344   | 0        | 236      | 17      | 0            |
| 3   | R     | 344   | 0        | 236      | 17      | 0            |
| 3   | S     | 344   | 0        | 236      | 15      | 0            |
| 3   | T     | 344   | 0        | 236      | 15      | 0            |
| 3   | U     | 344   | 0        | 236      | 17      | 0            |
| 3   | V     | 344   | 0        | 236      | 16      | 0            |
| 3   | W     | 344   | 0        | 236      | 18      | 0            |
| 3   | X     | 344   | 0        | 236      | 16      | 0            |
| 4   | A     | 15    | 0        | 0        | 0       | 0            |
| 4   | B     | 10    | 0        | 0        | 1       | 0            |
| 4   | C     | 15    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | D     | 5     | 0        | 0        | 0       | 0            |
| 4   | E     | 10    | 0        | 0        | 0       | 0            |
| 4   | F     | 10    | 0        | 0        | 0       | 0            |
| 4   | G     | 30    | 0        | 0        | 3       | 0            |
| 4   | H     | 25    | 0        | 0        | 1       | 0            |
| 4   | I     | 20    | 0        | 0        | 0       | 0            |
| 4   | J     | 15    | 0        | 0        | 2       | 0            |
| 4   | K     | 15    | 0        | 0        | 0       | 0            |
| 4   | L     | 20    | 0        | 0        | 1       | 0            |
| 4   | M     | 20    | 0        | 0        | 0       | 0            |
| 4   | N     | 15    | 0        | 0        | 1       | 0            |
| 4   | O     | 15    | 0        | 0        | 0       | 0            |
| 4   | P     | 5     | 0        | 0        | 0       | 0            |
| 4   | Q     | 15    | 0        | 0        | 1       | 0            |
| 4   | R     | 15    | 0        | 0        | 0       | 0            |
| 4   | S     | 10    | 0        | 0        | 0       | 0            |
| 4   | T     | 5     | 0        | 0        | 0       | 0            |
| 4   | U     | 15    | 0        | 0        | 0       | 0            |
| 4   | V     | 15    | 0        | 0        | 0       | 0            |
| 4   | W     | 5     | 0        | 0        | 0       | 0            |
| 4   | X     | 15    | 0        | 0        | 1       | 0            |
| 4   | Y     | 10    | 0        | 0        | 0       | 0            |
| 4   | a     | 5     | 0        | 0        | 0       | 0            |
| 4   | c     | 5     | 0        | 0        | 0       | 0            |
| 5   | A     | 18    | 0        | 24       | 2       | 0            |
| 5   | D     | 6     | 0        | 8        | 0       | 0            |
| 5   | G     | 12    | 0        | 16       | 2       | 0            |
| 5   | H     | 12    | 0        | 16       | 20      | 0            |
| 5   | I     | 18    | 0        | 24       | 5       | 0            |
| 5   | J     | 12    | 0        | 16       | 3       | 0            |
| 5   | K     | 24    | 0        | 32       | 14      | 0            |
| 5   | L     | 6     | 0        | 8        | 1       | 0            |
| 6   | H     | 1     | 0        | 0        | 0       | 0            |
| 6   | K     | 1     | 0        | 0        | 0       | 0            |
| 6   | Q     | 1     | 0        | 0        | 0       | 0            |
| 6   | X     | 1     | 0        | 0        | 0       | 0            |
| 7   | A     | 33    | 0        | 0        | 3       | 0            |
| 7   | B     | 40    | 0        | 0        | 2       | 0            |
| 7   | C     | 36    | 0        | 0        | 0       | 0            |
| 7   | D     | 21    | 0        | 0        | 0       | 0            |
| 7   | E     | 21    | 0        | 0        | 2       | 0            |
| 7   | F     | 24    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 7   | G     | 78     | 0        | 0        | 8       | 0            |
| 7   | H     | 70     | 0        | 0        | 4       | 0            |
| 7   | I     | 62     | 0        | 0        | 1       | 0            |
| 7   | J     | 78     | 0        | 0        | 4       | 0            |
| 7   | K     | 57     | 0        | 0        | 5       | 0            |
| 7   | L     | 69     | 0        | 0        | 1       | 0            |
| 7   | M     | 27     | 0        | 0        | 1       | 0            |
| 7   | N     | 37     | 0        | 0        | 0       | 0            |
| 7   | O     | 40     | 0        | 0        | 0       | 0            |
| 7   | P     | 50     | 0        | 0        | 3       | 0            |
| 7   | Q     | 48     | 0        | 0        | 4       | 0            |
| 7   | R     | 49     | 0        | 0        | 5       | 0            |
| 7   | S     | 4      | 0        | 0        | 0       | 0            |
| 7   | T     | 15     | 0        | 0        | 1       | 0            |
| 7   | U     | 15     | 0        | 0        | 0       | 0            |
| 7   | V     | 17     | 0        | 0        | 0       | 0            |
| 7   | W     | 12     | 0        | 0        | 0       | 0            |
| 7   | X     | 13     | 0        | 0        | 0       | 0            |
| 7   | Y     | 2      | 0        | 0        | 0       | 0            |
| 7   | Z     | 1      | 0        | 0        | 0       | 0            |
| 7   | a     | 2      | 0        | 0        | 0       | 0            |
| 7   | b     | 2      | 0        | 0        | 0       | 0            |
| 7   | c     | 2      | 0        | 0        | 0       | 0            |
| 7   | d     | 2      | 0        | 0        | 0       | 0            |
| 7   | e     | 2      | 0        | 0        | 0       | 0            |
| 7   | f     | 2      | 0        | 0        | 0       | 0            |
| 7   | g     | 1      | 0        | 0        | 0       | 0            |
| 7   | i     | 2      | 0        | 0        | 0       | 0            |
| 7   | j     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 118753 | 0        | 107910   | 1271    | 3            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1271 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:H:267:HIS:HD1 | 5:H:614:GOL:H11 | 1.06                     | 1.14              |
| 1:H:267:HIS:ND1 | 5:H:614:GOL:H11 | 1.65                     | 1.12              |
| 1:H:267:HIS:HD1 | 5:H:614:GOL:C1  | 1.74                     | 1.01              |
| 1:H:267:HIS:CE1 | 5:H:614:GOL:H31 | 2.01                     | 0.96              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:I:406:ILE:H | 1:I:410:HIS:HD2 | 1.14                     | 0.95              |

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

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:A:491:LYS:O  | 1:R:496:SER:OG[1_545] | 1.83                     | 0.37              |
| 1:G:42:HIS:NE2 | 1:J:496:SER:CB[2_555] | 2.03                     | 0.17              |
| 1:G:496:SER:OG | 1:Q:491:LYS:O[1_655]  | 2.18                     | 0.02              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 529/582 (91%) | 513 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | B     | 529/582 (91%) | 514 (97%) | 15 (3%) | 0        | 100         | 100 |
| 1   | C     | 529/582 (91%) | 512 (97%) | 17 (3%) | 0        | 100         | 100 |
| 1   | D     | 529/582 (91%) | 491 (93%) | 36 (7%) | 2 (0%)   | 34          | 66  |
| 1   | E     | 529/582 (91%) | 512 (97%) | 17 (3%) | 0        | 100         | 100 |
| 1   | F     | 529/582 (91%) | 515 (97%) | 14 (3%) | 0        | 100         | 100 |
| 1   | G     | 529/582 (91%) | 516 (98%) | 13 (2%) | 0        | 100         | 100 |
| 1   | H     | 529/582 (91%) | 513 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | I     | 525/582 (90%) | 502 (96%) | 23 (4%) | 0        | 100         | 100 |
| 1   | J     | 529/582 (91%) | 516 (98%) | 13 (2%) | 0        | 100         | 100 |
| 1   | K     | 529/582 (91%) | 513 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | L     | 529/582 (91%) | 513 (97%) | 16 (3%) | 0        | 100         | 100 |
| 1   | M     | 529/582 (91%) | 515 (97%) | 14 (3%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | N     | 529/582 (91%)     | 513 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | O     | 529/582 (91%)     | 513 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | P     | 529/582 (91%)     | 513 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | Q     | 529/582 (91%)     | 514 (97%)   | 15 (3%)  | 0        | 100         | 100 |
| 1   | R     | 530/582 (91%)     | 515 (97%)   | 15 (3%)  | 0        | 100         | 100 |
| 1   | S     | 529/582 (91%)     | 513 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | T     | 529/582 (91%)     | 511 (97%)   | 18 (3%)  | 0        | 100         | 100 |
| 1   | U     | 529/582 (91%)     | 513 (97%)   | 16 (3%)  | 0        | 100         | 100 |
| 1   | V     | 529/582 (91%)     | 512 (97%)   | 17 (3%)  | 0        | 100         | 100 |
| 1   | W     | 529/582 (91%)     | 512 (97%)   | 17 (3%)  | 0        | 100         | 100 |
| 1   | X     | 529/582 (91%)     | 515 (97%)   | 14 (3%)  | 0        | 100         | 100 |
| 2   | Y     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | Z     | 84/114 (74%)      | 82 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 2   | a     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | b     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | c     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | d     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | e     | 84/114 (74%)      | 82 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 2   | f     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | g     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | h     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | i     | 84/114 (74%)      | 83 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 2   | j     | 84/114 (74%)      | 79 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| All | All   | 13701/15336 (89%) | 13279 (97%) | 420 (3%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 256 | HIS  |
| 1   | D     | 106 | VAL  |



### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | B     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | C     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | D     | 451/491 (92%) | 432 (96%) | 19 (4%)  | 30          | 63 |
| 1   | E     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | F     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | G     | 451/491 (92%) | 448 (99%) | 3 (1%)   | 84          | 95 |
| 1   | H     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | I     | 449/491 (91%) | 433 (96%) | 16 (4%)  | 35          | 69 |
| 1   | J     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | K     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | L     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | M     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | N     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | O     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | P     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | Q     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | R     | 452/491 (92%) | 448 (99%) | 4 (1%)   | 78          | 94 |
| 1   | S     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | T     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | U     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | V     | 451/491 (92%) | 446 (99%) | 5 (1%)   | 73          | 92 |
| 1   | W     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 1   | X     | 451/491 (92%) | 447 (99%) | 4 (1%)   | 78          | 94 |
| 2   | Y     | 68/86 (79%)   | 65 (96%)  | 3 (4%)   | 28          | 61 |
| 2   | Z     | 68/86 (79%)   | 65 (96%)  | 3 (4%)   | 28          | 61 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|----------|-------------|----|
| 2   | a     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | b     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | c     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | d     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | e     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | f     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | g     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | h     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | i     | 68/86 (79%)       | 65 (96%)    | 3 (4%)   | 28          | 61 |
| 2   | j     | 68/86 (79%)       | 67 (98%)    | 1 (2%)   | 65          | 89 |
| All | All   | 11639/12816 (91%) | 11475 (99%) | 164 (1%) | 67          | 90 |

5 of 164 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 86  | TRP  |
| 1   | P     | 78  | TYR  |
| 2   | f     | 54  | GLU  |
| 1   | L     | 472 | TRP  |
| 1   | N     | 231 | HIS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 263 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 479 | ASN  |
| 1   | N     | 246 | GLN  |
| 1   | W     | 185 | GLN  |
| 1   | L     | 179 | GLN  |
| 1   | M     | 179 | GLN  |

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 286 ligands modelled in this entry, 4 are monoatomic - leaving 282 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 |
| 3   | HEC  | W     | 605 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.60 | 4 (22%)  |
| 4   | SO4  | K     | 610 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.10 | 0        |
| 4   | SO4  | V     | 610 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.12 | 0        |
| 3   | HEC  | N     | 600 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.21 | 2 (11%)  |
| 4   | SO4  | Y     | 202 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.11 | 0        |
| 3   | HEC  | I     | 601 | 1    | 26,50,50     | 1.68 | 4 (15%)  | 18,82,82    | 1.18 | 1 (5%)   |
| 3   | HEC  | X     | 603 | 1,7  | 26,50,50     | 2.66 | 9 (34%)  | 18,82,82    | 2.76 | 6 (33%)  |
| 3   | HEC  | V     | 602 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.36 | 2 (11%)  |
| 3   | HEC  | T     | 605 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.69 | 5 (27%)  |
| 3   | HEC  | X     | 600 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.23 | 2 (11%)  |
| 3   | HEC  | F     | 605 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.57 | 3 (16%)  |
| 3   | HEC  | L     | 606 | 1    | 26,50,50     | 1.55 | 4 (15%)  | 18,82,82    | 1.39 | 3 (16%)  |
| 3   | HEC  | D     | 601 | 1    | 26,50,50     | 1.64 | 4 (15%)  | 18,82,82    | 1.06 | 1 (5%)   |
| 4   | SO4  | O     | 609 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.08 | 0        |
| 3   | HEC  | L     | 602 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.38 | 2 (11%)  |
| 3   | HEC  | Q     | 600 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.11 | 2 (11%)  |
| 3   | HEC  | V     | 600 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.15 | 2 (11%)  |
| 3   | HEC  | D     | 605 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.80 | 4 (22%)  |
| 3   | HEC  | Q     | 601 | 1    | 26,50,50     | 1.64 | 4 (15%)  | 18,82,82    | 1.23 | 1 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SO4  | L     | 609 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.13 | 0        |
| 3   | HEC  | X     | 602 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.40 | 2 (11%)  |
| 4   | SO4  | I     | 609 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.34 | 0        |
| 3   | HEC  | C     | 606 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.30 | 2 (11%)  |
| 3   | HEC  | X     | 607 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.10 | 1 (5%)   |
| 3   | HEC  | K     | 602 | 1    | 26,50,50     | 1.55 | 4 (15%)  | 18,82,82    | 1.37 | 2 (11%)  |
| 5   | GOL  | J     | 612 | -    | 5,5,5        | 0.50 | 0        | 5,5,5       | 0.57 | 0        |
| 3   | HEC  | X     | 604 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.77 | 2 (11%)  |
| 3   | HEC  | Q     | 607 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.26 | 1 (5%)   |
| 3   | HEC  | G     | 606 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.33 | 3 (16%)  |
| 3   | HEC  | U     | 606 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.30 | 2 (11%)  |
| 3   | HEC  | P     | 604 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.87 | 3 (16%)  |
| 3   | HEC  | R     | 601 | 1    | 26,50,50     | 1.67 | 4 (15%)  | 18,82,82    | 1.26 | 1 (5%)   |
| 3   | HEC  | D     | 602 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.43 | 3 (16%)  |
| 4   | SO4  | Q     | 610 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.11 | 0        |
| 3   | HEC  | I     | 602 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.53 | 3 (16%)  |
| 3   | HEC  | N     | 604 | 1    | 26,50,50     | 1.63 | 4 (15%)  | 18,82,82    | 1.79 | 2 (11%)  |
| 3   | HEC  | Q     | 605 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.59 | 4 (22%)  |
| 3   | HEC  | P     | 602 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.33 | 2 (11%)  |
| 3   | HEC  | U     | 600 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.14 | 2 (11%)  |
| 5   | GOL  | L     | 613 | -    | 5,5,5        | 0.25 | 0        | 5,5,5       | 0.35 | 0        |
| 3   | HEC  | O     | 606 | 1    | 26,50,50     | 1.51 | 4 (15%)  | 18,82,82    | 1.39 | 1 (5%)   |
| 3   | HEC  | S     | 603 | 1,7  | 26,50,50     | 2.71 | 11 (42%) | 18,82,82    | 2.72 | 6 (33%)  |
| 3   | HEC  | R     | 600 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.21 | 2 (11%)  |
| 5   | GOL  | I     | 614 | -    | 5,5,5        | 0.23 | 0        | 5,5,5       | 0.19 | 0        |
| 3   | HEC  | G     | 601 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.30 | 2 (11%)  |
| 3   | HEC  | H     | 603 | 1,7  | 26,50,50     | 2.67 | 10 (38%) | 18,82,82    | 2.65 | 8 (44%)  |
| 3   | HEC  | V     | 604 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.84 | 2 (11%)  |
| 3   | HEC  | S     | 606 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.30 | 1 (5%)   |
| 3   | HEC  | T     | 600 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.15 | 2 (11%)  |
| 3   | HEC  | U     | 602 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.39 | 2 (11%)  |
| 3   | HEC  | H     | 600 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.21 | 1 (5%)   |
| 3   | HEC  | M     | 606 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.32 | 2 (11%)  |
| 3   | HEC  | S     | 601 | 1    | 26,50,50     | 1.67 | 4 (15%)  | 18,82,82    | 1.26 | 1 (5%)   |
| 4   | SO4  | X     | 609 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.14 | 0        |
| 3   | HEC  | X     | 606 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.32 | 1 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SO4  | N     | 609 | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.13 | 0        |
| 3   | HEC  | W     | 604 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.82 | 3 (16%)  |
| 3   | HEC  | T     | 606 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.32 | 1 (5%)   |
| 5   | GOL  | K     | 613 | -    | 5,5,5        | 0.23 | 0        | 5,5,5       | 0.34 | 0        |
| 4   | SO4  | L     | 612 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.10 | 0        |
| 3   | HEC  | T     | 602 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.39 | 2 (11%)  |
| 4   | SO4  | F     | 609 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.13 | 0        |
| 3   | HEC  | V     | 603 | 1,7  | 26,50,50     | 2.65 | 10 (38%) | 18,82,82    | 2.68 | 9 (50%)  |
| 3   | HEC  | S     | 607 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.08 | 0        |
| 4   | SO4  | O     | 611 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.08 | 0        |
| 3   | HEC  | H     | 606 | 1    | 26,50,50     | 1.68 | 4 (15%)  | 18,82,82    | 1.27 | 1 (5%)   |
| 5   | GOL  | K     | 612 | -    | 5,5,5        | 0.39 | 0        | 5,5,5       | 0.33 | 0        |
| 3   | HEC  | L     | 607 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.08 | 0        |
| 3   | HEC  | W     | 602 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.27 | 3 (16%)  |
| 3   | HEC  | K     | 607 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.08 | 0        |
| 4   | SO4  | U     | 609 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.26 | 0        |
| 5   | GOL  | D     | 610 | -    | 5,5,5        | 0.29 | 0        | 5,5,5       | 0.23 | 0        |
| 3   | HEC  | H     | 604 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.89 | 3 (16%)  |
| 3   | HEC  | V     | 601 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.22 | 1 (5%)   |
| 3   | HEC  | E     | 604 | 1    | 26,50,50     | 1.66 | 4 (15%)  | 18,82,82    | 1.83 | 3 (16%)  |
| 4   | SO4  | C     | 609 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.14 | 0        |
| 4   | SO4  | P     | 609 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.14 | 0        |
| 3   | HEC  | K     | 601 | 1    | 26,50,50     | 1.66 | 4 (15%)  | 18,82,82    | 1.26 | 1 (5%)   |
| 3   | HEC  | L     | 601 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.20 | 1 (5%)   |
| 3   | HEC  | A     | 606 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.36 | 2 (11%)  |
| 4   | SO4  | Y     | 201 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.11 | 0        |
| 3   | HEC  | T     | 607 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.11 | 0        |
| 4   | SO4  | M     | 612 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.14 | 0        |
| 3   | HEC  | A     | 605 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.59 | 3 (16%)  |
| 4   | SO4  | R     | 611 | -    | 4,4,4        | 0.31 | 0        | 6,6,6       | 0.06 | 0        |
| 4   | SO4  | U     | 611 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.08 | 0        |
| 3   | HEC  | C     | 600 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.19 | 2 (11%)  |
| 3   | HEC  | E     | 600 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.22 | 2 (11%)  |
| 3   | HEC  | L     | 603 | 1,7  | 26,50,50     | 2.67 | 9 (34%)  | 18,82,82    | 2.78 | 9 (50%)  |
| 3   | HEC  | D     | 607 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.02 | 0        |
| 3   | HEC  | L     | 600 | 1    | 26,50,50     | 1.53 | 4 (15%)  | 18,82,82    | 1.15 | 1 (5%)   |
| 5   | GOL  | A     | 613 | -    | 5,5,5        | 0.41 | 0        | 5,5,5       | 0.35 | 0        |
| 3   | HEC  | N     | 607 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.13 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SO4  | L     | 611 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | HEC  | K     | 604 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.87 | 3 (16%)  |
| 3   | HEC  | O     | 605 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.55 | 3 (16%)  |
| 4   | SO4  | C     | 610 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.12 | 0        |
| 4   | SO4  | a     | 201 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.08 | 0        |
| 3   | HEC  | N     | 606 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.30 | 1 (5%)   |
| 4   | SO4  | J     | 610 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.13 | 0        |
| 3   | HEC  | C     | 601 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.21 | 1 (5%)   |
| 3   | HEC  | J     | 606 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.28 | 1 (5%)   |
| 3   | HEC  | U     | 604 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.81 | 2 (11%)  |
| 3   | HEC  | B     | 602 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.43 | 2 (11%)  |
| 3   | HEC  | M     | 607 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.06 | 0        |
| 4   | SO4  | G     | 614 | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.15 | 0        |
| 3   | HEC  | I     | 600 | 1    | 26,50,50     | 1.48 | 4 (15%)  | 18,82,82    | 1.38 | 4 (22%)  |
| 3   | HEC  | F     | 603 | 1,7  | 26,50,50     | 2.64 | 10 (38%) | 18,82,82    | 2.90 | 8 (44%)  |
| 3   | HEC  | X     | 601 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.26 | 1 (5%)   |
| 4   | SO4  | J     | 609 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.09 | 0        |
| 4   | SO4  | R     | 609 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.25 | 0        |
| 4   | SO4  | H     | 611 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.21 | 0        |
| 4   | SO4  | R     | 610 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.10 | 0        |
| 3   | HEC  | B     | 604 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.84 | 2 (11%)  |
| 3   | HEC  | O     | 604 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.82 | 2 (11%)  |
| 4   | SO4  | K     | 609 | -    | 4,4,4        | 0.21 | 0        | 6,6,6       | 0.34 | 0        |
| 3   | HEC  | R     | 604 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.76 | 3 (16%)  |
| 3   | HEC  | U     | 603 | 1,7  | 26,50,50     | 2.64 | 10 (38%) | 18,82,82    | 2.73 | 8 (44%)  |
| 3   | HEC  | F     | 606 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.30 | 1 (5%)   |
| 5   | GOL  | A     | 612 | -    | 5,5,5        | 0.28 | 0        | 5,5,5       | 0.28 | 0        |
| 4   | SO4  | A     | 610 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.14 | 0        |
| 4   | SO4  | X     | 611 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.07 | 0        |
| 3   | HEC  | K     | 606 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.39 | 2 (11%)  |
| 3   | HEC  | G     | 603 | 1,7  | 26,50,50     | 2.70 | 9 (34%)  | 18,82,82    | 2.56 | 7 (38%)  |
| 3   | HEC  | R     | 605 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.54 | 3 (16%)  |
| 3   | HEC  | A     | 600 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.28 | 2 (11%)  |
| 4   | SO4  | U     | 610 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.07 | 0        |
| 3   | HEC  | R     | 607 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.13 | 1 (5%)   |
| 3   | HEC  | H     | 605 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.60 | 4 (22%)  |
| 3   | HEC  | A     | 601 | 1    | 26,50,50     | 1.66 | 4 (15%)  | 18,82,82    | 1.27 | 1 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | HEC  | V     | 607 | 1    | 26,50,50     | 1.55 | 4 (15%)  | 18,82,82    | 1.07 | 0        |
| 5   | GOL  | G     | 615 | -    | 5,5,5        | 0.45 | 0        | 5,5,5       | 0.34 | 0        |
| 3   | HEC  | L     | 605 | 1    | 26,50,50     | 1.53 | 4 (15%)  | 18,82,82    | 1.63 | 5 (27%)  |
| 4   | SO4  | E     | 610 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.10 | 0        |
| 3   | HEC  | D     | 606 | 1    | 26,50,50     | 1.55 | 4 (15%)  | 18,82,82    | 1.24 | 1 (5%)   |
| 3   | HEC  | M     | 603 | 1,7  | 26,50,50     | 2.68 | 10 (38%) | 18,82,82    | 2.74 | 7 (38%)  |
| 3   | HEC  | J     | 602 | 1    | 26,50,50     | 1.63 | 4 (15%)  | 18,82,82    | 1.36 | 2 (11%)  |
| 4   | SO4  | C     | 611 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.16 | 0        |
| 4   | SO4  | I     | 610 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.05 | 0        |
| 4   | SO4  | G     | 611 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.10 | 0        |
| 4   | SO4  | G     | 613 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.37 | 0        |
| 5   | GOL  | H     | 614 | -    | 5,5,5        | 0.41 | 0        | 5,5,5       | 0.77 | 0        |
| 4   | SO4  | M     | 611 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.11 | 0        |
| 3   | HEC  | W     | 600 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.19 | 2 (11%)  |
| 3   | HEC  | W     | 603 | 1,7  | 26,50,50     | 2.63 | 9 (34%)  | 18,82,82    | 2.63 | 6 (33%)  |
| 3   | HEC  | O     | 600 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.17 | 2 (11%)  |
| 4   | SO4  | Q     | 611 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.14 | 0        |
| 3   | HEC  | Q     | 602 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.31 | 2 (11%)  |
| 4   | SO4  | Q     | 609 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.14 | 0        |
| 3   | HEC  | X     | 605 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.62 | 4 (22%)  |
| 4   | SO4  | W     | 609 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.10 | 0        |
| 4   | SO4  | N     | 610 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.13 | 0        |
| 5   | GOL  | I     | 615 | -    | 5,5,5        | 0.33 | 0        | 5,5,5       | 0.36 | 0        |
| 4   | SO4  | X     | 610 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.05 | 0        |
| 3   | HEC  | B     | 607 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.21 | 0        |
| 3   | HEC  | D     | 603 | 1,7  | 26,50,50     | 2.66 | 10 (38%) | 18,82,82    | 2.89 | 10 (55%) |
| 4   | SO4  | T     | 609 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.08 | 0        |
| 4   | SO4  | A     | 609 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.12 | 0        |
| 3   | HEC  | E     | 606 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.31 | 2 (11%)  |
| 3   | HEC  | M     | 604 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.78 | 2 (11%)  |
| 3   | HEC  | Q     | 603 | 1,7  | 26,50,50     | 2.69 | 11 (42%) | 18,82,82    | 2.84 | 9 (50%)  |
| 3   | HEC  | B     | 605 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.51 | 2 (11%)  |
| 3   | HEC  | P     | 600 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.16 | 1 (5%)   |
| 4   | SO4  | V     | 611 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.05 | 0        |
| 3   | HEC  | G     | 607 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.07 | 0        |
| 5   | GOL  | K     | 615 | -    | 5,5,5        | 0.33 | 0        | 5,5,5       | 0.20 | 0        |
| 3   | HEC  | T     | 601 | 1    | 26,50,50     | 1.66 | 4 (15%)  | 18,82,82    | 1.19 | 1 (5%)   |
| 3   | HEC  | R     | 603 | 1    | 26,50,50     | 2.68 | 9 (34%)  | 18,82,82    | 2.51 | 8 (44%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | HEC  | A     | 607 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.08 | 0        |
| 3   | HEC  | S     | 602 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.40 | 2 (11%)  |
| 3   | HEC  | S     | 600 | 1    | 26,50,50     | 1.65 | 4 (15%)  | 18,82,82    | 1.13 | 2 (11%)  |
| 4   | SO4  | J     | 611 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | HEC  | I     | 605 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.68 | 4 (22%)  |
| 3   | HEC  | N     | 601 | 1    | 26,50,50     | 1.65 | 4 (15%)  | 18,82,82    | 1.24 | 1 (5%)   |
| 3   | HEC  | P     | 606 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.30 | 2 (11%)  |
| 4   | SO4  | c     | 201 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | HEC  | G     | 605 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.66 | 4 (22%)  |
| 4   | SO4  | L     | 610 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.16 | 0        |
| 3   | HEC  | N     | 602 | 1    | 26,50,50     | 1.64 | 4 (15%)  | 18,82,82    | 1.42 | 2 (11%)  |
| 3   | HEC  | M     | 602 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.39 | 2 (11%)  |
| 5   | GOL  | K     | 614 | -    | 5,5,5        | 0.18 | 0        | 5,5,5       | 0.37 | 0        |
| 3   | HEC  | H     | 601 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.23 | 1 (5%)   |
| 3   | HEC  | T     | 604 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.86 | 2 (11%)  |
| 3   | HEC  | E     | 603 | 1,7  | 26,50,50     | 2.71 | 9 (34%)  | 18,82,82    | 2.79 | 6 (33%)  |
| 3   | HEC  | I     | 607 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.12 | 1 (5%)   |
| 4   | SO4  | A     | 611 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.16 | 0        |
| 3   | HEC  | U     | 601 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.27 | 1 (5%)   |
| 3   | HEC  | C     | 604 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.87 | 3 (16%)  |
| 5   | GOL  | J     | 613 | -    | 5,5,5        | 0.27 | 0        | 5,5,5       | 0.49 | 0        |
| 4   | SO4  | G     | 612 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.12 | 0        |
| 3   | HEC  | W     | 606 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.27 | 1 (5%)   |
| 3   | HEC  | R     | 606 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.31 | 1 (5%)   |
| 3   | HEC  | S     | 604 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.86 | 2 (11%)  |
| 3   | HEC  | B     | 603 | 1    | 26,50,50     | 2.65 | 10 (38%) | 18,82,82    | 2.65 | 8 (44%)  |
| 3   | HEC  | W     | 607 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.13 | 0        |
| 3   | HEC  | B     | 601 | 1    | 26,50,50     | 1.63 | 4 (15%)  | 18,82,82    | 1.32 | 1 (5%)   |
| 3   | HEC  | H     | 602 | 1    | 26,50,50     | 1.64 | 4 (15%)  | 18,82,82    | 1.37 | 2 (11%)  |
| 4   | SO4  | H     | 613 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.23 | 0        |
| 4   | SO4  | I     | 612 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.06 | 0        |
| 3   | HEC  | K     | 603 | 1,7  | 26,50,50     | 2.68 | 9 (34%)  | 18,82,82    | 2.58 | 8 (44%)  |
| 4   | SO4  | D     | 609 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.11 | 0        |
| 4   | SO4  | H     | 612 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.07 | 0        |
| 3   | HEC  | A     | 603 | 1,7  | 26,50,50     | 2.65 | 9 (34%)  | 18,82,82    | 2.85 | 8 (44%)  |
| 3   | HEC  | O     | 602 | 1    | 26,50,50     | 1.53 | 4 (15%)  | 18,82,82    | 1.42 | 2 (11%)  |
| 3   | HEC  | J     | 601 | 1    | 26,50,50     | 1.67 | 4 (15%)  | 18,82,82    | 1.19 | 1 (5%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SO4  | K     | 611 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.06 | 0        |
| 5   | GOL  | A     | 614 | -    | 5,5,5        | 0.35 | 0        | 5,5,5       | 0.18 | 0        |
| 4   | SO4  | H     | 609 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.10 | 0        |
| 3   | HEC  | K     | 605 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.64 | 4 (22%)  |
| 3   | HEC  | F     | 607 | 1    | 26,50,50     | 1.52 | 4 (15%)  | 18,82,82    | 1.09 | 0        |
| 3   | HEC  | E     | 605 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.57 | 3 (16%)  |
| 3   | HEC  | K     | 600 | 1    | 26,50,50     | 1.55 | 4 (15%)  | 18,82,82    | 1.24 | 1 (5%)   |
| 3   | HEC  | J     | 603 | 1,7  | 26,50,50     | 2.61 | 9 (34%)  | 18,82,82    | 2.74 | 8 (44%)  |
| 5   | GOL  | I     | 613 | -    | 5,5,5        | 0.26 | 0        | 5,5,5       | 0.24 | 0        |
| 4   | SO4  | B     | 609 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.13 | 0        |
| 3   | HEC  | C     | 602 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.40 | 2 (11%)  |
| 3   | HEC  | O     | 607 | 1    | 26,50,50     | 1.52 | 4 (15%)  | 18,82,82    | 1.18 | 1 (5%)   |
| 3   | HEC  | J     | 607 | 1    | 26,50,50     | 1.63 | 4 (15%)  | 18,82,82    | 1.04 | 0        |
| 3   | HEC  | I     | 603 | 1,7  | 26,50,50     | 2.64 | 9 (34%)  | 18,82,82    | 4.33 | 7 (38%)  |
| 3   | HEC  | O     | 603 | 1,7  | 26,50,50     | 2.68 | 10 (38%) | 18,82,82    | 2.72 | 8 (44%)  |
| 3   | HEC  | M     | 601 | 1    | 26,50,50     | 1.65 | 4 (15%)  | 18,82,82    | 1.20 | 1 (5%)   |
| 3   | HEC  | C     | 603 | 1    | 26,50,50     | 2.65 | 11 (42%) | 18,82,82    | 2.61 | 8 (44%)  |
| 3   | HEC  | E     | 607 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.13 | 0        |
| 3   | HEC  | P     | 605 | 1    | 26,50,50     | 1.53 | 4 (15%)  | 18,82,82    | 1.61 | 4 (22%)  |
| 3   | HEC  | S     | 605 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.58 | 4 (22%)  |
| 3   | HEC  | M     | 605 | 1    | 26,50,50     | 1.53 | 4 (15%)  | 18,82,82    | 1.58 | 4 (22%)  |
| 3   | HEC  | N     | 605 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.61 | 4 (22%)  |
| 3   | HEC  | D     | 600 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.19 | 2 (11%)  |
| 3   | HEC  | J     | 605 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.62 | 4 (22%)  |
| 3   | HEC  | O     | 601 | 1    | 26,50,50     | 1.68 | 4 (15%)  | 18,82,82    | 1.30 | 1 (5%)   |
| 4   | SO4  | I     | 611 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.07 | 0        |
| 4   | SO4  | F     | 610 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.08 | 0        |
| 3   | HEC  | I     | 604 | 1    | 26,50,50     | 1.68 | 4 (15%)  | 18,82,82    | 1.71 | 3 (16%)  |
| 3   | HEC  | E     | 601 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.29 | 1 (5%)   |
| 3   | HEC  | P     | 607 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.16 | 0        |
| 3   | HEC  | C     | 605 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.57 | 3 (16%)  |
| 3   | HEC  | G     | 604 | 1    | 26,50,50     | 1.66 | 4 (15%)  | 18,82,82    | 1.80 | 3 (16%)  |
| 3   | HEC  | N     | 603 | 1,7  | 26,50,50     | 2.69 | 10 (38%) | 18,82,82    | 2.70 | 7 (38%)  |
| 3   | HEC  | B     | 606 | 1    | 26,50,50     | 1.54 | 4 (15%)  | 18,82,82    | 1.41 | 2 (11%)  |
| 3   | HEC  | Q     | 606 | 1    | 26,50,50     | 1.52 | 4 (15%)  | 18,82,82    | 1.30 | 1 (5%)   |
| 3   | HEC  | U     | 605 | 1    | 26,50,50     | 1.52 | 4 (15%)  | 18,82,82    | 1.63 | 4 (22%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | SO4  | O     | 610 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.10 | 0        |
| 3   | HEC  | J     | 600 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.15 | 2 (11%)  |
| 3   | HEC  | C     | 607 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.09 | 0        |
| 3   | HEC  | I     | 606 | 1    | 26,50,50     | 1.51 | 4 (15%)  | 18,82,82    | 1.38 | 3 (16%)  |
| 3   | HEC  | W     | 601 | 1    | 26,50,50     | 1.67 | 4 (15%)  | 18,82,82    | 1.18 | 1 (5%)   |
| 4   | SO4  | S     | 609 | -    | 4,4,4        | 0.34 | 0        | 6,6,6       | 0.05 | 0        |
| 3   | HEC  | V     | 606 | 1    | 26,50,50     | 1.63 | 4 (15%)  | 18,82,82    | 1.29 | 3 (16%)  |
| 4   | SO4  | B     | 610 | -    | 4,4,4        | 0.37 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | HEC  | B     | 600 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.24 | 2 (11%)  |
| 3   | HEC  | G     | 602 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.38 | 2 (11%)  |
| 4   | SO4  | E     | 609 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.36 | 0        |
| 3   | HEC  | U     | 607 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.16 | 0        |
| 3   | HEC  | M     | 600 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.21 | 2 (11%)  |
| 3   | HEC  | T     | 603 | 1    | 26,50,50     | 2.74 | 10 (38%) | 18,82,82    | 2.77 | 8 (44%)  |
| 4   | SO4  | H     | 610 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.05 | 0        |
| 3   | HEC  | A     | 602 | 1    | 26,50,50     | 1.59 | 4 (15%)  | 18,82,82    | 1.42 | 2 (11%)  |
| 3   | HEC  | F     | 602 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.37 | 2 (11%)  |
| 3   | HEC  | G     | 600 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.26 | 2 (11%)  |
| 3   | HEC  | E     | 602 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.35 | 2 (11%)  |
| 4   | SO4  | M     | 609 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | HEC  | J     | 604 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.83 | 3 (16%)  |
| 3   | HEC  | R     | 602 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.28 | 2 (11%)  |
| 3   | HEC  | D     | 604 | 1    | 26,50,50     | 1.60 | 5 (19%)  | 18,82,82    | 1.76 | 3 (16%)  |
| 4   | SO4  | S     | 610 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.08 | 0        |
| 3   | HEC  | F     | 604 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.84 | 2 (11%)  |
| 4   | SO4  | V     | 609 | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.28 | 0        |
| 4   | SO4  | G     | 609 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.08 | 0        |
| 3   | HEC  | F     | 600 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.09 | 1 (5%)   |
| 3   | HEC  | P     | 601 | 1    | 26,50,50     | 1.60 | 4 (15%)  | 18,82,82    | 1.27 | 1 (5%)   |
| 5   | GOL  | H     | 615 | -    | 5,5,5        | 0.46 | 0        | 5,5,5       | 0.57 | 0        |
| 3   | HEC  | P     | 603 | 1,7  | 26,50,50     | 2.64 | 9 (34%)  | 18,82,82    | 2.77 | 8 (44%)  |
| 4   | SO4  | N     | 611 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.09 | 0        |
| 3   | HEC  | F     | 601 | 1    | 26,50,50     | 1.66 | 4 (15%)  | 18,82,82    | 1.24 | 1 (5%)   |
| 4   | SO4  | M     | 610 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.09 | 0        |
| 5   | GOL  | G     | 616 | -    | 5,5,5        | 0.19 | 0        | 5,5,5       | 0.42 | 0        |
| 3   | HEC  | Q     | 604 | 1    | 26,50,50     | 1.57 | 4 (15%)  | 18,82,82    | 1.86 | 2 (11%)  |
| 4   | SO4  | G     | 610 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.09 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | HEC  | A     | 604 | 1    | 26,50,50     | 1.62 | 4 (15%)  | 18,82,82    | 1.80 | 2 (11%)  |
| 3   | HEC  | H     | 607 | 1    | 26,50,50     | 1.58 | 4 (15%)  | 18,82,82    | 1.17 | 0        |
| 3   | HEC  | L     | 604 | 1    | 26,50,50     | 1.61 | 4 (15%)  | 18,82,82    | 1.80 | 3 (16%)  |
| 3   | HEC  | V     | 605 | 1    | 26,50,50     | 1.56 | 4 (15%)  | 18,82,82    | 1.60 | 4 (22%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 3   | HEC  | W     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | J     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | N     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | I     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | X     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | V     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | T     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | X     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | F     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | L     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | D     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | L     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | Q     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | V     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | D     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | Q     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | X     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | X     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | C     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | X     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | K     | 602 | 1    | -       | 1/6/54/54 | -     |
| 5   | GOL  | J     | 612 | -    | -       | 4/4/4/4   | -     |
| 3   | HEC  | X     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | Q     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | G     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | U     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | P     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | R     | 601 | 1    | -       | 2/6/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 3   | HEC  | D     | 602 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | I     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | N     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | Q     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | P     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | U     | 600 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | L     | 613 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | O     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | S     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | M     | 607 | 1    | -       | 1/6/54/54 | -     |
| 5   | GOL  | I     | 614 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | G     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | H     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | V     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | S     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | T     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | U     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | H     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | M     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | S     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | X     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | W     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | T     | 606 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | K     | 613 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | T     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | V     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | S     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | H     | 606 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | K     | 612 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | L     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | W     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | K     | 607 | 1    | -       | 1/6/54/54 | -     |
| 5   | GOL  | D     | 610 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | H     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | V     | 601 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | E     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | J     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | K     | 601 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | L     | 601 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | A     | 606 | 1    | -       | 0/6/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 3   | HEC  | T     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | A     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | T     | 603 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | C     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | E     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | L     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | D     | 607 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | L     | 600 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | A     | 613 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | N     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | O     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | Q     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | N     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | C     | 601 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | J     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | U     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | B     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | R     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | I     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | F     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | B     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | O     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | U     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | F     | 606 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | A     | 612 | -    | -       | 0/4/4/4   | -     |
| 3   | HEC  | M     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | K     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | G     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | R     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | A     | 600 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | J     | 613 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | R     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | H     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | A     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | V     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | K     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | L     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | D     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | M     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 5   | GOL  | H     | 614 | -    | -       | 4/4/4/4   | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 3   | HEC  | W     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | W     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | O     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | Q     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | X     | 605 | 1    | -       | 2/6/54/54 | -     |
| 5   | GOL  | I     | 615 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | J     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | B     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | D     | 603 | 1,7  | -       | 2/6/54/54 | -     |
| 3   | HEC  | E     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | K     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | Q     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | B     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | P     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | C     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | G     | 607 | 1    | -       | 1/6/54/54 | -     |
| 5   | GOL  | K     | 615 | -    | -       | 4/4/4/4   | -     |
| 3   | HEC  | T     | 601 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | R     | 603 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | A     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | S     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | S     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | I     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | N     | 601 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | P     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | G     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | N     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | M     | 602 | 1    | -       | 1/6/54/54 | -     |
| 5   | GOL  | K     | 614 | -    | -       | 4/4/4/4   | -     |
| 3   | HEC  | H     | 601 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | T     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | E     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | I     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | U     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | W     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | R     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | S     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | B     | 603 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | W     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | B     | 601 | 1    | -       | 1/6/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 3   | HEC  | H     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | K     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | A     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | O     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | J     | 601 | 1    | -       | 2/6/54/54 | -     |
| 5   | GOL  | A     | 614 | -    | -       | 4/4/4/4   | -     |
| 3   | HEC  | K     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | F     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | E     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | C     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | O     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | J     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | I     | 603 | 1,7  | -       | 2/6/54/54 | -     |
| 3   | HEC  | O     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | M     | 601 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | C     | 603 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | E     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | P     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | S     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | M     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | N     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | D     | 600 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | I     | 613 | -    | -       | 4/4/4/4   | -     |
| 3   | HEC  | O     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | I     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | E     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | P     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | C     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | G     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | N     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | B     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | Q     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | U     | 605 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | J     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | C     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | I     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | W     | 601 | 1    | -       | 2/6/54/54 | -     |
| 3   | HEC  | V     | 606 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | B     | 600 | 1    | -       | 0/6/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 3   | HEC  | G     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | U     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | M     | 600 | 1    | -       | 0/6/54/54 | -     |
| 5   | GOL  | G     | 615 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | F     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | G     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | E     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | J     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | R     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | D     | 604 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | A     | 602 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | F     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | R     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | F     | 600 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | P     | 601 | 1    | -       | 1/6/54/54 | -     |
| 5   | GOL  | H     | 615 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | P     | 603 | 1,7  | -       | 0/6/54/54 | -     |
| 3   | HEC  | F     | 601 | 1    | -       | 1/6/54/54 | -     |
| 5   | GOL  | G     | 616 | -    | -       | 2/4/4/4   | -     |
| 3   | HEC  | A     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | H     | 607 | 1    | -       | 1/6/54/54 | -     |
| 3   | HEC  | L     | 604 | 1    | -       | 0/6/54/54 | -     |
| 3   | HEC  | V     | 605 | 1    | -       | 2/6/54/54 | -     |

The worst 5 of 905 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | T     | 603 | HEC  | C3B-C4B | 6.59 | 1.55        | 1.43     |
| 3   | X     | 603 | HEC  | C3B-C4B | 6.38 | 1.54        | 1.43     |
| 3   | O     | 603 | HEC  | C3B-C4B | 6.35 | 1.54        | 1.43     |
| 3   | A     | 603 | HEC  | C3B-C4B | 6.33 | 1.54        | 1.43     |
| 3   | E     | 603 | HEC  | C3B-C4B | 6.32 | 1.54        | 1.43     |

The worst 5 of 501 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | I     | 603 | HEC  | CBA-CAA-C2A | 16.22 | 142.36      | 112.48   |
| 3   | F     | 603 | HEC  | CAA-CBA-CGA | 8.64  | 127.17      | 112.67   |
| 3   | A     | 603 | HEC  | CAA-CBA-CGA | 8.59  | 127.09      | 112.67   |
| 3   | E     | 603 | HEC  | CAA-CBA-CGA | 8.56  | 127.03      | 112.67   |
| 3   | L     | 603 | HEC  | CAA-CBA-CGA | 8.44  | 126.82      | 112.67   |



There are no chirality outliers.

5 of 183 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | W     | 605 | HEC  | C2D-C3D-CAD-CBD |
| 3   | W     | 605 | HEC  | C4D-C3D-CAD-CBD |
| 3   | I     | 601 | HEC  | C1A-C2A-CAA-CBA |
| 3   | I     | 601 | HEC  | C3A-C2A-CAA-CBA |
| 3   | T     | 605 | HEC  | C2D-C3D-CAD-CBD |

There are no ring outliers.

171 monomers are involved in 453 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | W     | 605 | HEC  | 7       | 0            |
| 3   | N     | 600 | HEC  | 3       | 0            |
| 3   | I     | 601 | HEC  | 6       | 0            |
| 3   | T     | 605 | HEC  | 7       | 0            |
| 3   | X     | 600 | HEC  | 3       | 0            |
| 3   | F     | 605 | HEC  | 5       | 0            |
| 3   | L     | 606 | HEC  | 3       | 0            |
| 3   | D     | 601 | HEC  | 5       | 0            |
| 3   | Q     | 600 | HEC  | 3       | 0            |
| 3   | V     | 600 | HEC  | 3       | 0            |
| 3   | D     | 605 | HEC  | 7       | 0            |
| 3   | Q     | 601 | HEC  | 5       | 0            |
| 3   | C     | 606 | HEC  | 3       | 0            |
| 3   | X     | 607 | HEC  | 2       | 0            |
| 3   | K     | 602 | HEC  | 1       | 0            |
| 3   | X     | 604 | HEC  | 3       | 0            |
| 3   | Q     | 607 | HEC  | 3       | 0            |
| 3   | G     | 606 | HEC  | 3       | 0            |
| 3   | U     | 606 | HEC  | 3       | 0            |
| 3   | P     | 604 | HEC  | 3       | 0            |
| 3   | R     | 601 | HEC  | 4       | 0            |
| 3   | D     | 602 | HEC  | 1       | 0            |
| 3   | I     | 602 | HEC  | 1       | 0            |
| 3   | N     | 604 | HEC  | 3       | 0            |
| 3   | Q     | 605 | HEC  | 6       | 0            |
| 3   | U     | 600 | HEC  | 3       | 0            |
| 5   | L     | 613 | GOL  | 1       | 0            |
| 3   | O     | 606 | HEC  | 3       | 0            |
| 3   | R     | 600 | HEC  | 3       | 0            |
| 5   | I     | 614 | GOL  | 4       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | G     | 601 | HEC  | 4       | 0            |
| 3   | V     | 604 | HEC  | 3       | 0            |
| 3   | S     | 606 | HEC  | 2       | 0            |
| 3   | T     | 600 | HEC  | 3       | 0            |
| 3   | H     | 600 | HEC  | 3       | 0            |
| 3   | M     | 606 | HEC  | 2       | 0            |
| 3   | S     | 601 | HEC  | 5       | 0            |
| 3   | X     | 606 | HEC  | 3       | 0            |
| 3   | W     | 604 | HEC  | 3       | 0            |
| 3   | T     | 606 | HEC  | 2       | 0            |
| 5   | K     | 613 | GOL  | 1       | 0            |
| 3   | S     | 607 | HEC  | 1       | 0            |
| 3   | H     | 606 | HEC  | 4       | 0            |
| 3   | L     | 607 | HEC  | 3       | 0            |
| 3   | K     | 607 | HEC  | 3       | 0            |
| 3   | H     | 604 | HEC  | 3       | 0            |
| 3   | V     | 601 | HEC  | 4       | 0            |
| 3   | E     | 604 | HEC  | 3       | 0            |
| 3   | K     | 601 | HEC  | 7       | 0            |
| 3   | L     | 601 | HEC  | 4       | 0            |
| 3   | A     | 606 | HEC  | 3       | 0            |
| 3   | T     | 607 | HEC  | 2       | 0            |
| 3   | A     | 605 | HEC  | 5       | 0            |
| 3   | C     | 600 | HEC  | 4       | 0            |
| 3   | E     | 600 | HEC  | 3       | 0            |
| 3   | D     | 607 | HEC  | 1       | 0            |
| 3   | L     | 600 | HEC  | 3       | 0            |
| 5   | A     | 613 | GOL  | 1       | 0            |
| 3   | N     | 607 | HEC  | 3       | 0            |
| 3   | K     | 604 | HEC  | 3       | 0            |
| 3   | O     | 605 | HEC  | 6       | 0            |
| 3   | N     | 606 | HEC  | 3       | 0            |
| 3   | C     | 601 | HEC  | 4       | 0            |
| 3   | J     | 606 | HEC  | 2       | 0            |
| 3   | U     | 604 | HEC  | 3       | 0            |
| 3   | M     | 607 | HEC  | 3       | 0            |
| 3   | I     | 600 | HEC  | 5       | 0            |
| 3   | X     | 601 | HEC  | 5       | 0            |
| 3   | B     | 604 | HEC  | 3       | 0            |
| 3   | O     | 604 | HEC  | 2       | 0            |
| 3   | R     | 604 | HEC  | 3       | 0            |
| 3   | F     | 606 | HEC  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | A     | 612 | GOL  | 1       | 0            |
| 3   | K     | 606 | HEC  | 3       | 0            |
| 3   | R     | 605 | HEC  | 7       | 0            |
| 3   | A     | 600 | HEC  | 3       | 0            |
| 3   | R     | 607 | HEC  | 3       | 0            |
| 3   | H     | 605 | HEC  | 7       | 0            |
| 3   | A     | 601 | HEC  | 4       | 0            |
| 3   | V     | 607 | HEC  | 3       | 0            |
| 5   | G     | 615 | GOL  | 1       | 0            |
| 3   | L     | 605 | HEC  | 5       | 0            |
| 3   | D     | 606 | HEC  | 3       | 0            |
| 5   | H     | 614 | GOL  | 11      | 0            |
| 3   | W     | 600 | HEC  | 3       | 0            |
| 3   | O     | 600 | HEC  | 4       | 0            |
| 4   | Q     | 609 | SO4  | 1       | 0            |
| 3   | X     | 605 | HEC  | 6       | 0            |
| 4   | N     | 610 | SO4  | 1       | 0            |
| 5   | I     | 615 | GOL  | 1       | 0            |
| 4   | X     | 610 | SO4  | 1       | 0            |
| 3   | B     | 607 | HEC  | 2       | 0            |
| 3   | D     | 603 | HEC  | 2       | 0            |
| 3   | E     | 606 | HEC  | 2       | 0            |
| 3   | M     | 604 | HEC  | 2       | 0            |
| 3   | B     | 605 | HEC  | 6       | 0            |
| 3   | P     | 600 | HEC  | 3       | 0            |
| 3   | G     | 607 | HEC  | 3       | 0            |
| 5   | K     | 615 | GOL  | 3       | 0            |
| 3   | T     | 601 | HEC  | 4       | 0            |
| 3   | A     | 607 | HEC  | 3       | 0            |
| 3   | S     | 600 | HEC  | 3       | 0            |
| 4   | J     | 611 | SO4  | 2       | 0            |
| 3   | I     | 605 | HEC  | 8       | 0            |
| 3   | N     | 601 | HEC  | 4       | 0            |
| 3   | P     | 606 | HEC  | 3       | 0            |
| 3   | G     | 605 | HEC  | 5       | 0            |
| 4   | L     | 610 | SO4  | 1       | 0            |
| 5   | K     | 614 | GOL  | 10      | 0            |
| 3   | H     | 601 | HEC  | 4       | 0            |
| 3   | T     | 604 | HEC  | 3       | 0            |
| 3   | I     | 607 | HEC  | 2       | 0            |
| 3   | U     | 601 | HEC  | 5       | 0            |
| 3   | C     | 604 | HEC  | 3       | 0            |

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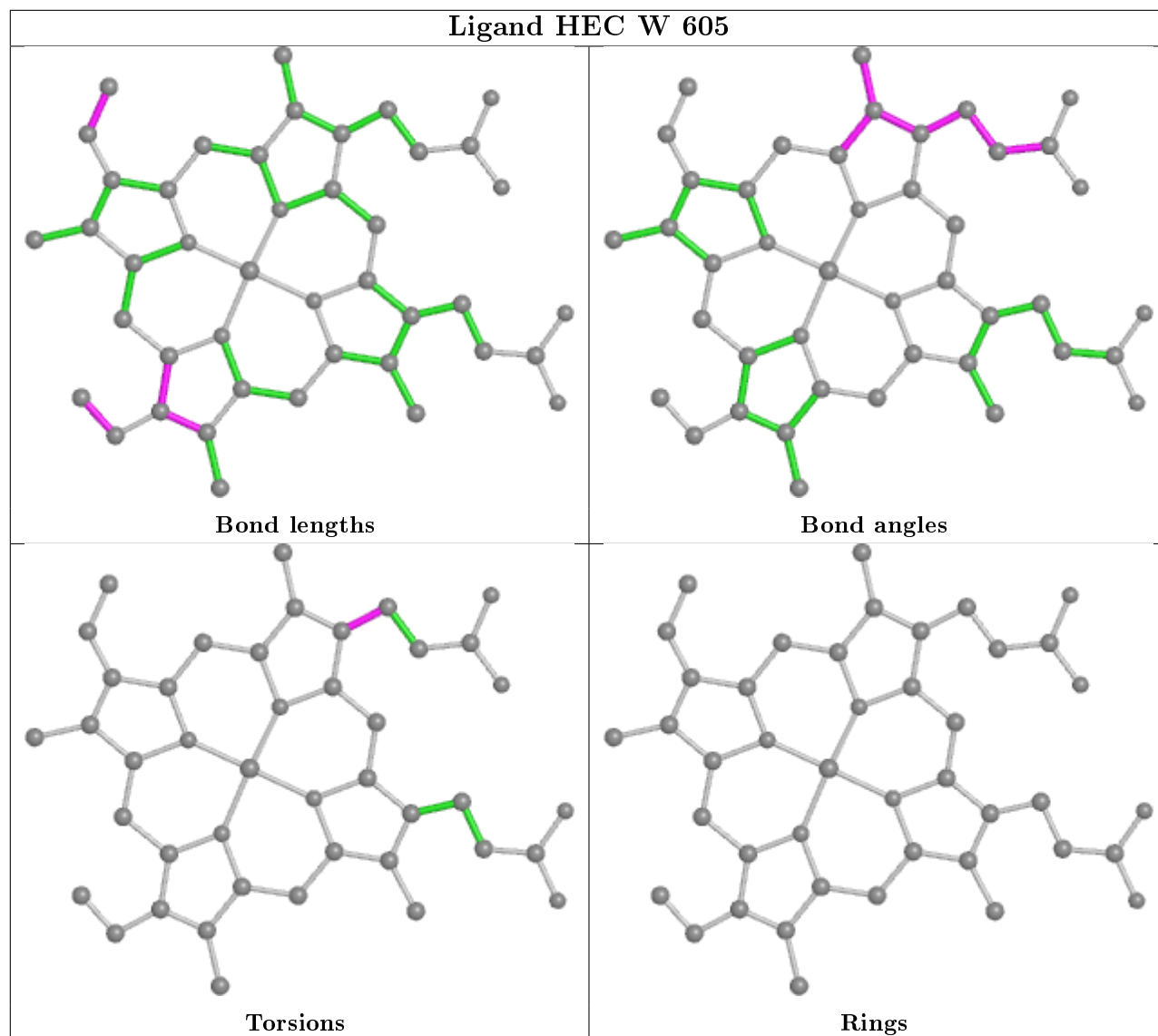
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5   | J     | 613 | GOL  | 3       | 0            |
| 3   | W     | 606 | HEC  | 3       | 0            |
| 3   | R     | 606 | HEC  | 3       | 0            |
| 3   | S     | 604 | HEC  | 3       | 0            |
| 3   | W     | 607 | HEC  | 3       | 0            |
| 3   | B     | 601 | HEC  | 4       | 0            |
| 3   | J     | 601 | HEC  | 4       | 0            |
| 4   | H     | 609 | SO4  | 1       | 0            |
| 3   | K     | 605 | HEC  | 6       | 0            |
| 3   | F     | 607 | HEC  | 1       | 0            |
| 3   | E     | 605 | HEC  | 6       | 0            |
| 3   | K     | 600 | HEC  | 3       | 0            |
| 4   | B     | 609 | SO4  | 1       | 0            |
| 3   | O     | 607 | HEC  | 2       | 0            |
| 3   | J     | 607 | HEC  | 3       | 0            |
| 3   | I     | 603 | HEC  | 3       | 0            |
| 3   | M     | 601 | HEC  | 4       | 0            |
| 3   | E     | 607 | HEC  | 1       | 0            |
| 3   | P     | 605 | HEC  | 7       | 0            |
| 3   | S     | 605 | HEC  | 6       | 0            |
| 3   | M     | 605 | HEC  | 5       | 0            |
| 3   | N     | 605 | HEC  | 6       | 0            |
| 3   | D     | 600 | HEC  | 3       | 0            |
| 3   | J     | 605 | HEC  | 5       | 0            |
| 3   | O     | 601 | HEC  | 5       | 0            |
| 3   | I     | 604 | HEC  | 3       | 0            |
| 3   | E     | 601 | HEC  | 5       | 0            |
| 3   | P     | 607 | HEC  | 2       | 0            |
| 3   | C     | 605 | HEC  | 7       | 0            |
| 3   | G     | 604 | HEC  | 2       | 0            |
| 3   | B     | 606 | HEC  | 3       | 0            |
| 3   | Q     | 606 | HEC  | 3       | 0            |
| 3   | U     | 605 | HEC  | 7       | 0            |
| 3   | J     | 600 | HEC  | 3       | 0            |
| 3   | C     | 607 | HEC  | 3       | 0            |
| 3   | I     | 606 | HEC  | 4       | 0            |
| 3   | W     | 601 | HEC  | 5       | 0            |
| 3   | V     | 606 | HEC  | 3       | 0            |
| 3   | B     | 600 | HEC  | 3       | 0            |
| 3   | U     | 607 | HEC  | 2       | 0            |
| 3   | M     | 600 | HEC  | 3       | 0            |
| 3   | G     | 600 | HEC  | 3       | 0            |

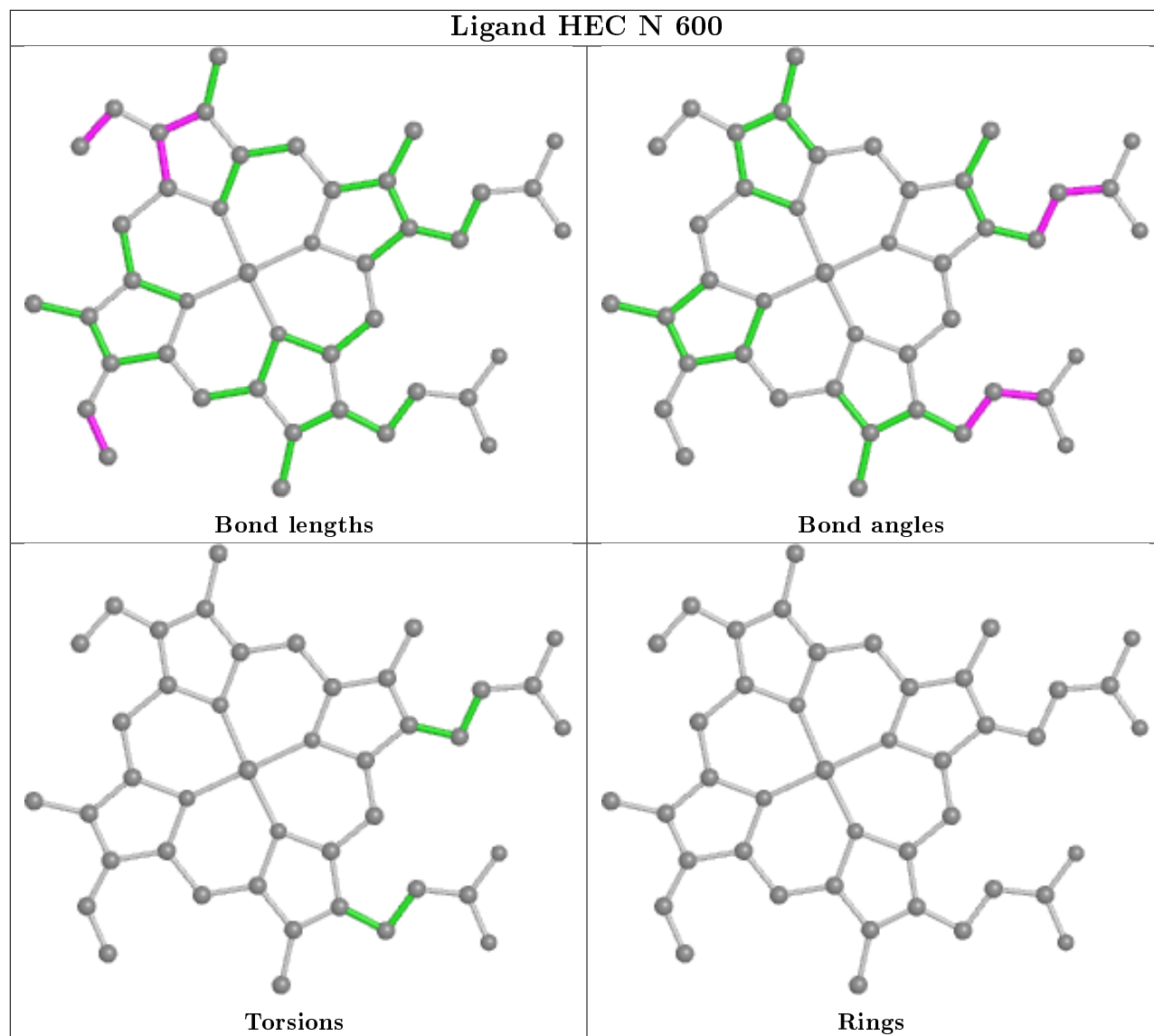
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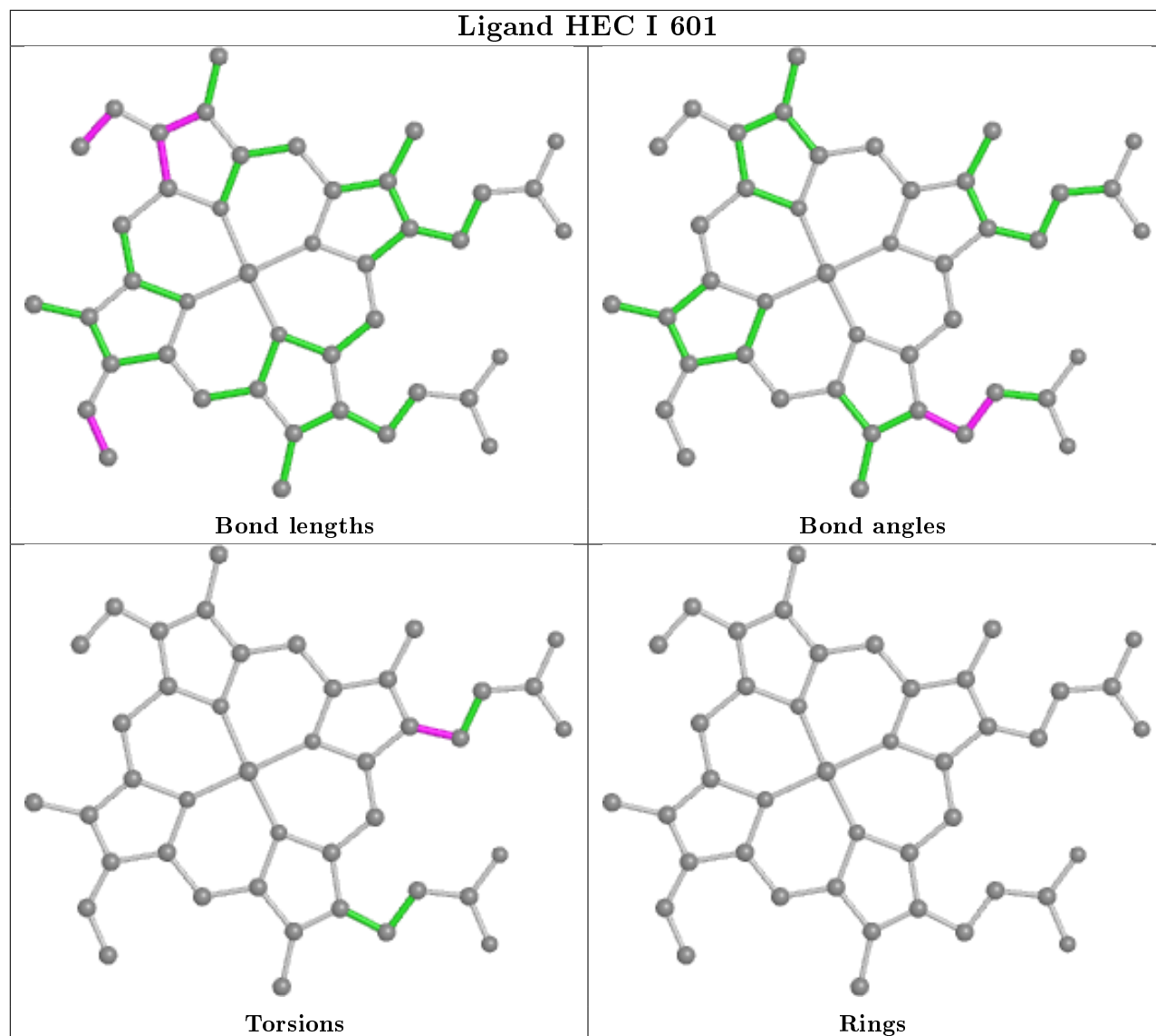
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | J     | 604 | HEC  | 3       | 0            |
| 3   | D     | 604 | HEC  | 3       | 0            |
| 3   | F     | 604 | HEC  | 3       | 0            |
| 4   | G     | 609 | SO4  | 1       | 0            |
| 3   | F     | 600 | HEC  | 4       | 0            |
| 3   | P     | 601 | HEC  | 4       | 0            |
| 5   | H     | 615 | GOL  | 9       | 0            |
| 3   | F     | 601 | HEC  | 4       | 0            |
| 5   | G     | 616 | GOL  | 1       | 0            |
| 3   | Q     | 604 | HEC  | 3       | 0            |
| 4   | G     | 610 | SO4  | 2       | 0            |
| 3   | A     | 604 | HEC  | 2       | 0            |
| 3   | H     | 607 | HEC  | 1       | 0            |
| 3   | L     | 604 | HEC  | 3       | 0            |
| 3   | V     | 605 | HEC  | 6       | 0            |

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

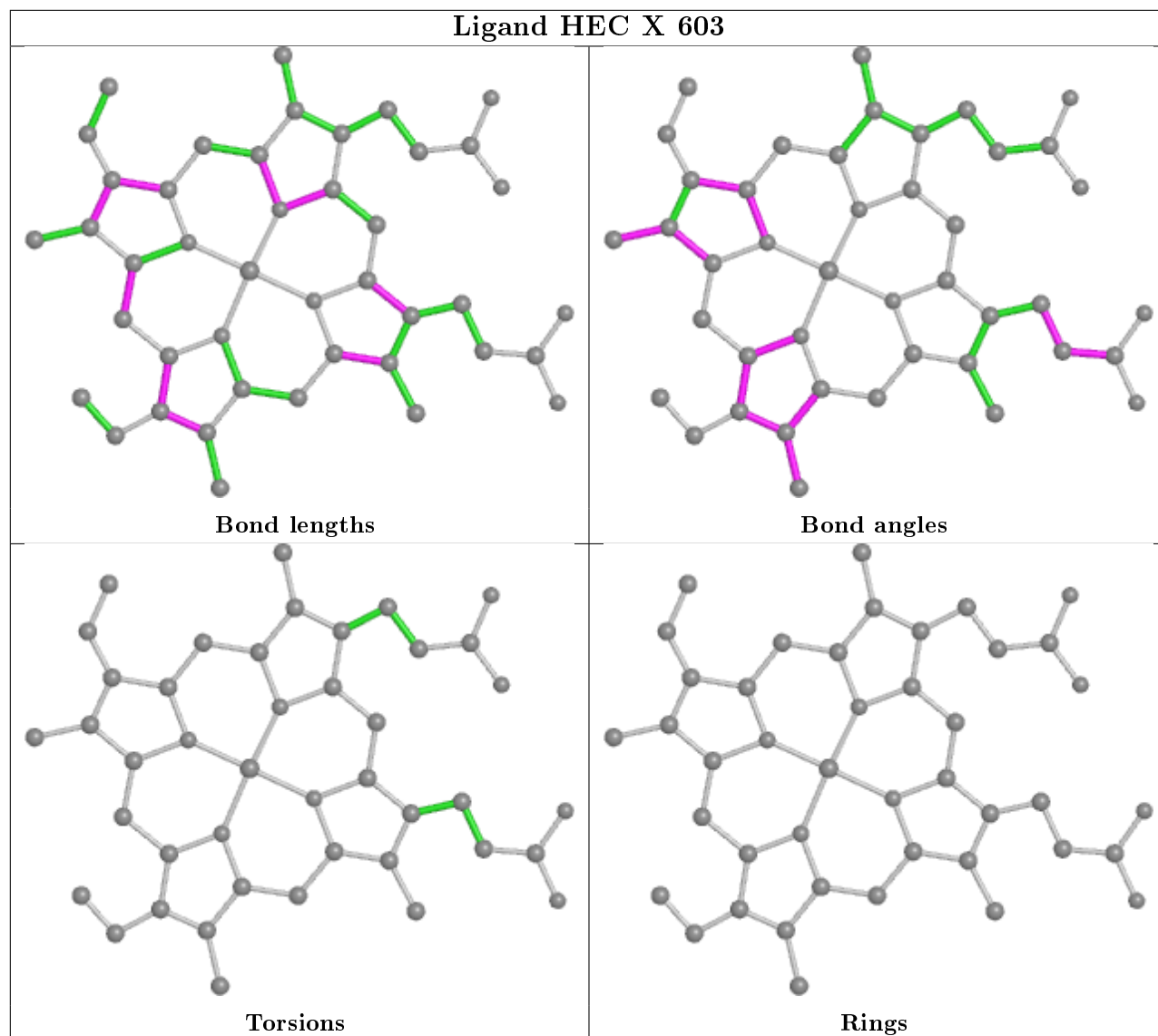


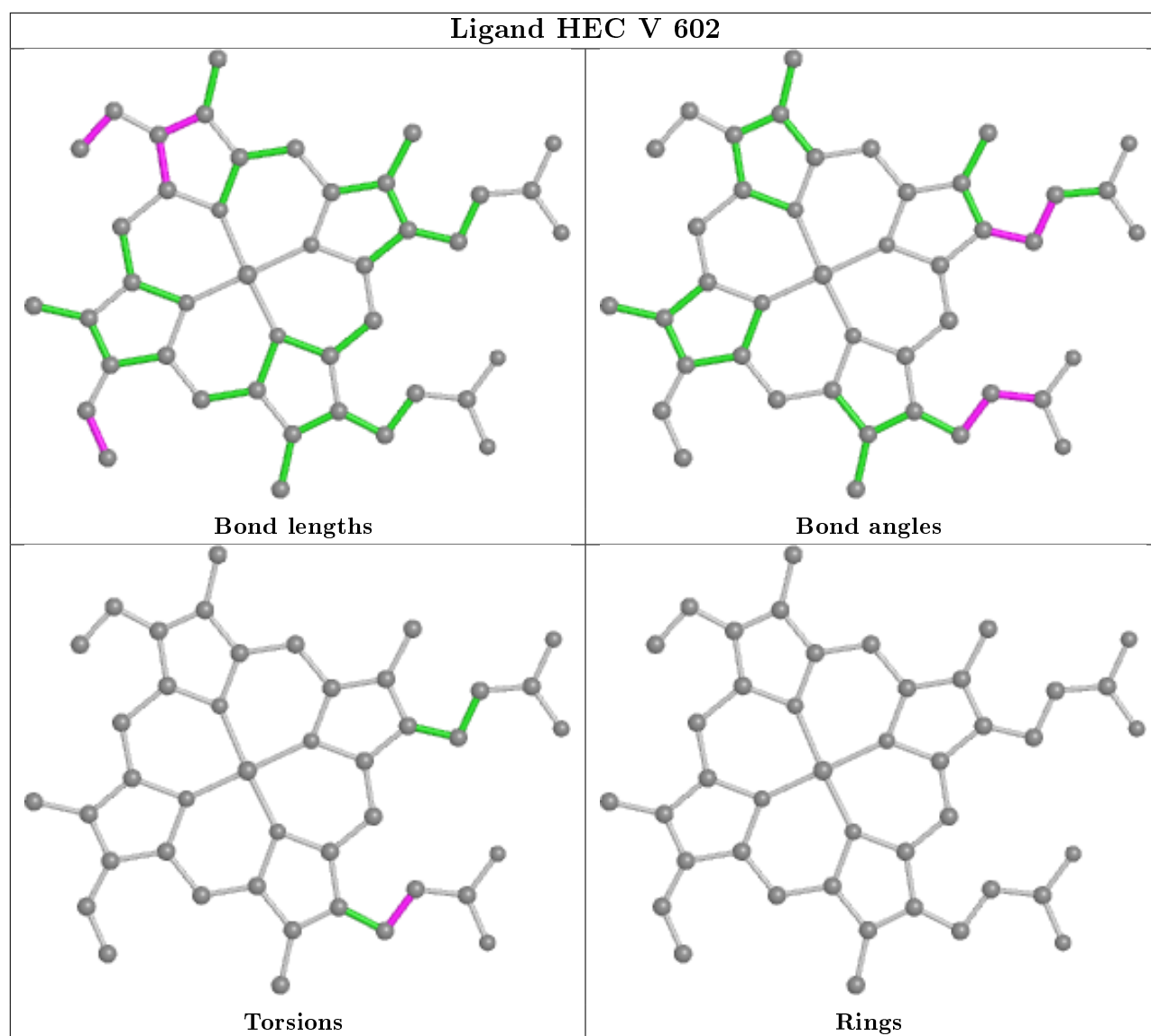


## Ligand HEC I 601

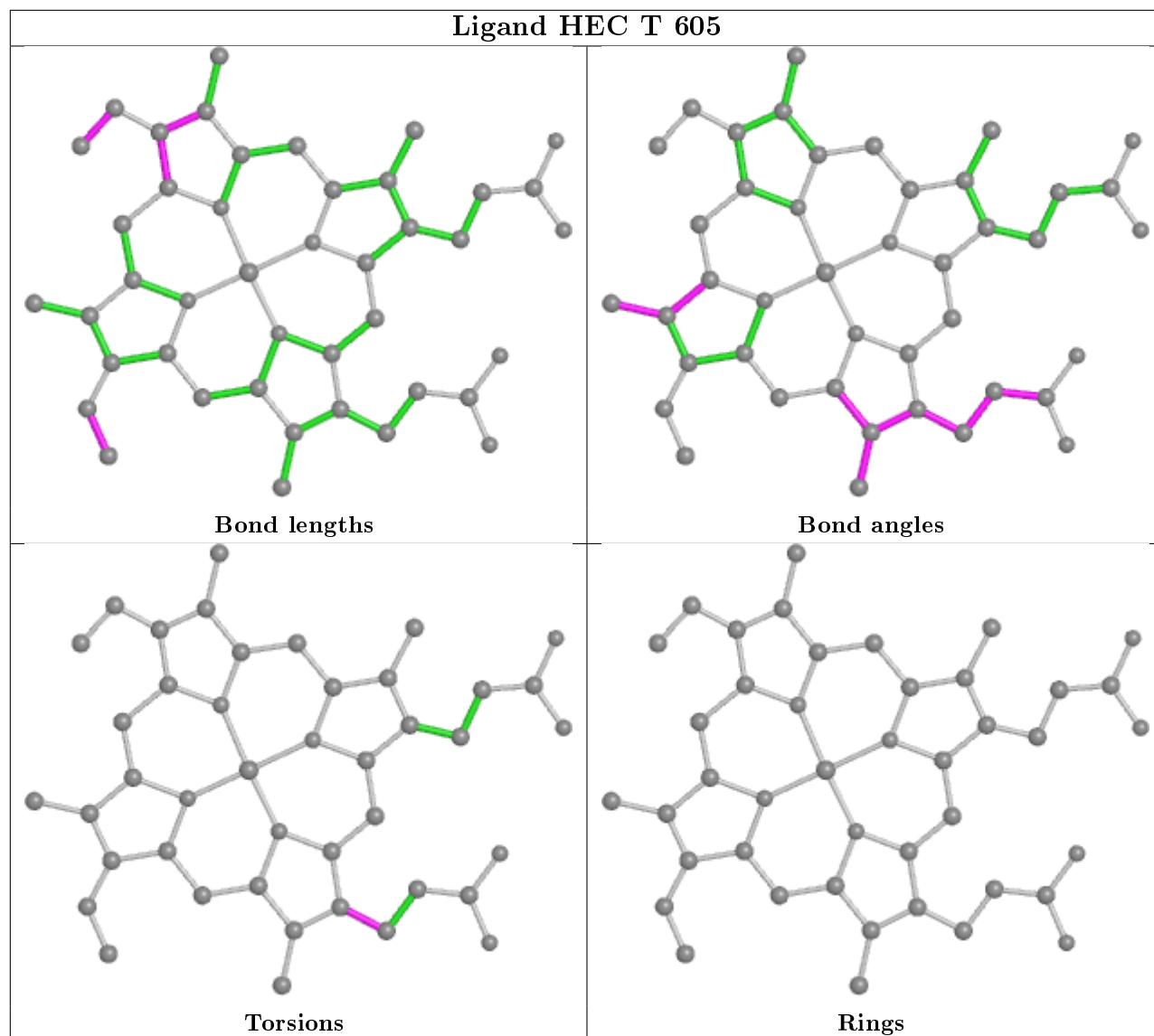


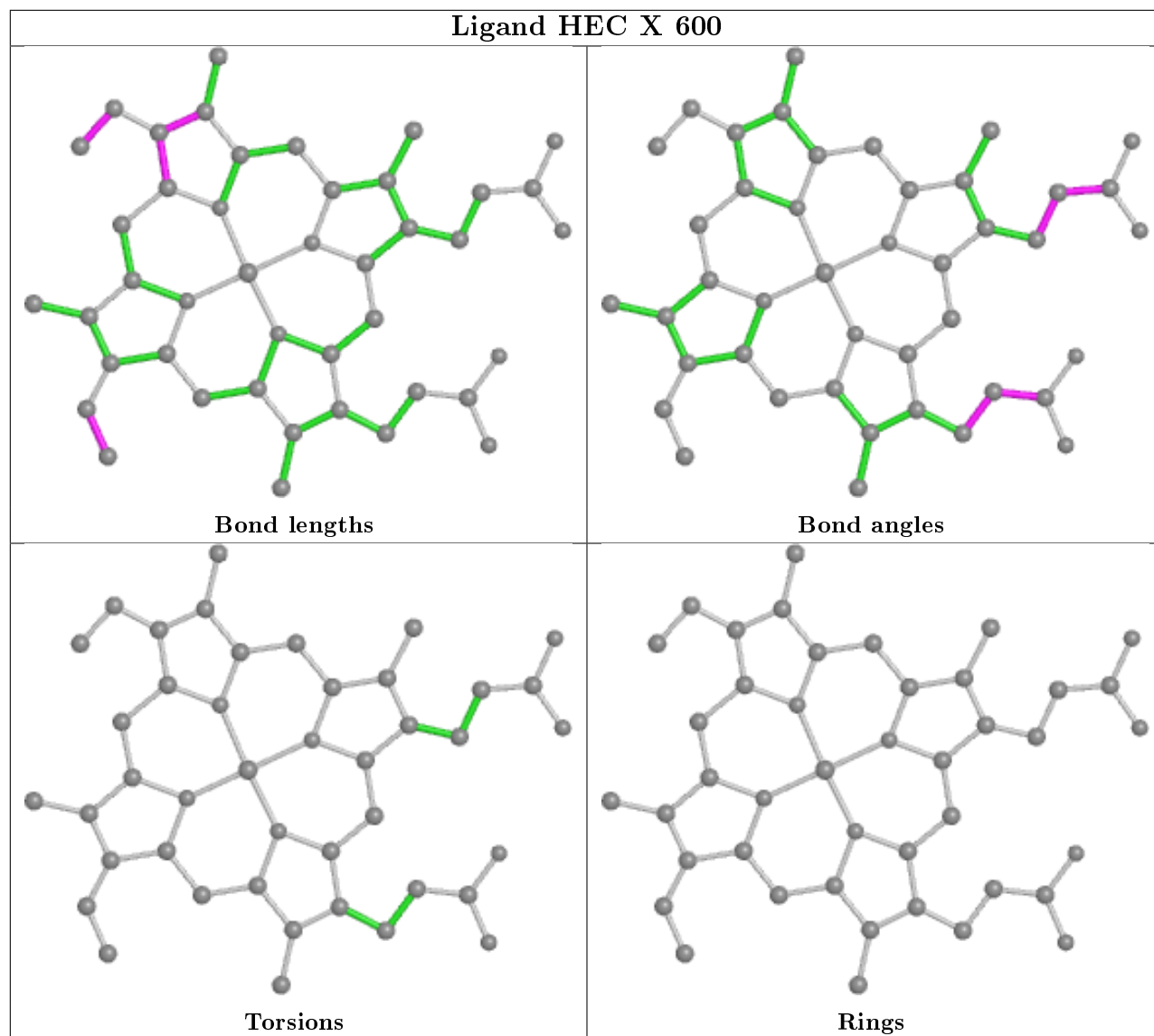




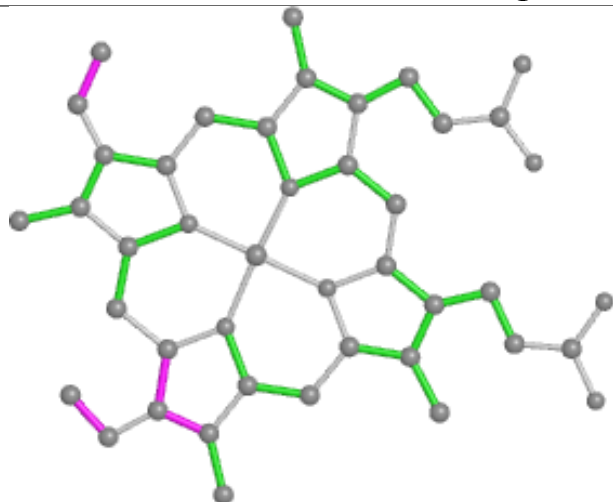


## Ligand HEC T 605

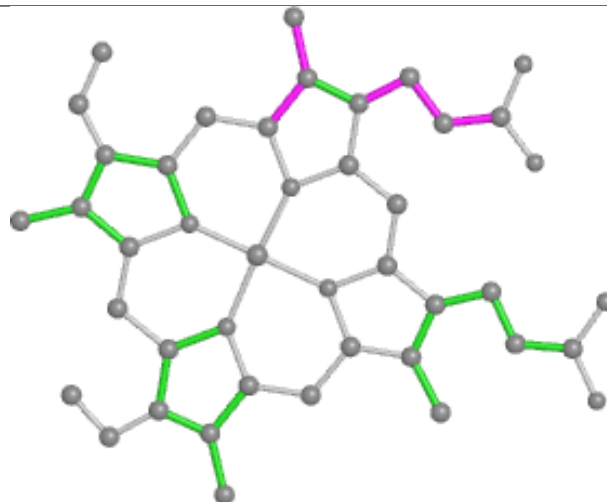




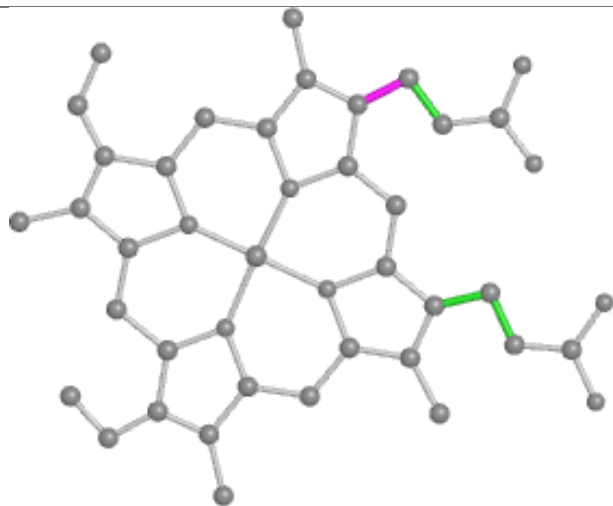
## Ligand HEC F 605



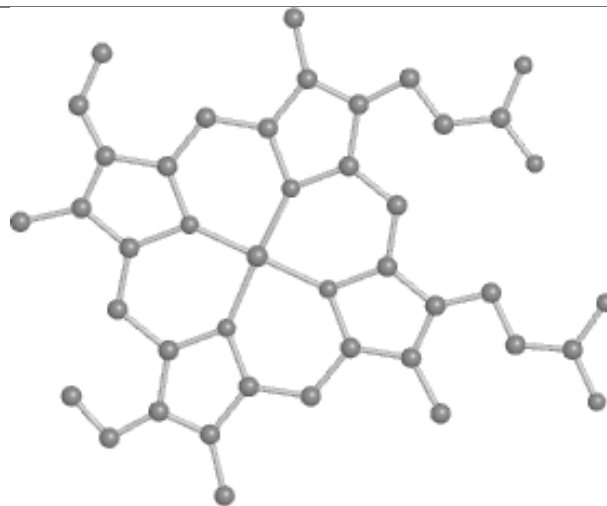
Bond lengths



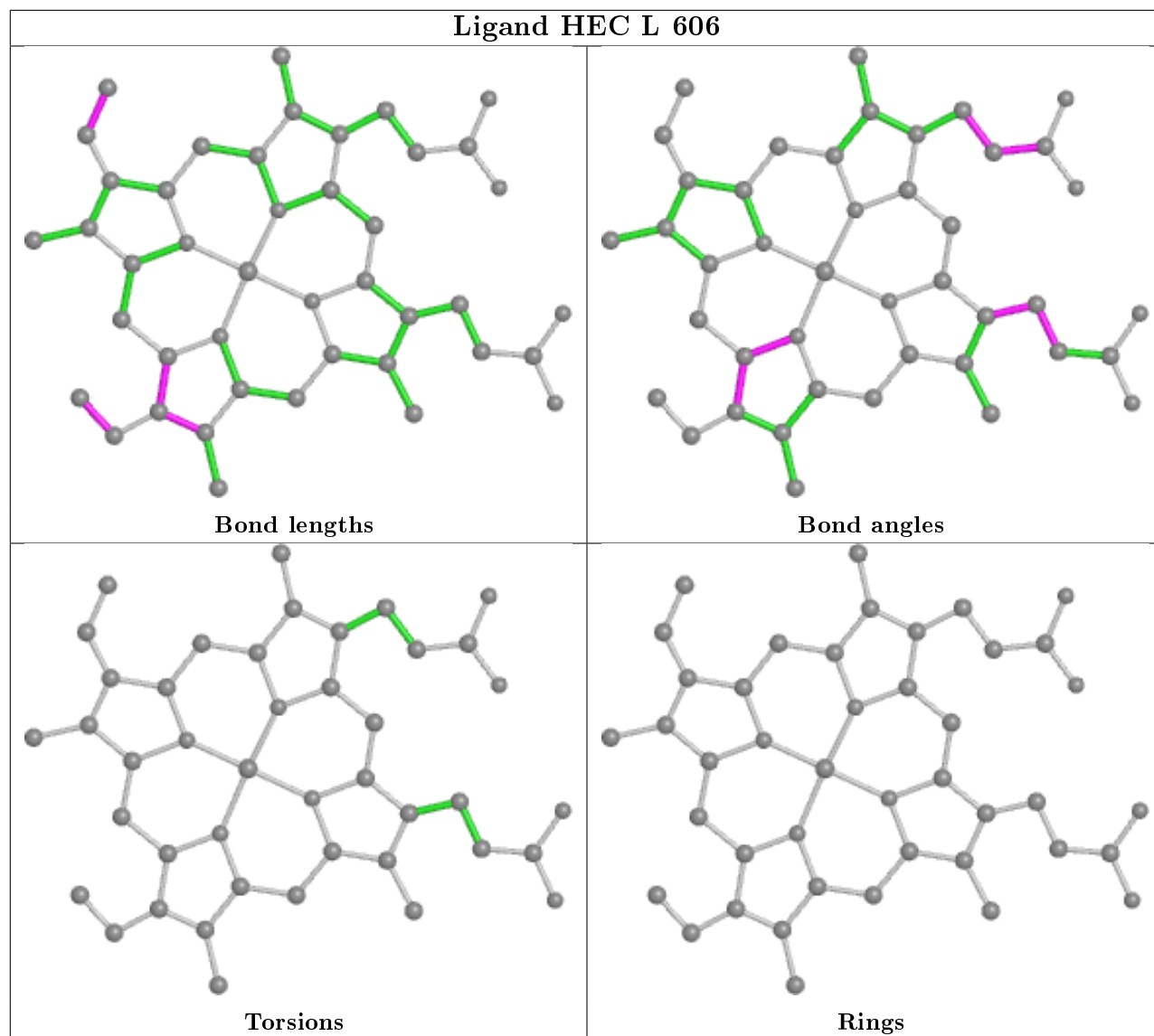
Bond angles

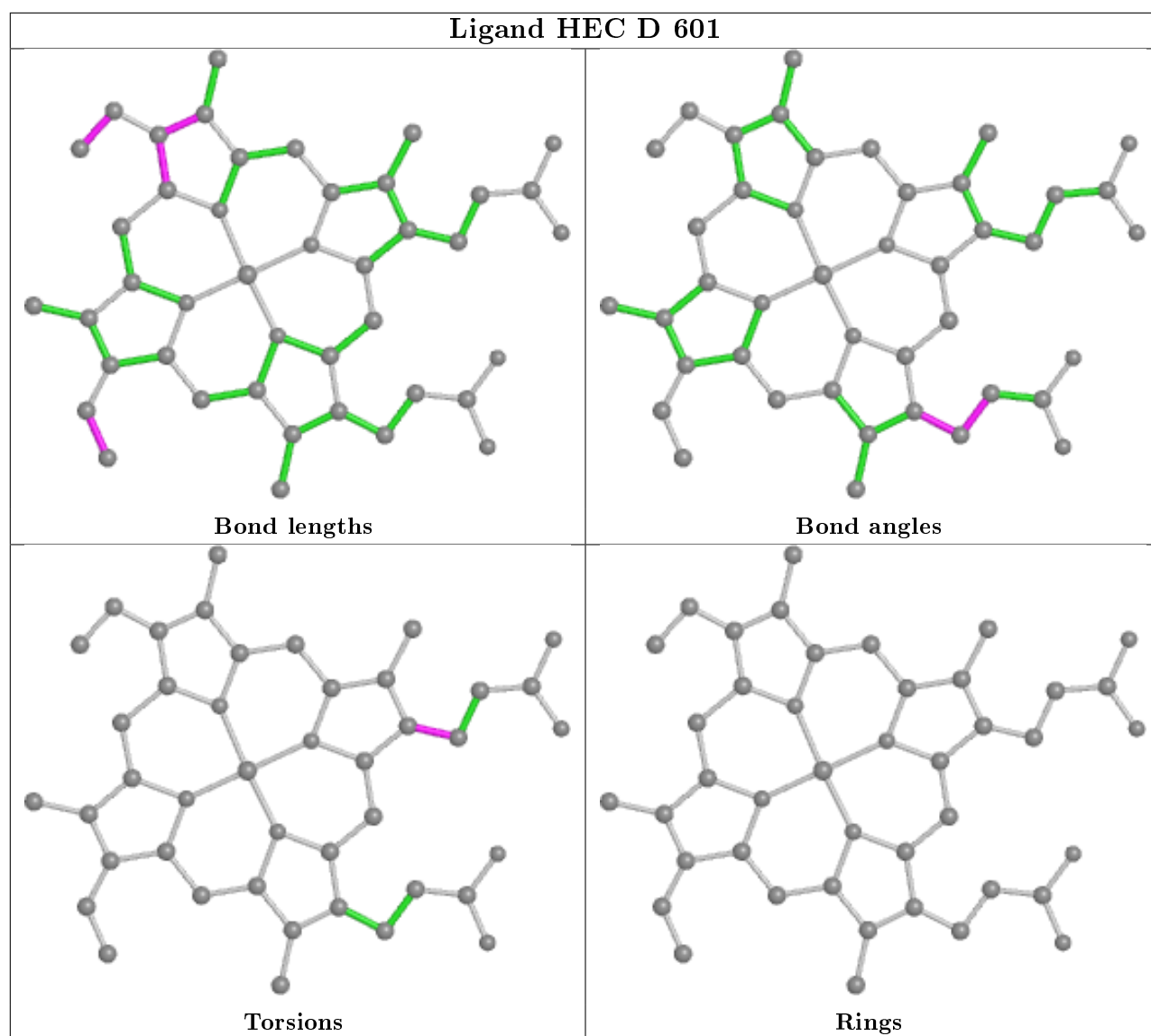


Torsions

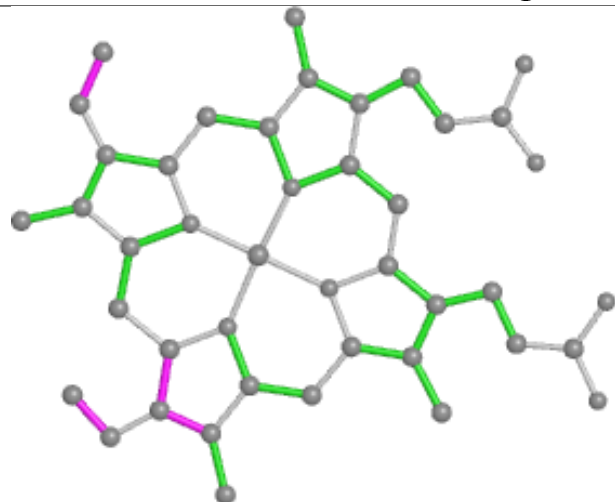


Rings

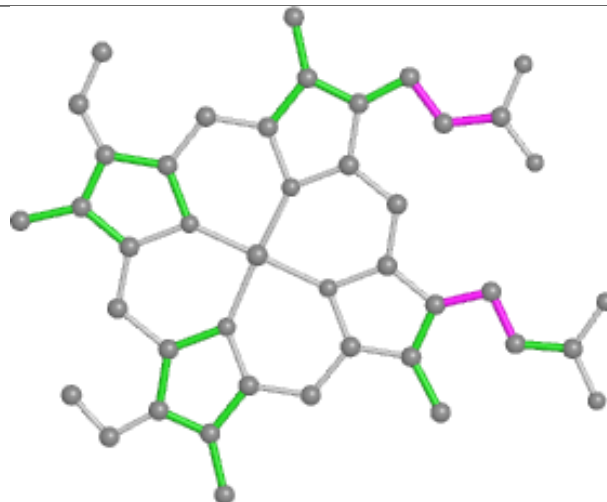




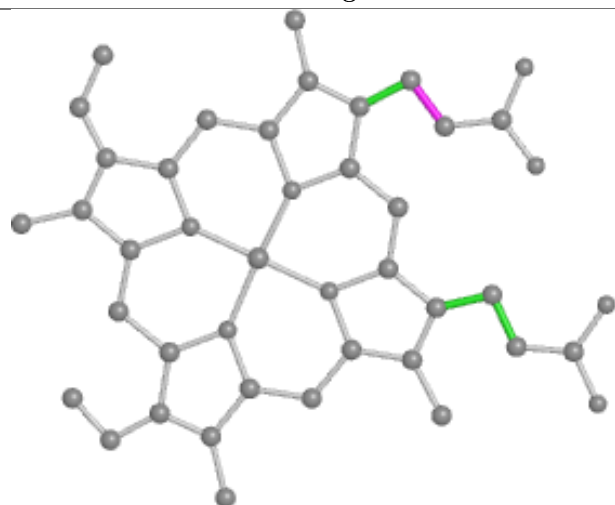
## Ligand HEC L 602



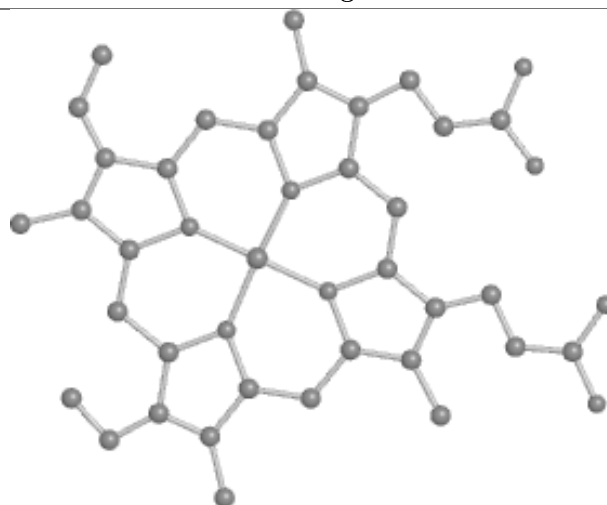
Bond lengths



Bond angles

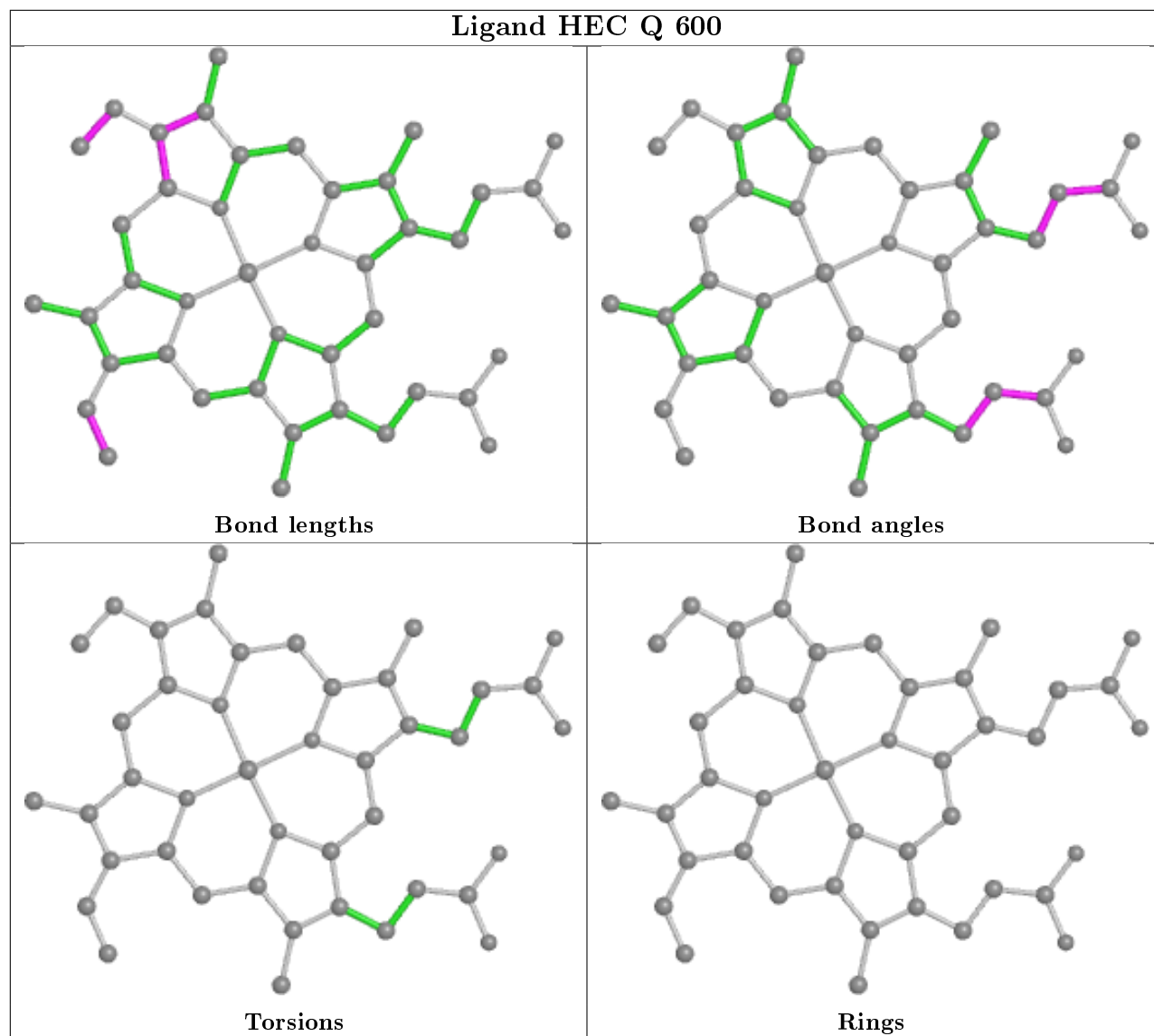


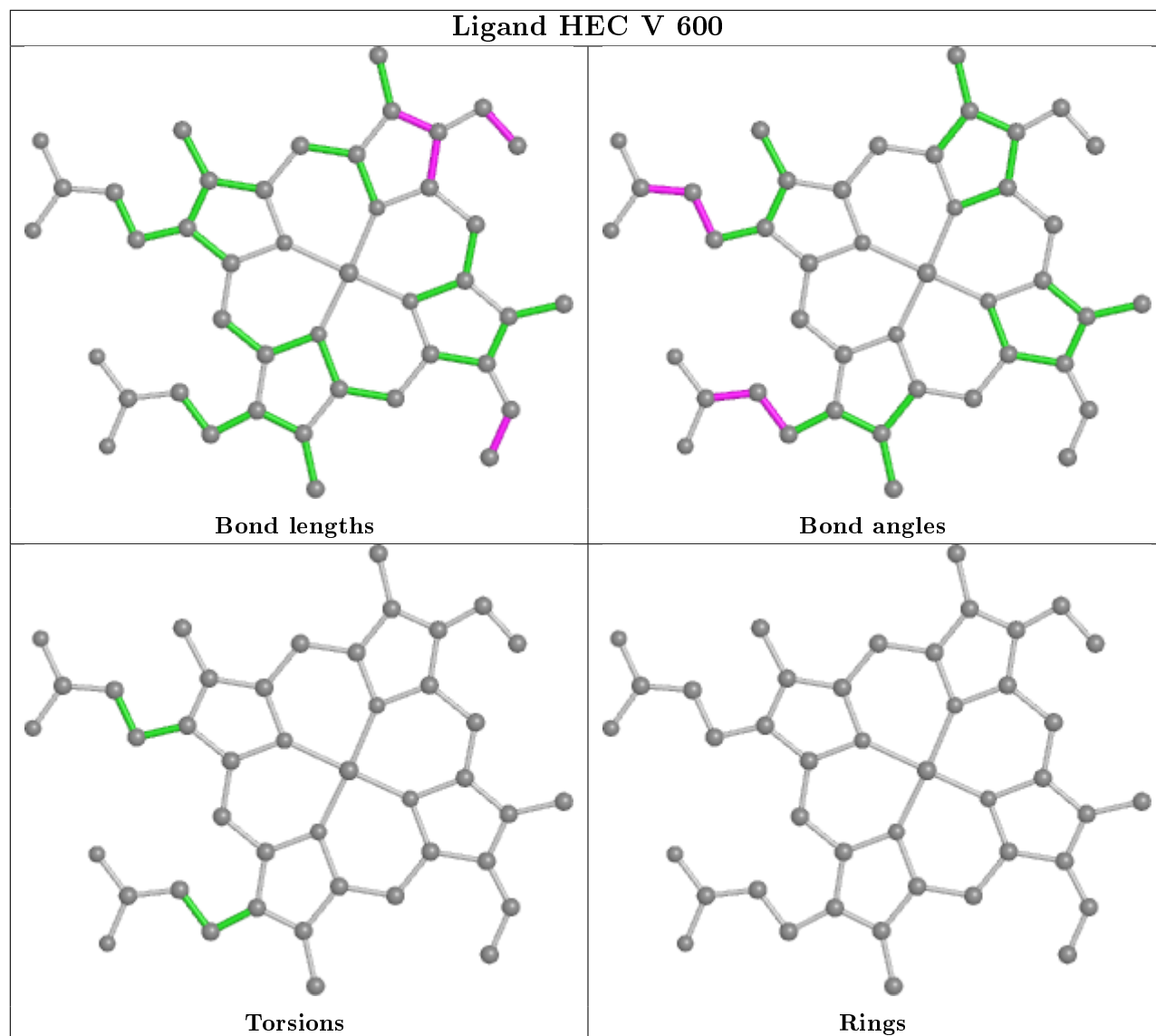
Torsions

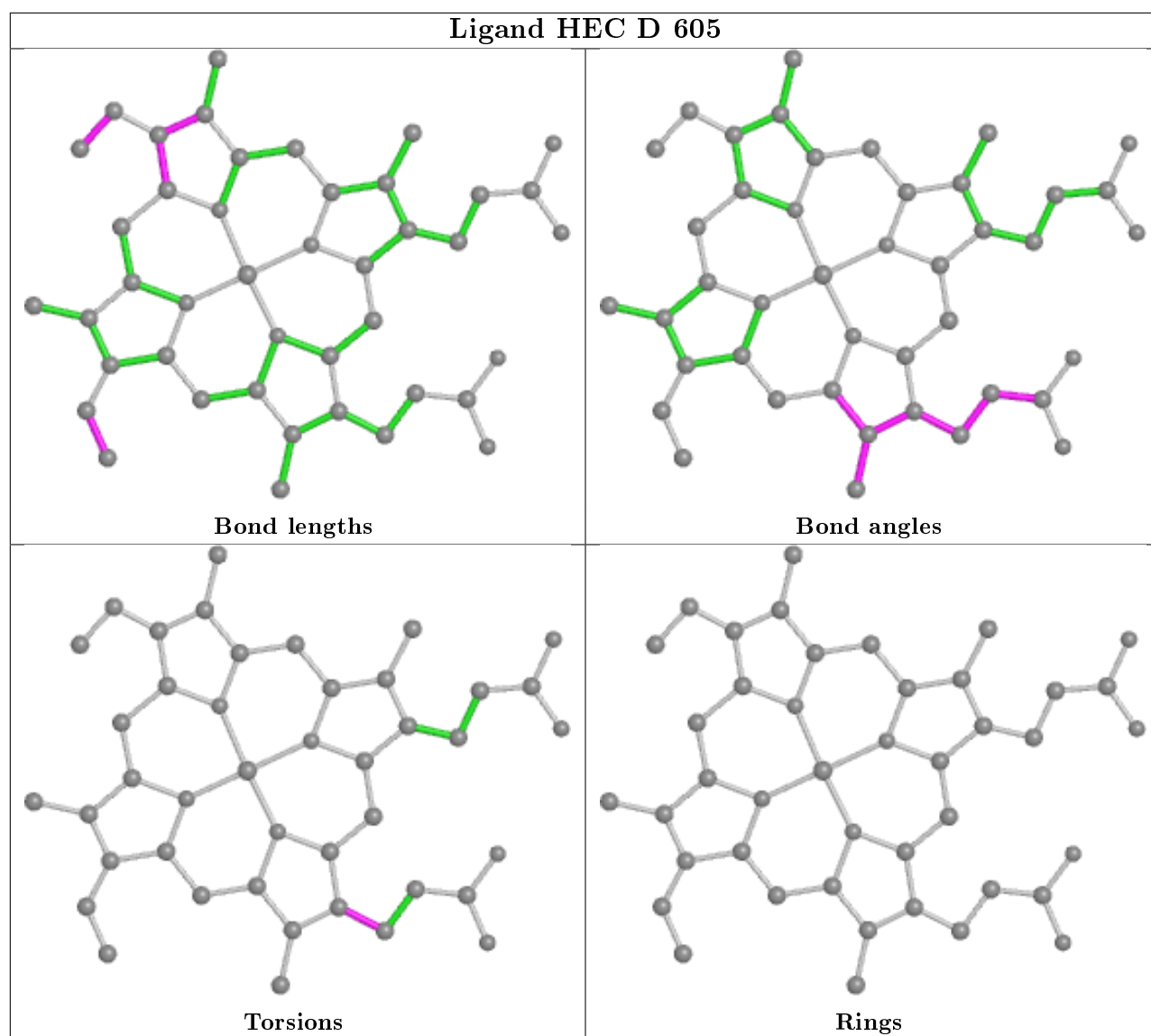


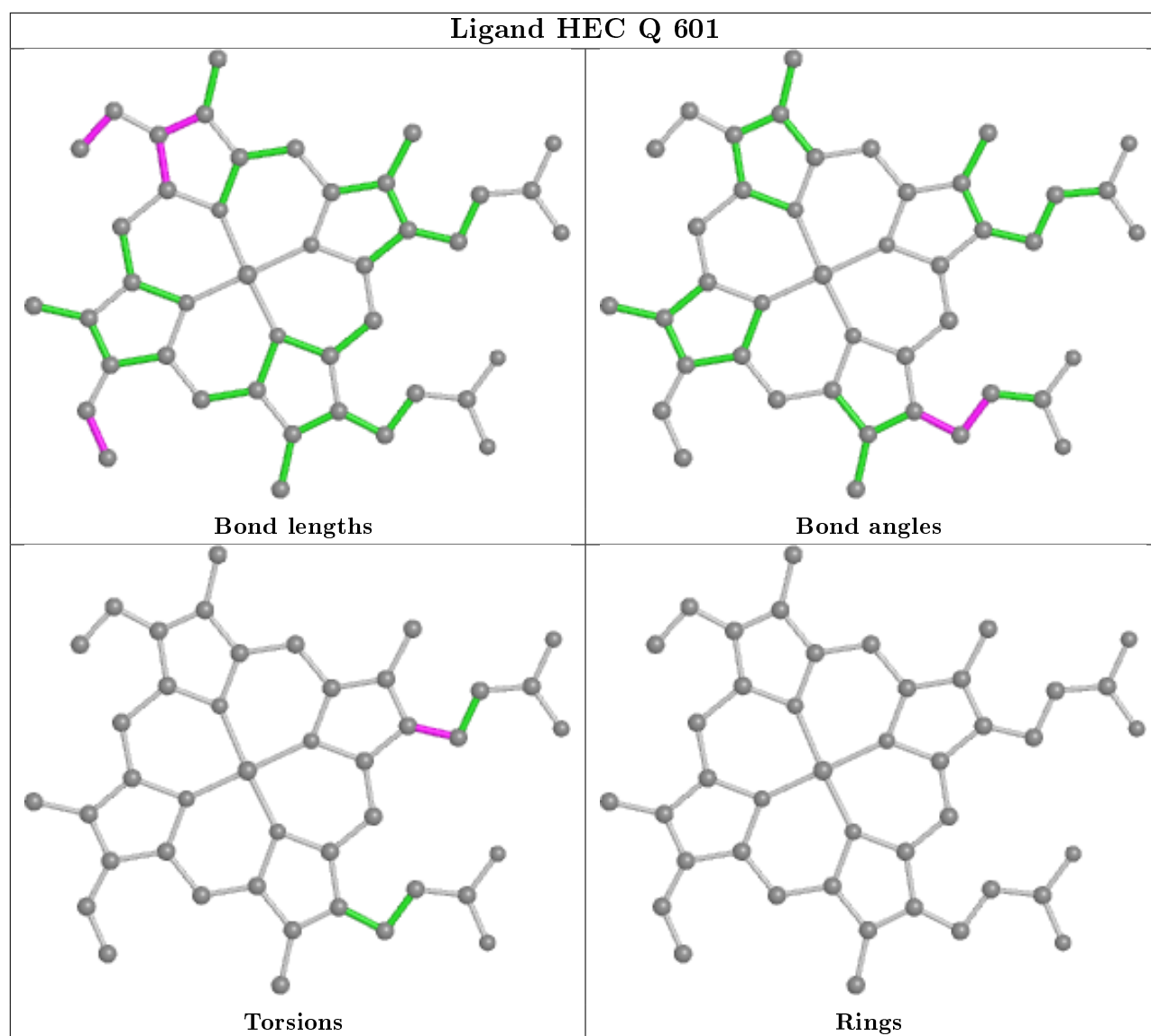
Rings

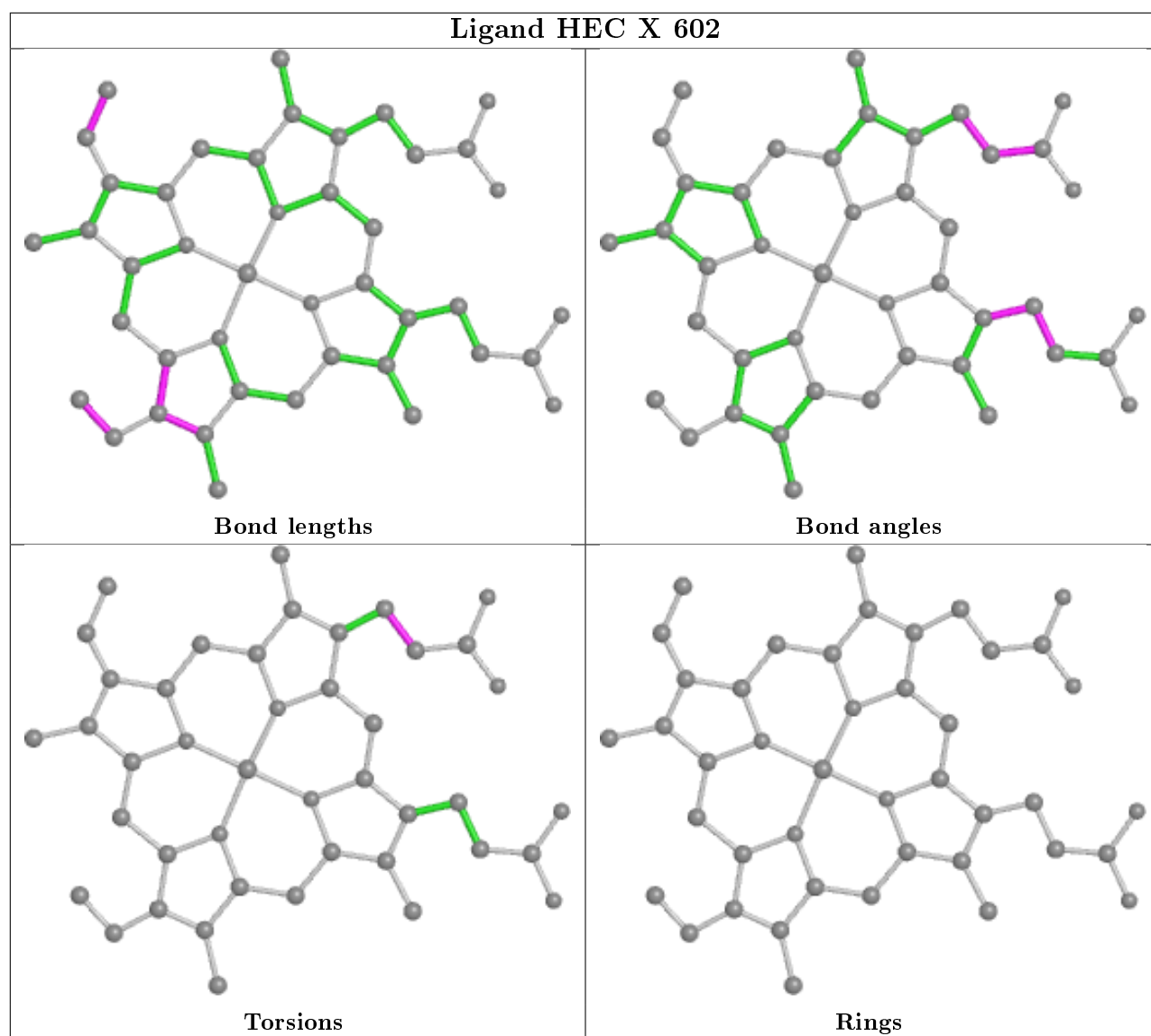


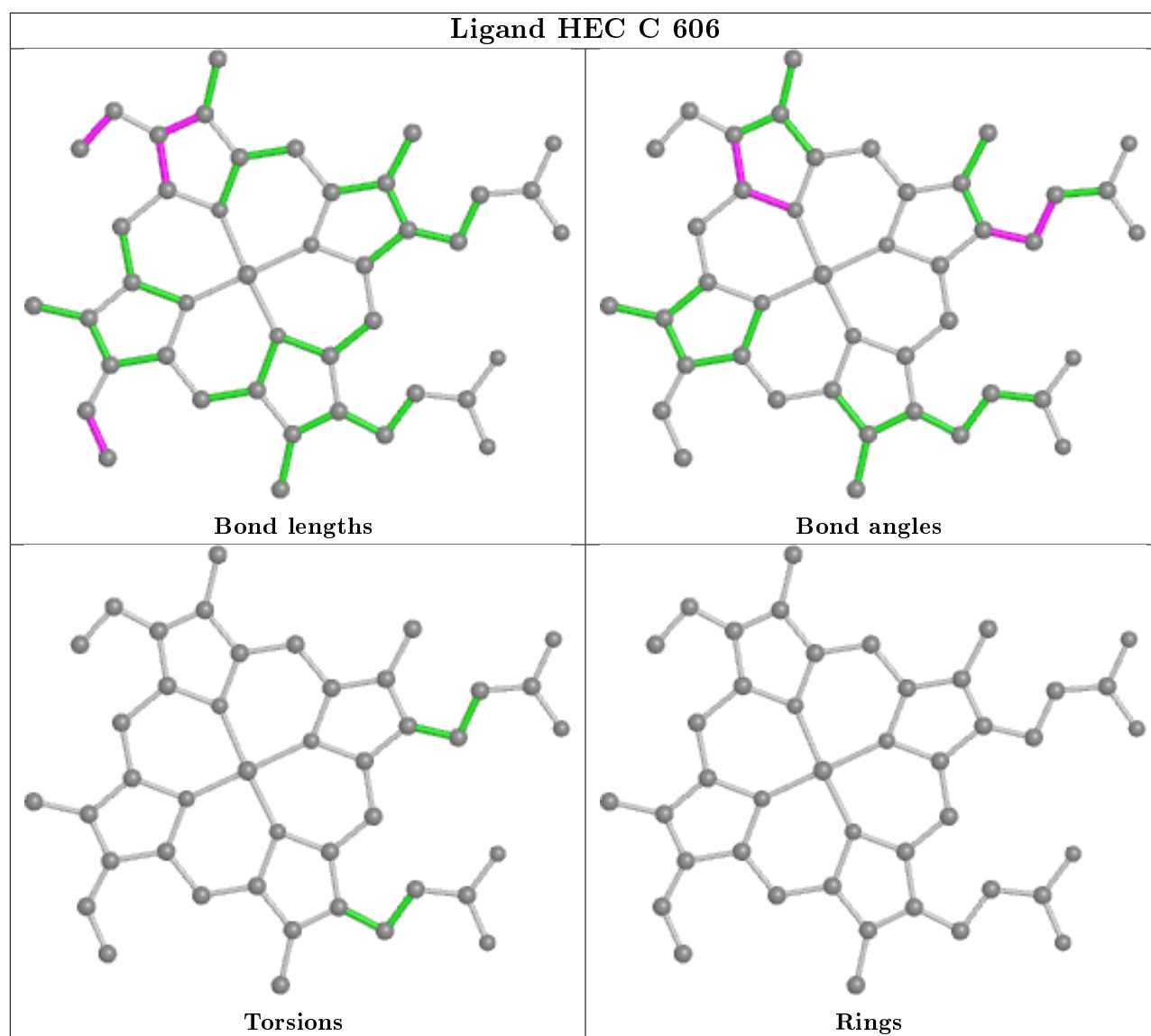


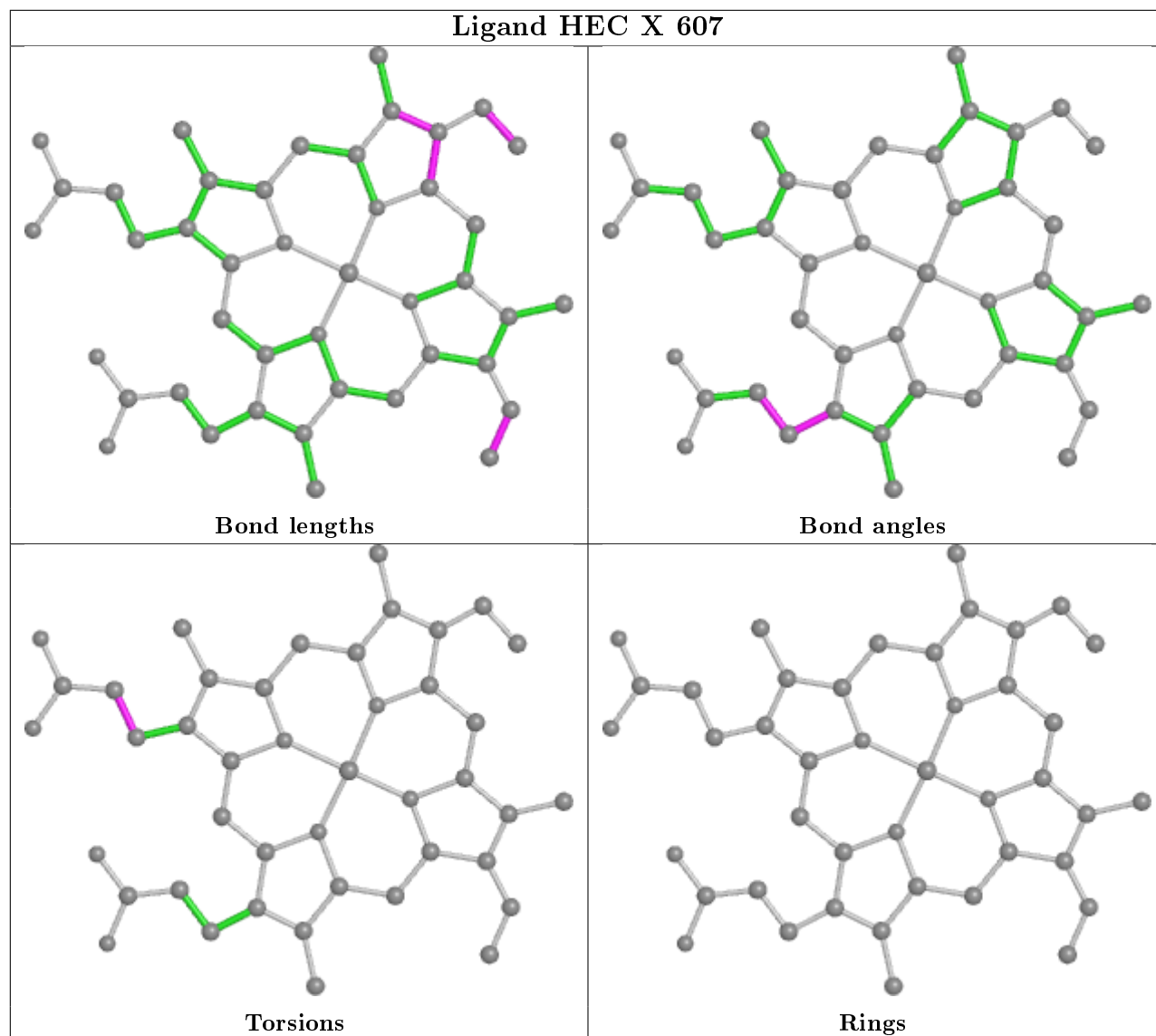


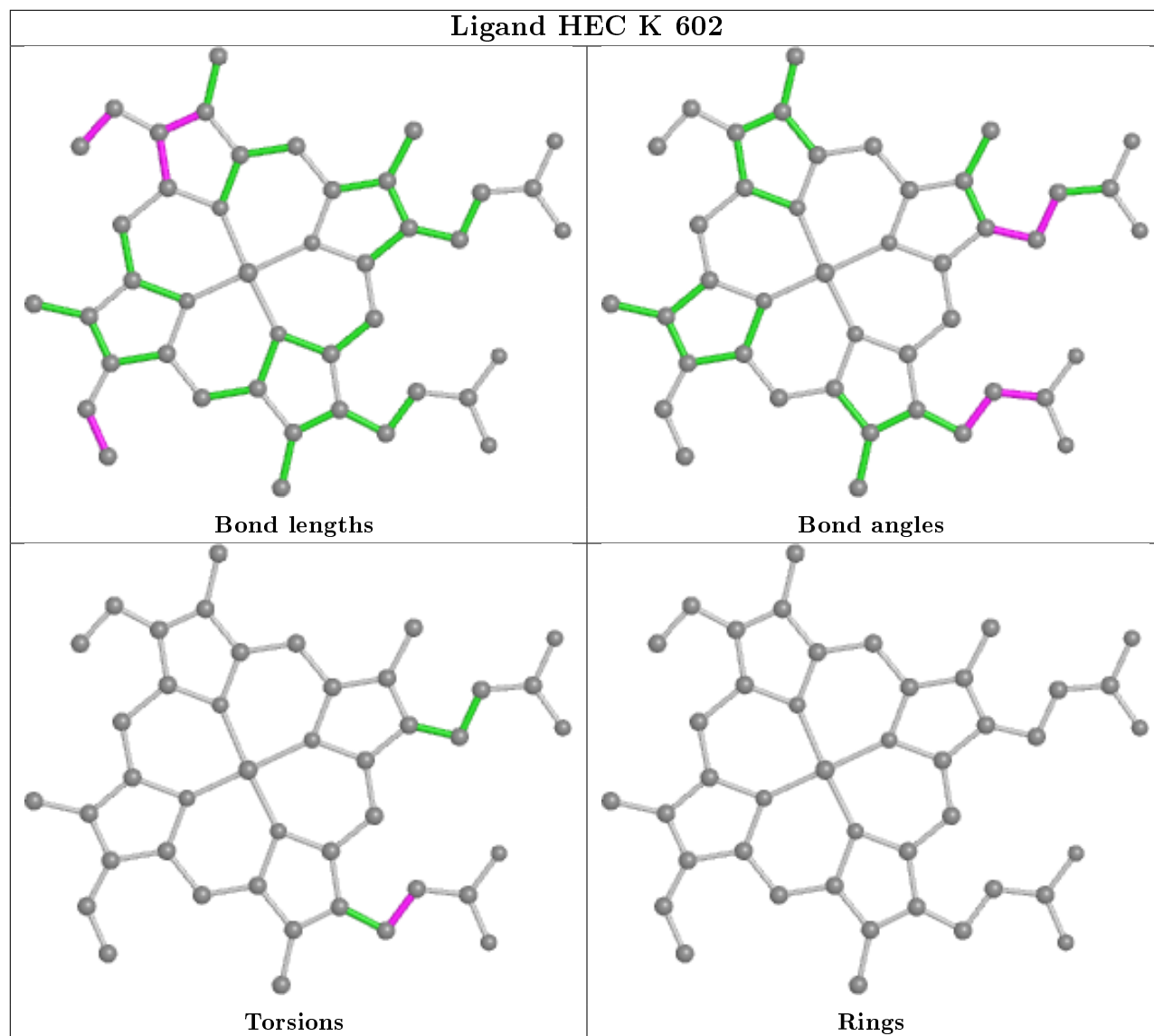




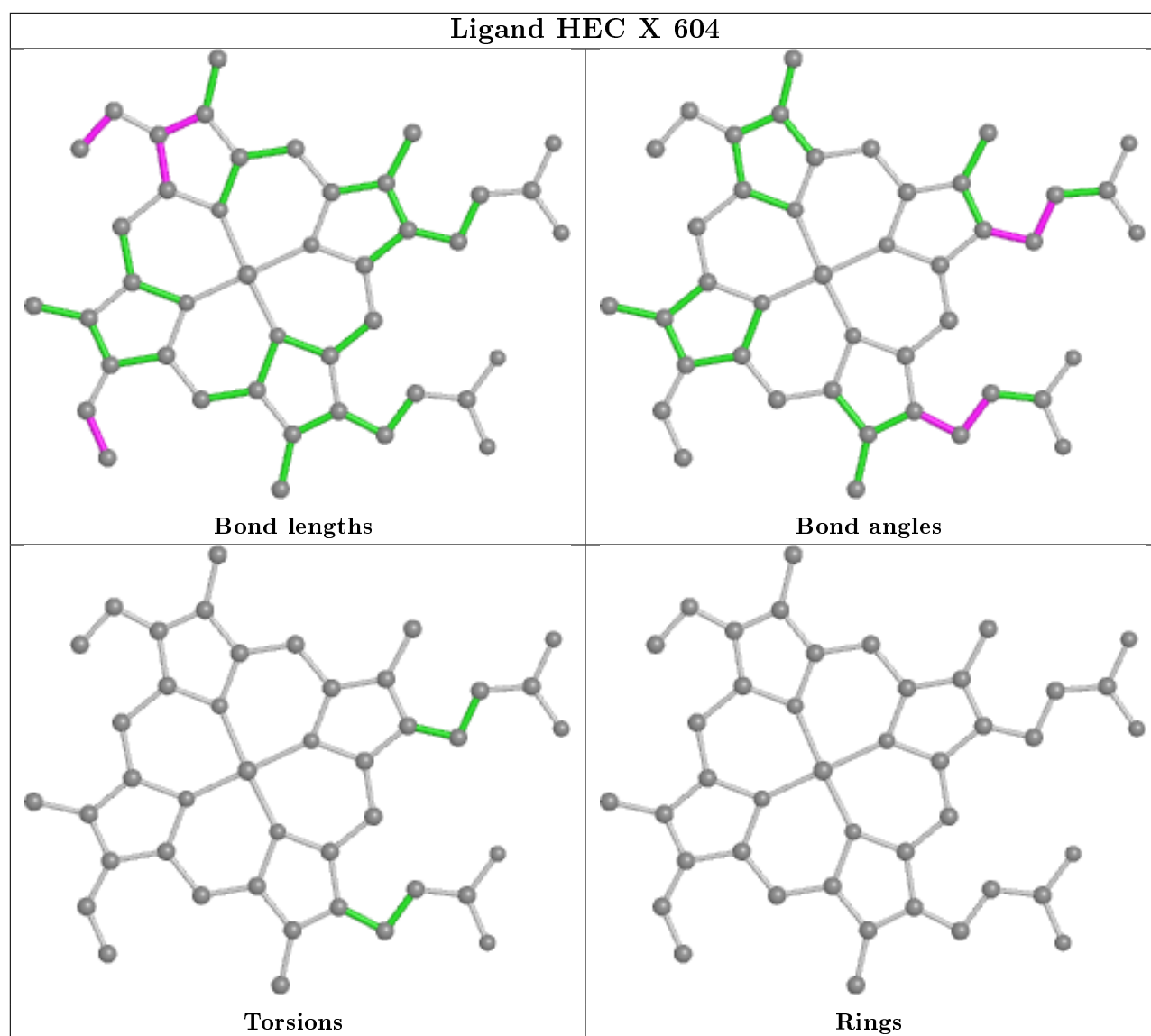


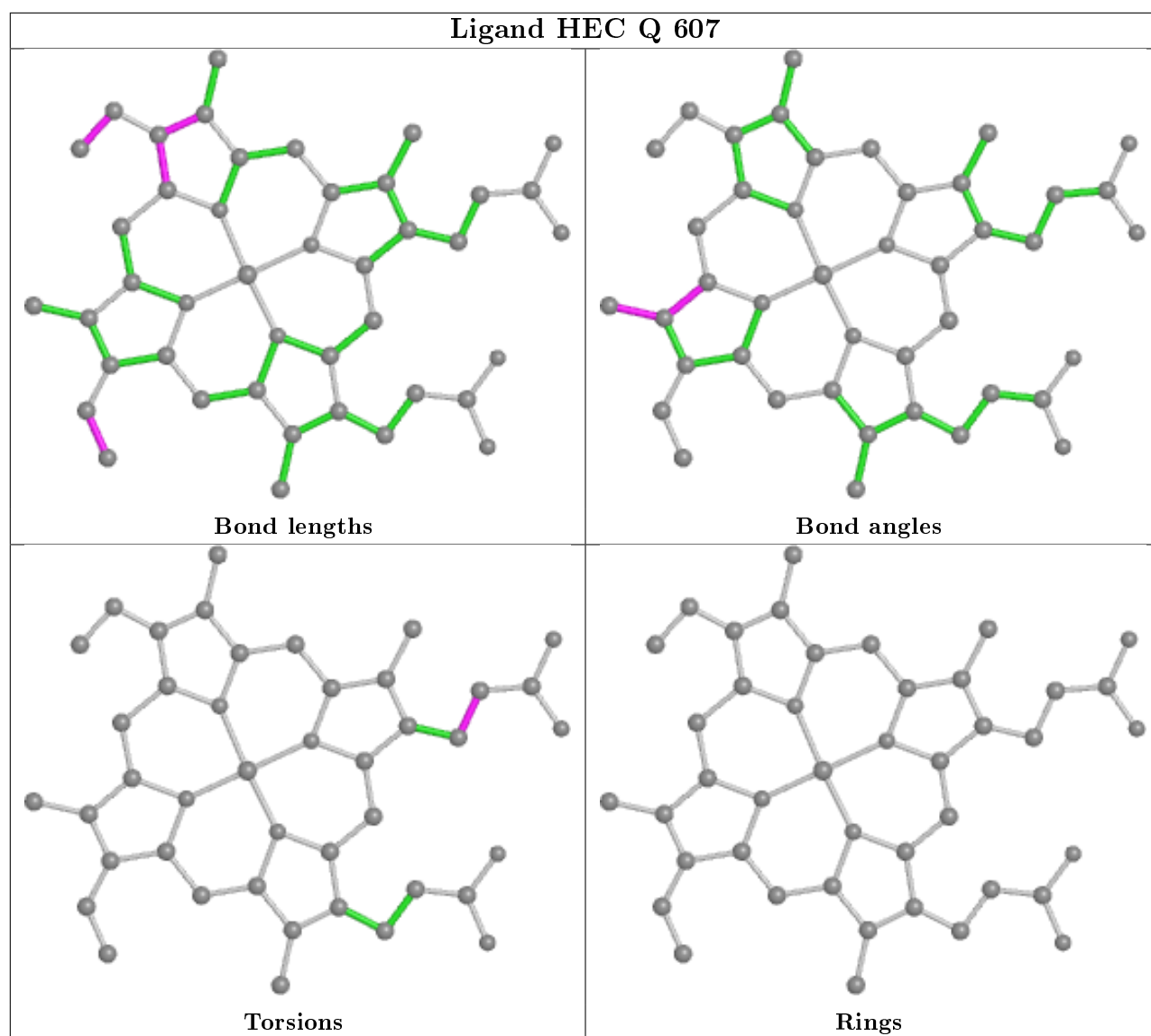


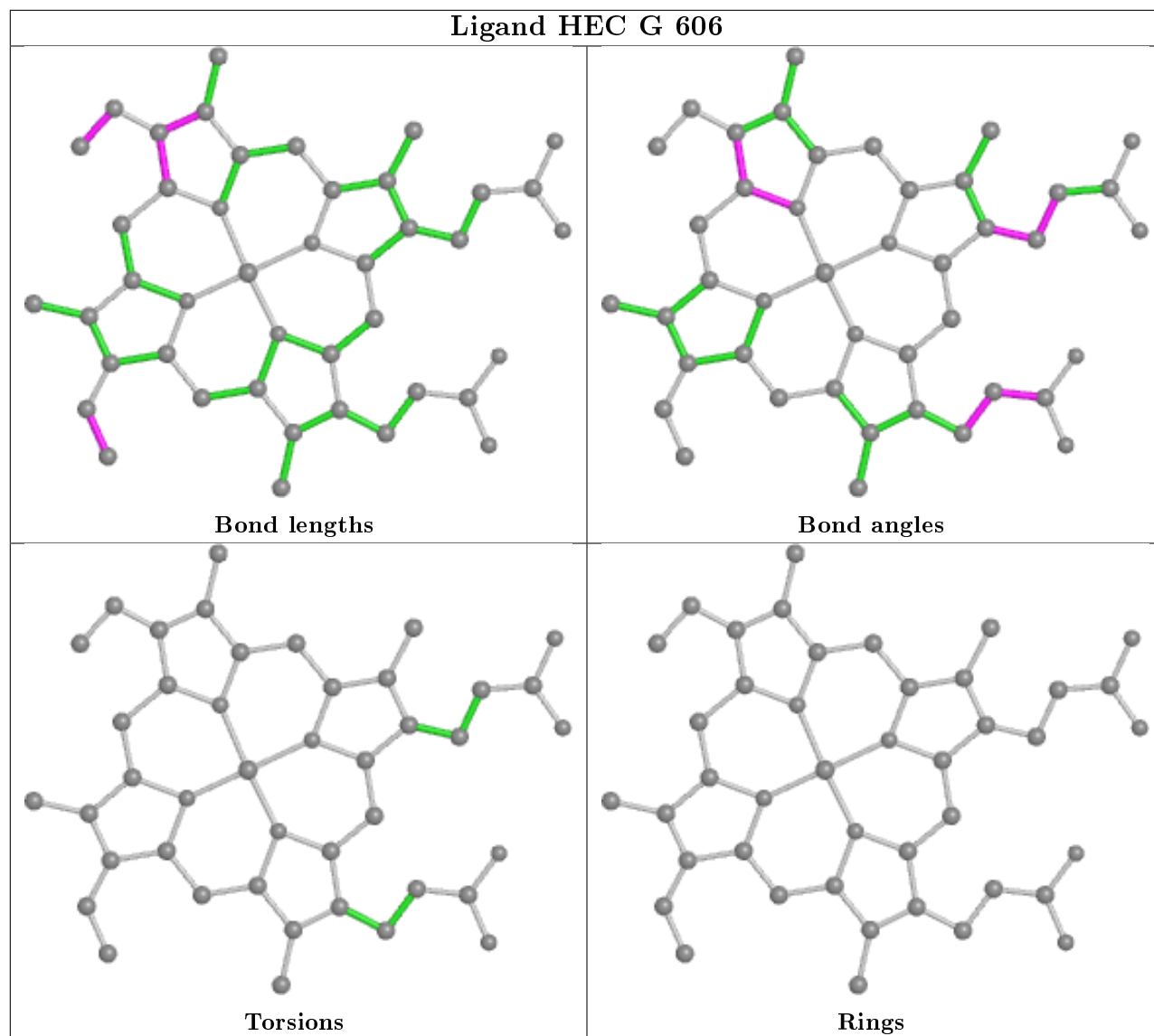


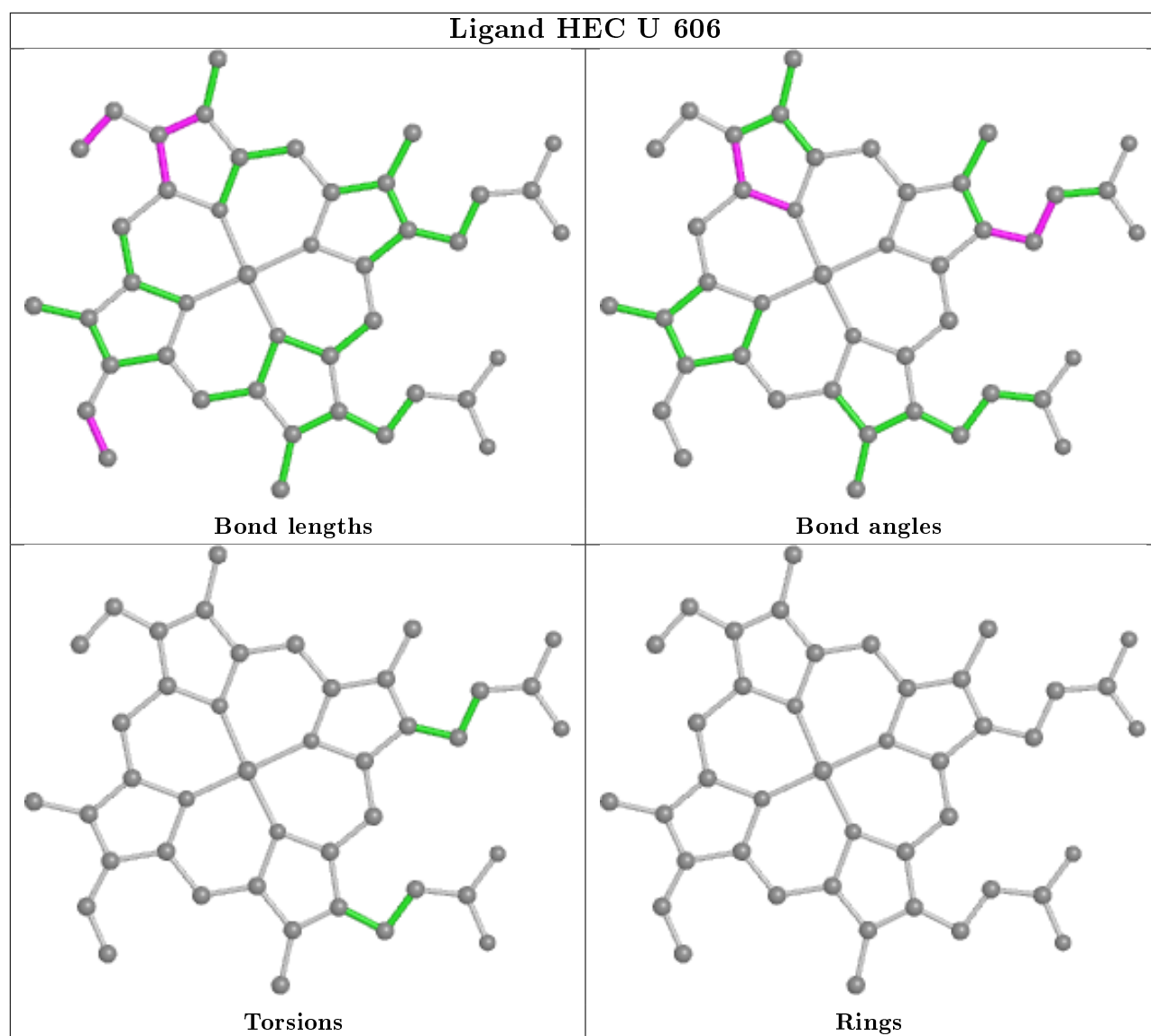




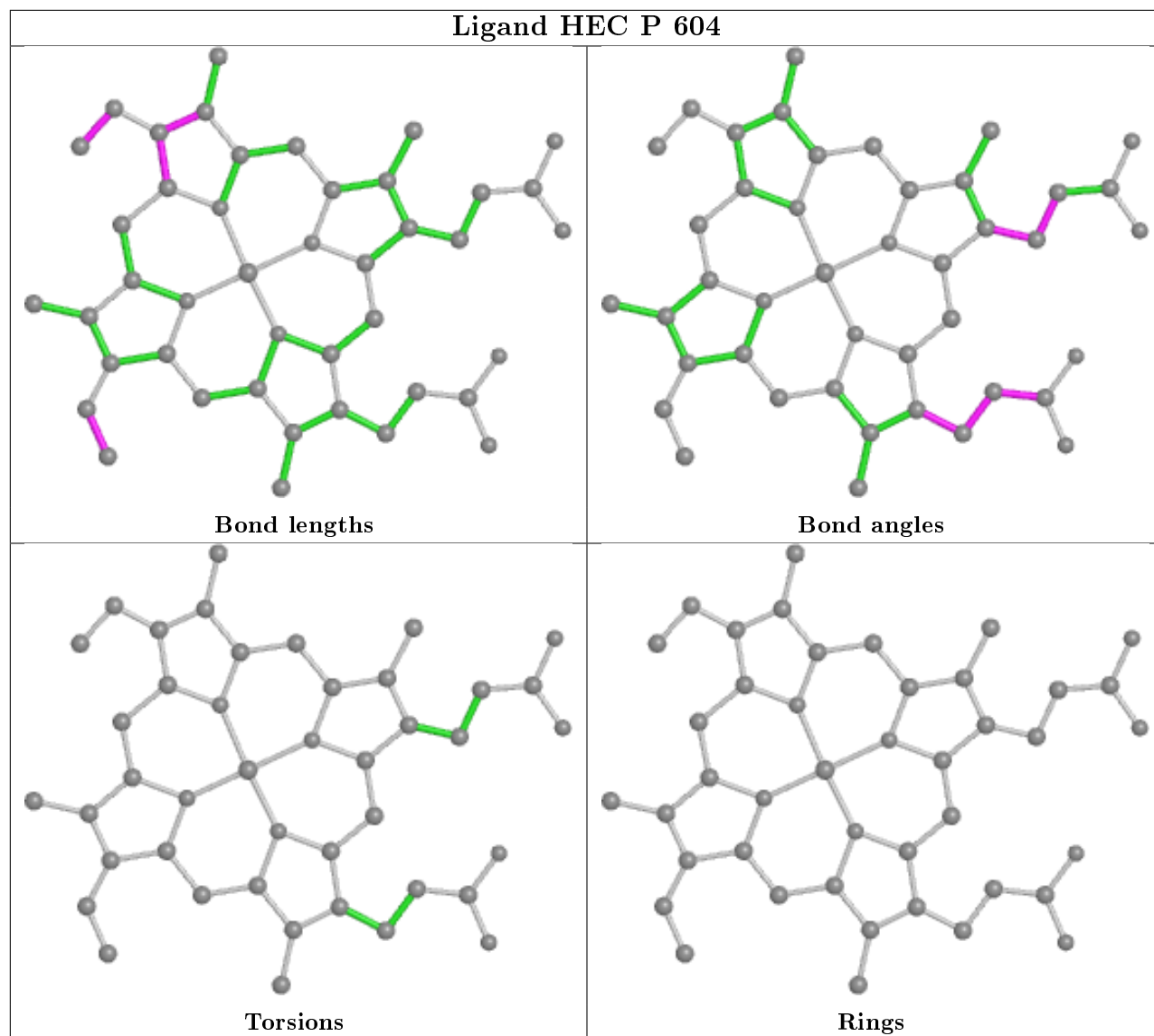


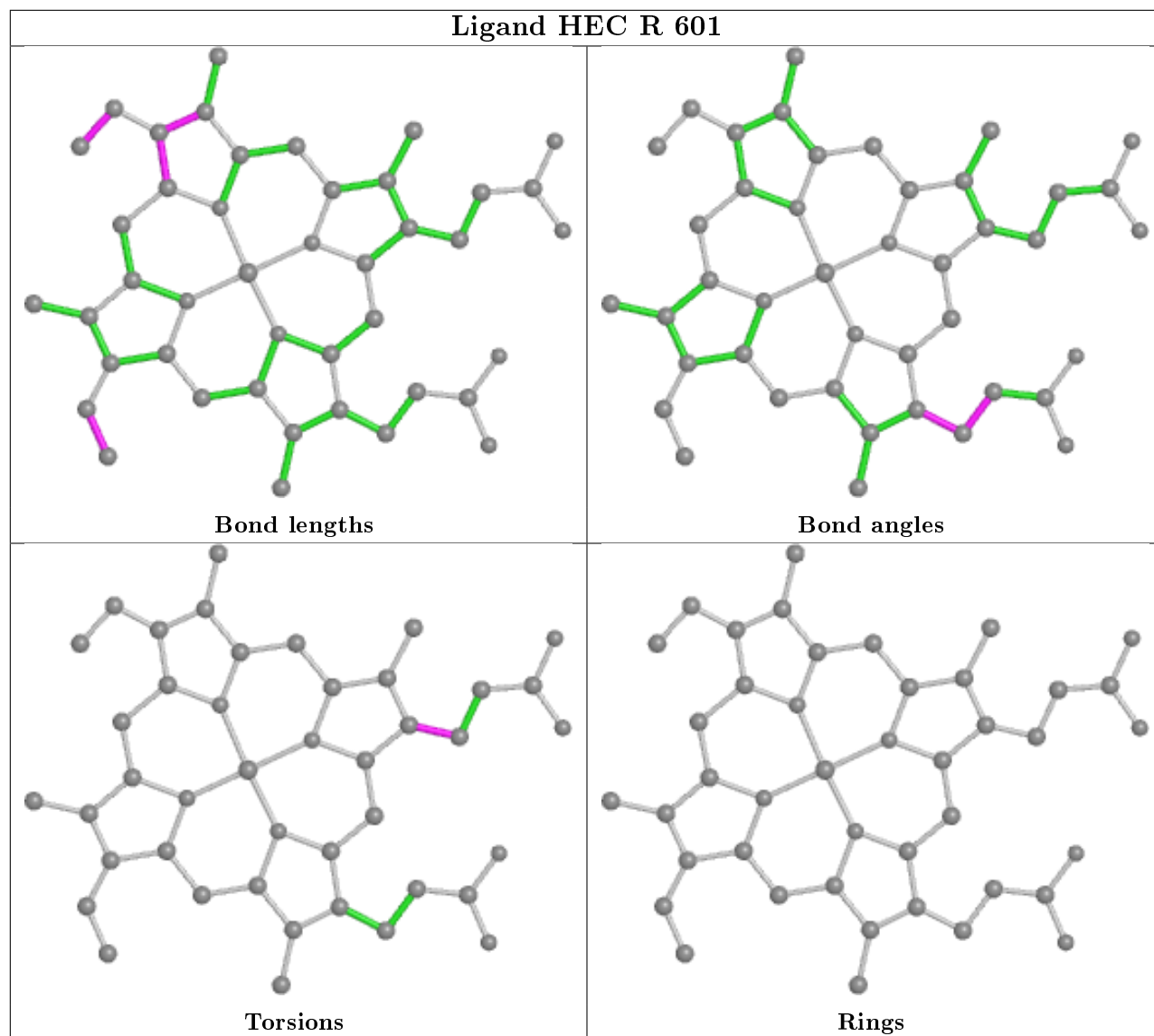


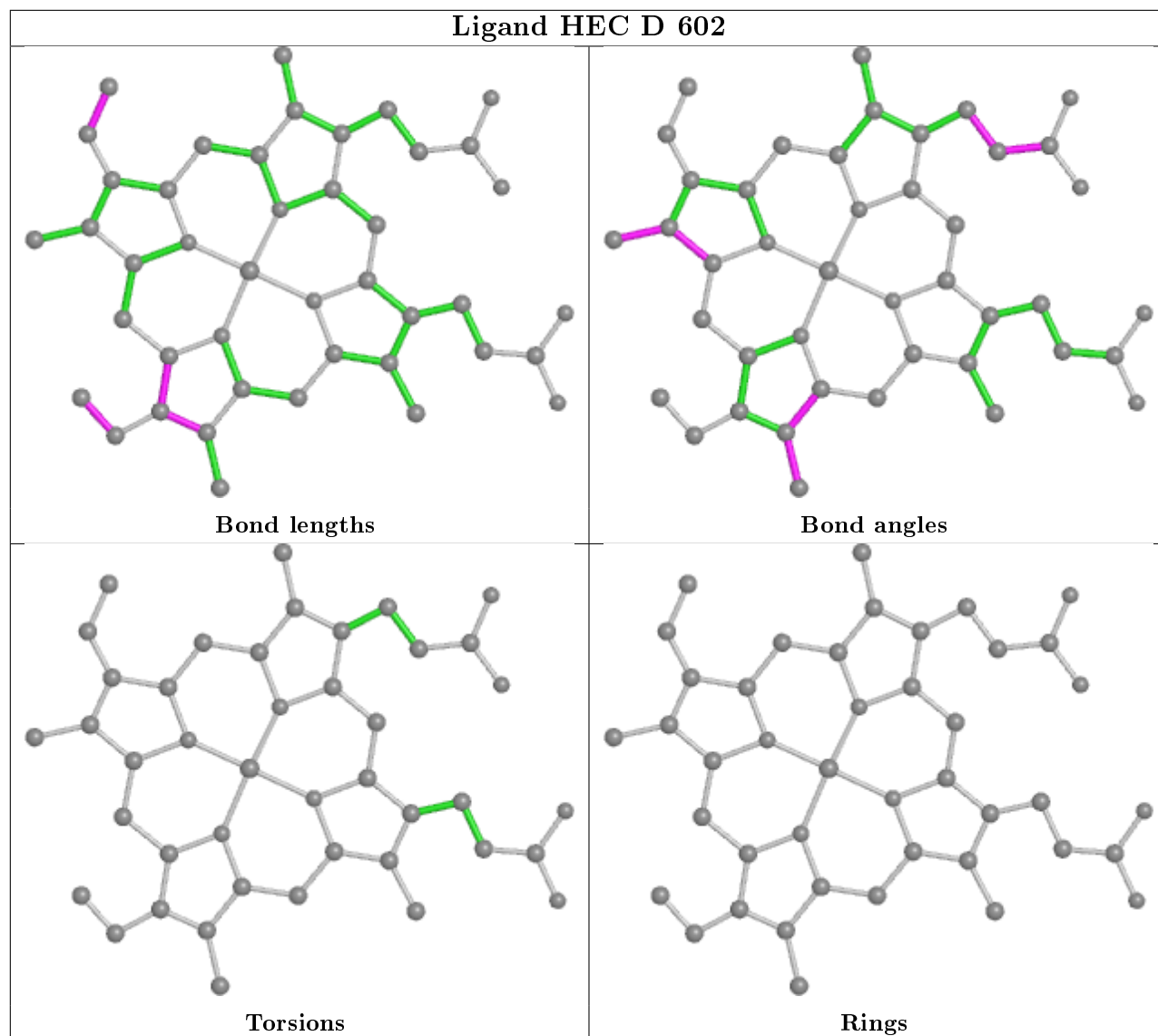




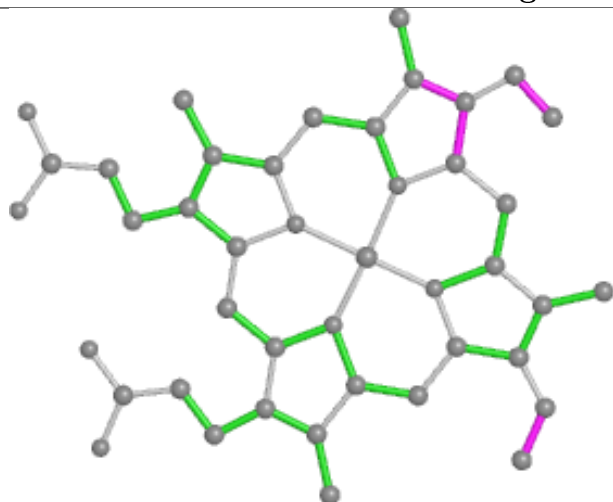
## Ligand HEC P 604



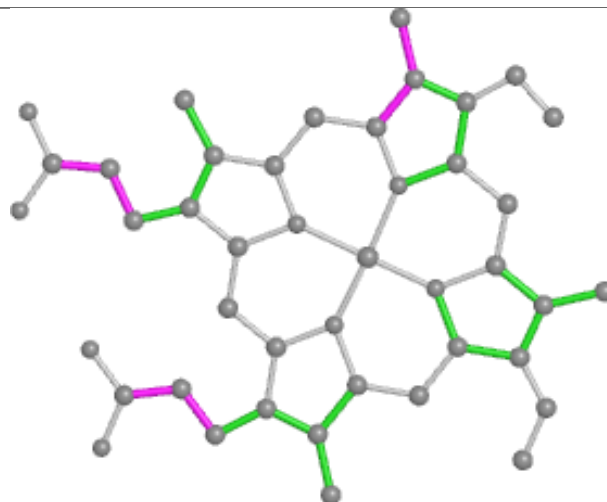




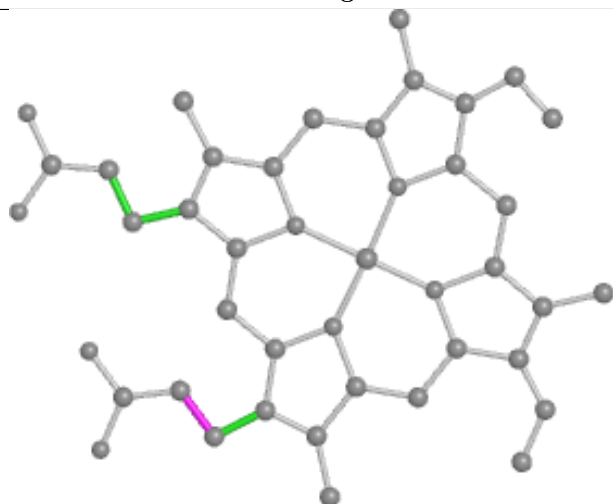
## Ligand HEC I 602



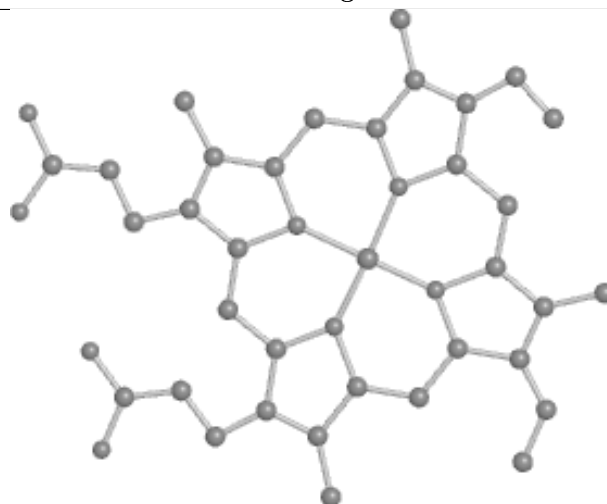
Bond lengths



Bond angles

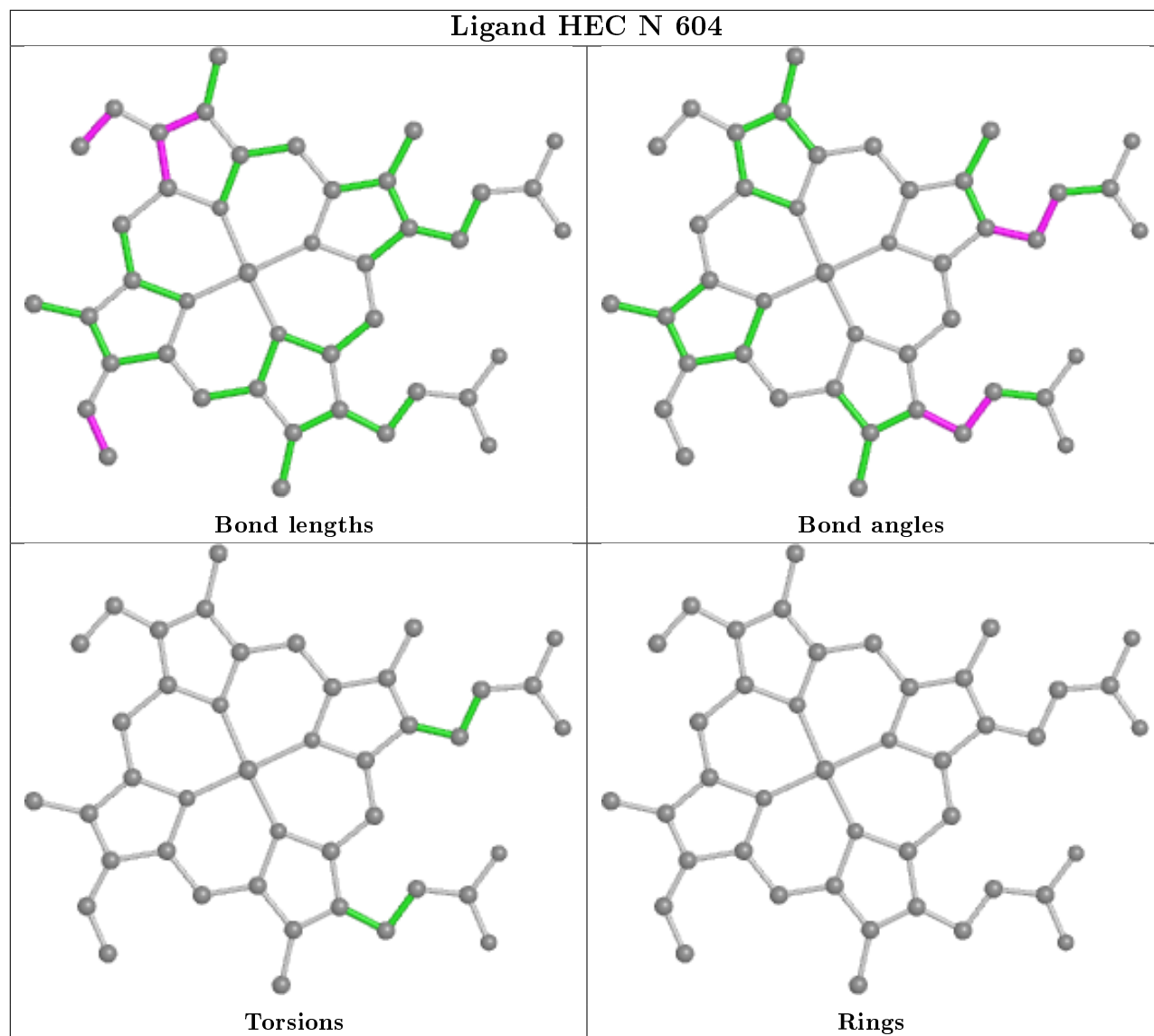


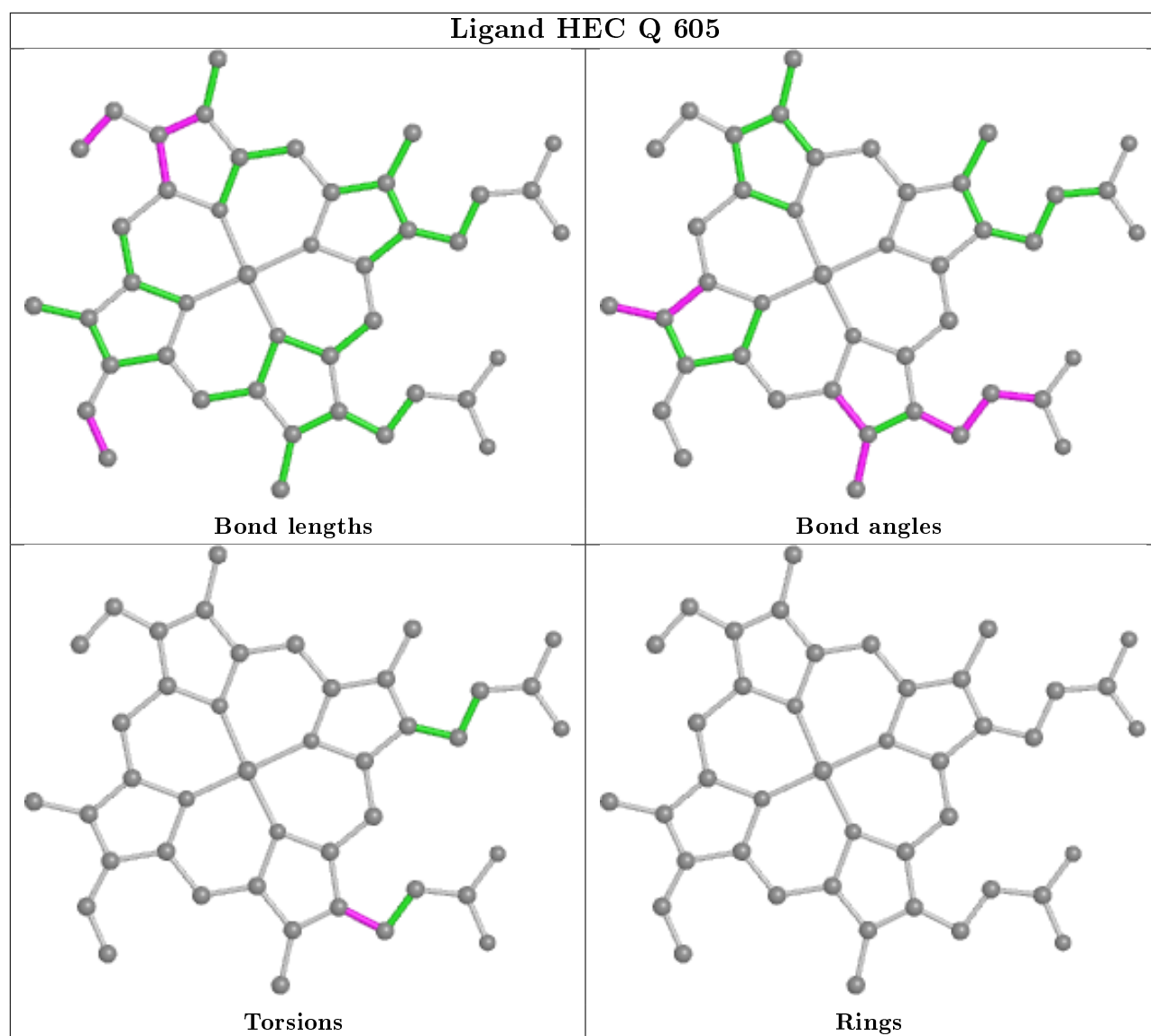
Torsions



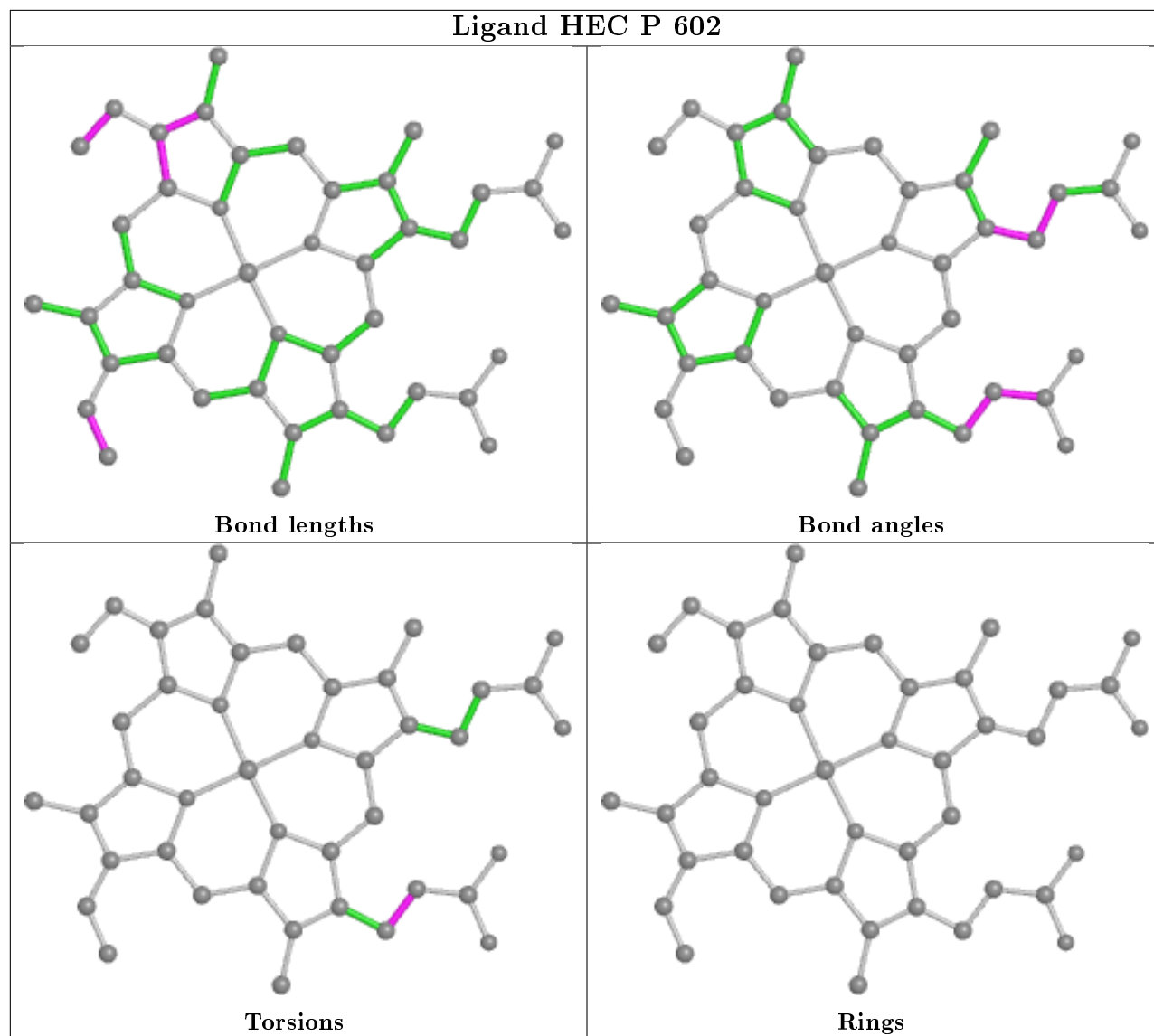
Rings

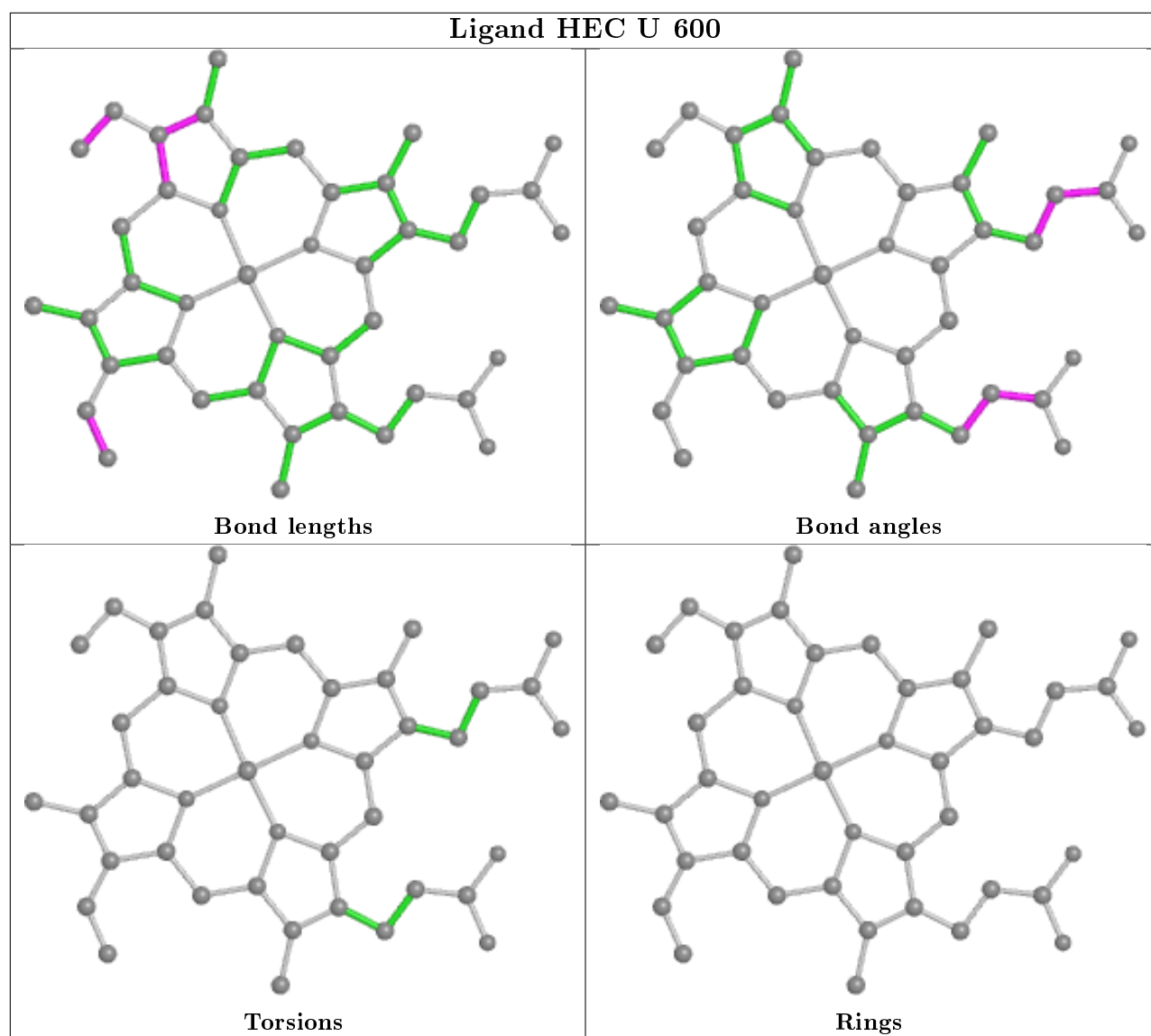


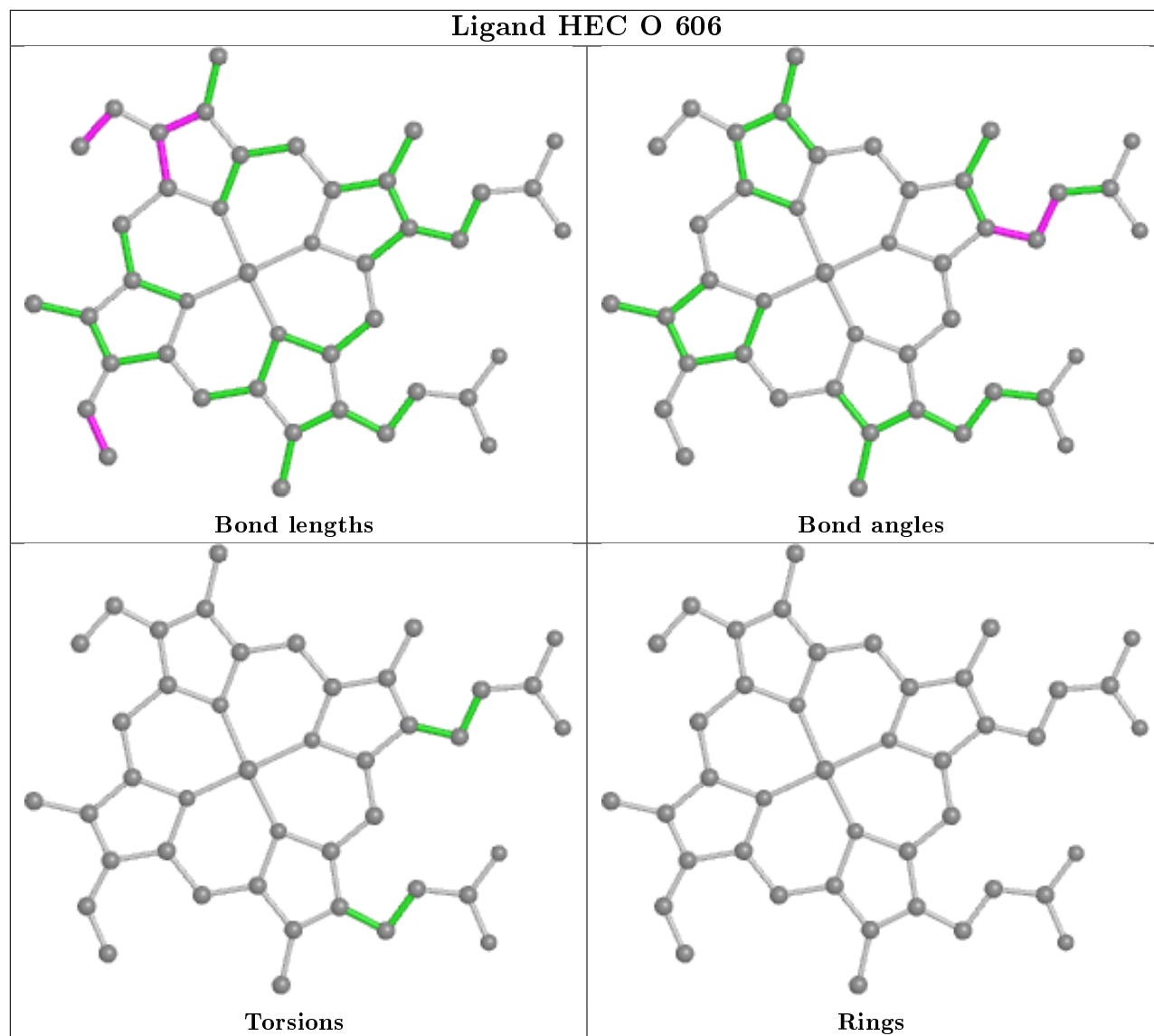




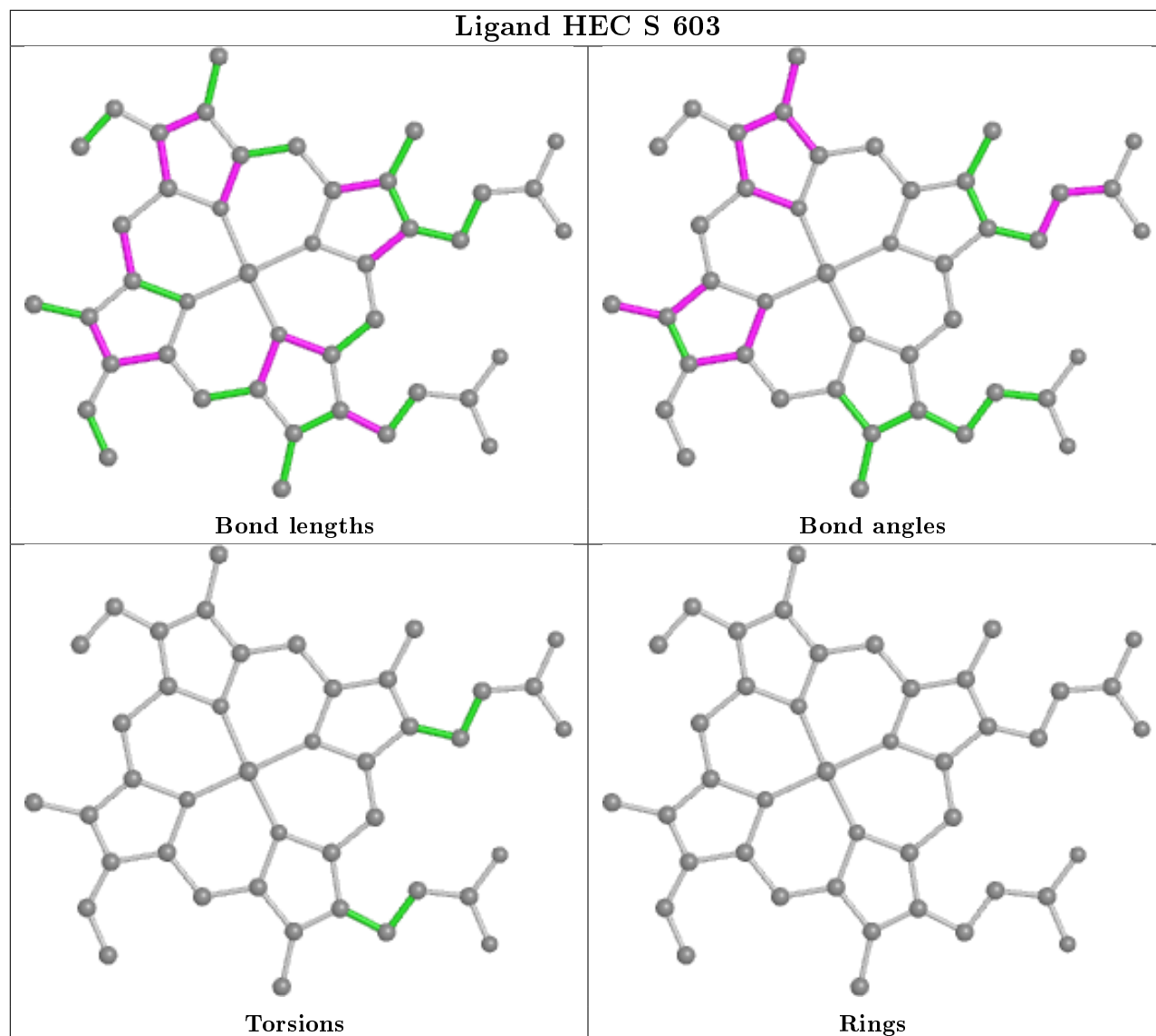
## Ligand HEC P 602

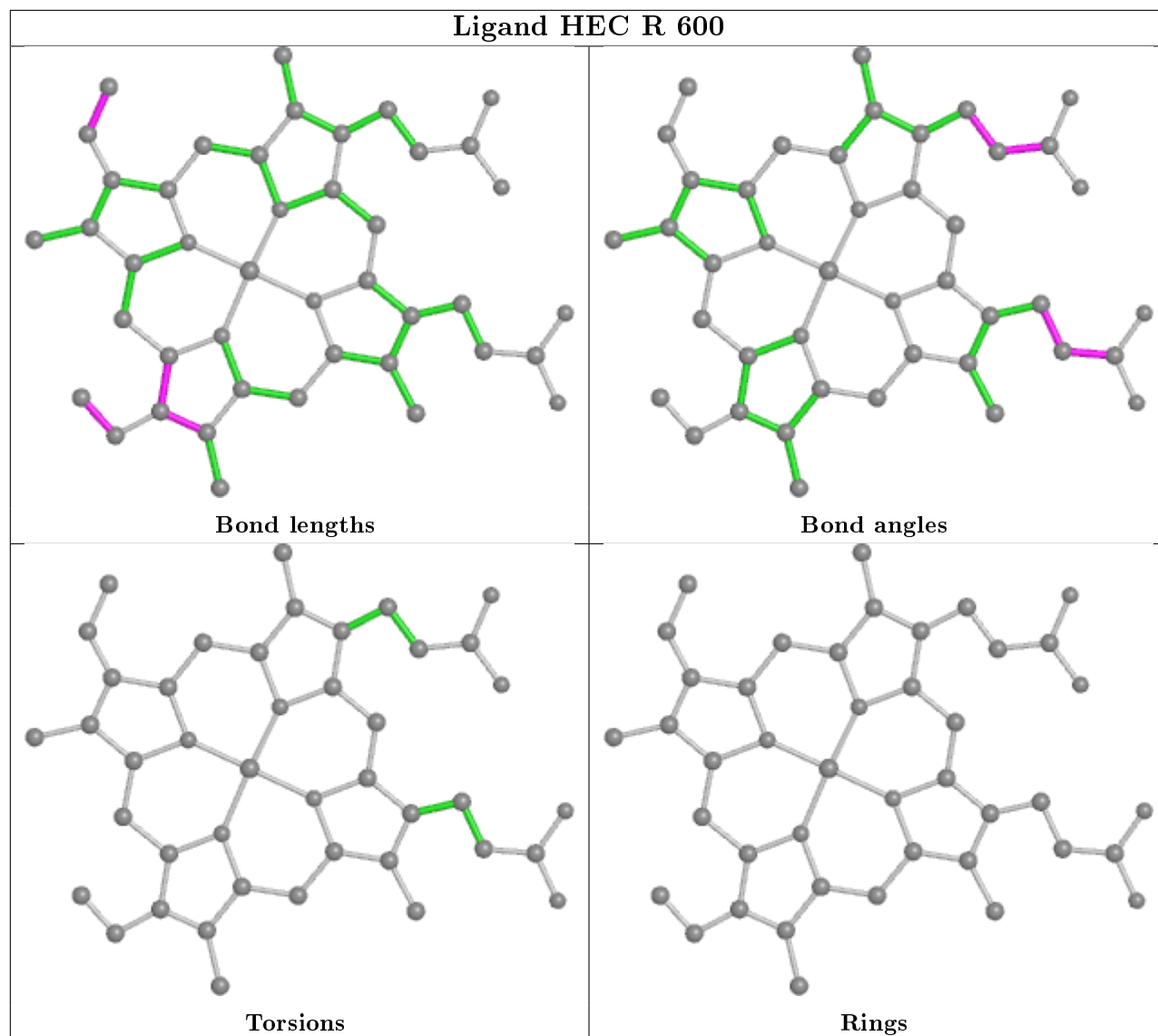


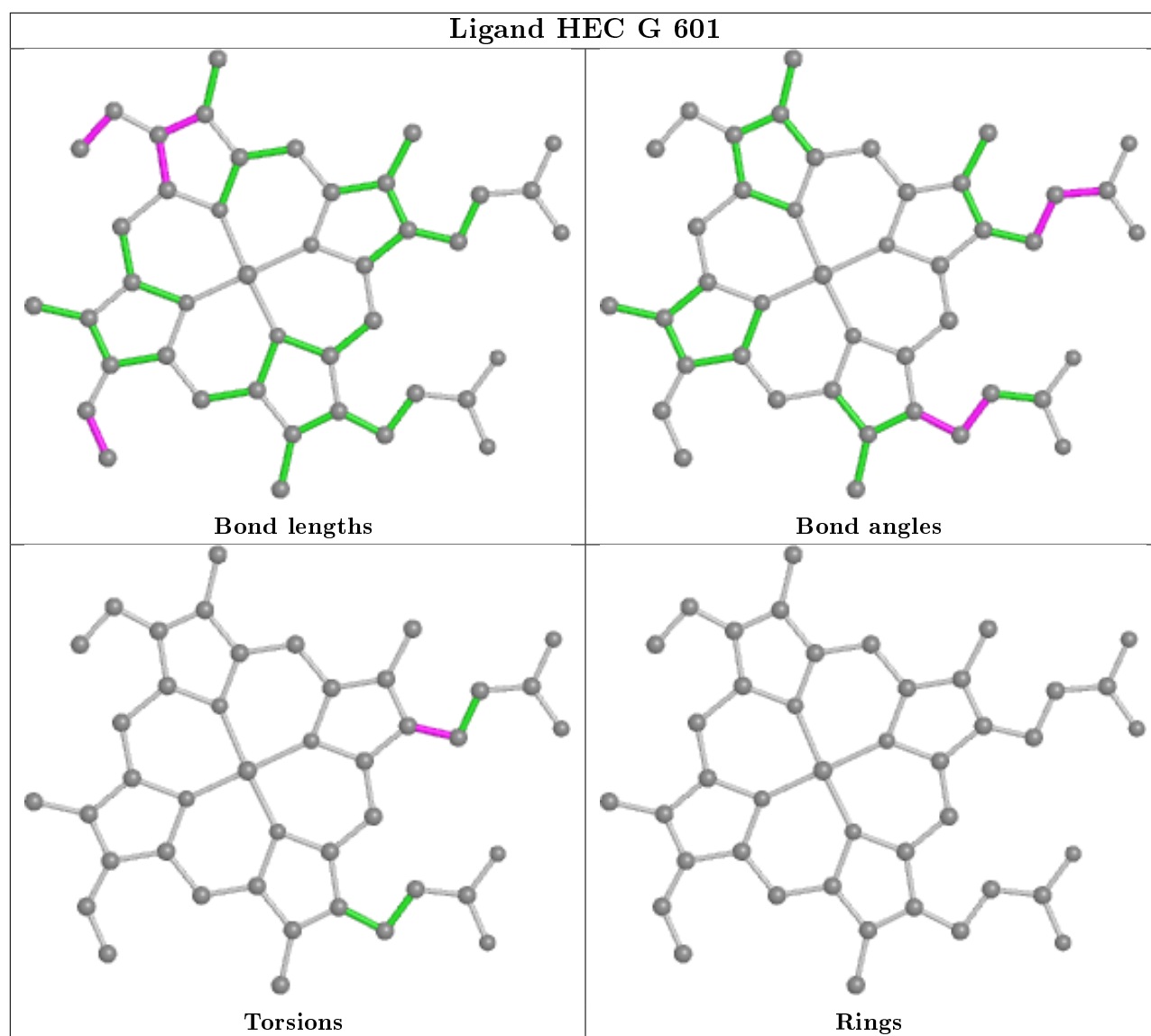




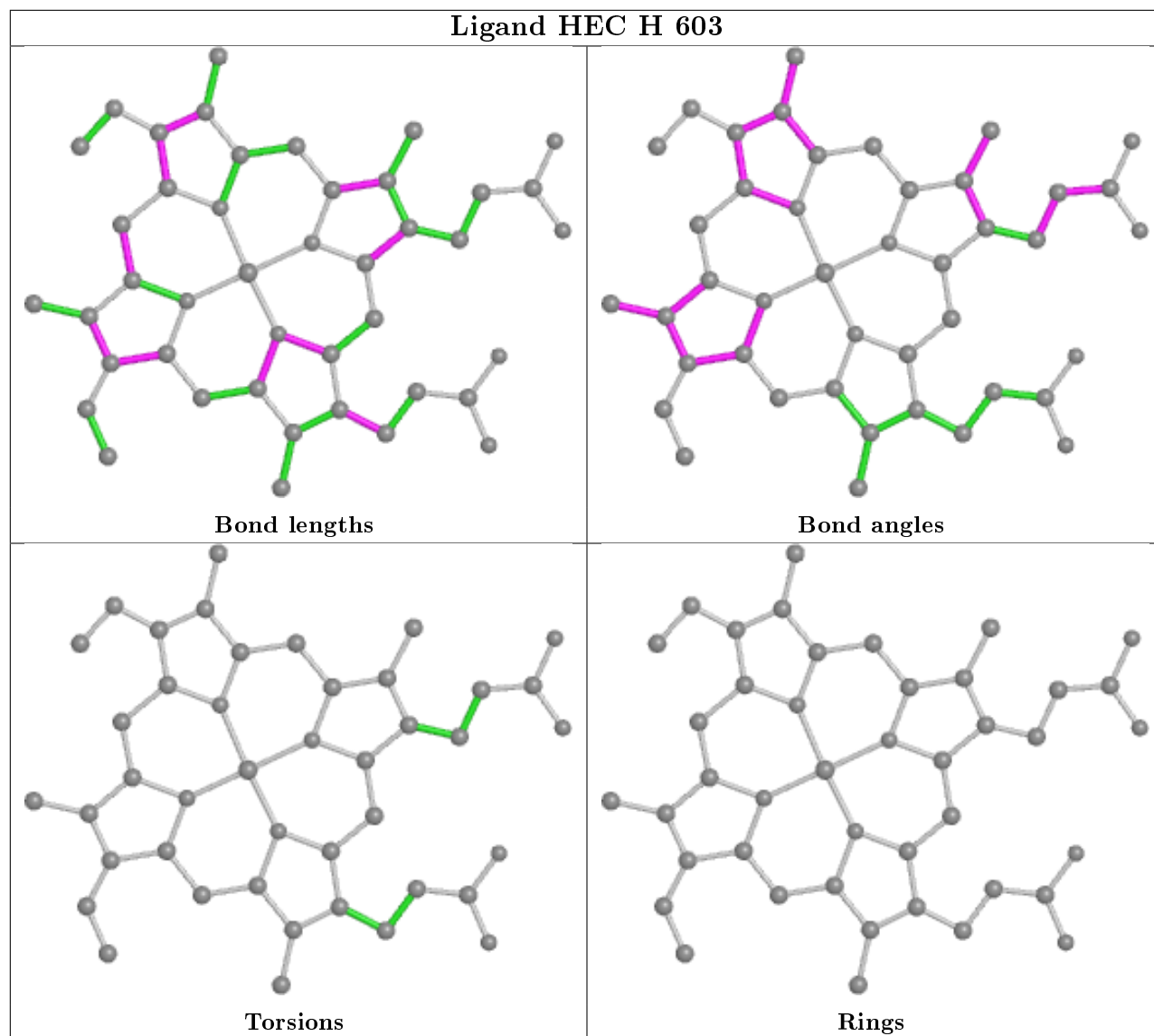
## Ligand HEC S 603

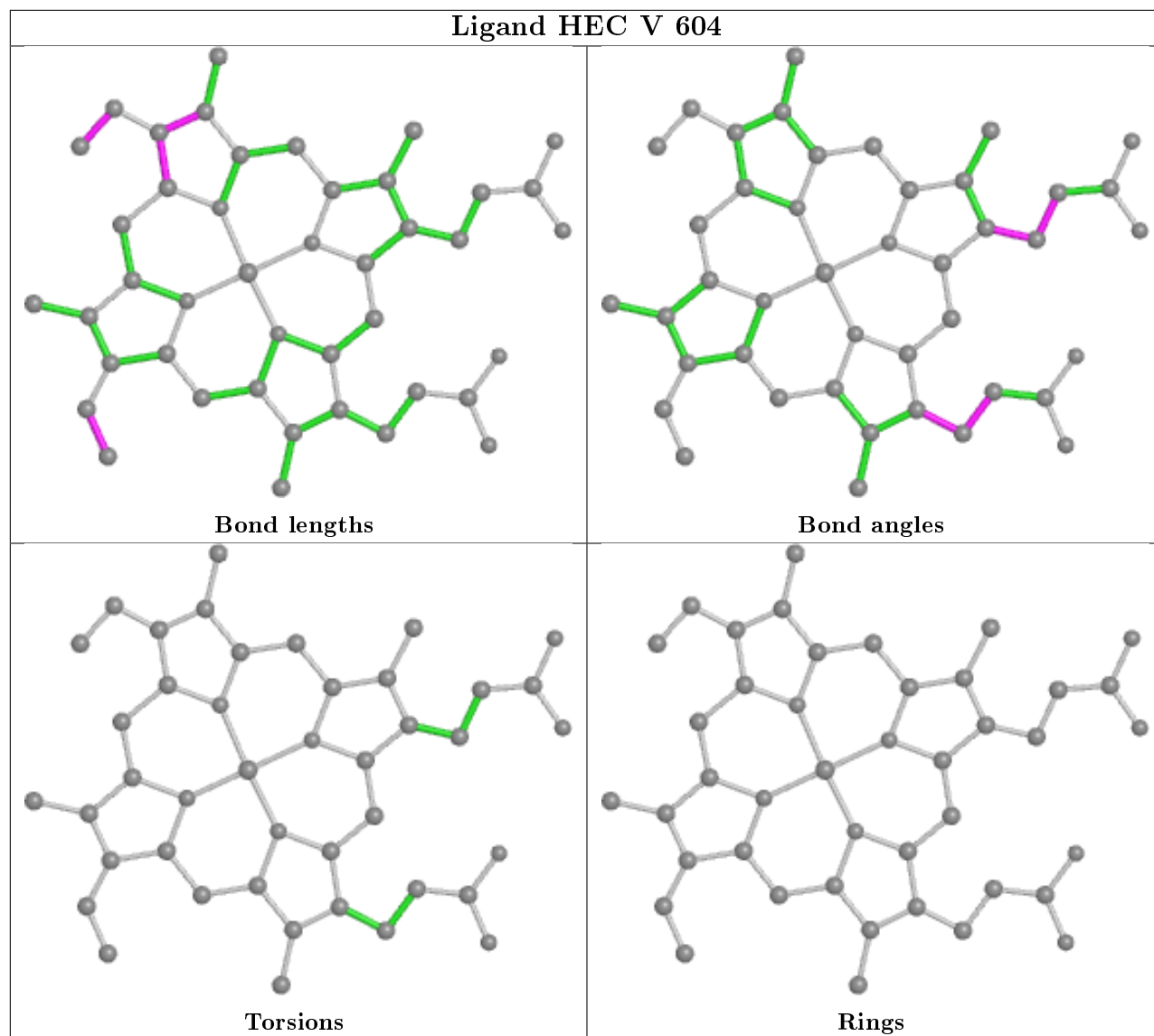




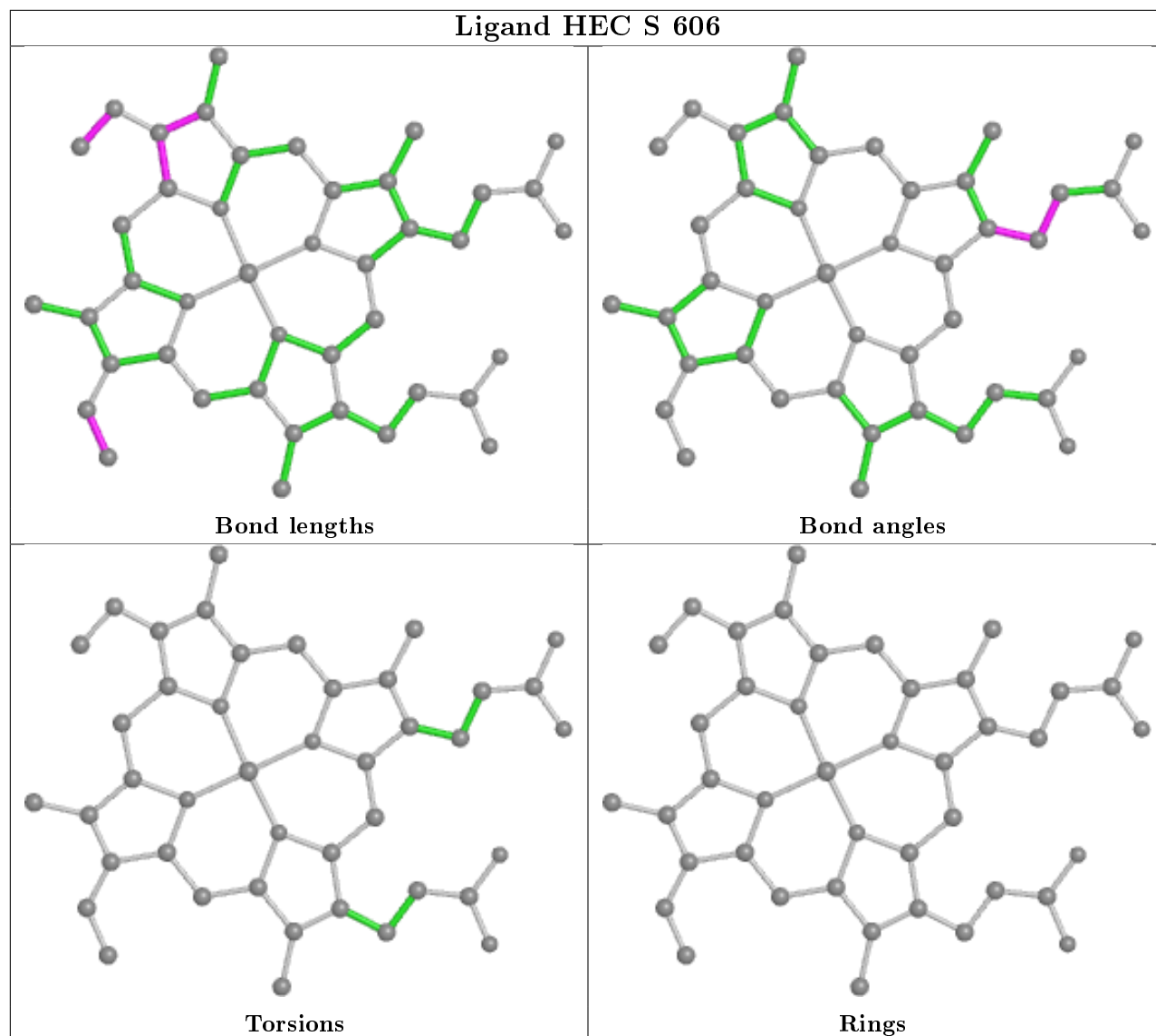


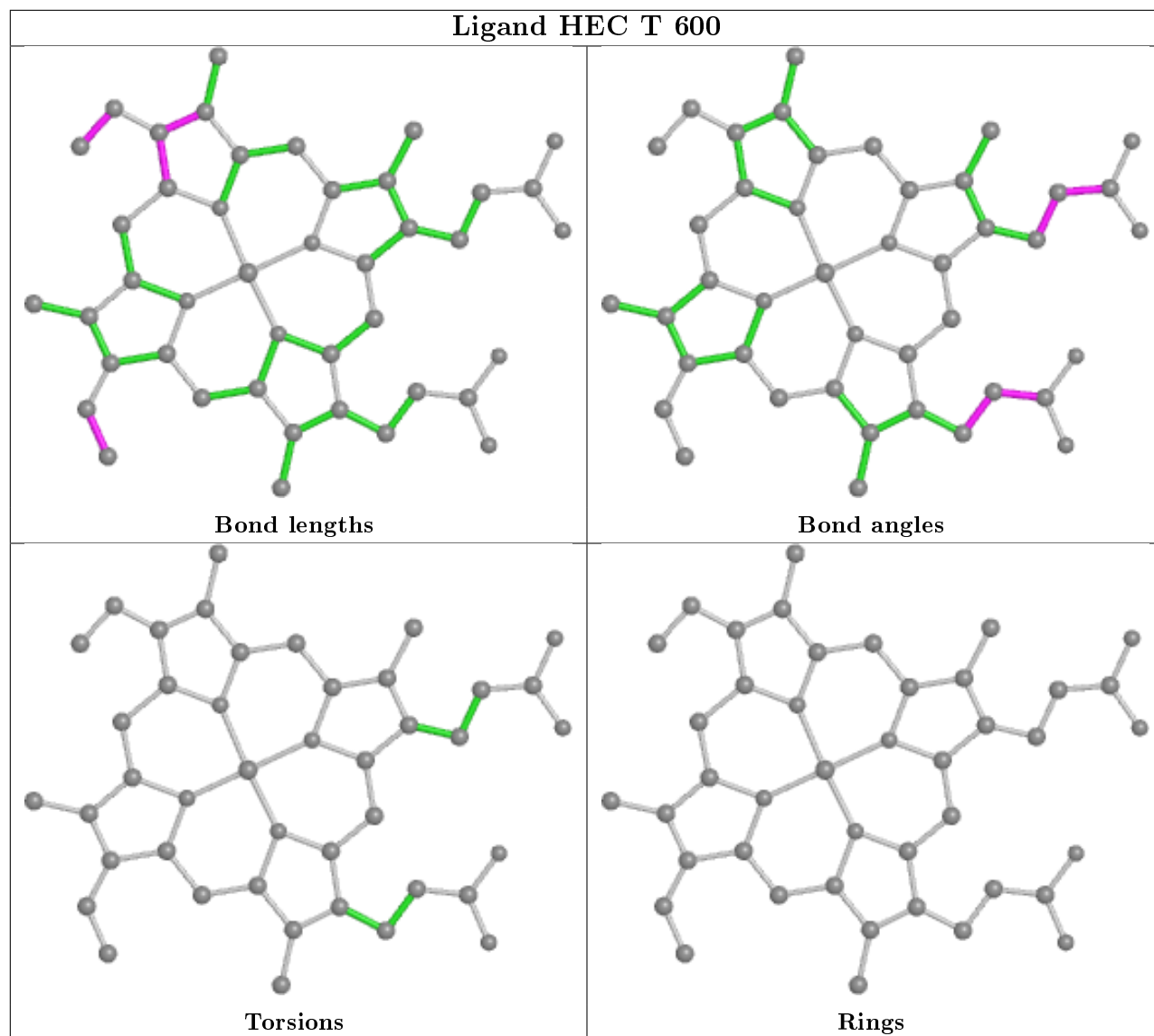


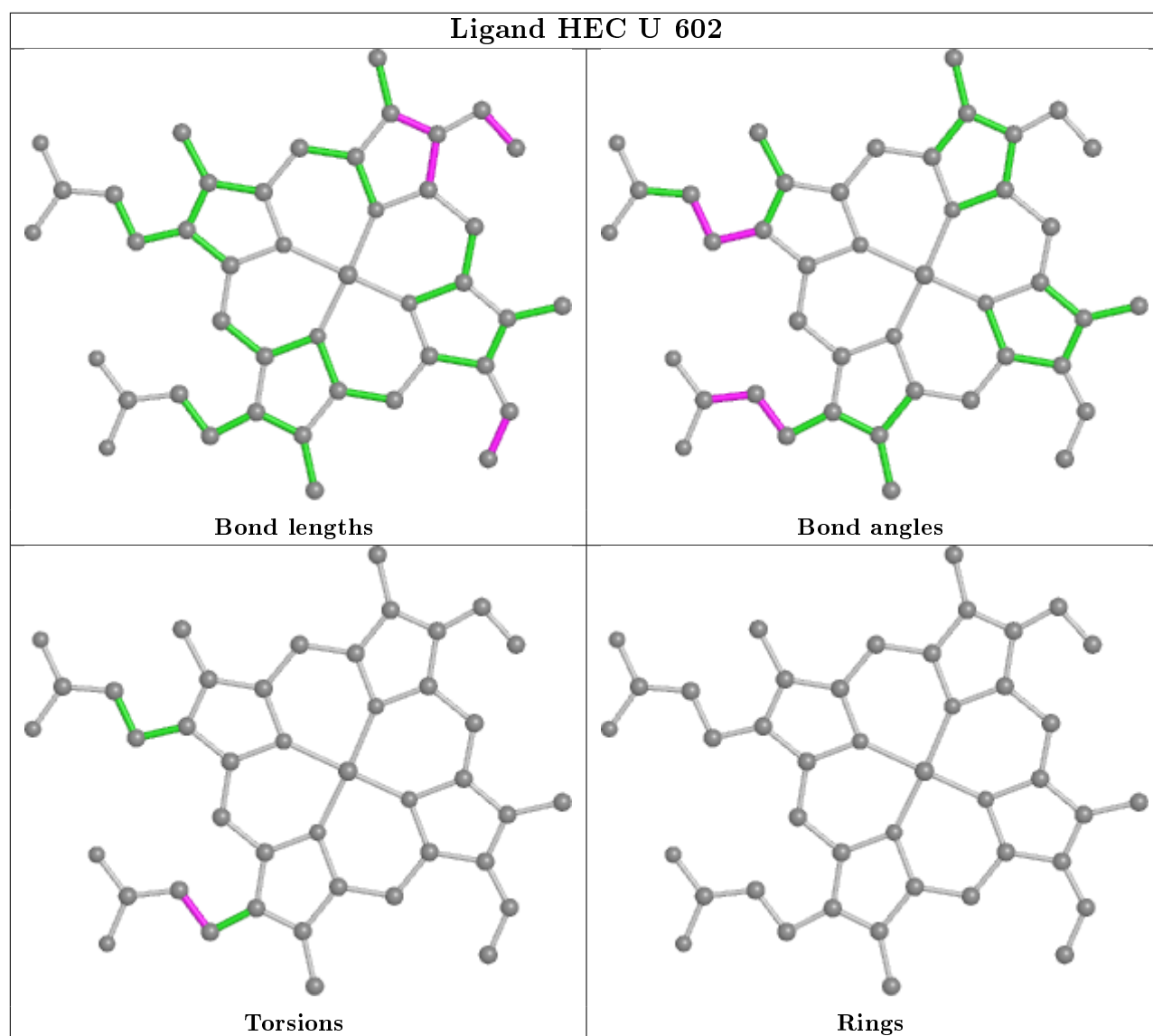


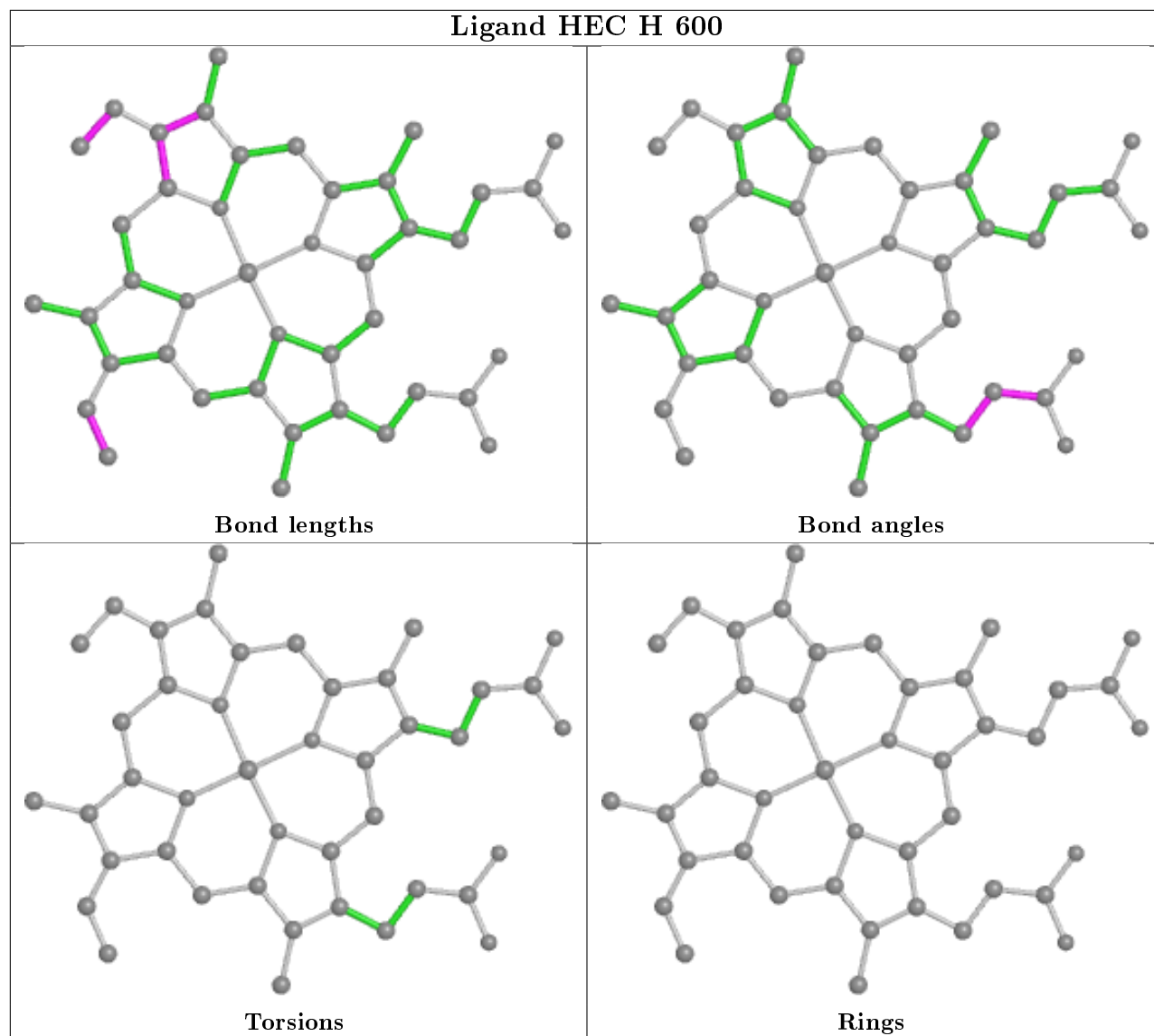


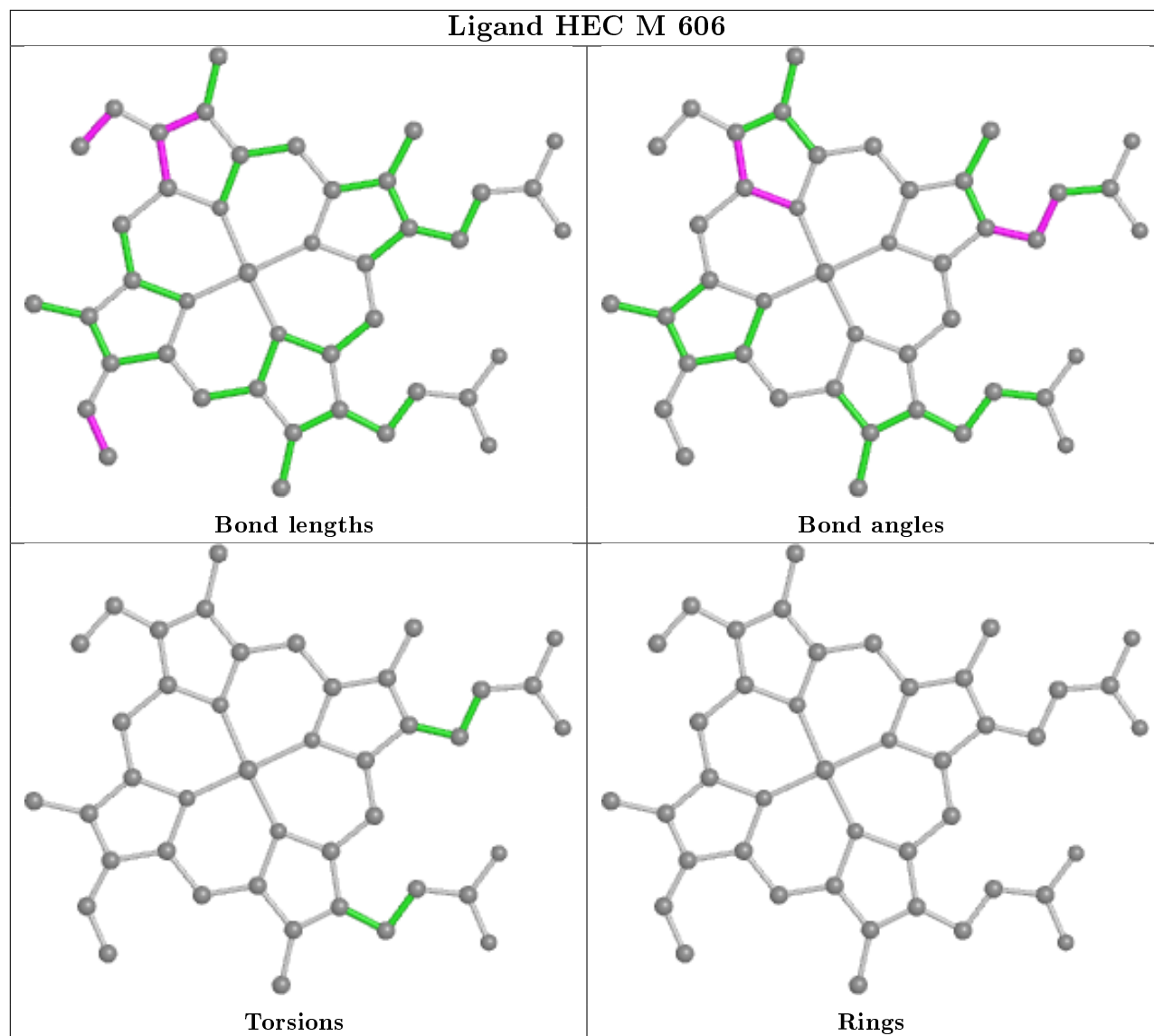
## Ligand HEC S 606



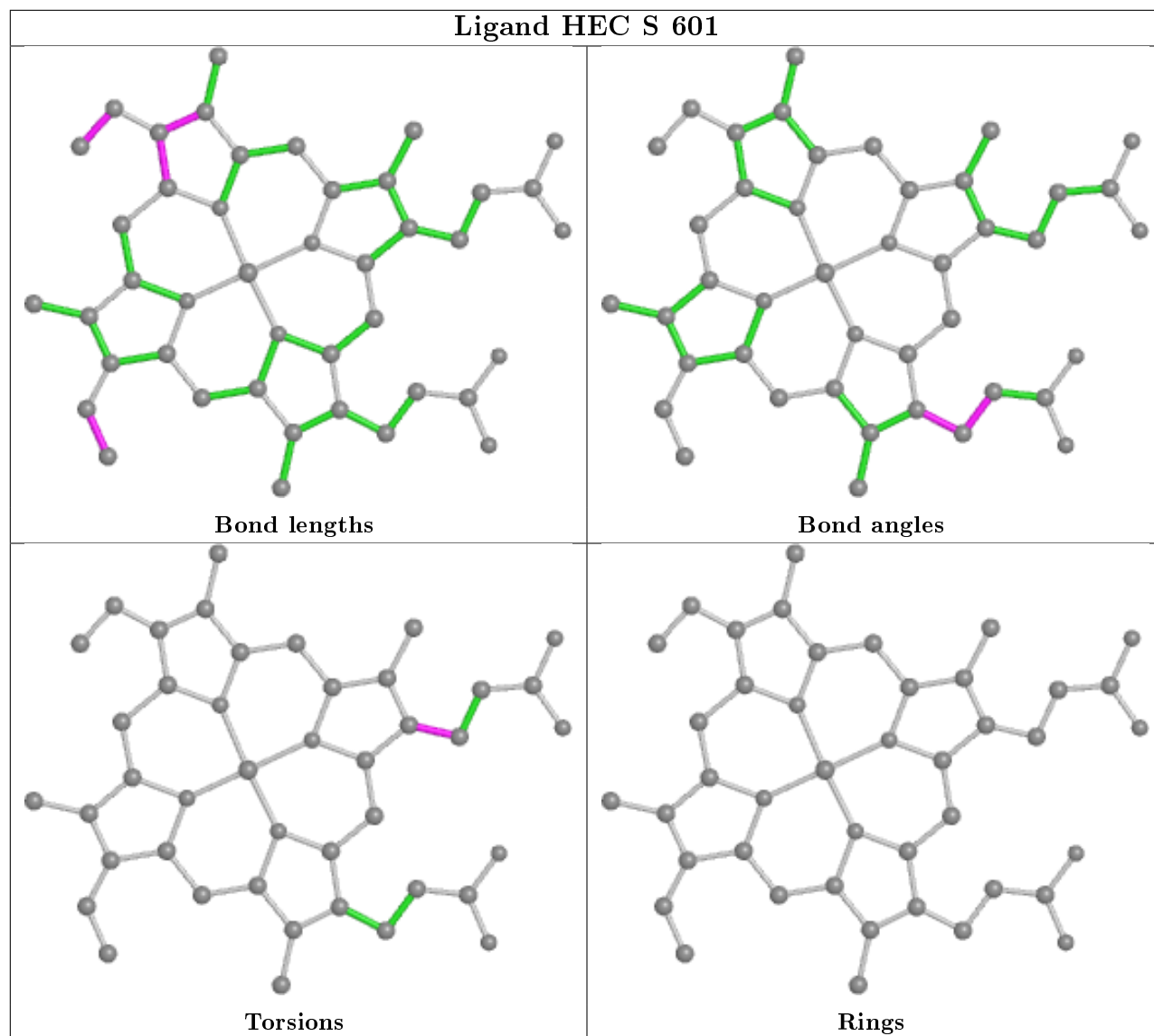




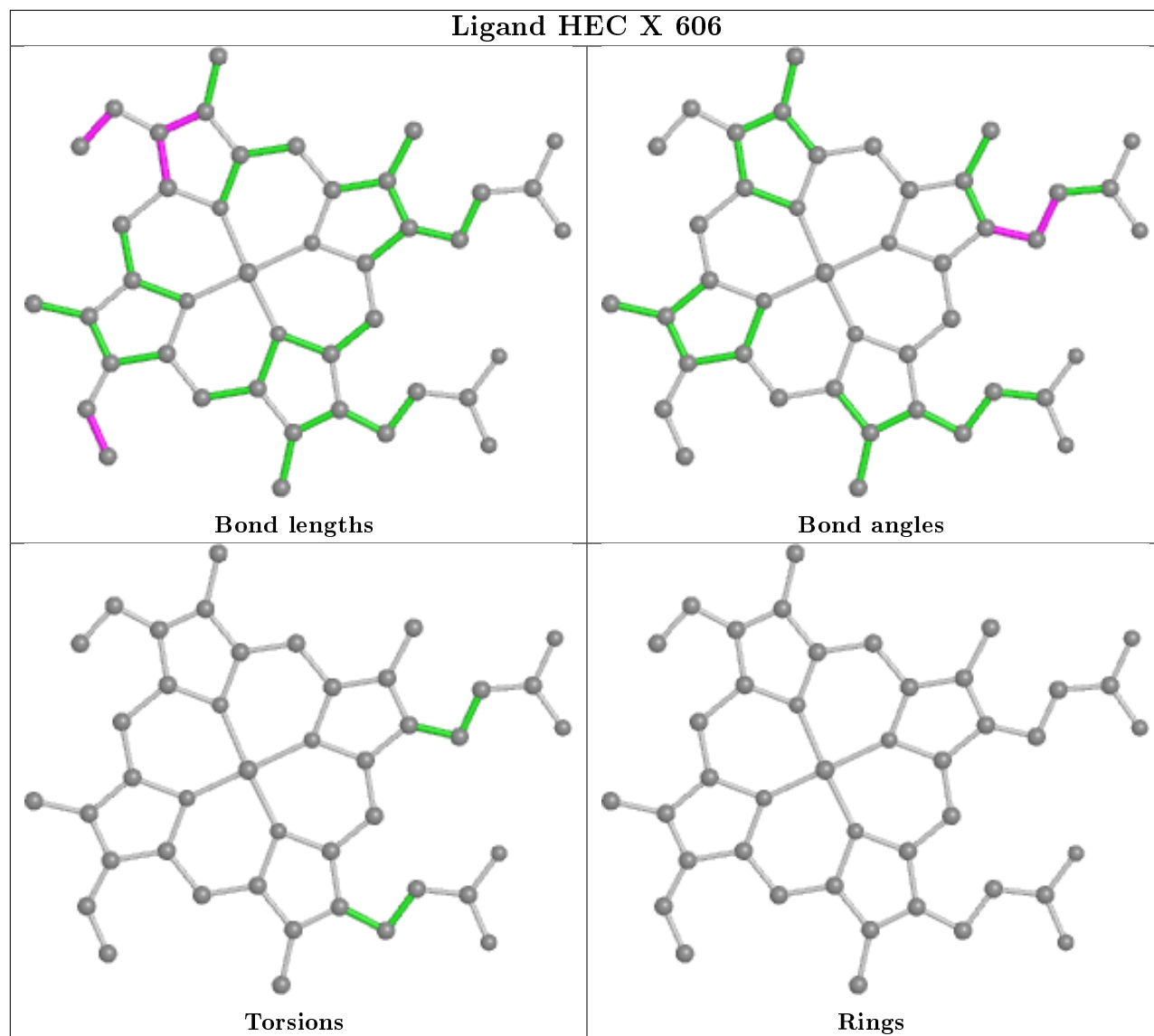


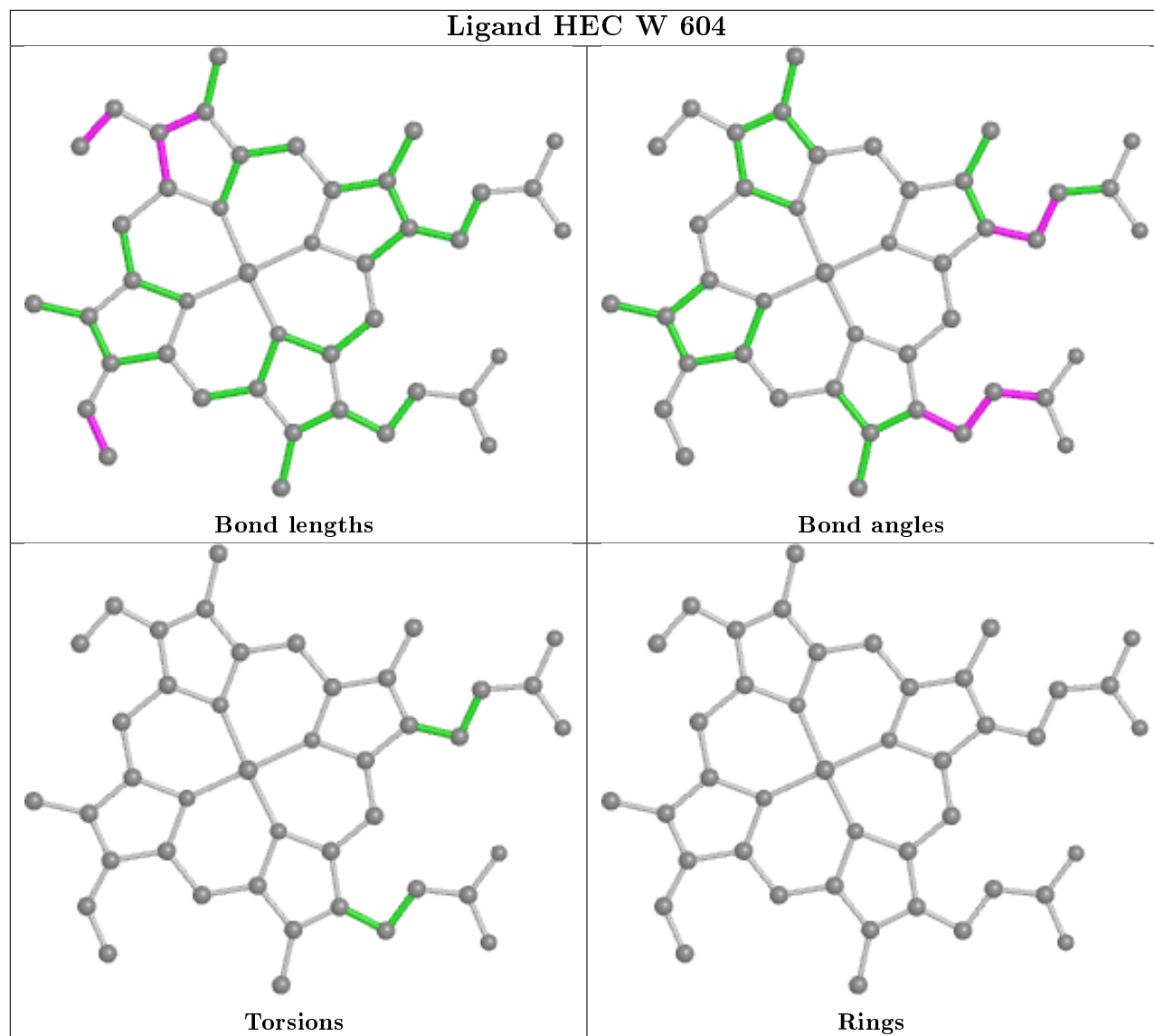


## Ligand HEC S 601

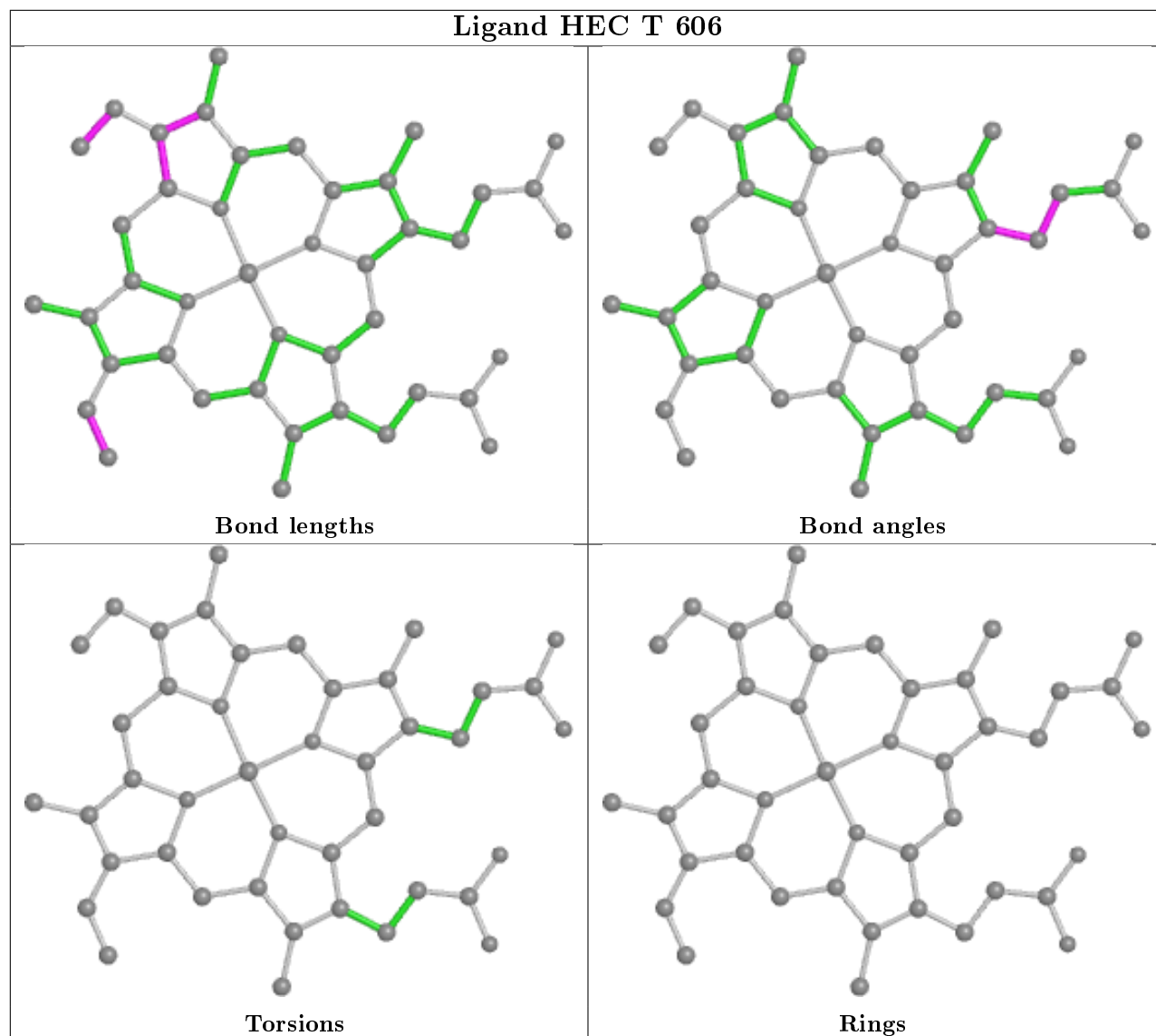




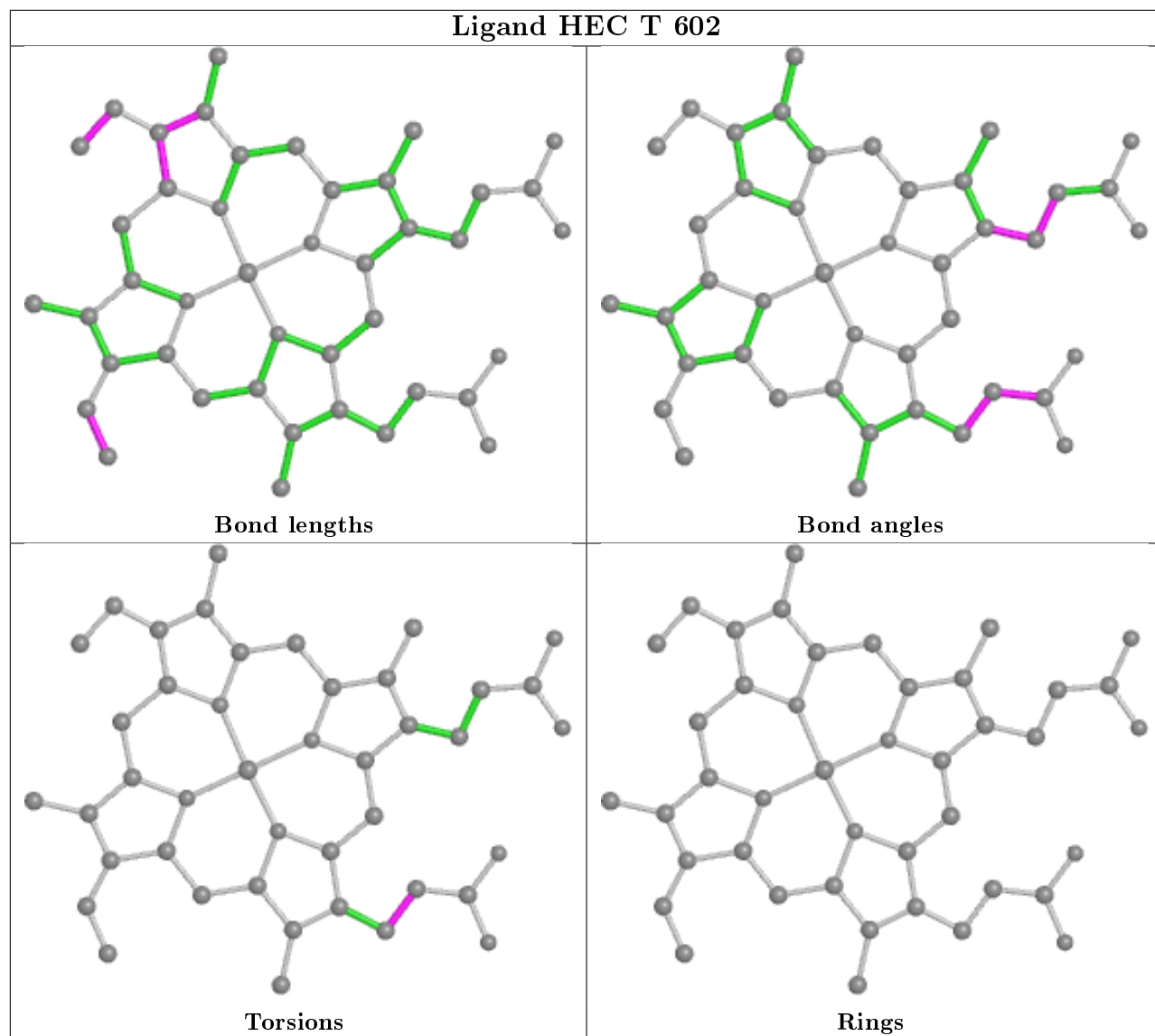




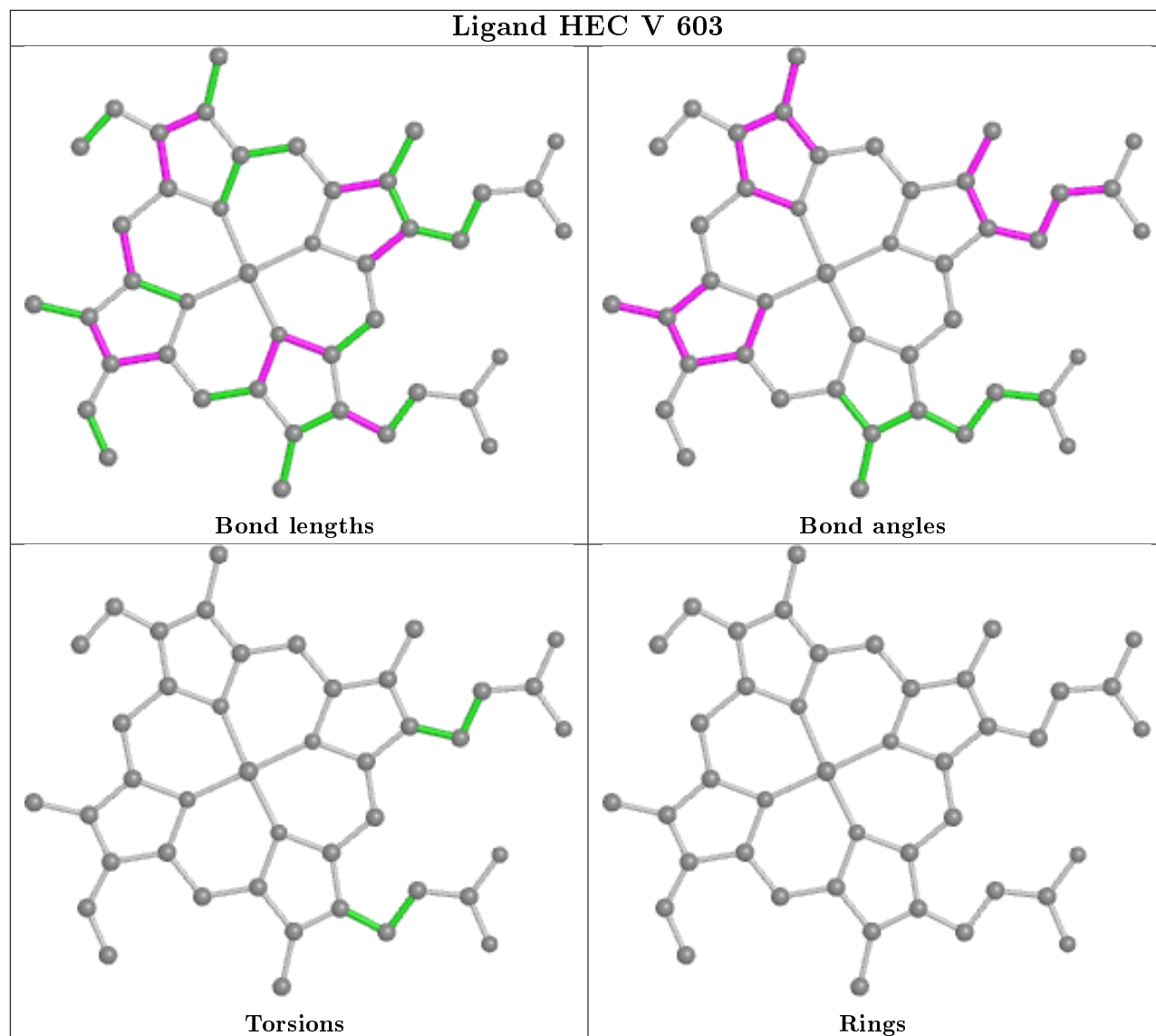
## Ligand HEC T 606



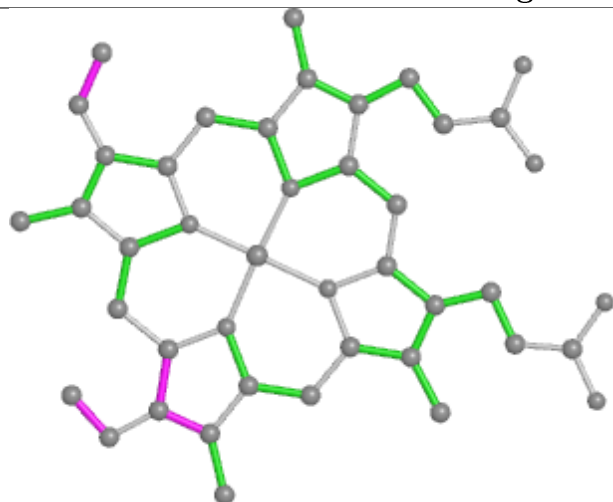
## Ligand HEC T 602



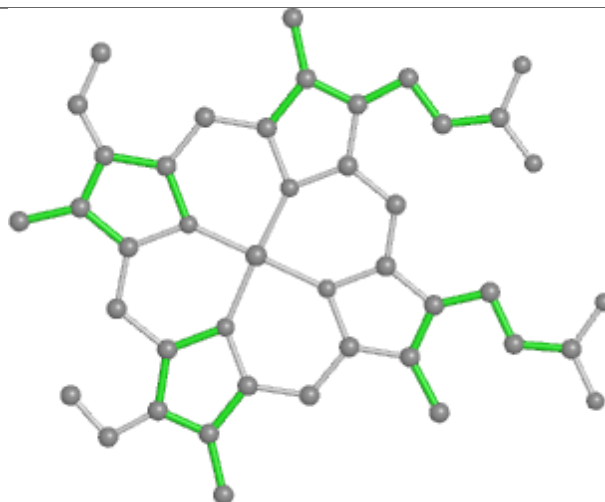
## Ligand HEC V 603



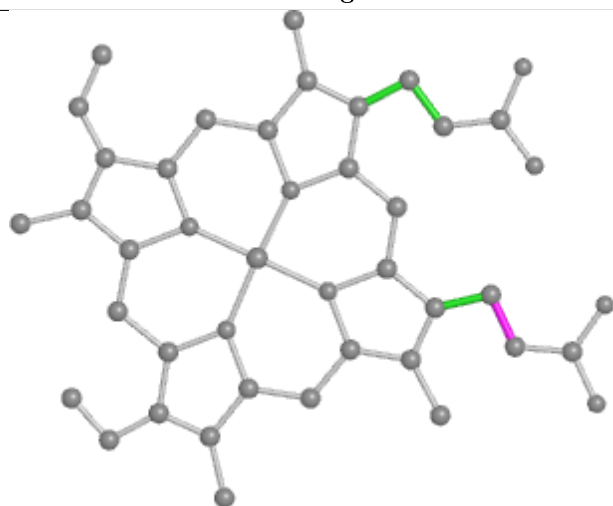
## Ligand HEC S 607



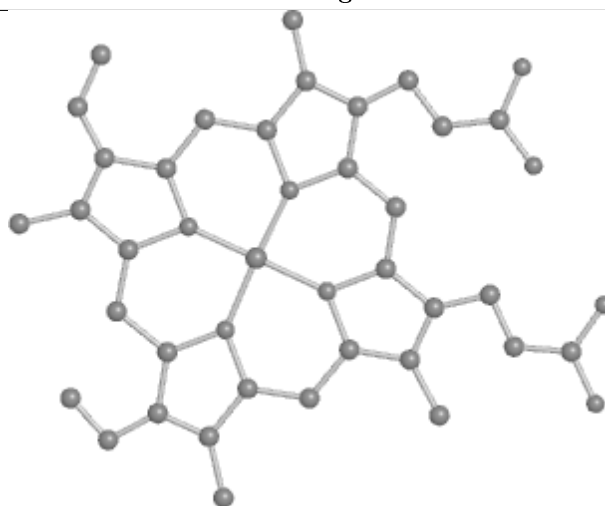
Bond lengths



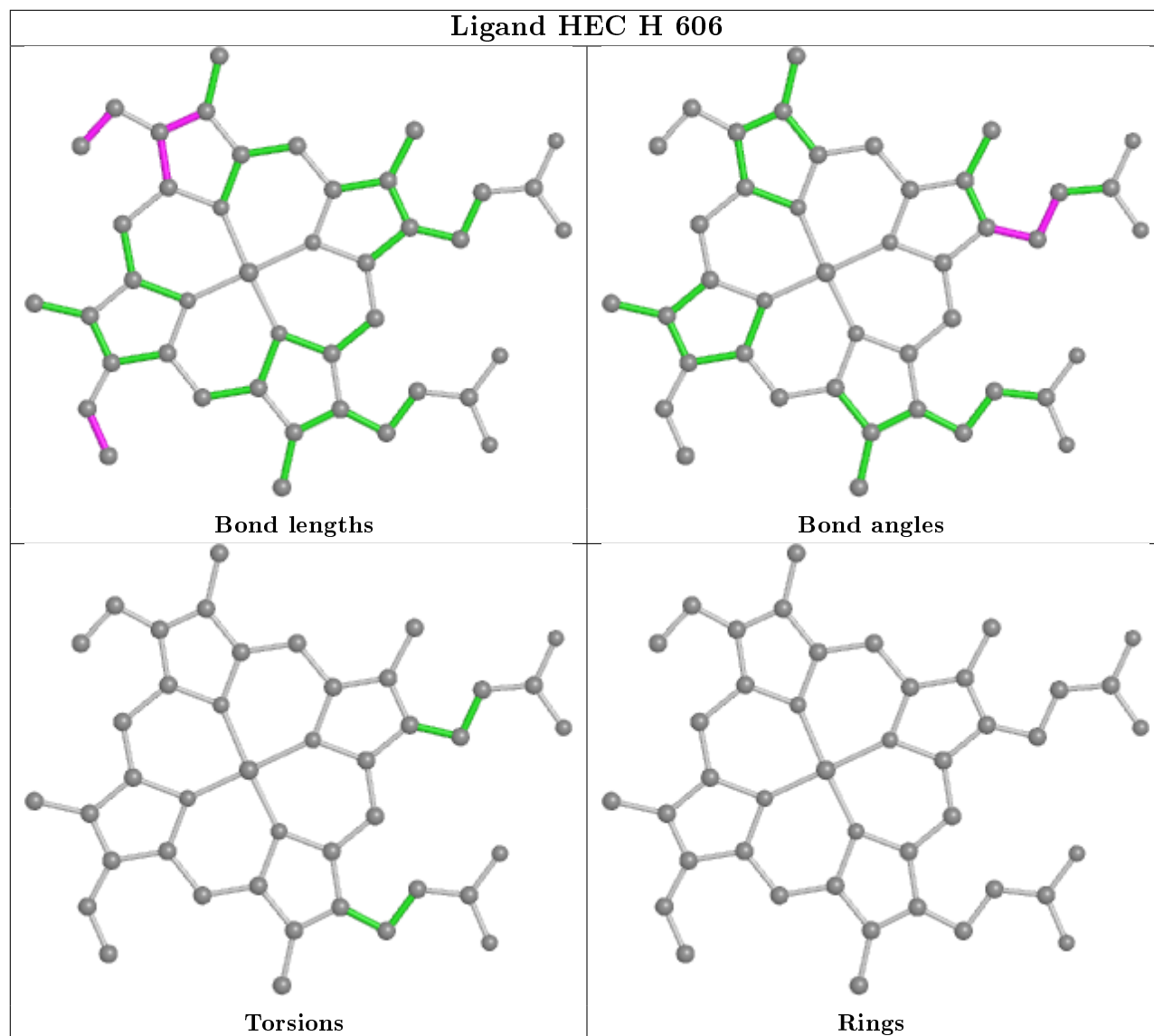
Bond angles



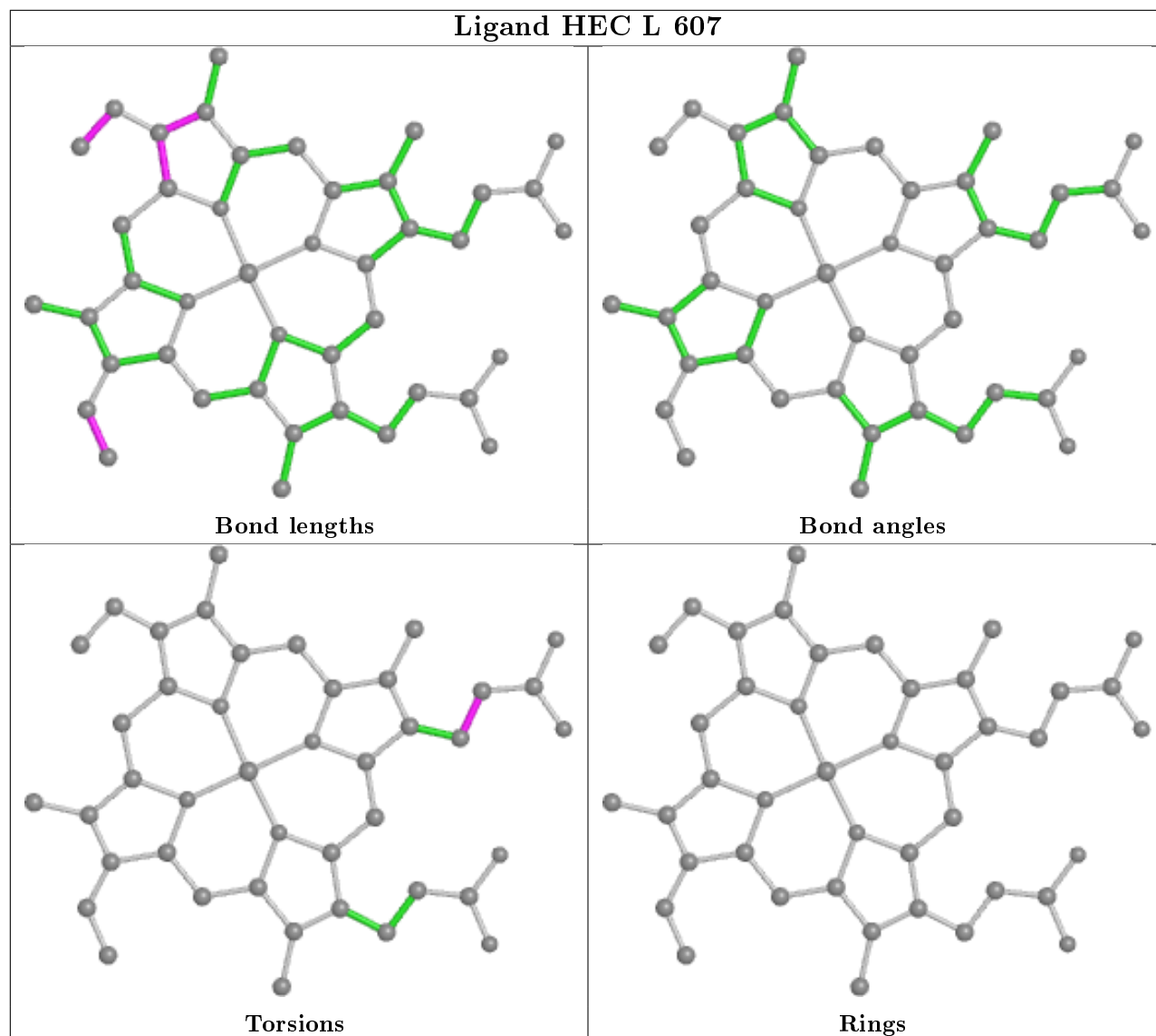
Torsions



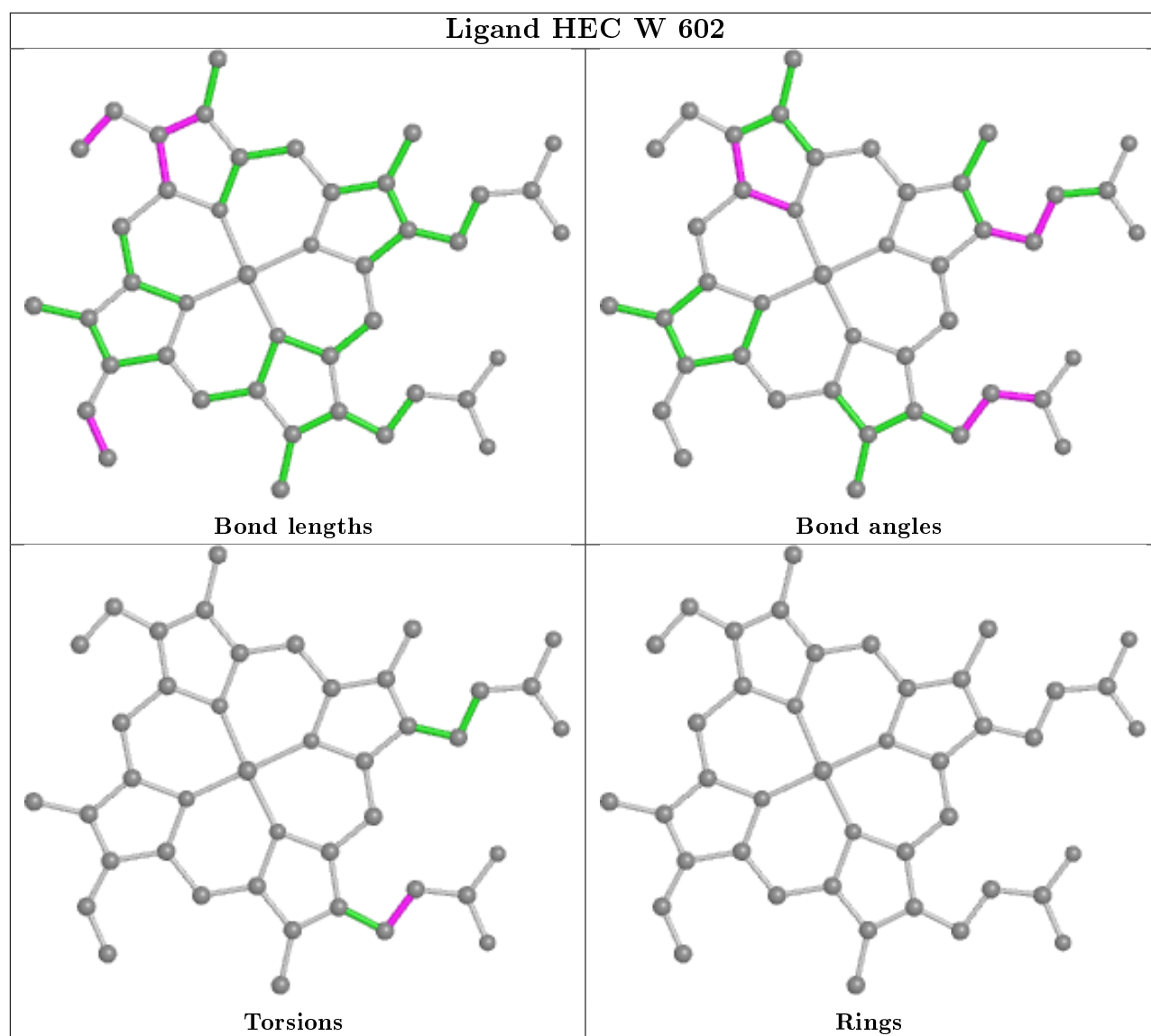
Rings

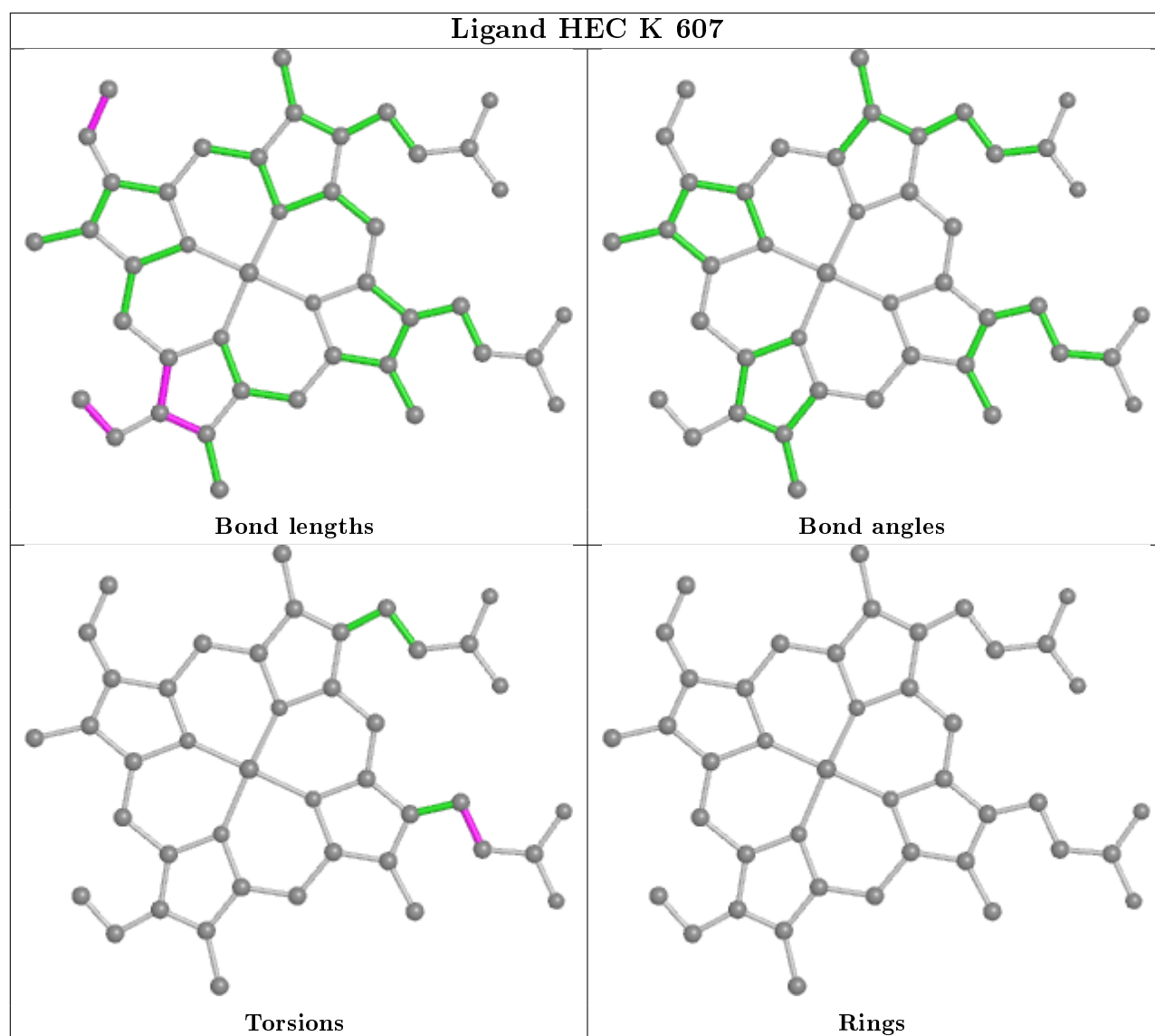


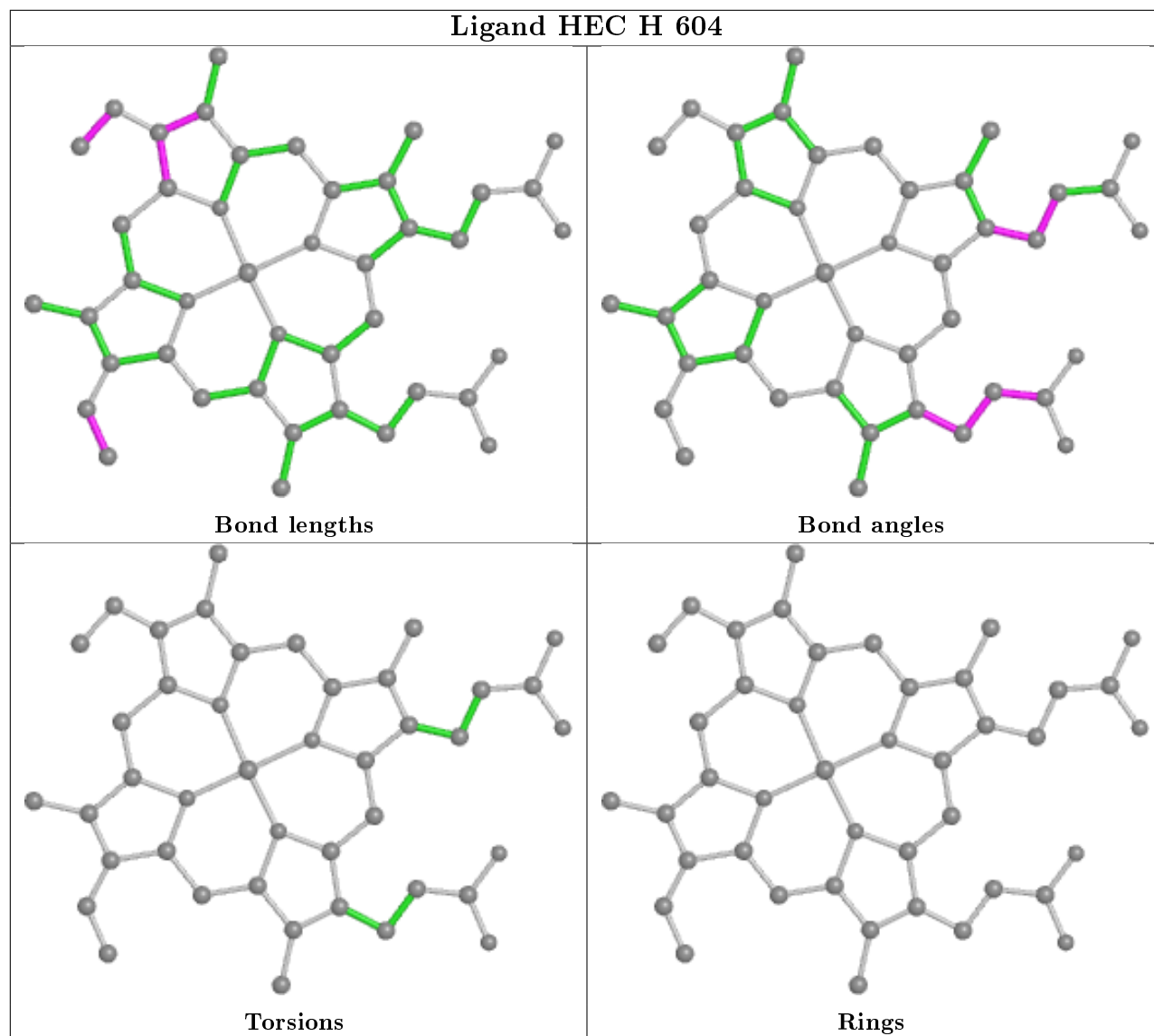
## Ligand HEC L 607

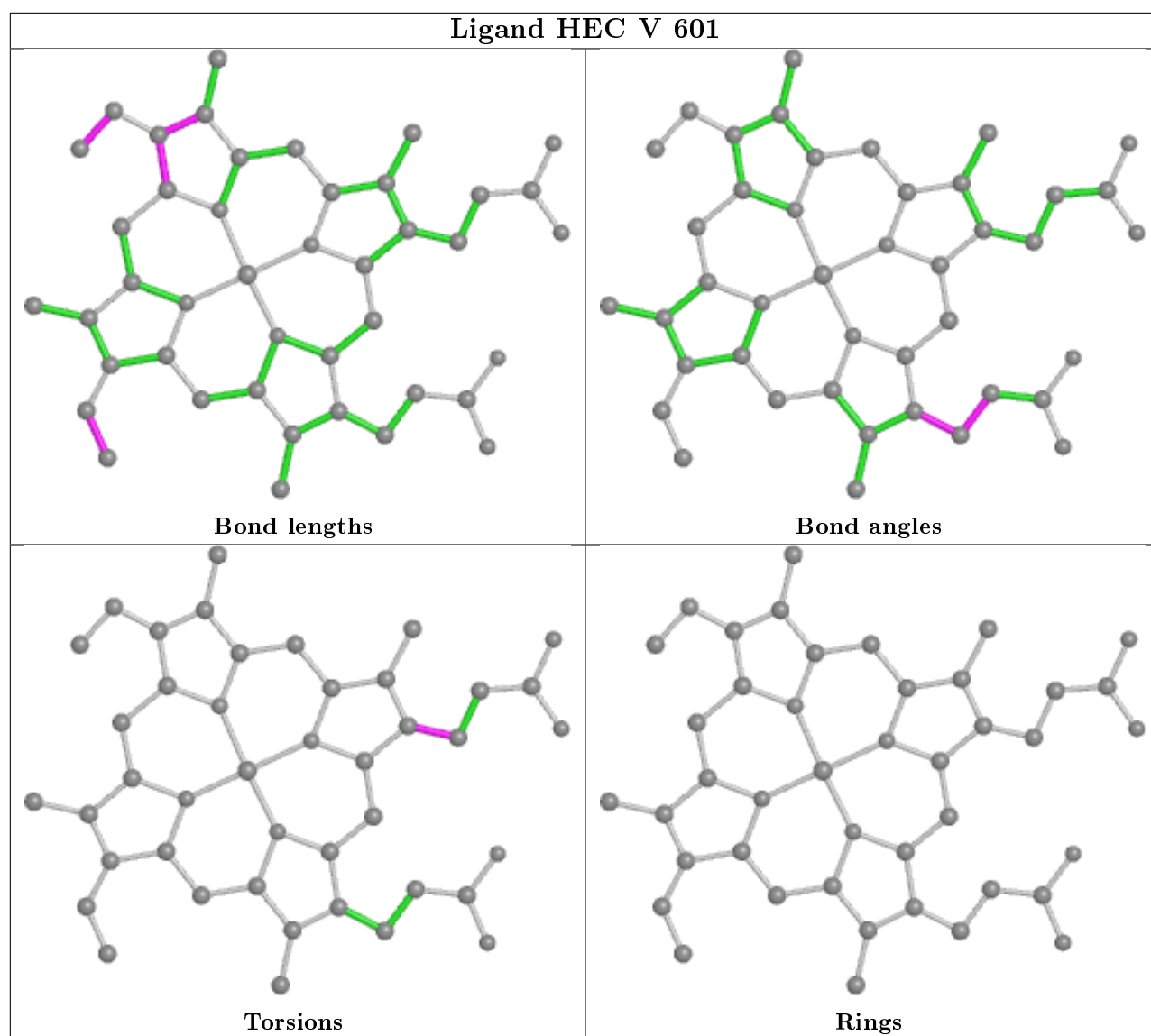




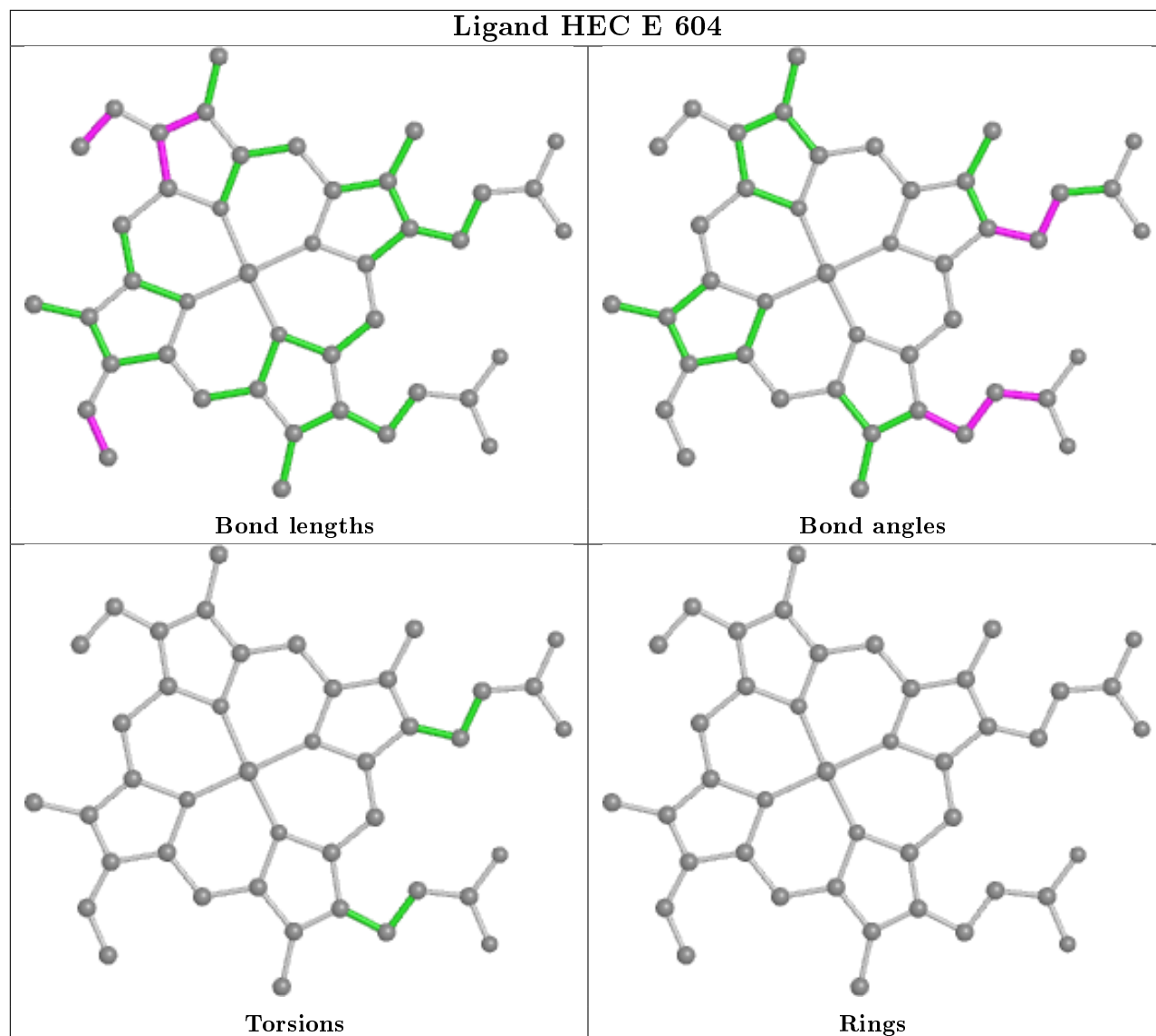


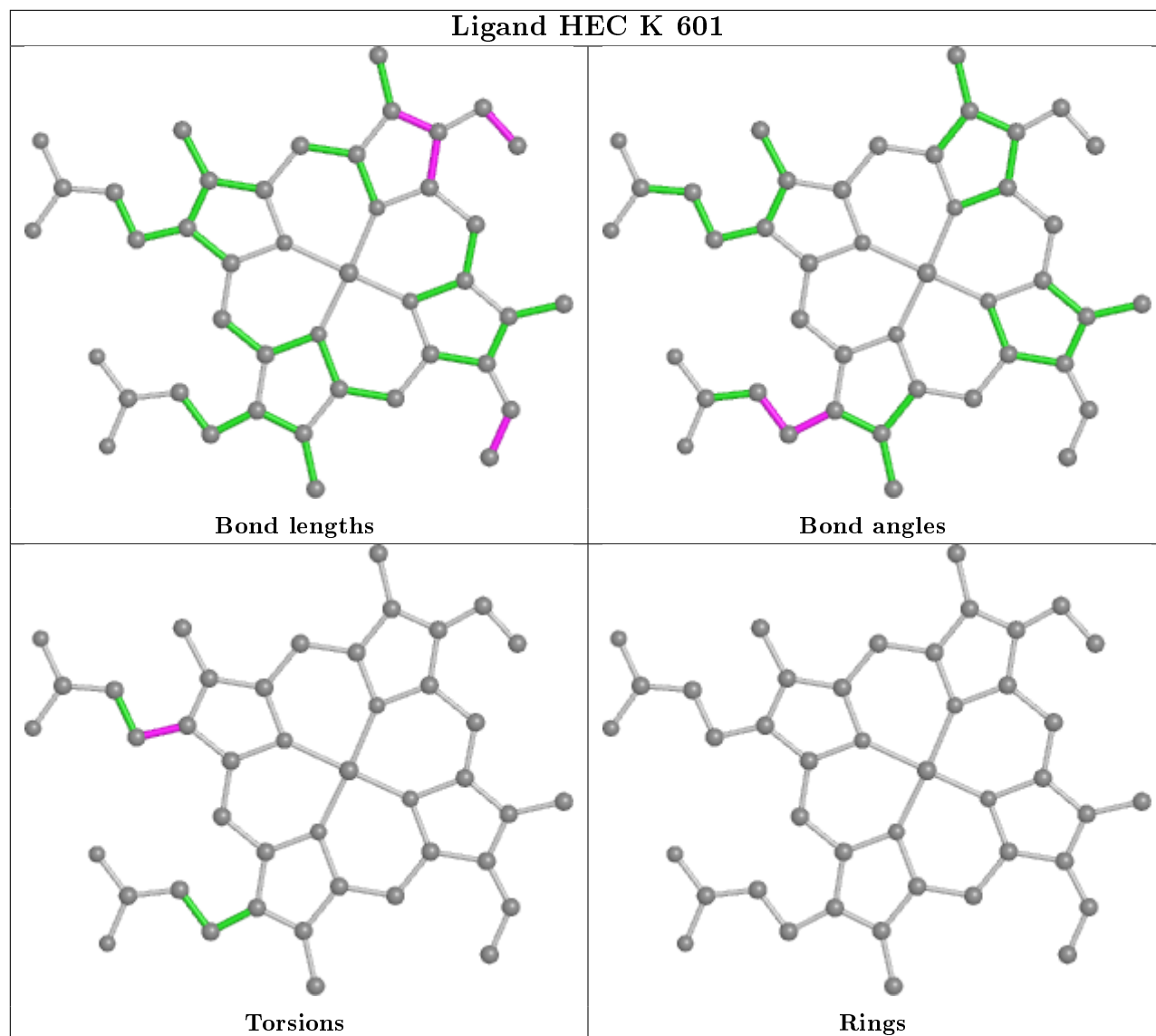




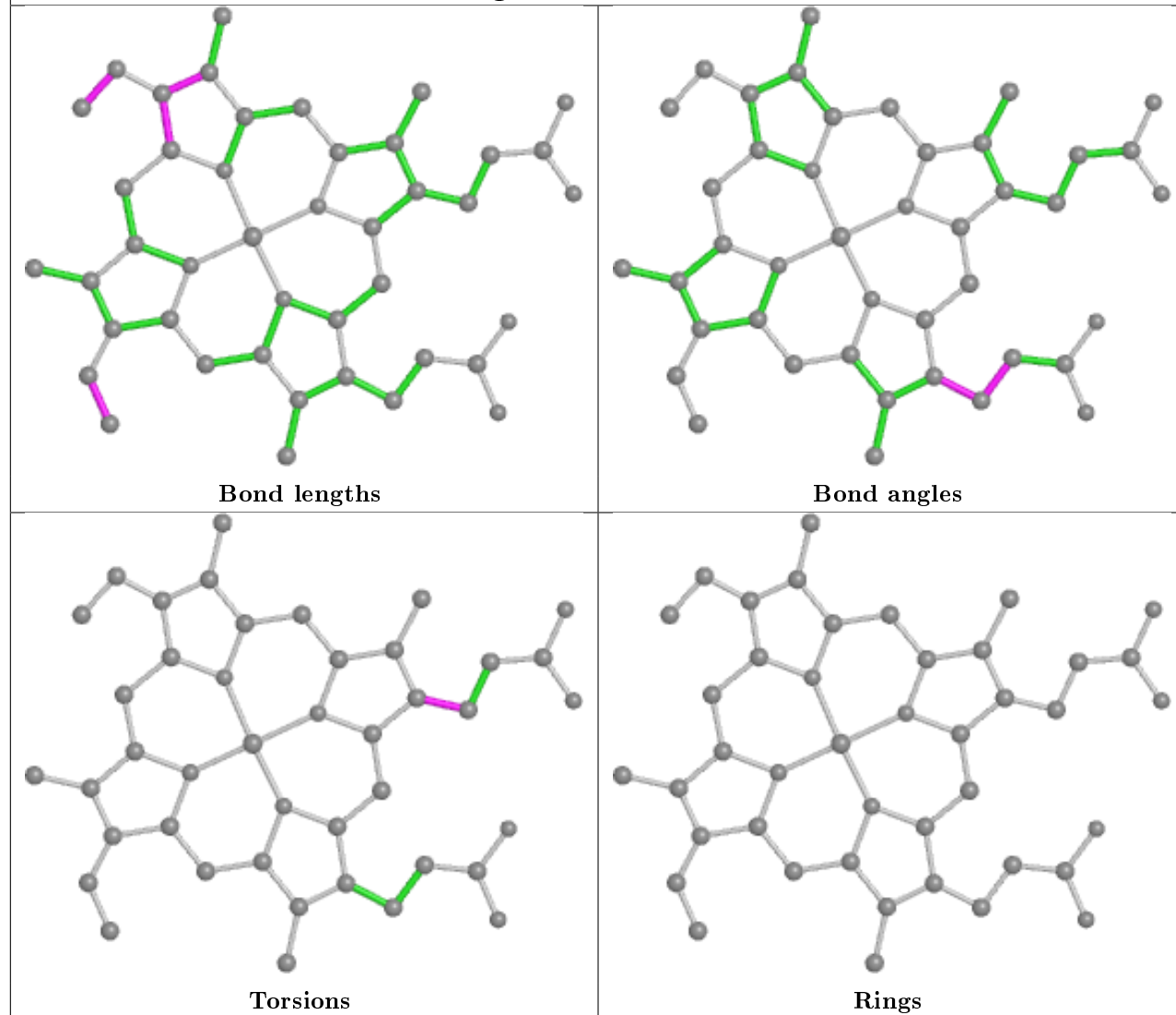


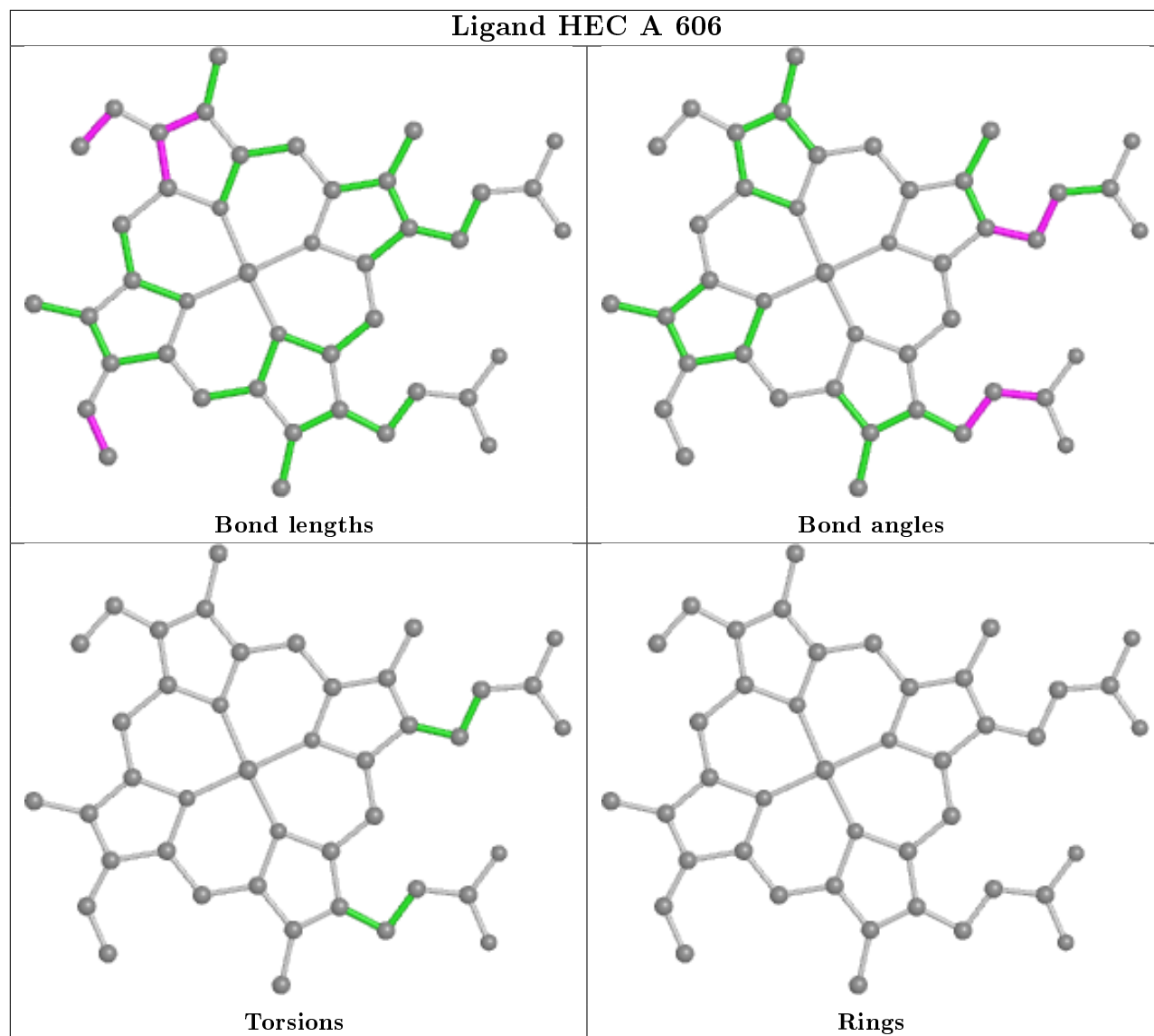
## Ligand HEC E 604



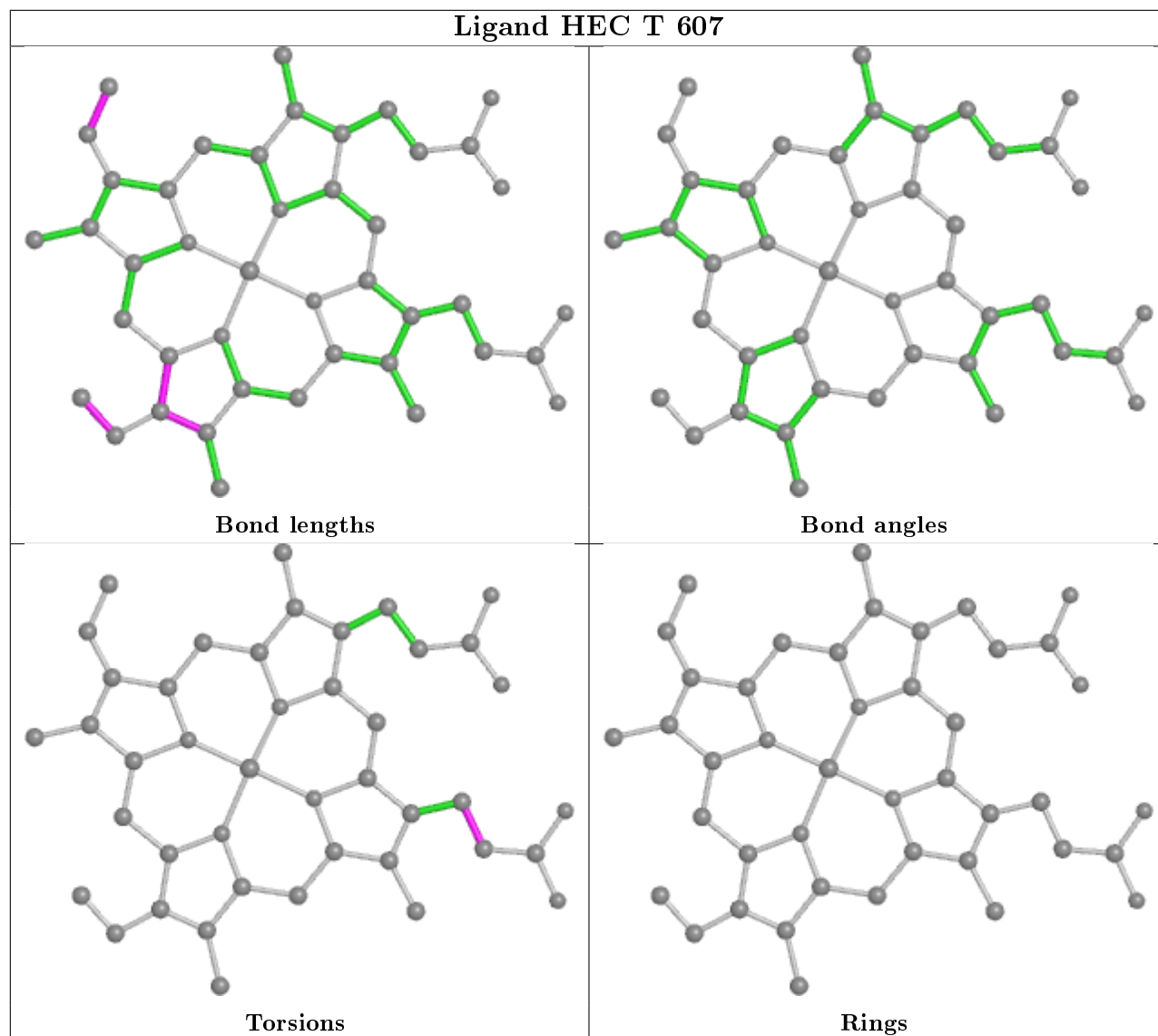


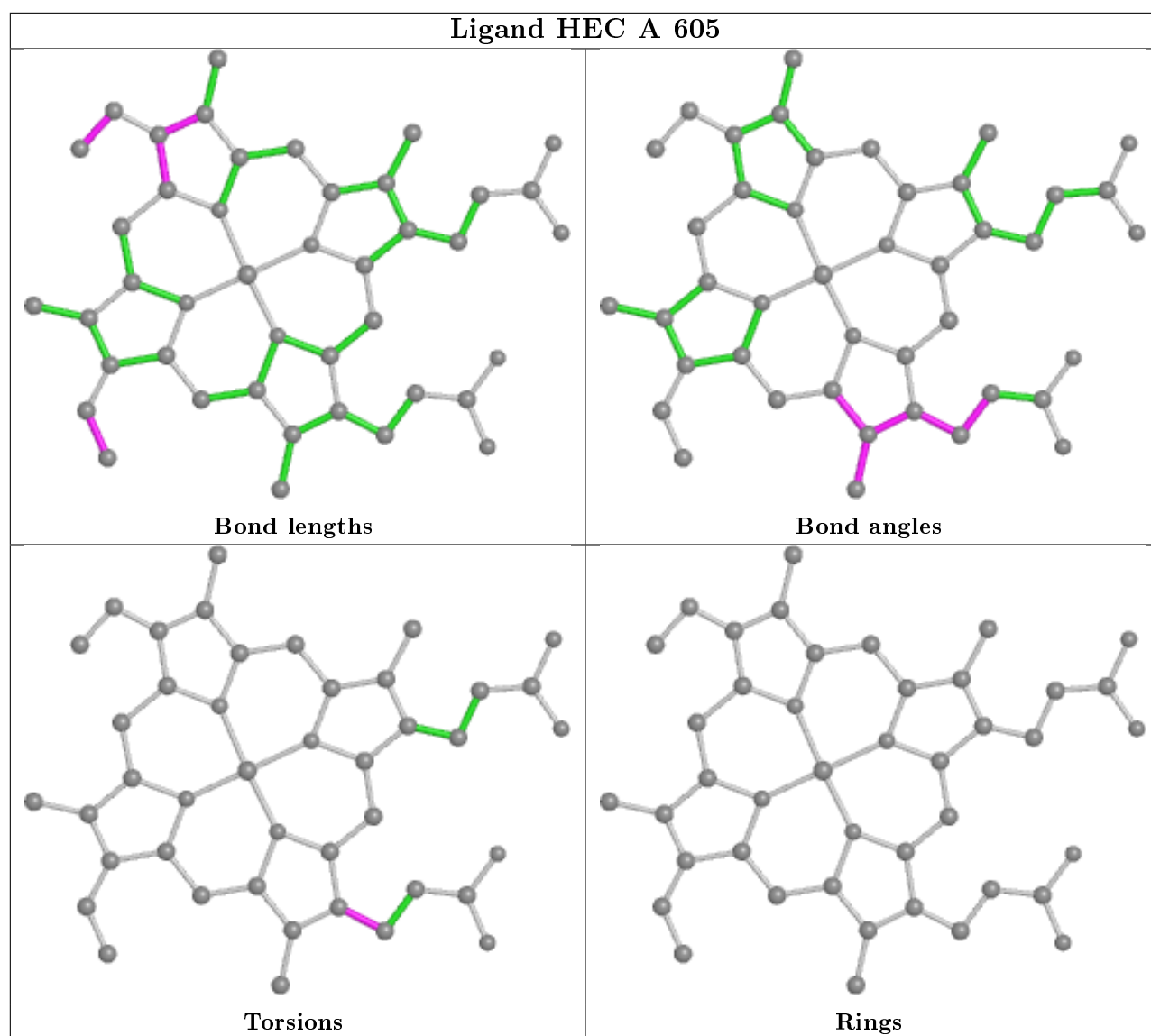
## Ligand HEC L 601

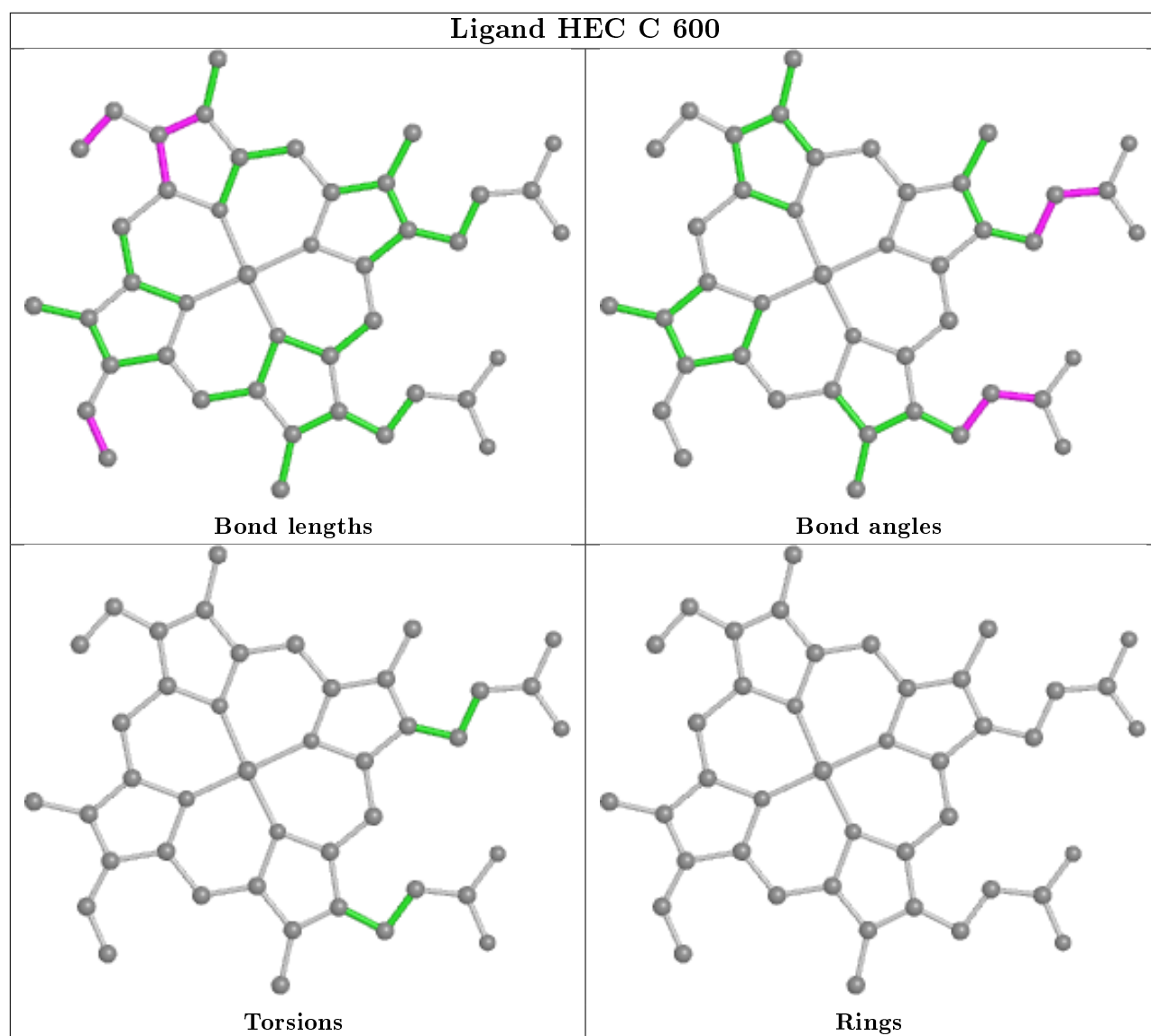


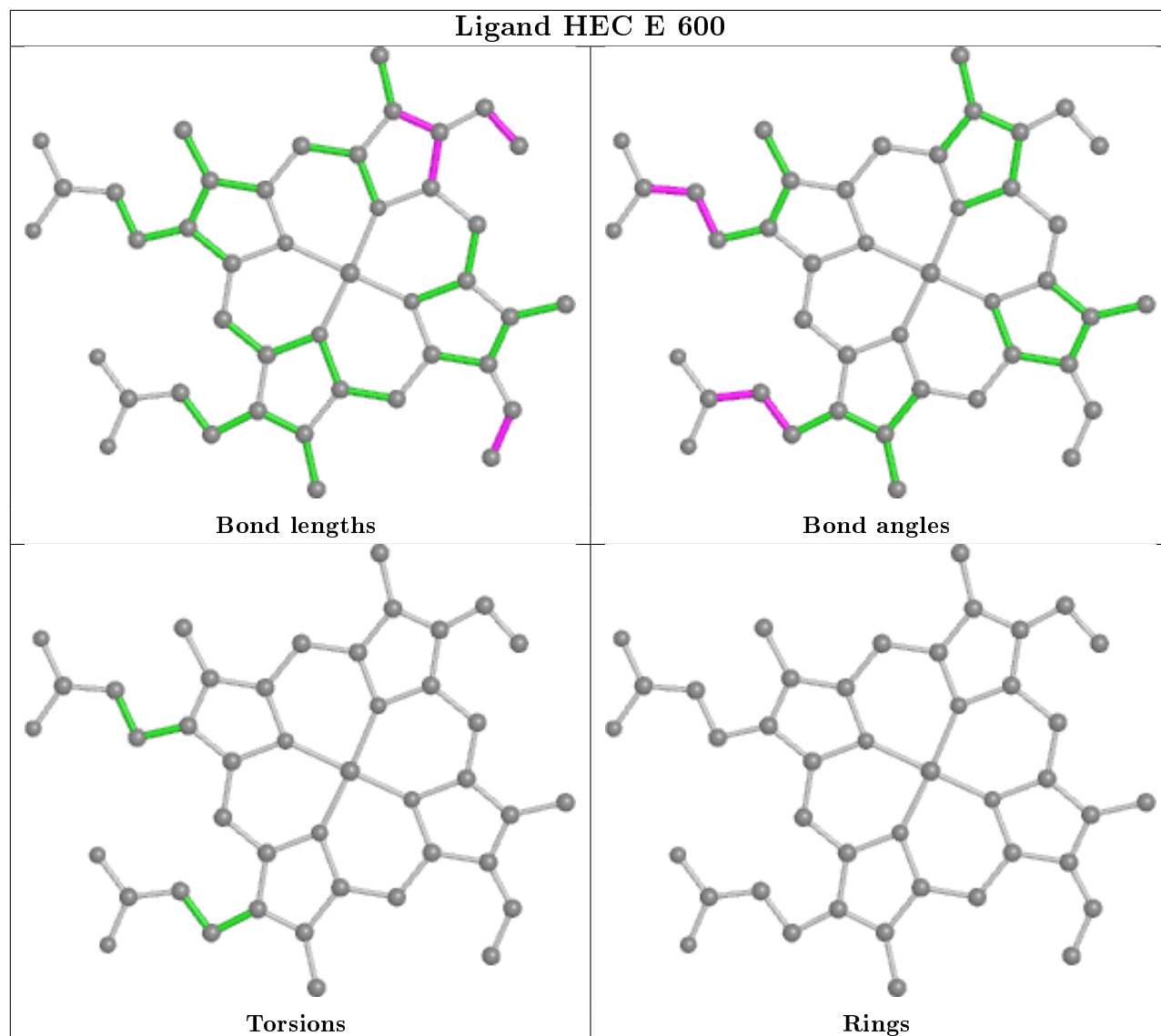




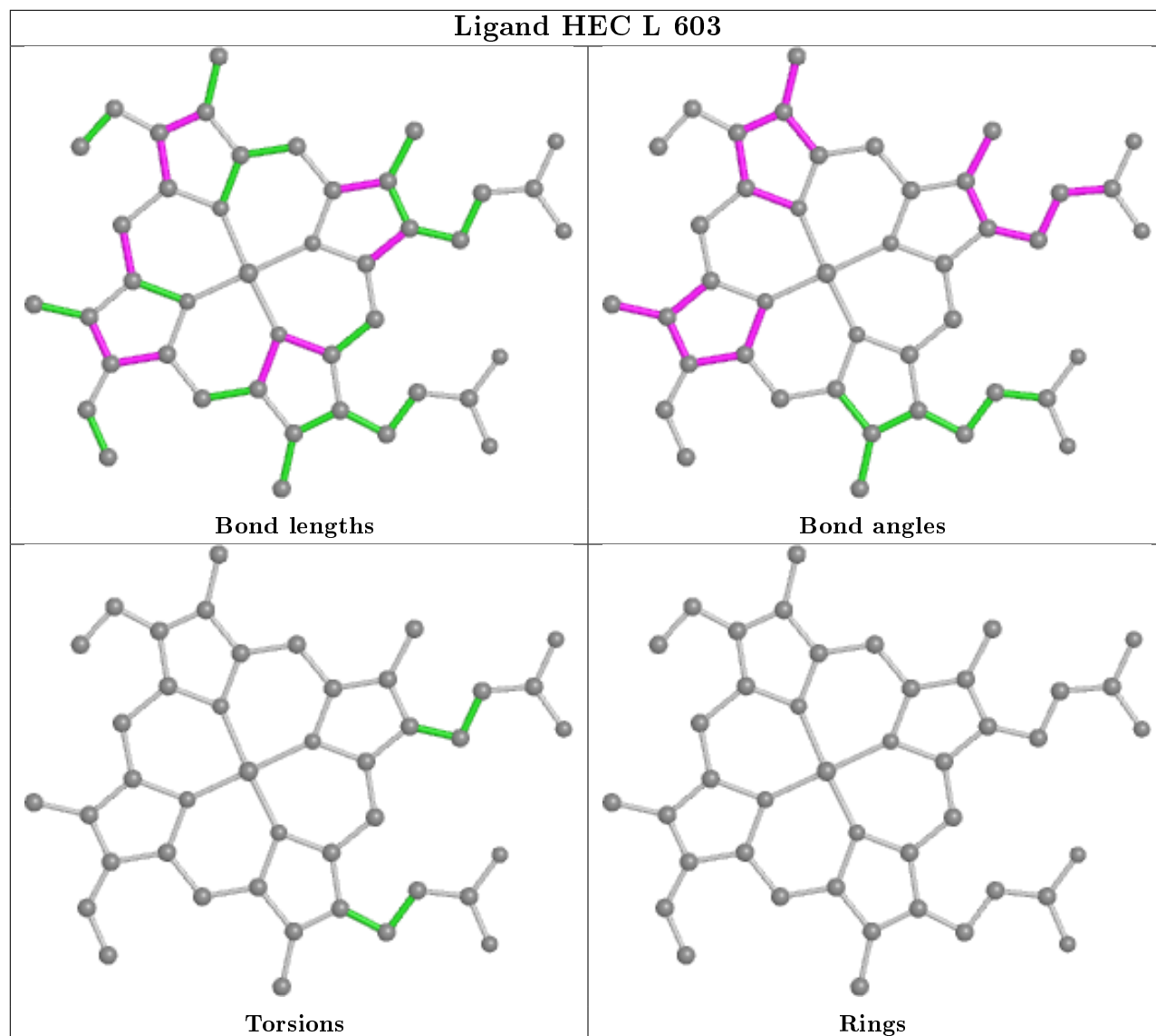


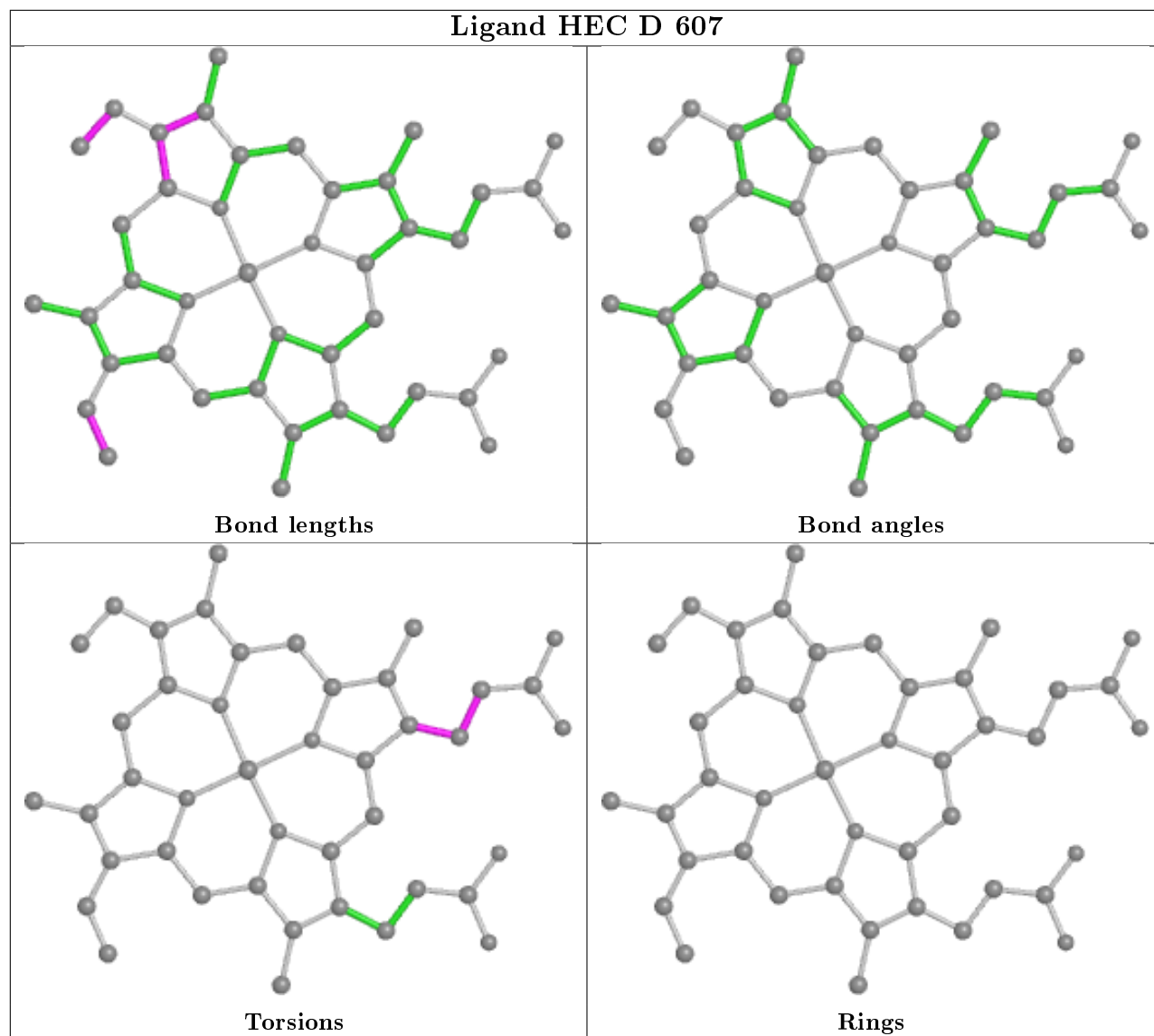




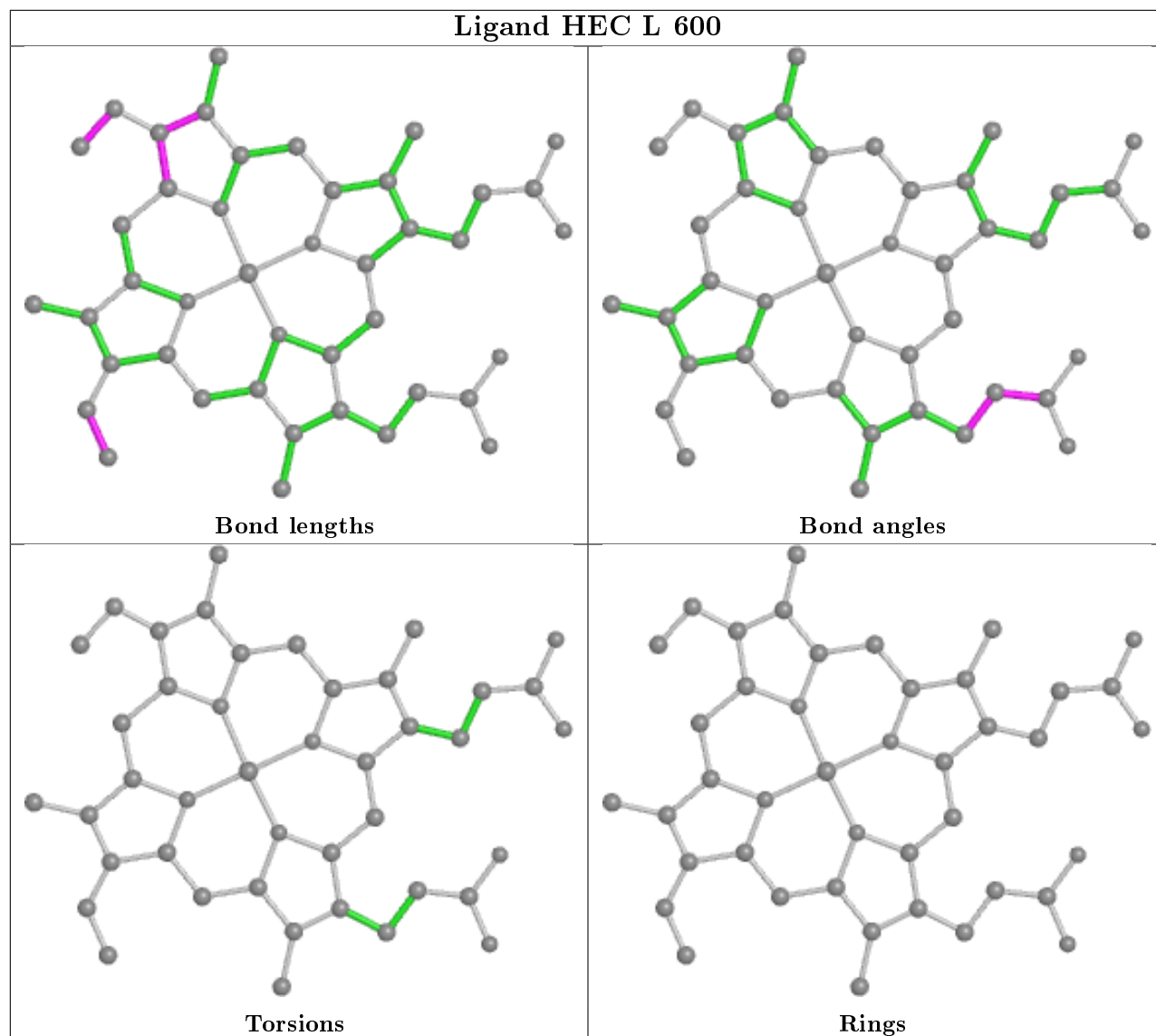


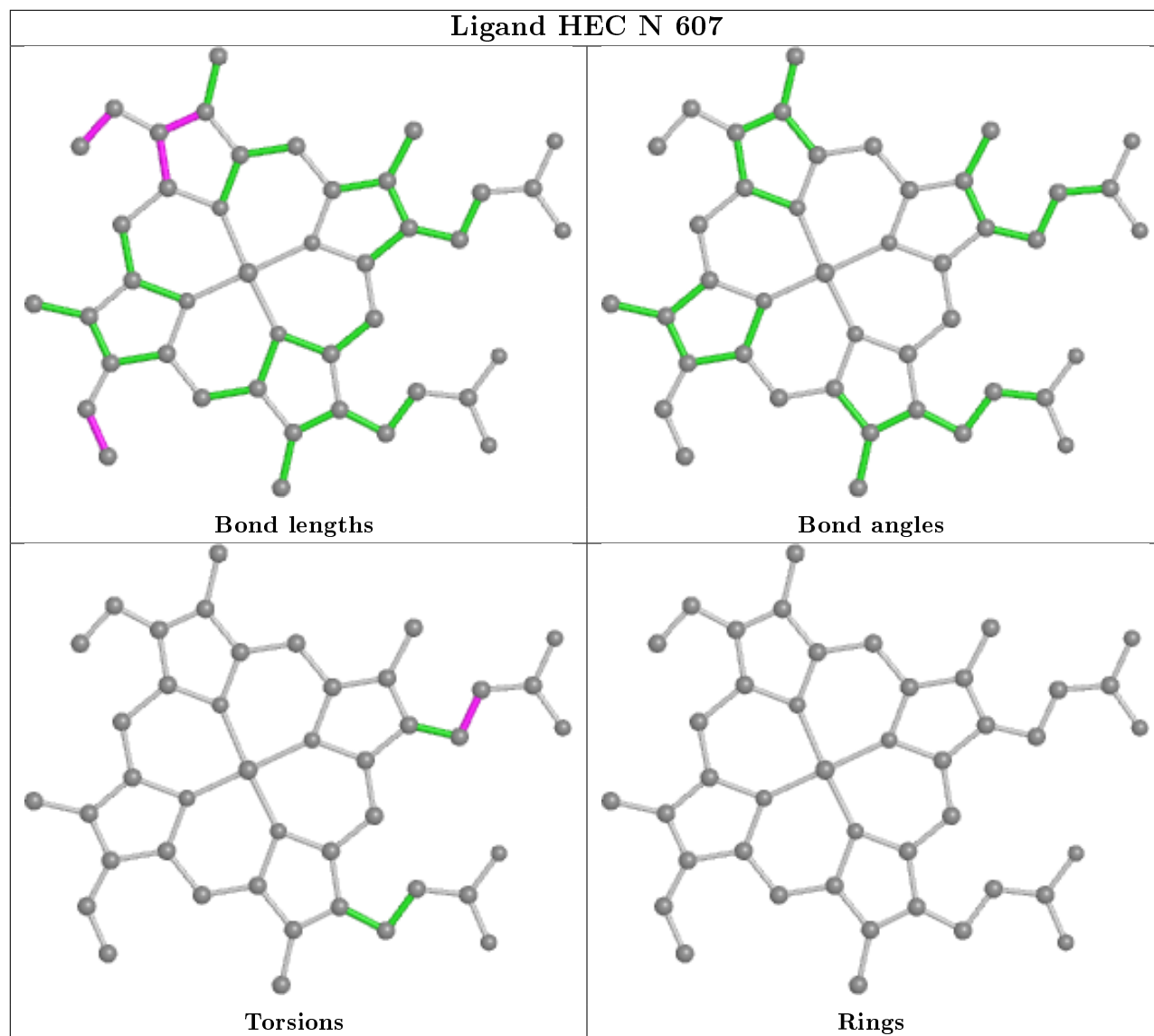
## Ligand HEC L 603



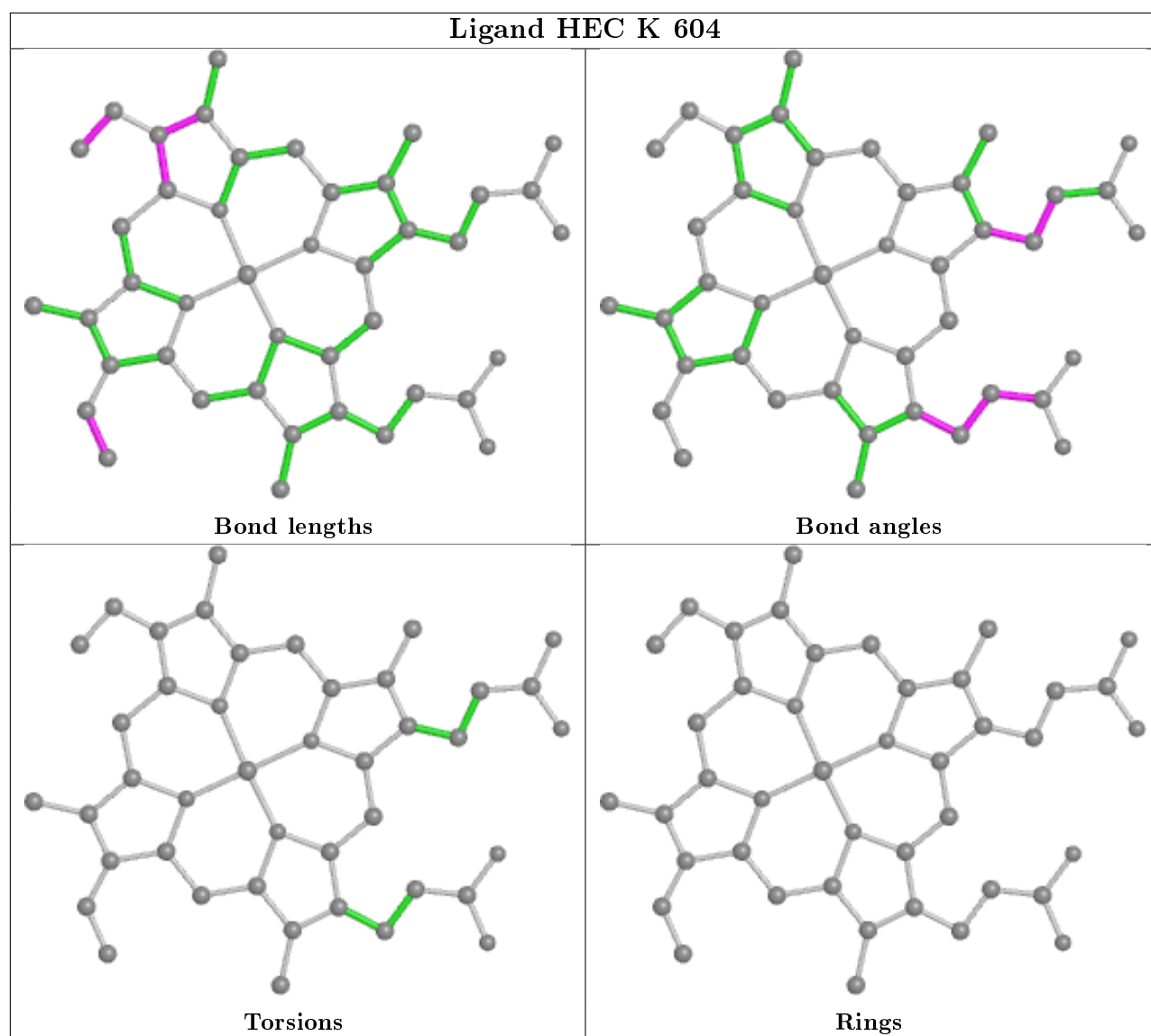


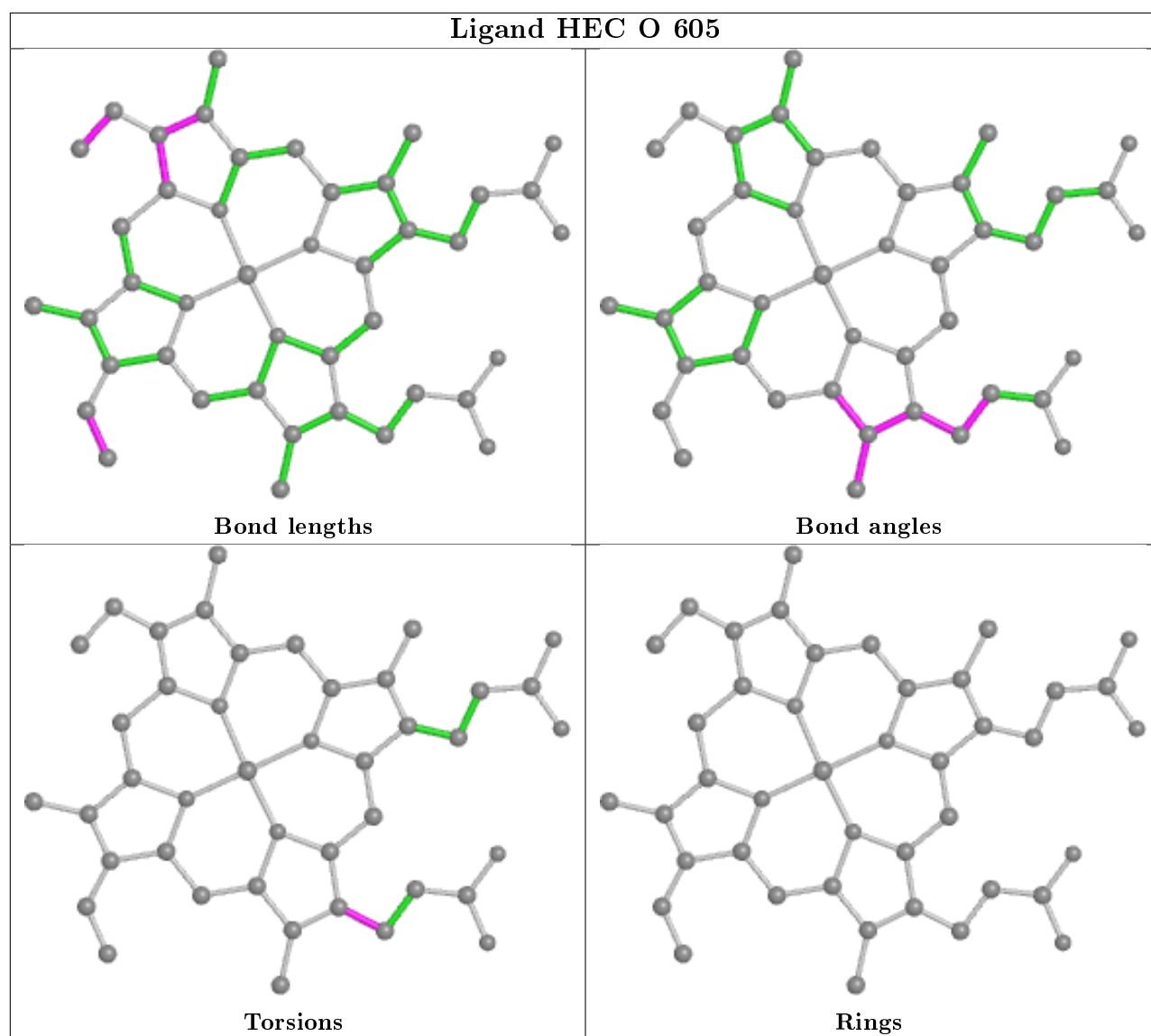
## Ligand HEC L 600

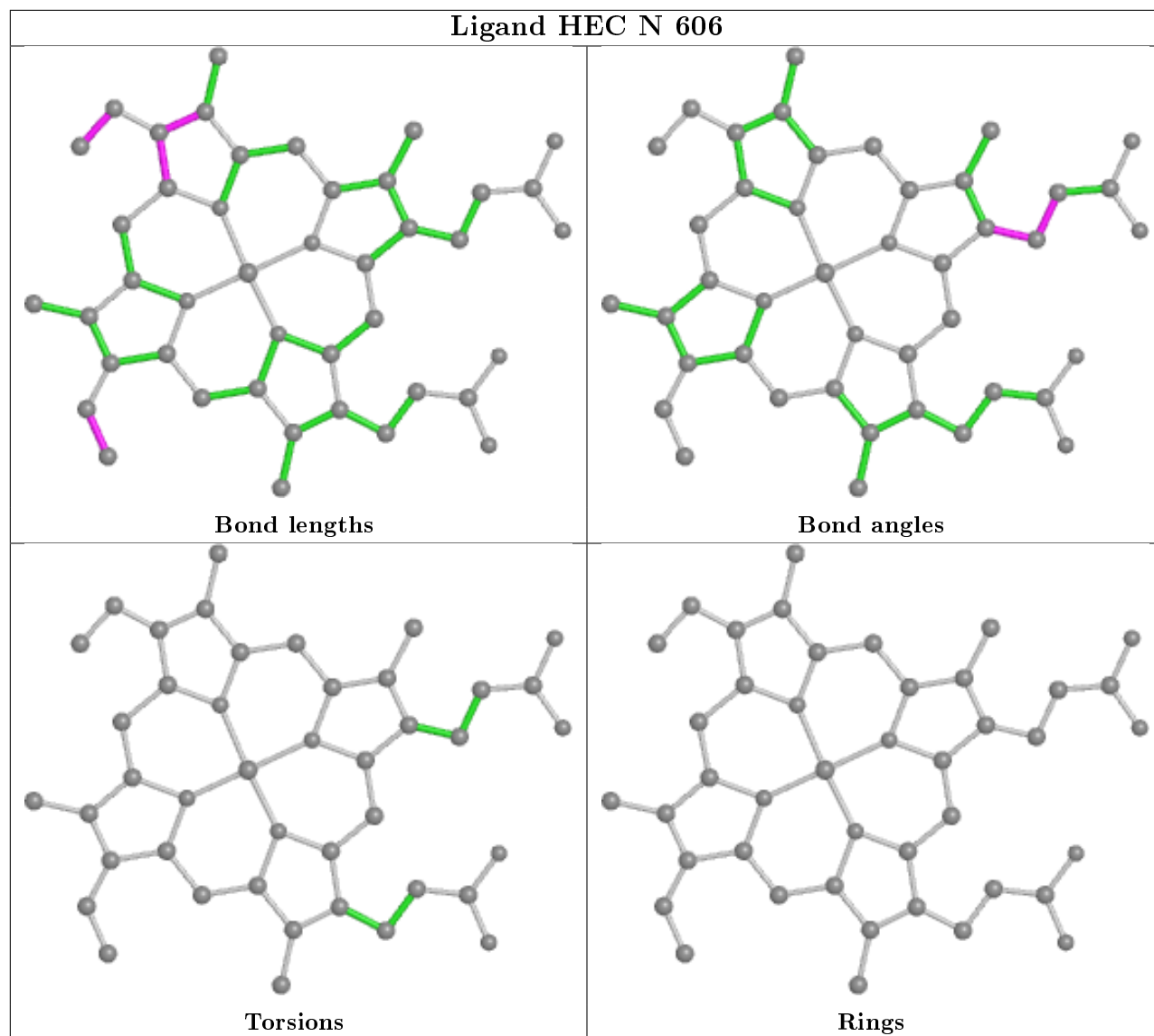


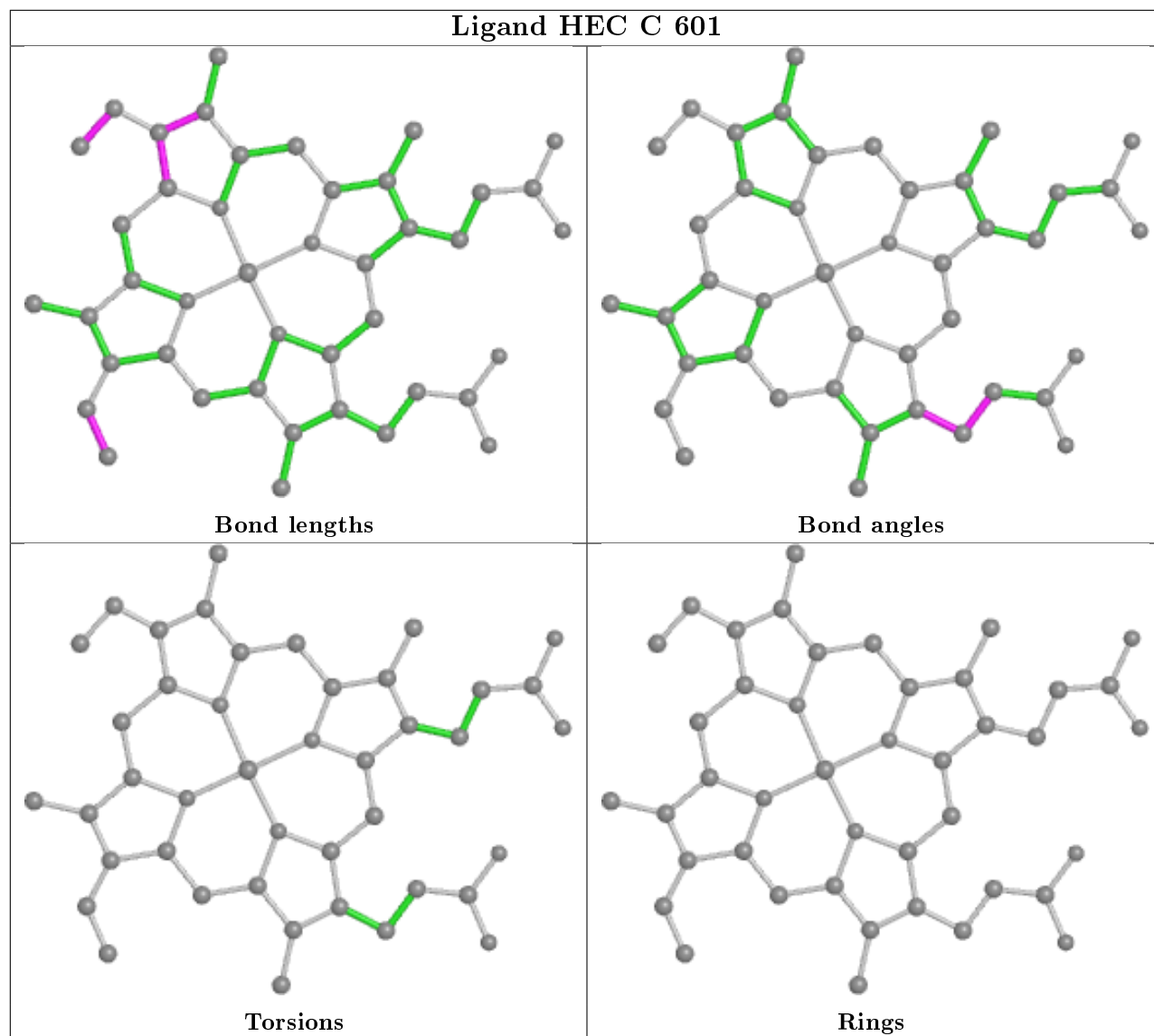




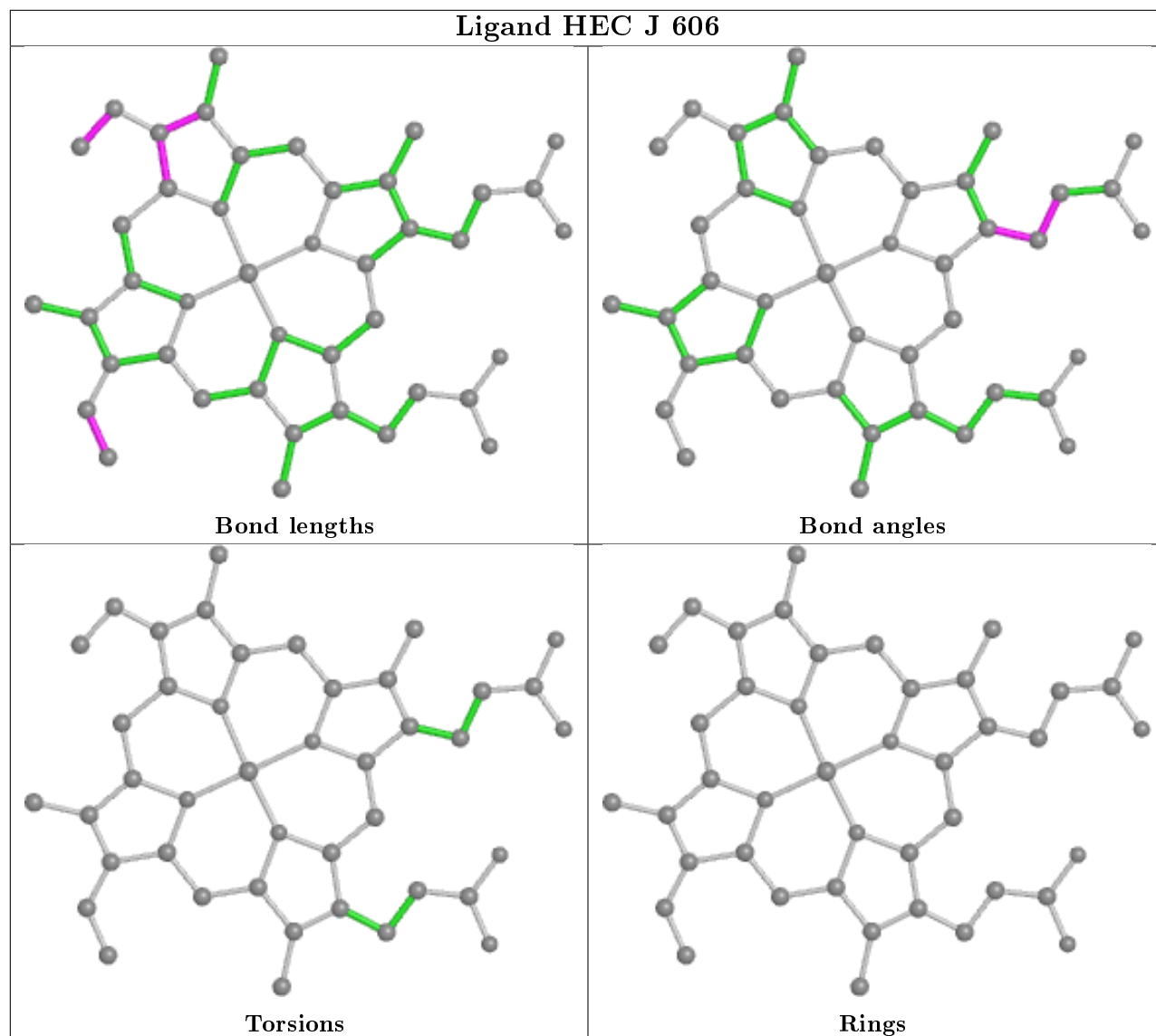


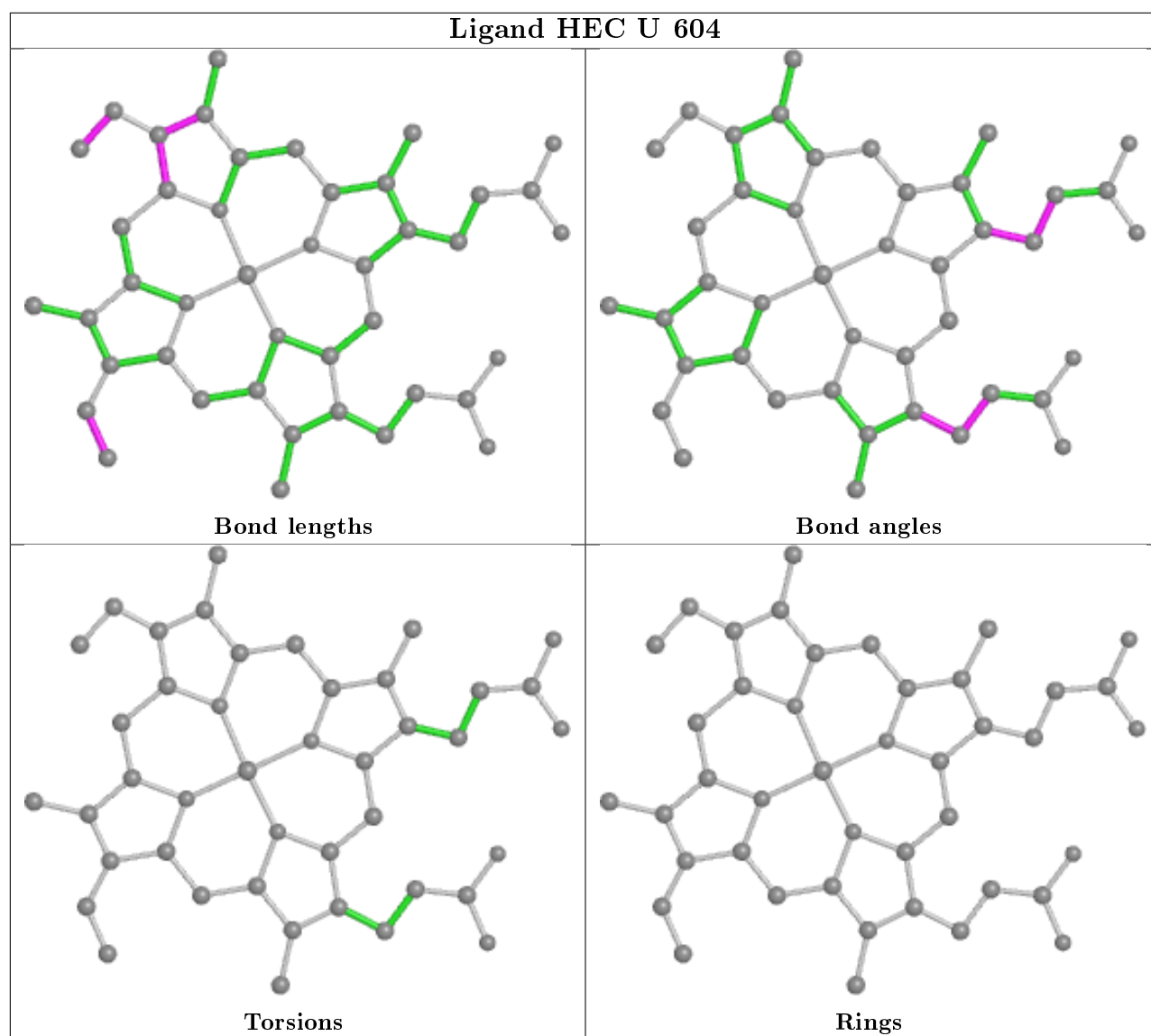




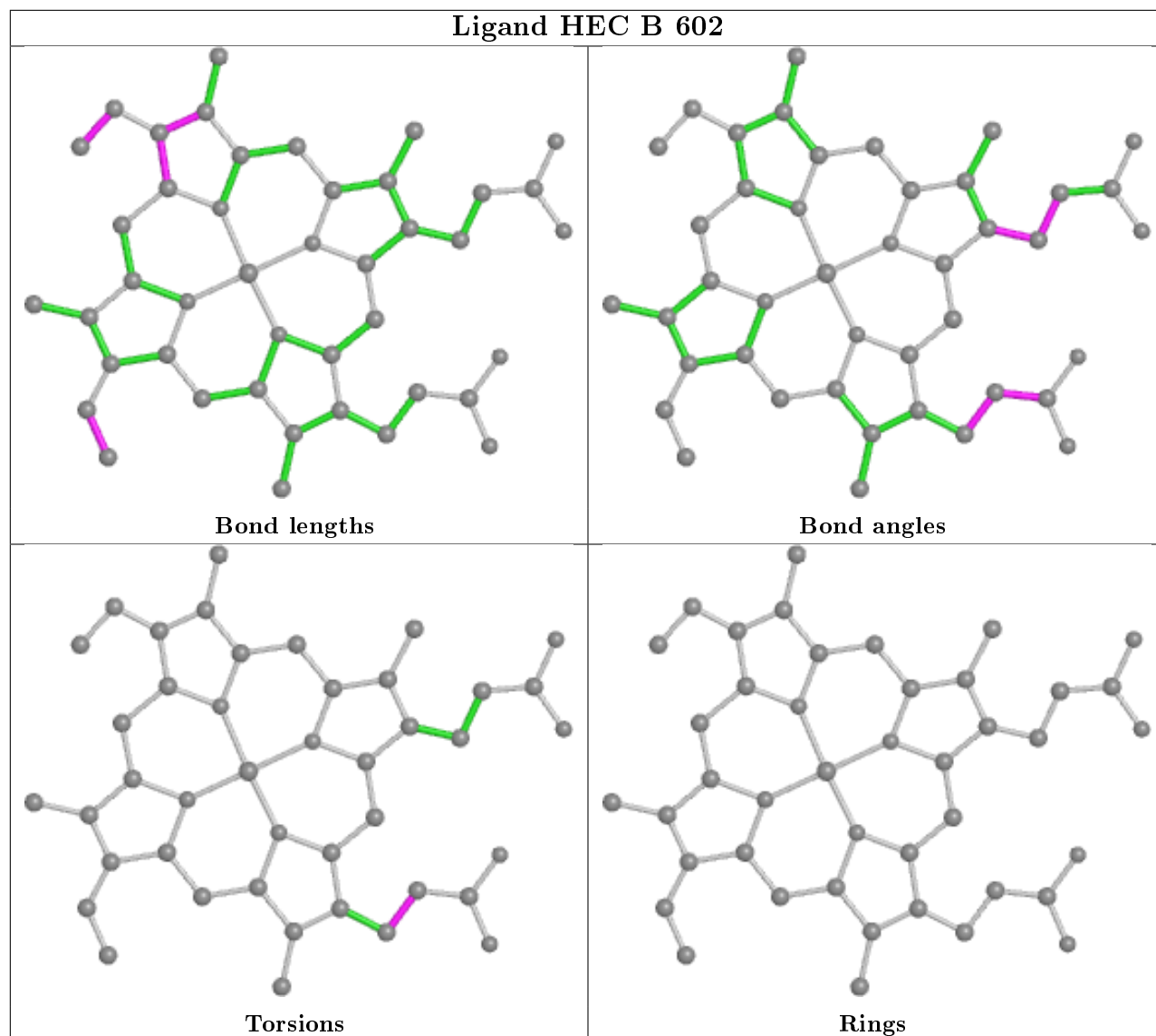


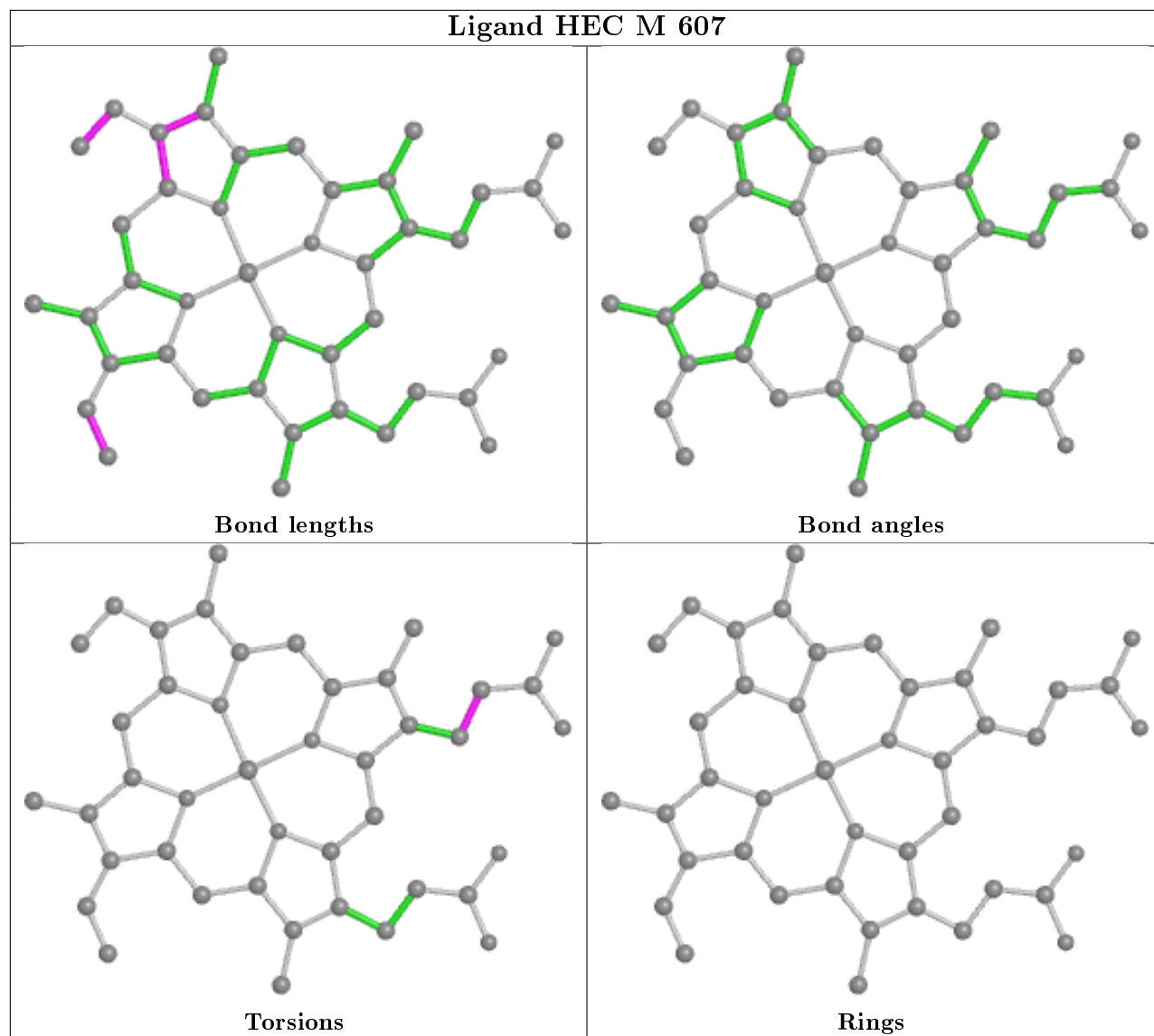
## Ligand HEC J 606





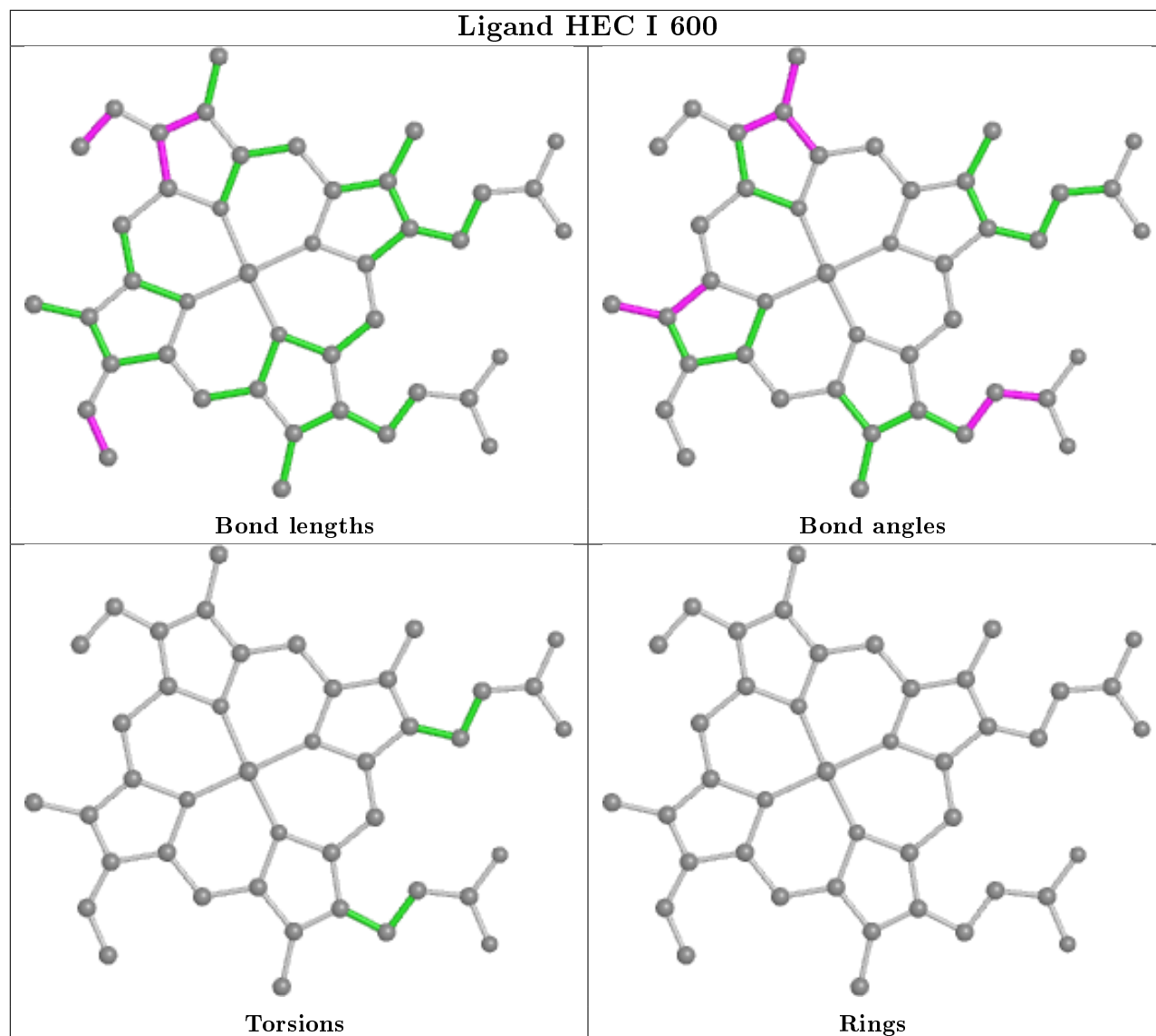
## Ligand HEC B 602



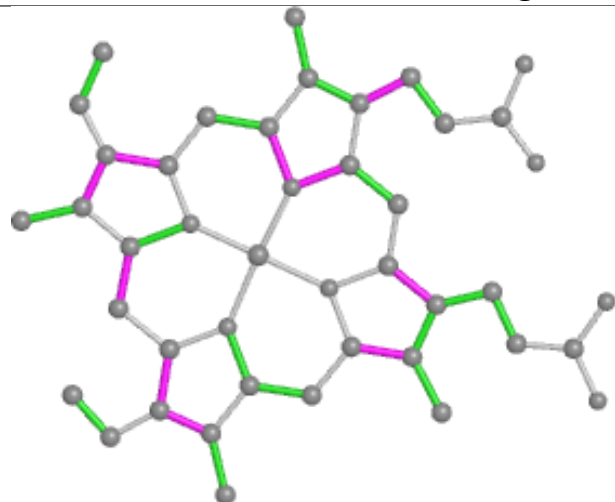




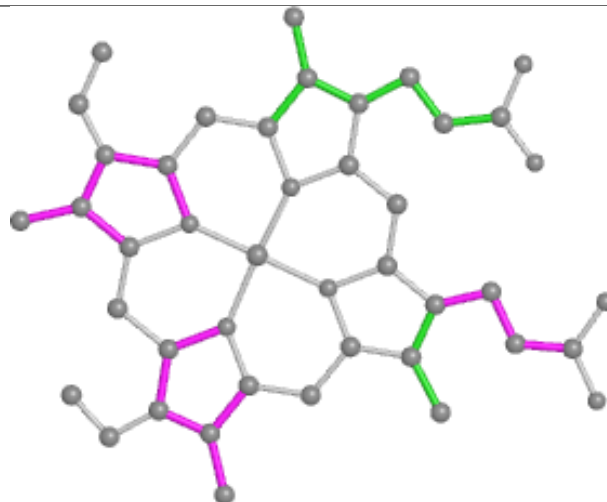
## Ligand HEC I 600



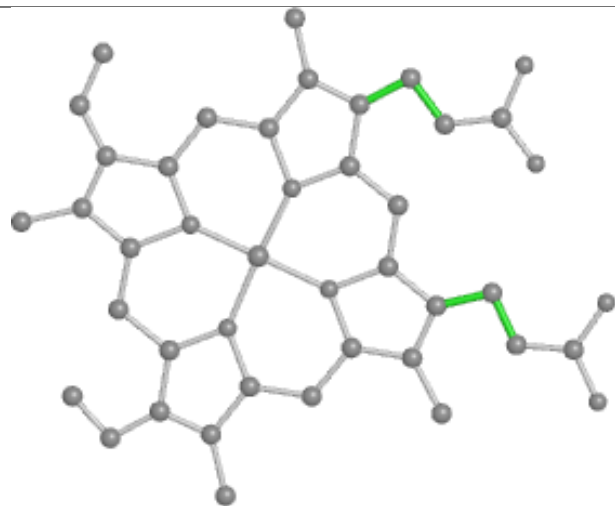
## Ligand HEC F 603



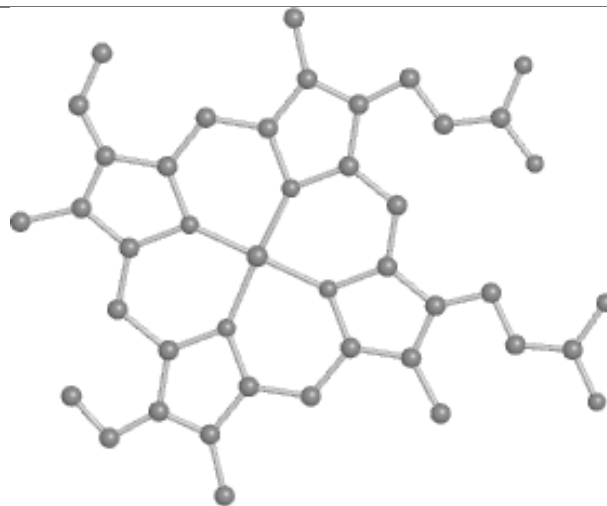
Bond lengths



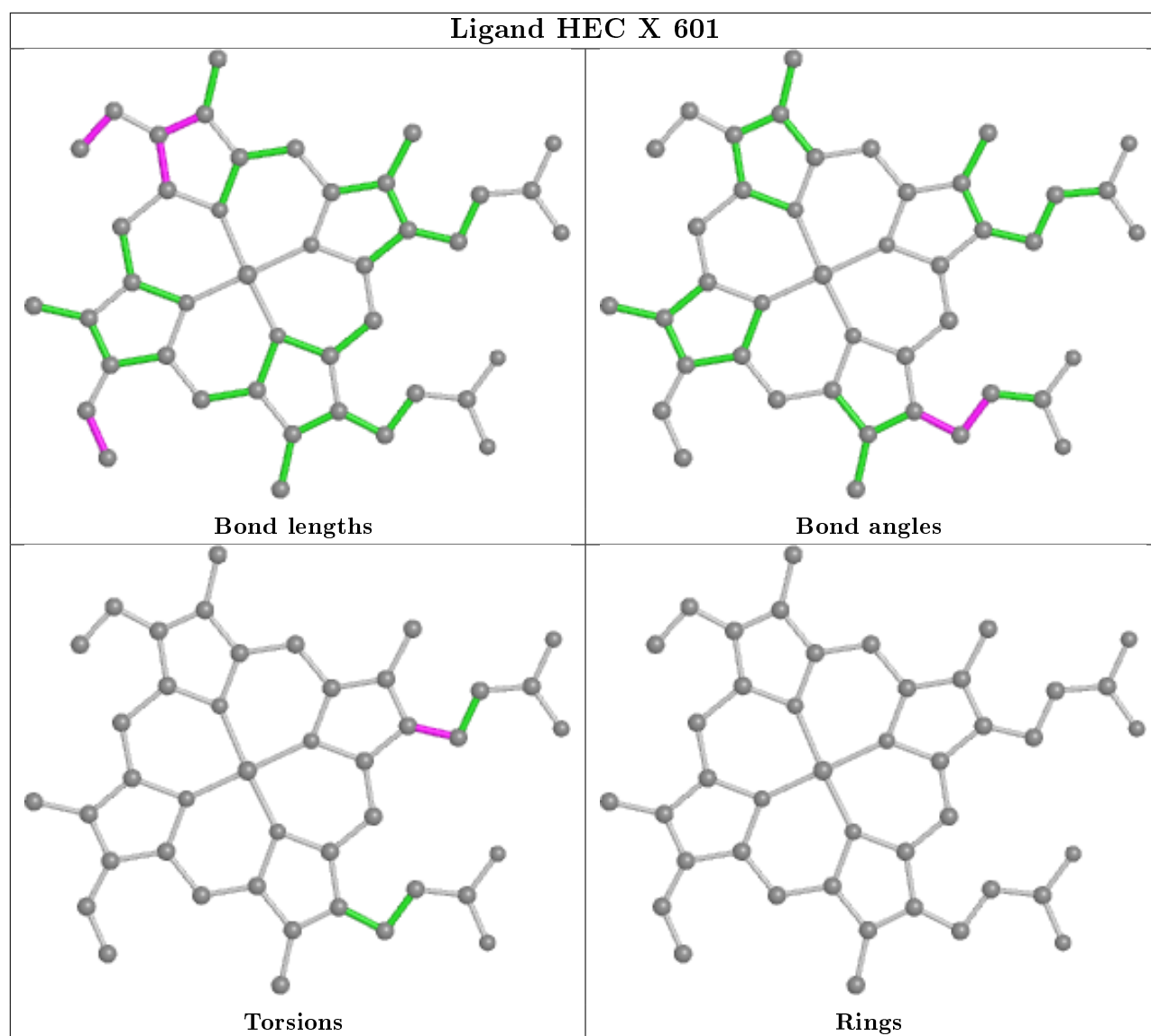
Bond angles

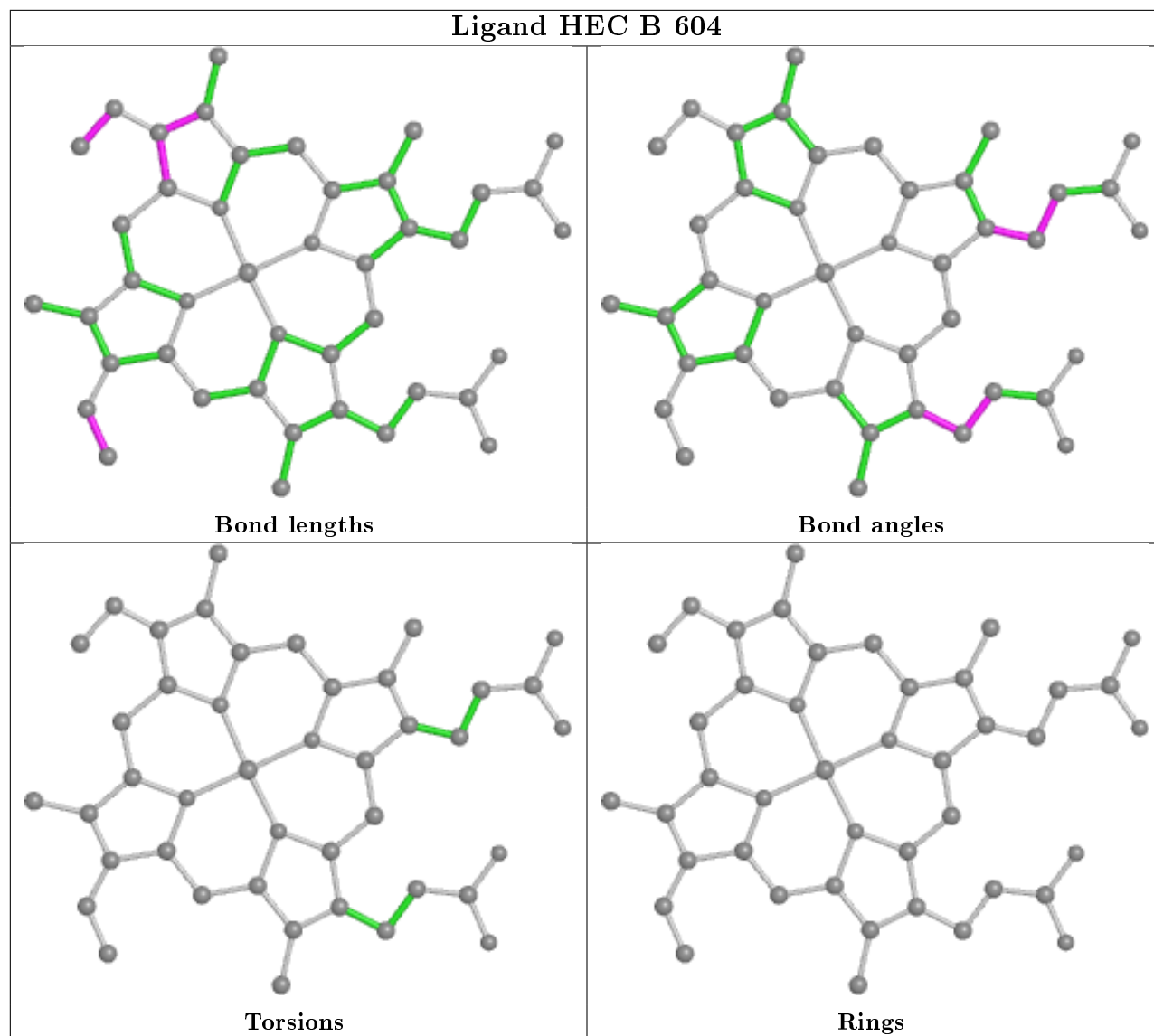


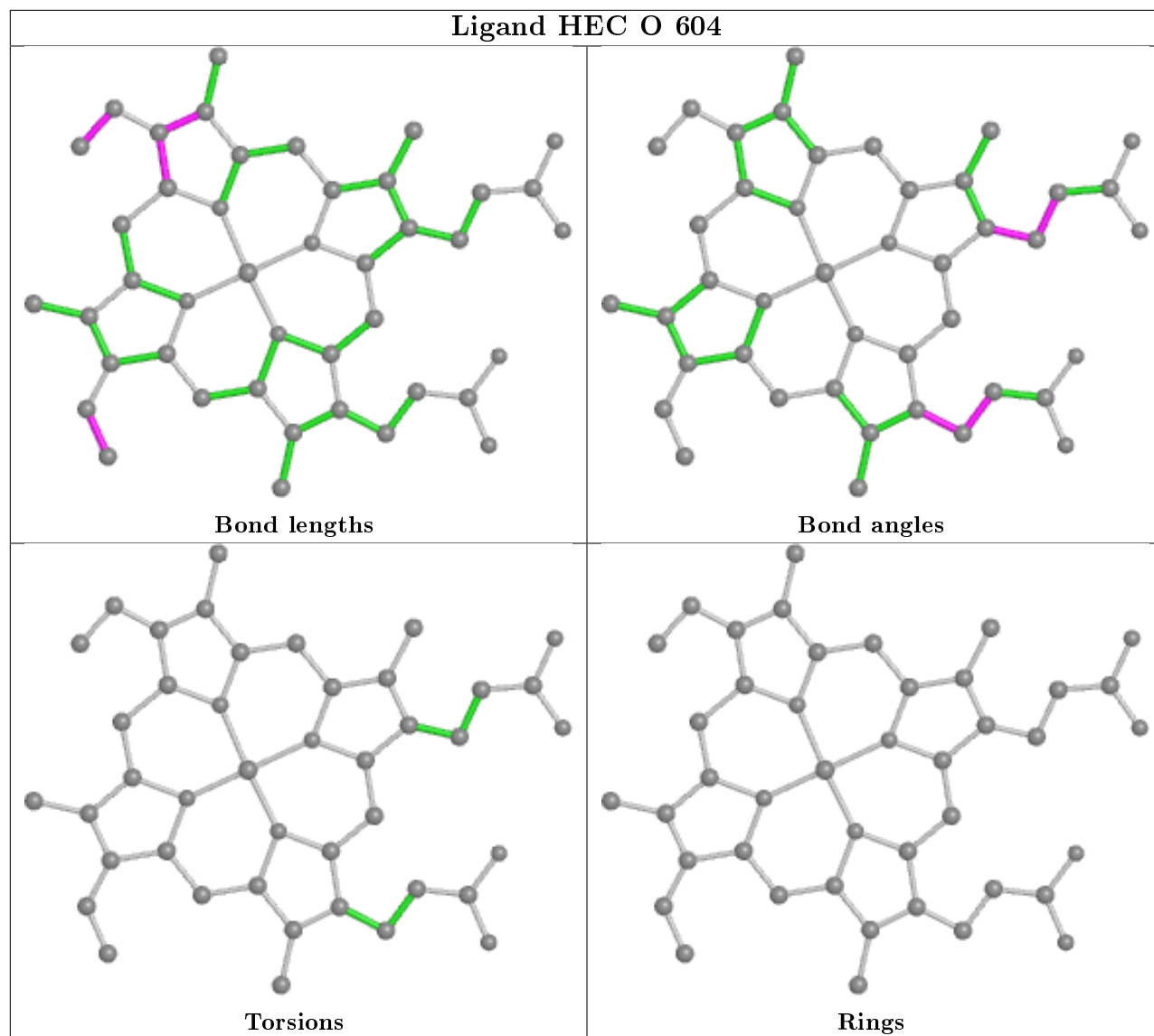
Torsions

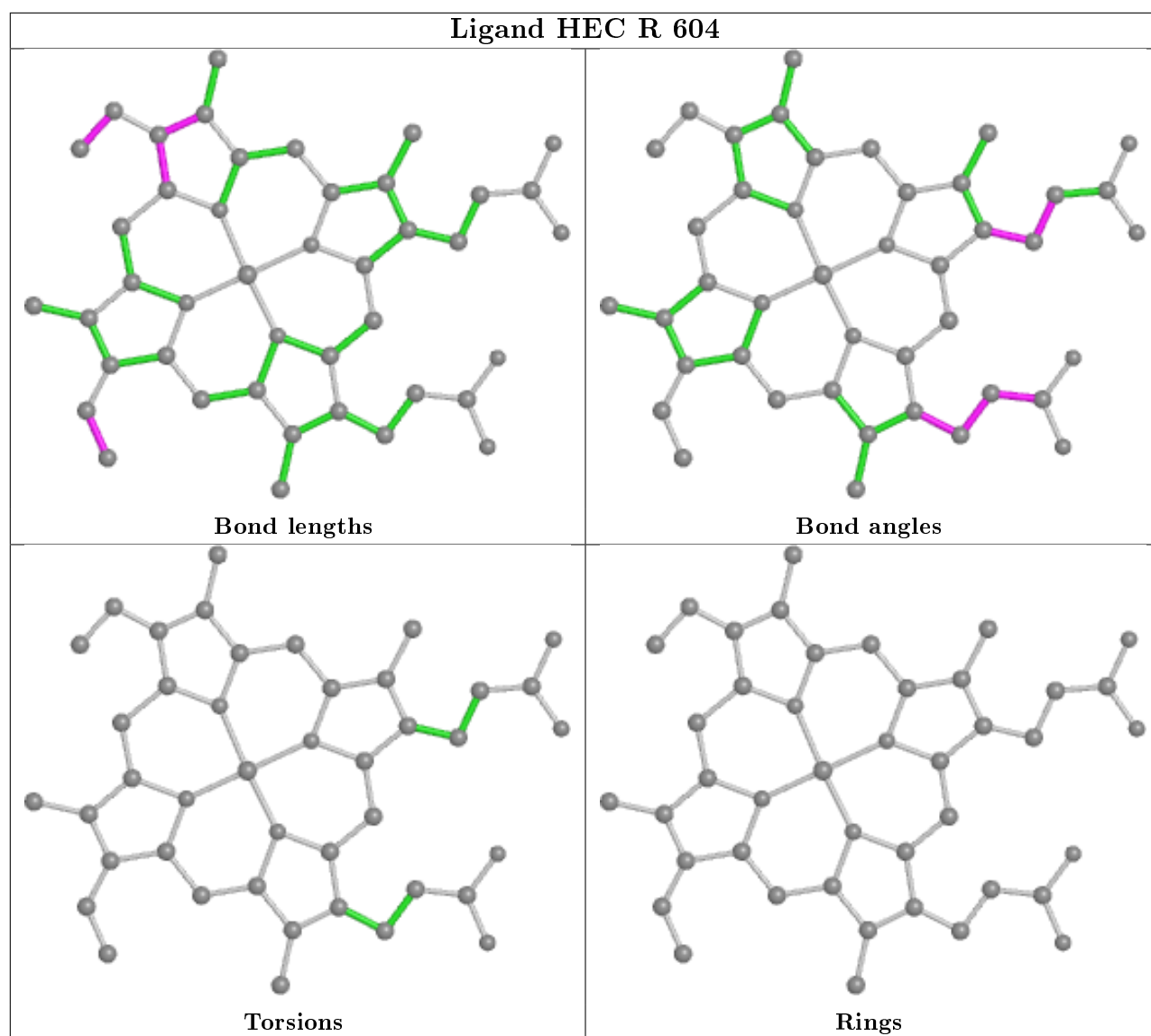


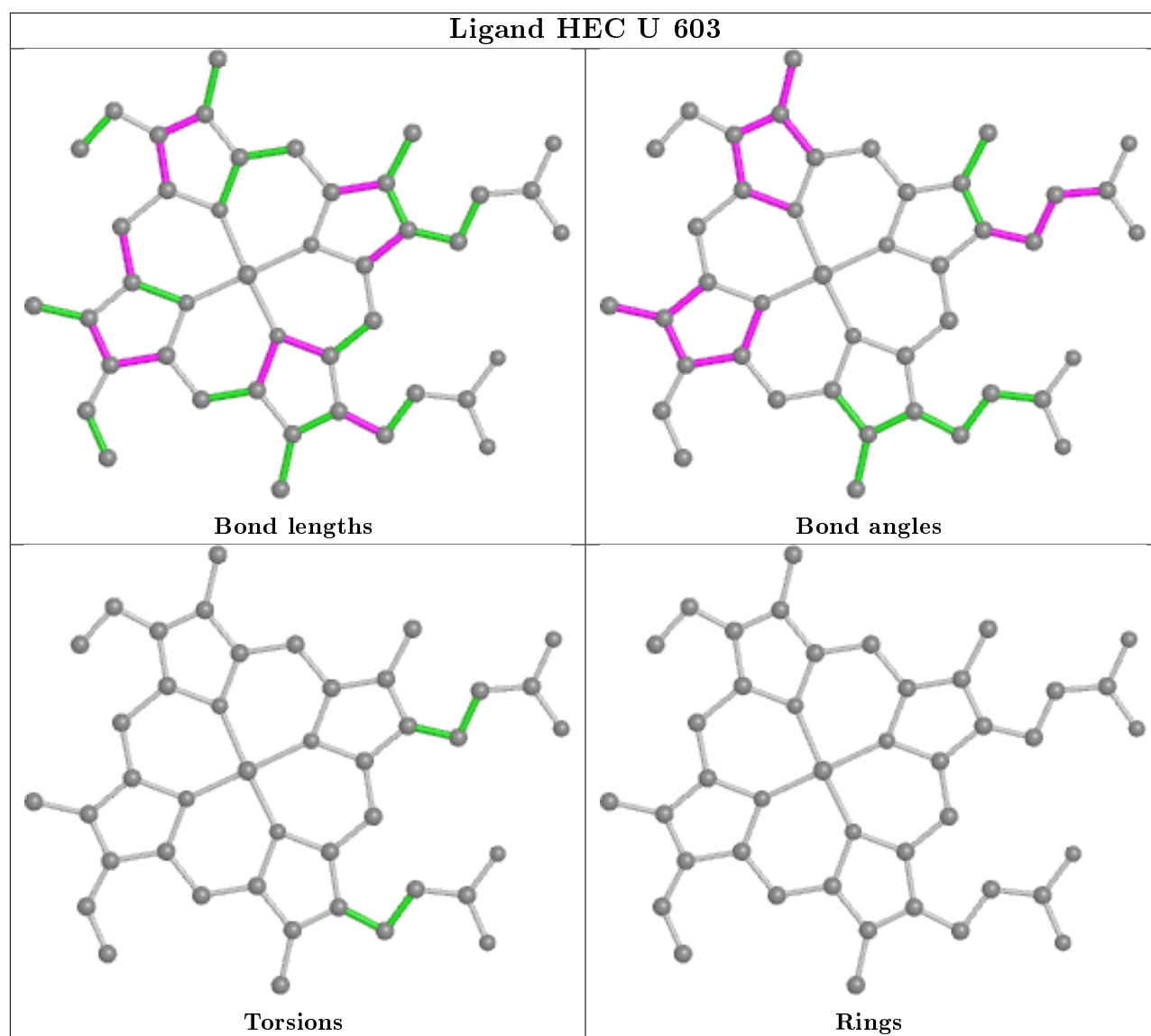
Rings



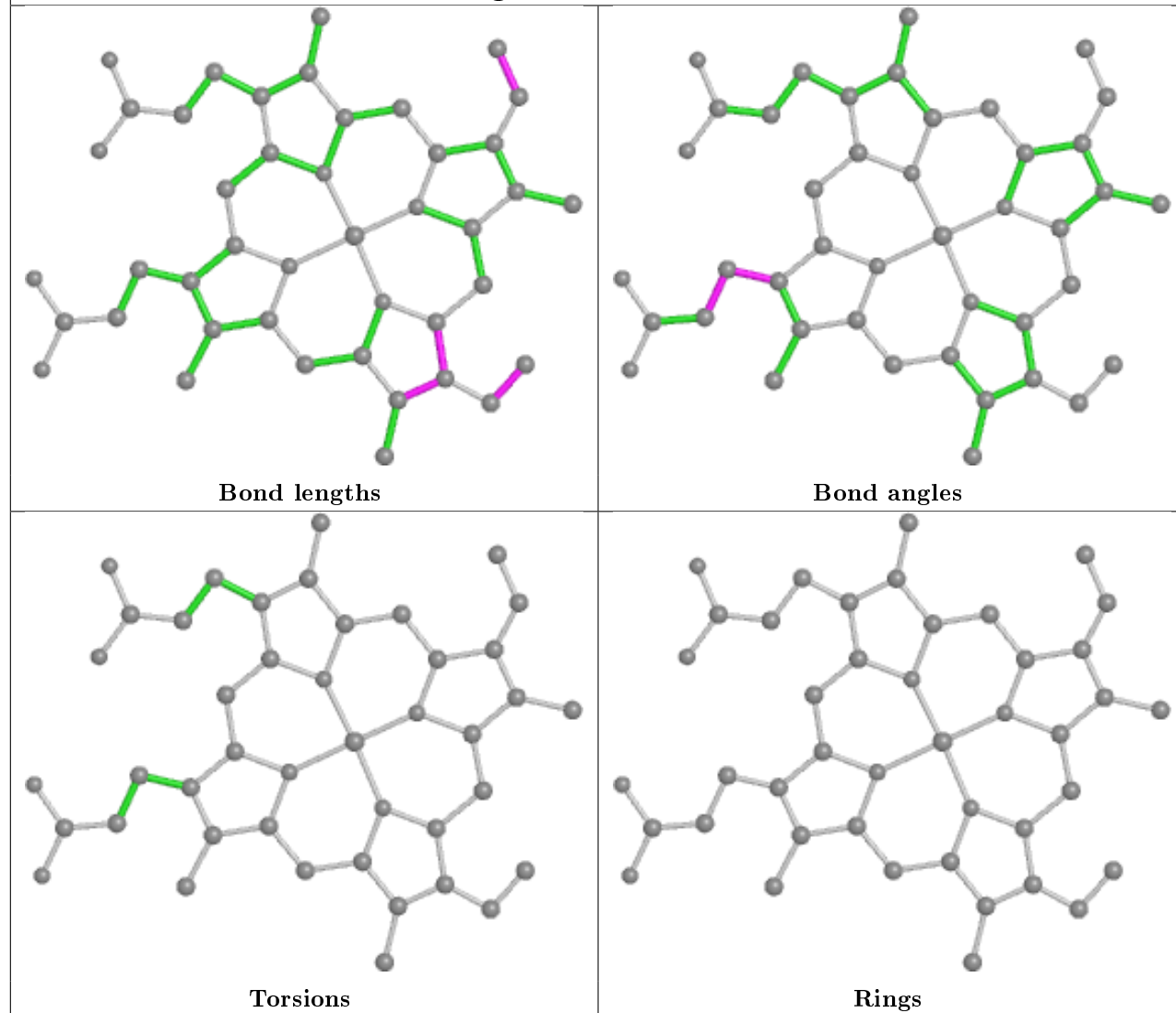




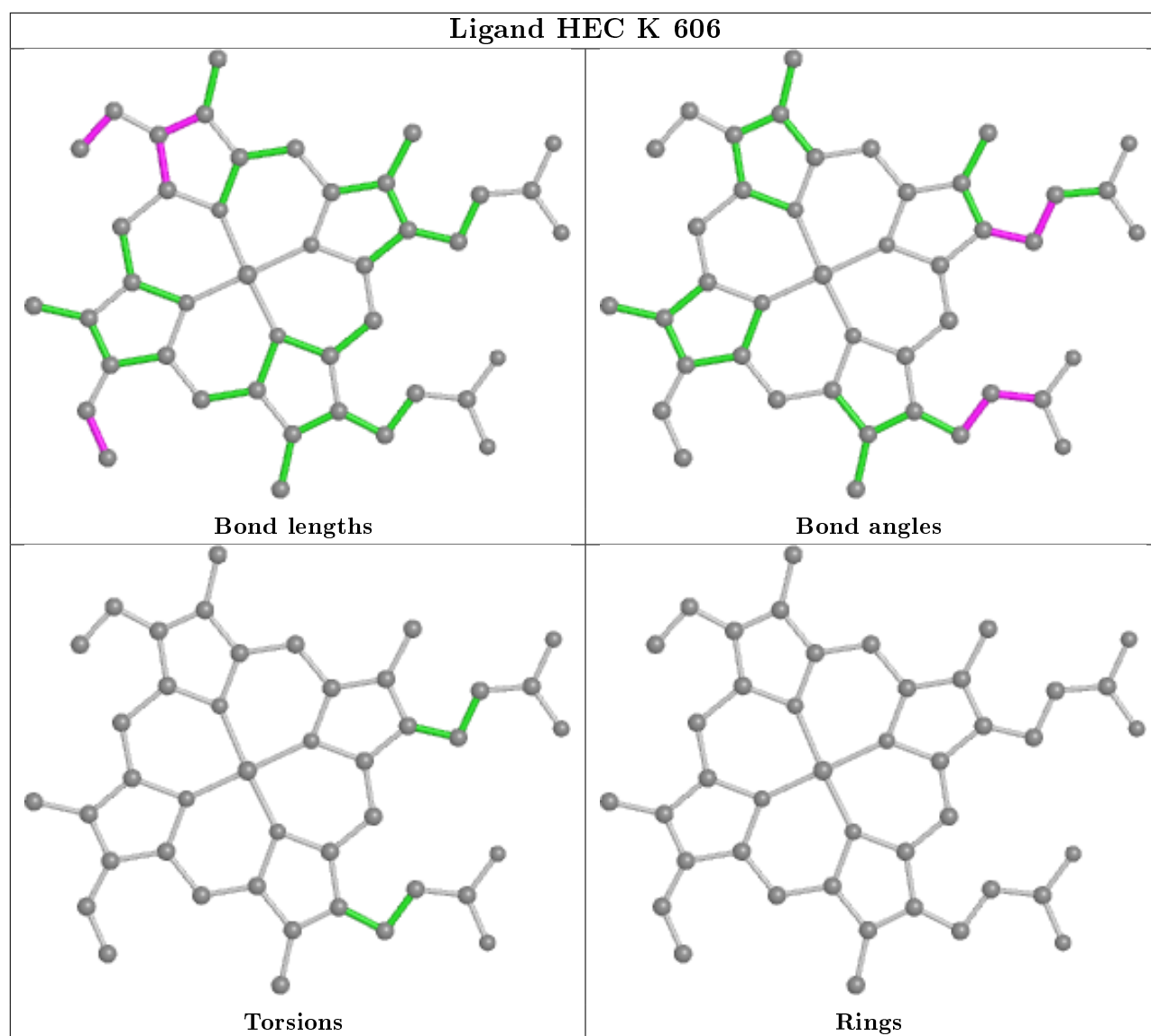


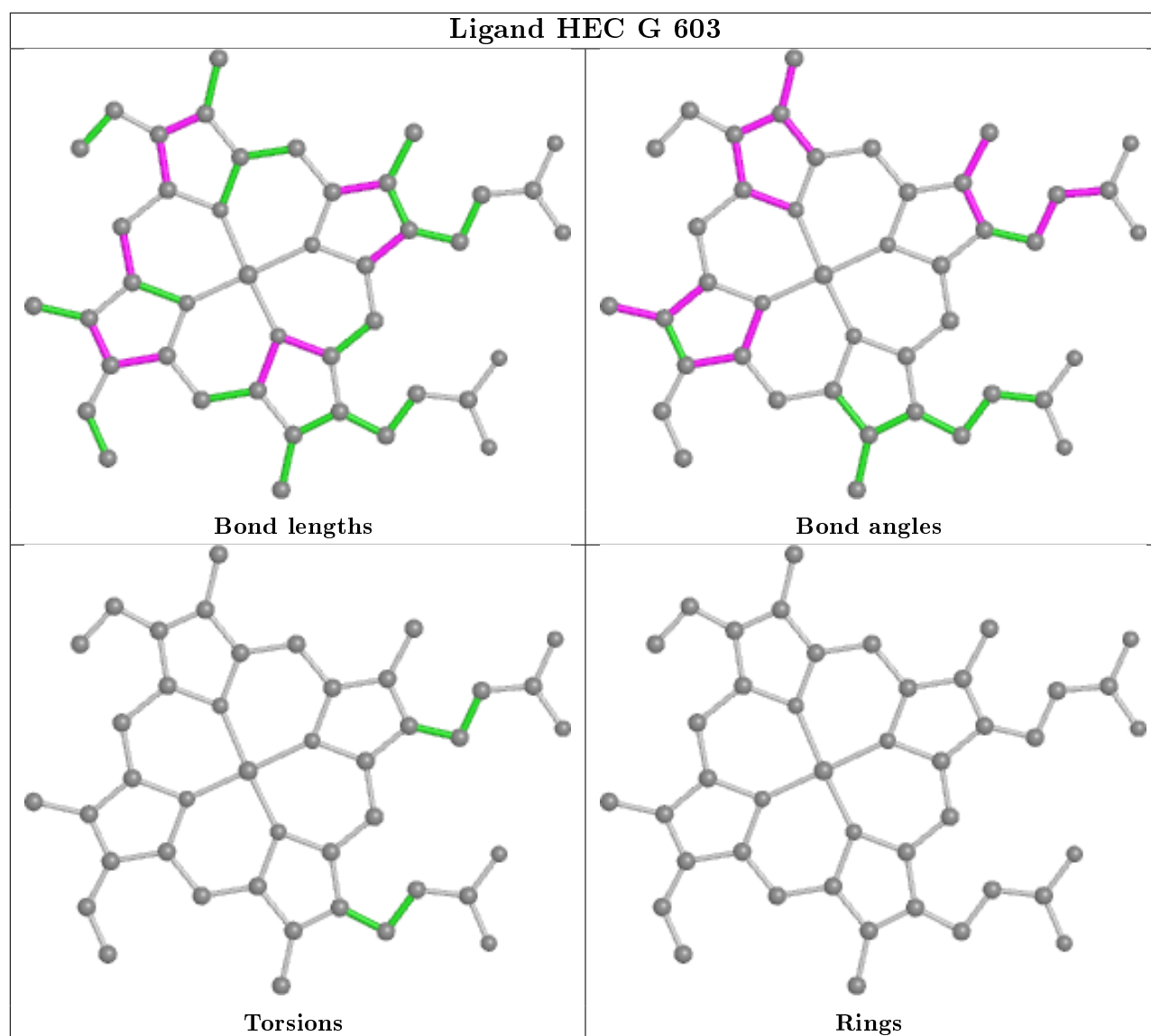


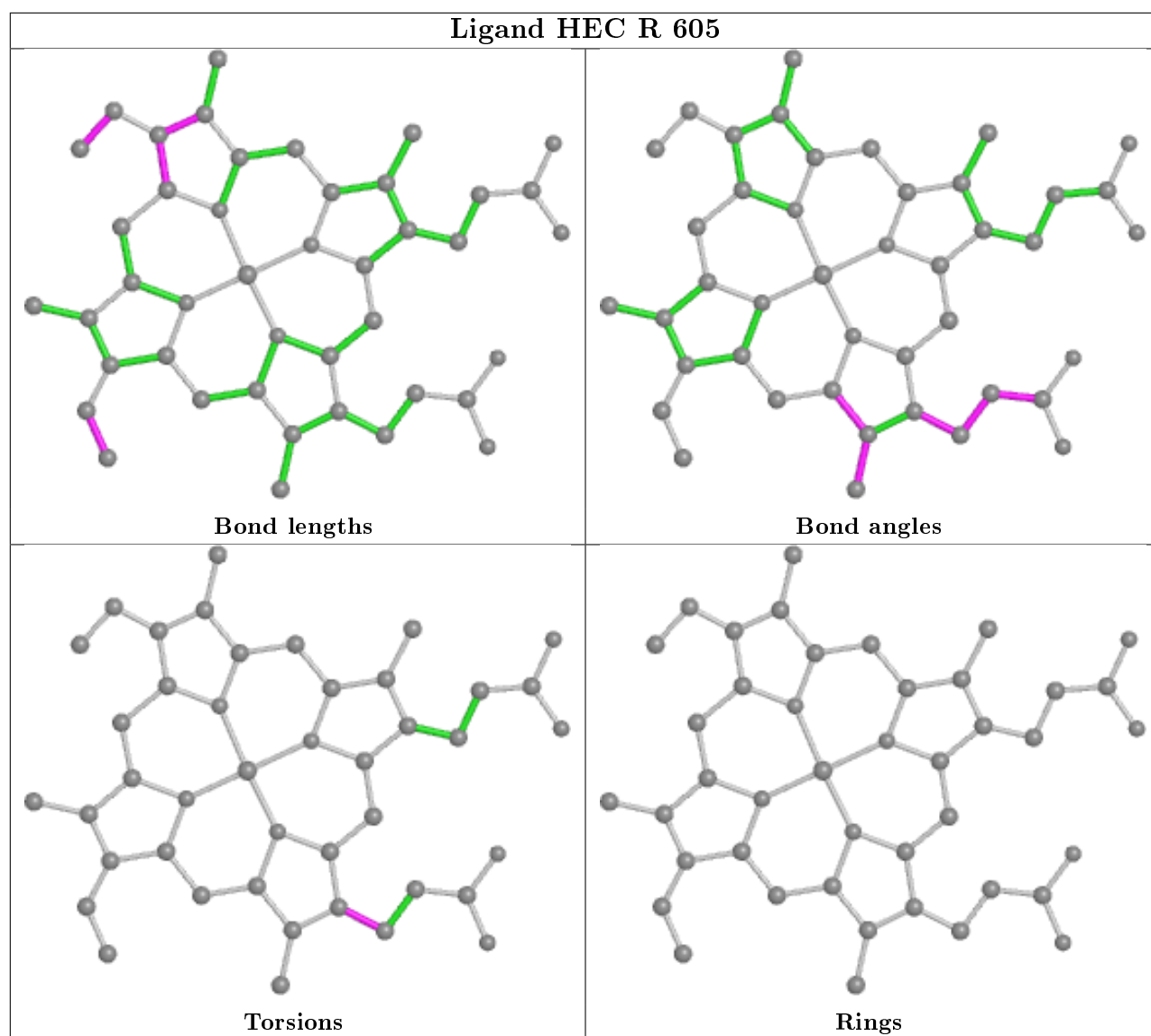
## Ligand HEC F 606

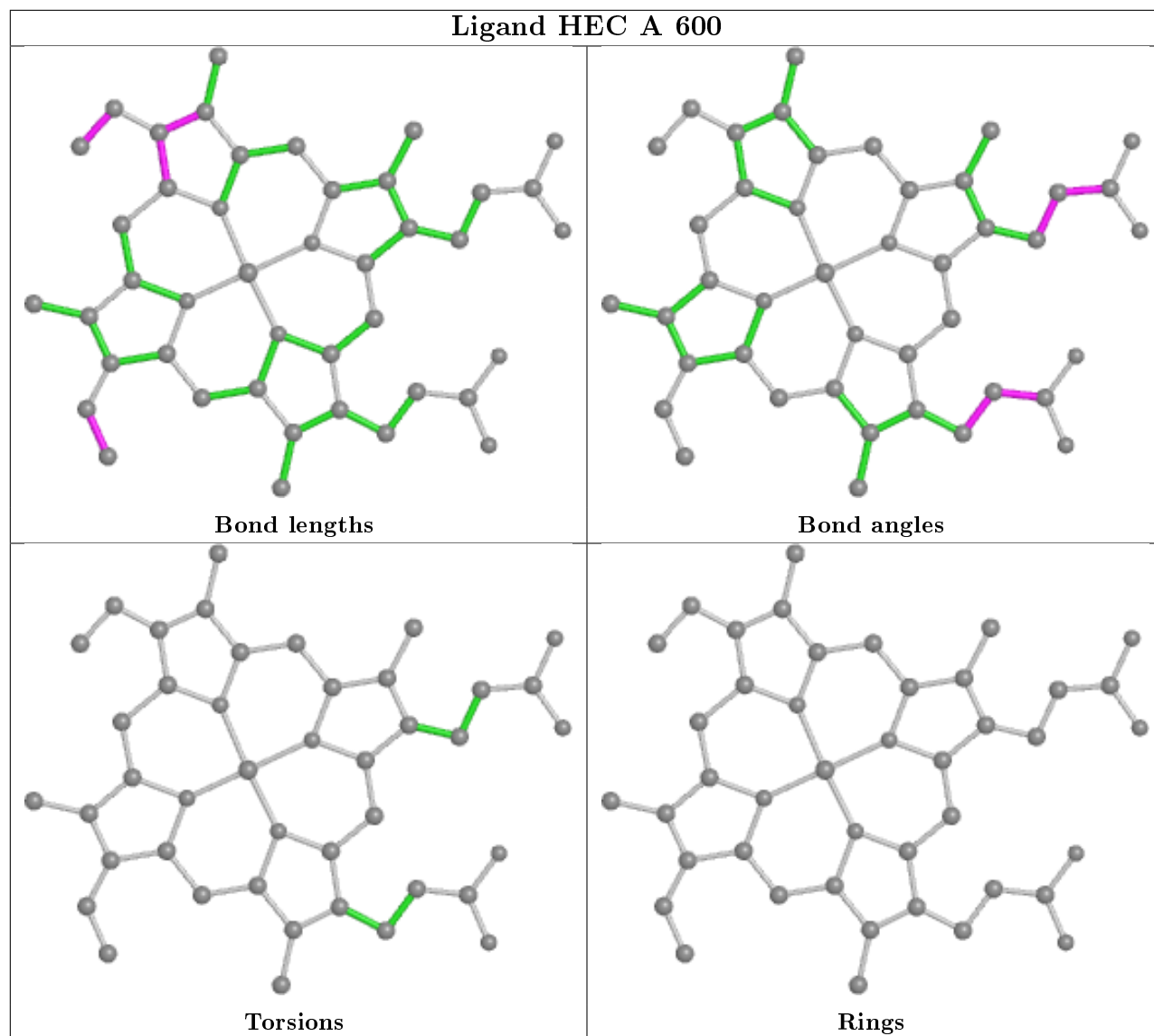




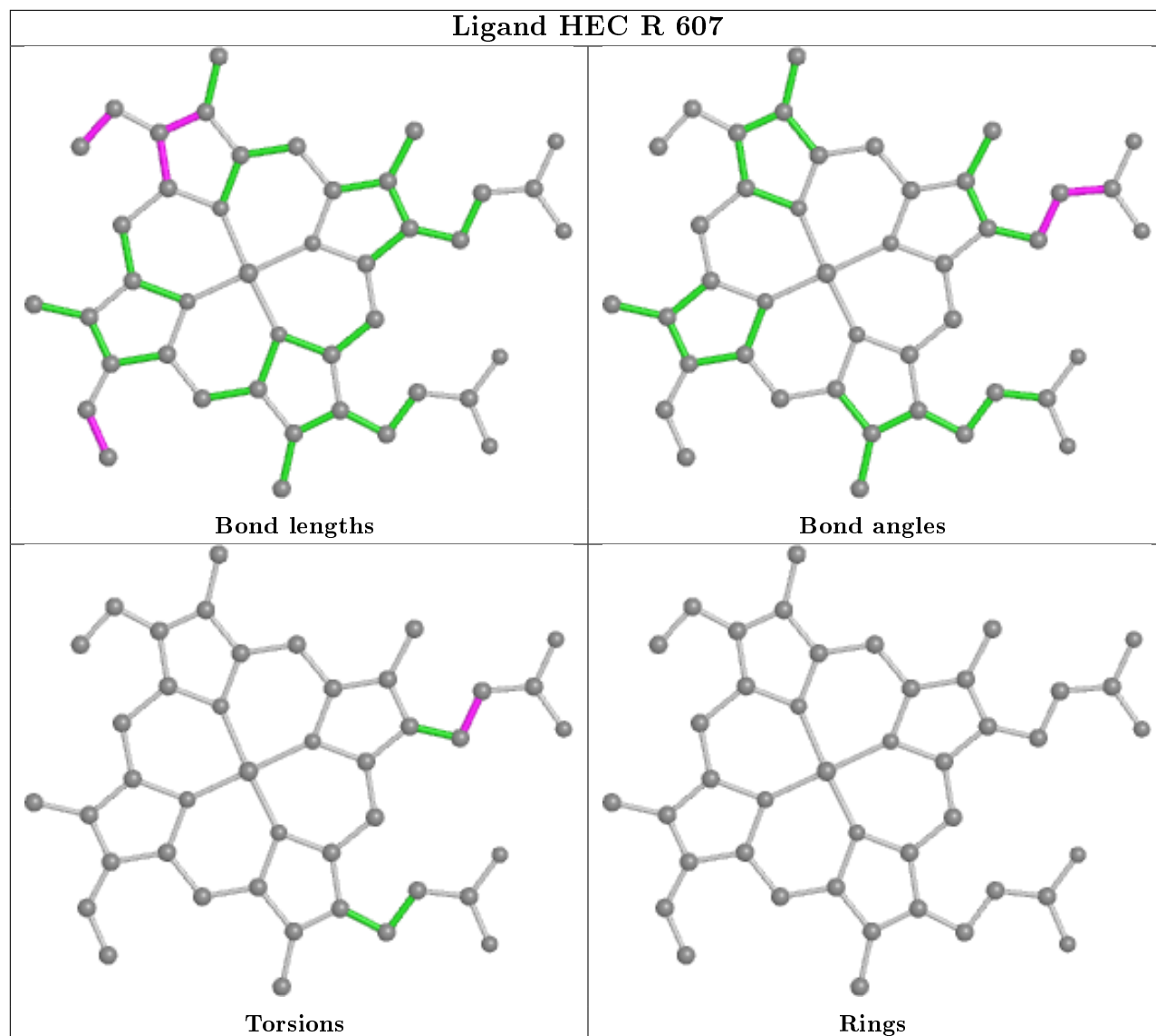


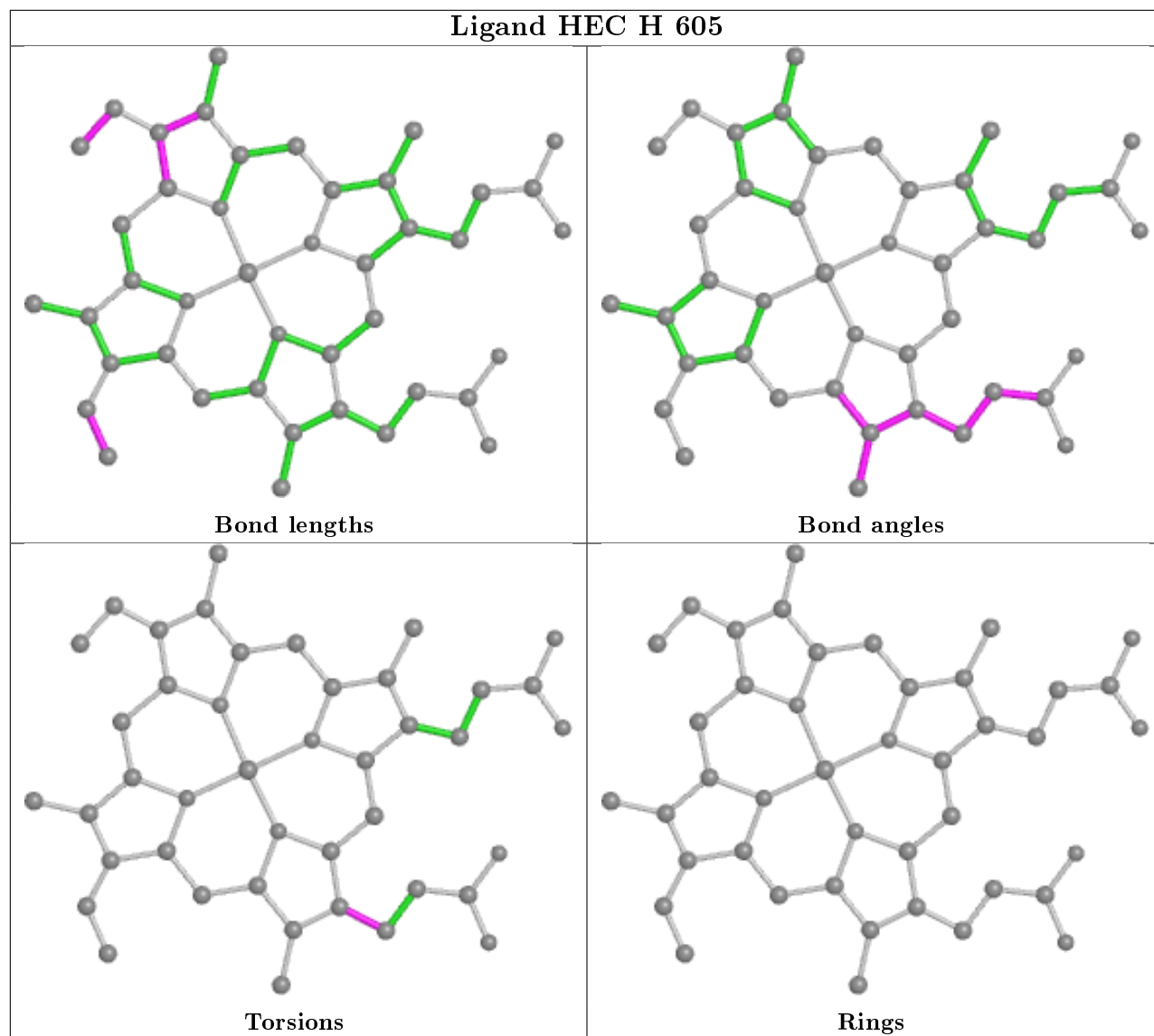


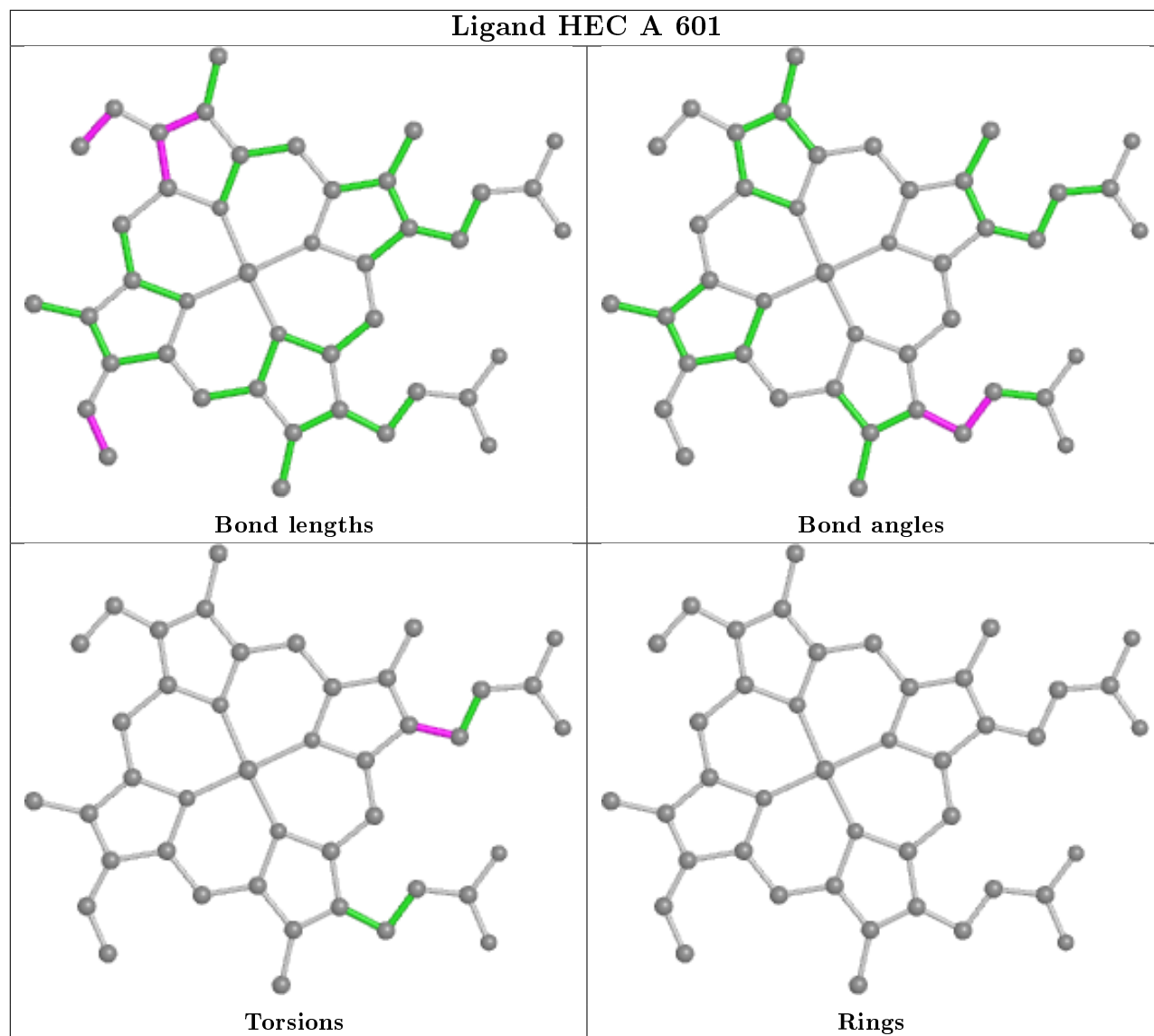


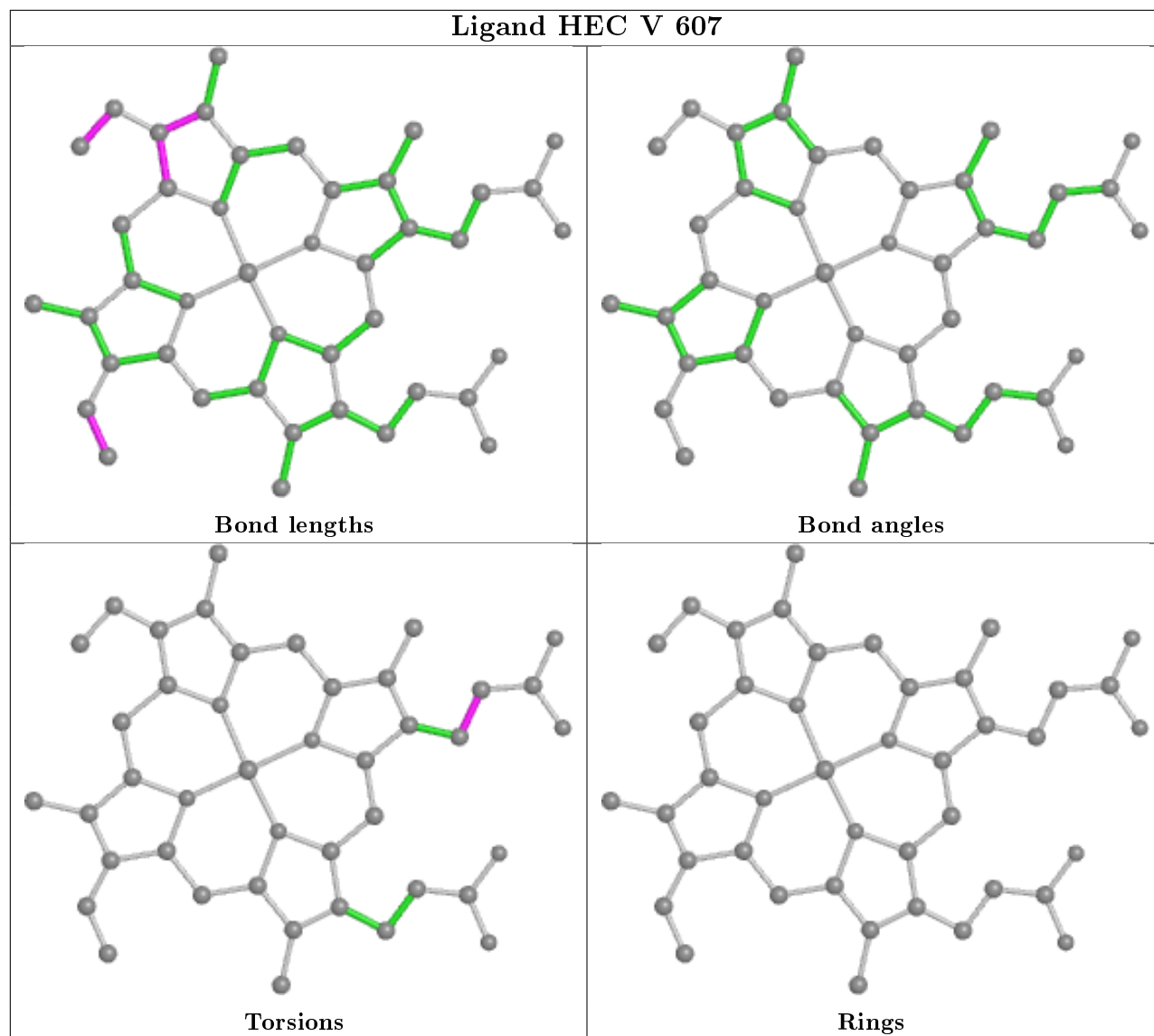


## Ligand HEC R 607



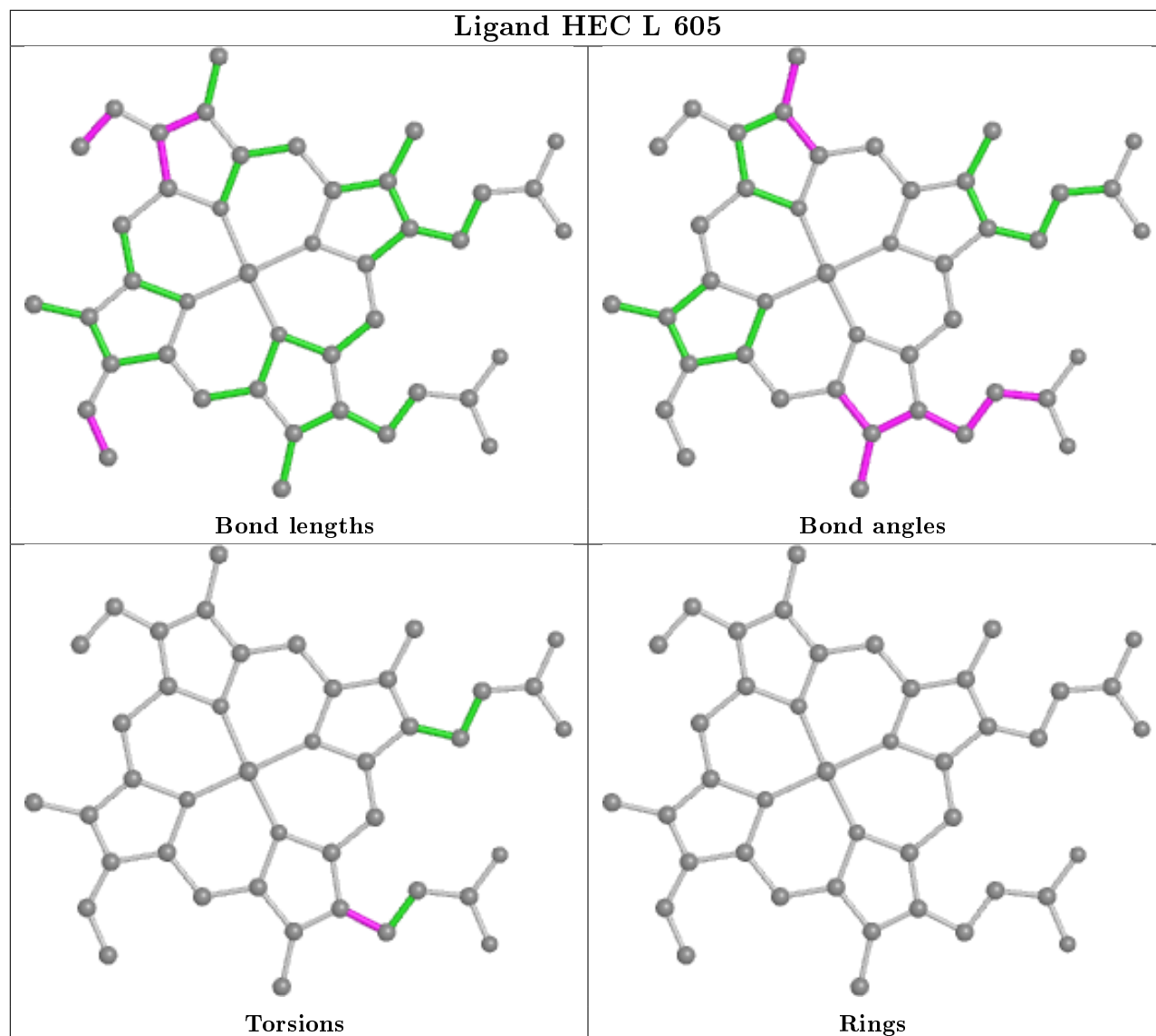


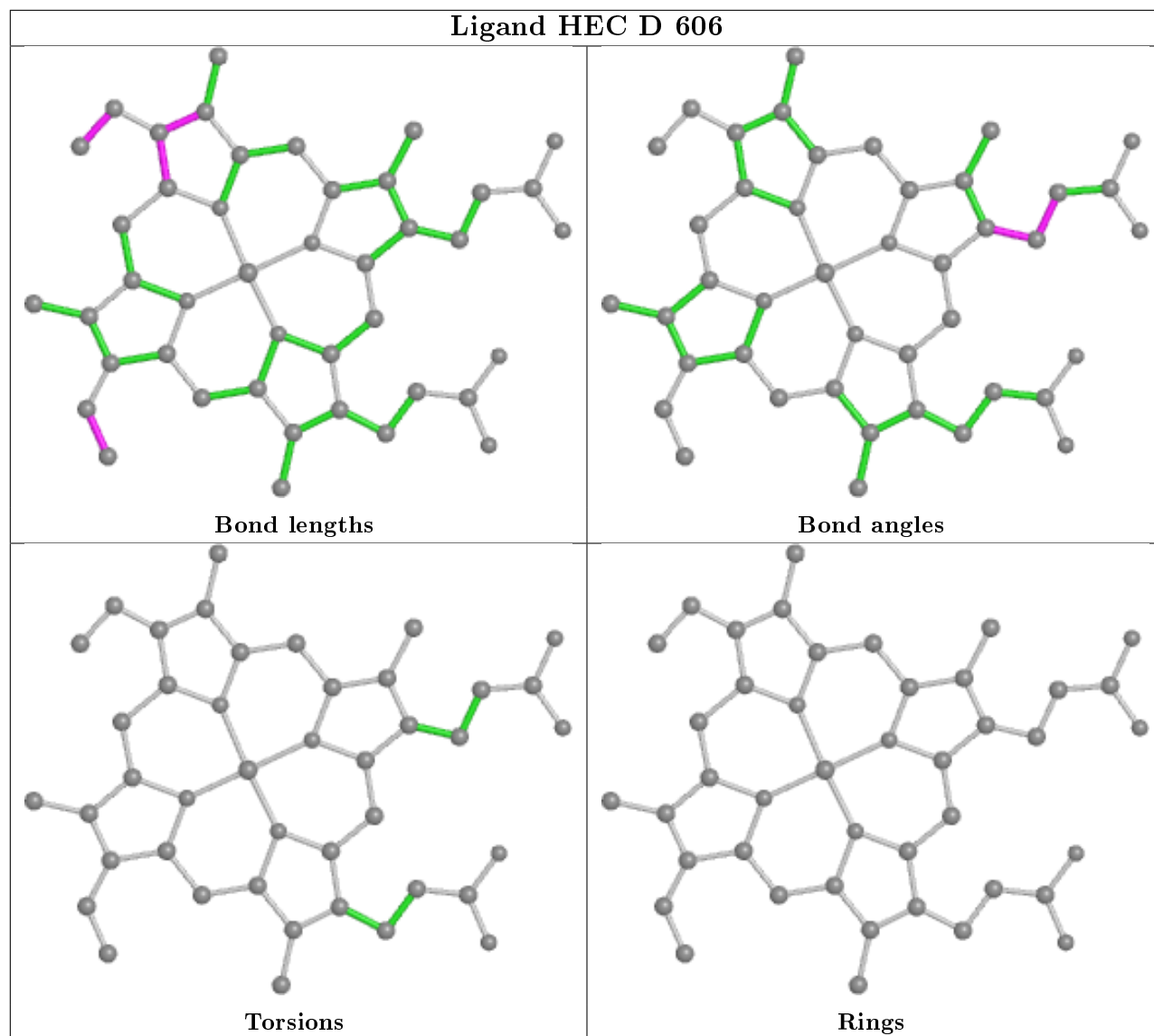


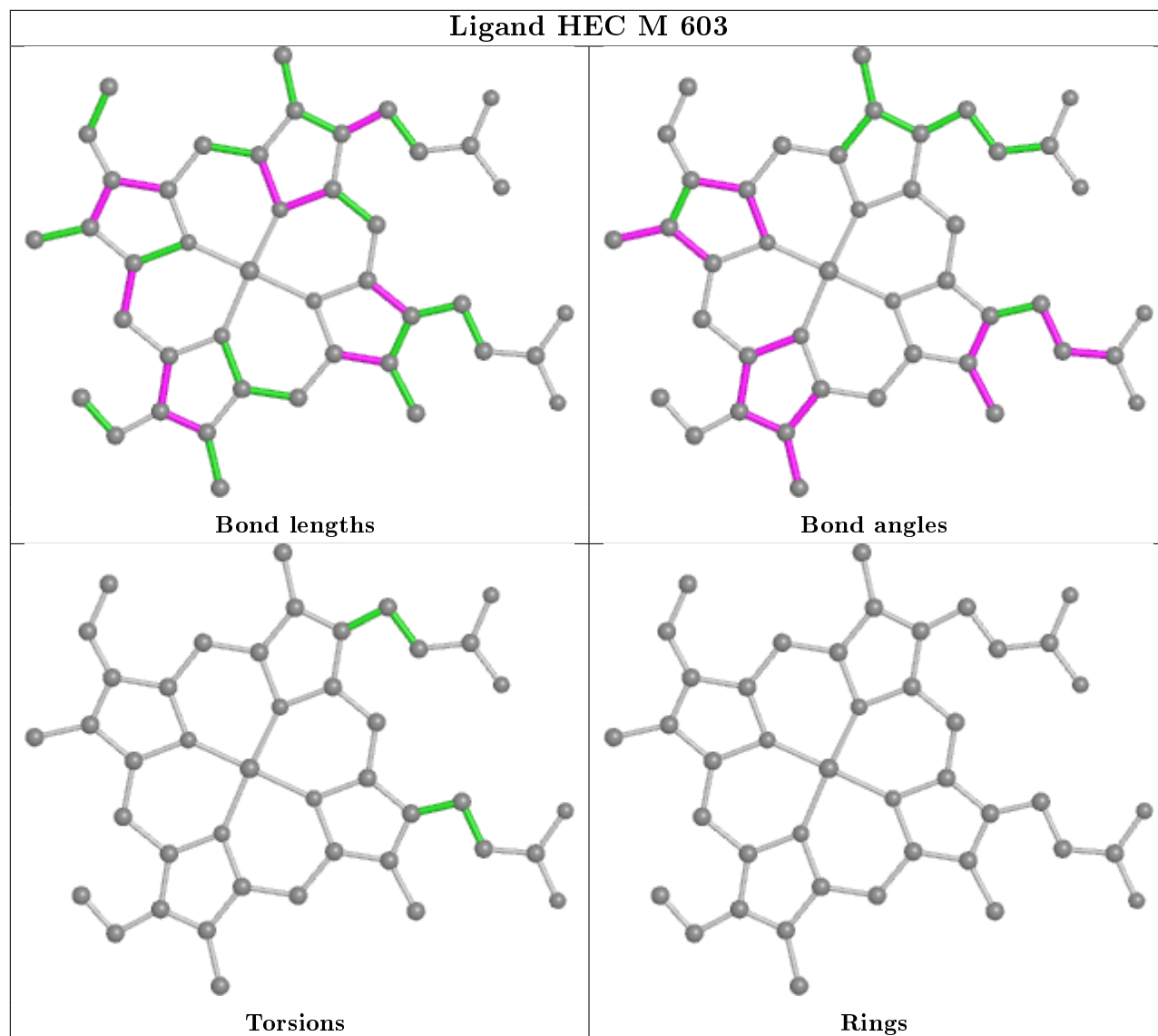




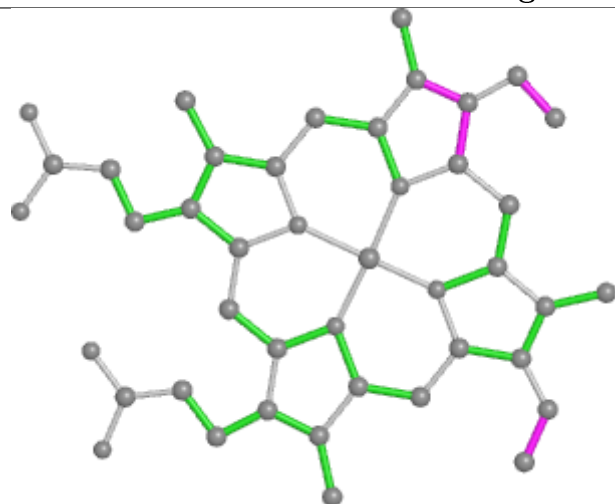
## Ligand HEC L 605



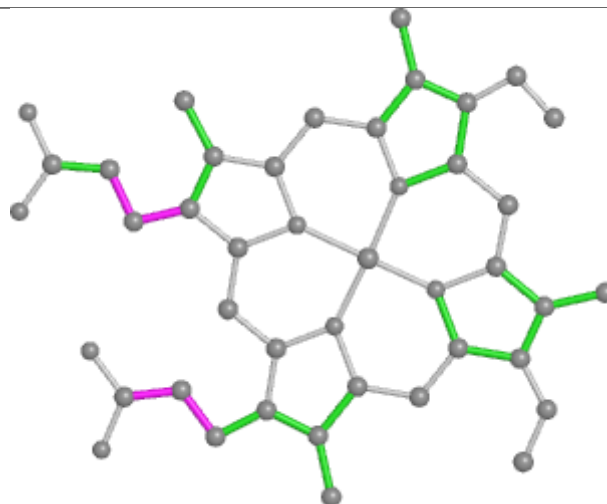




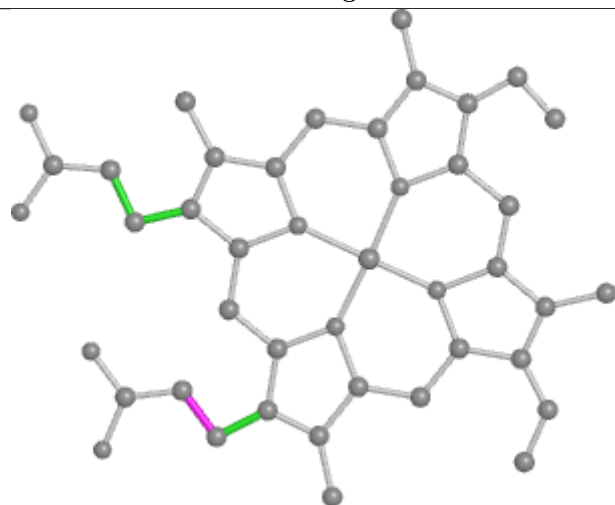
## Ligand HEC J 602



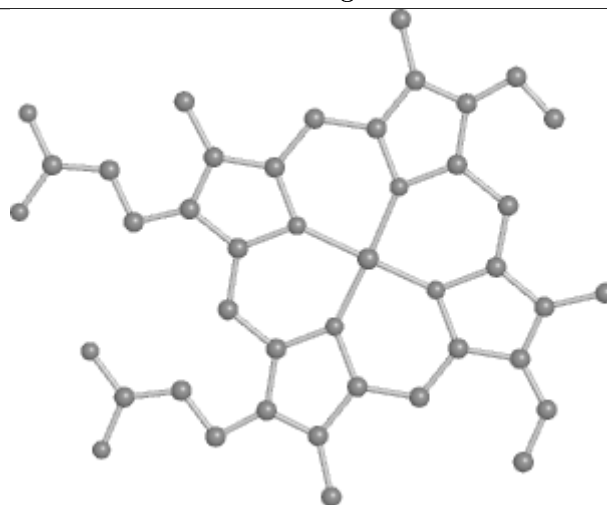
Bond lengths



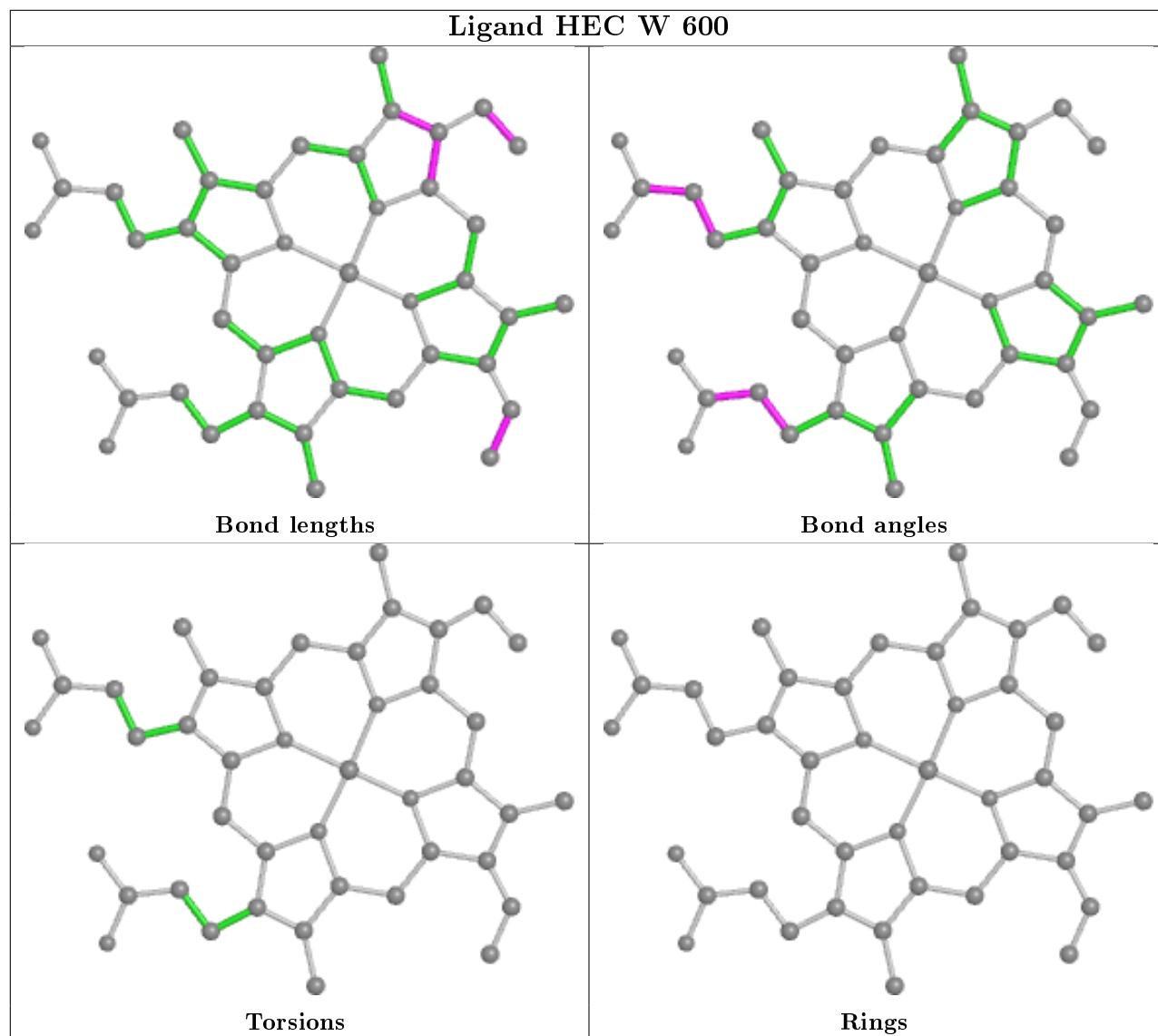
Bond angles

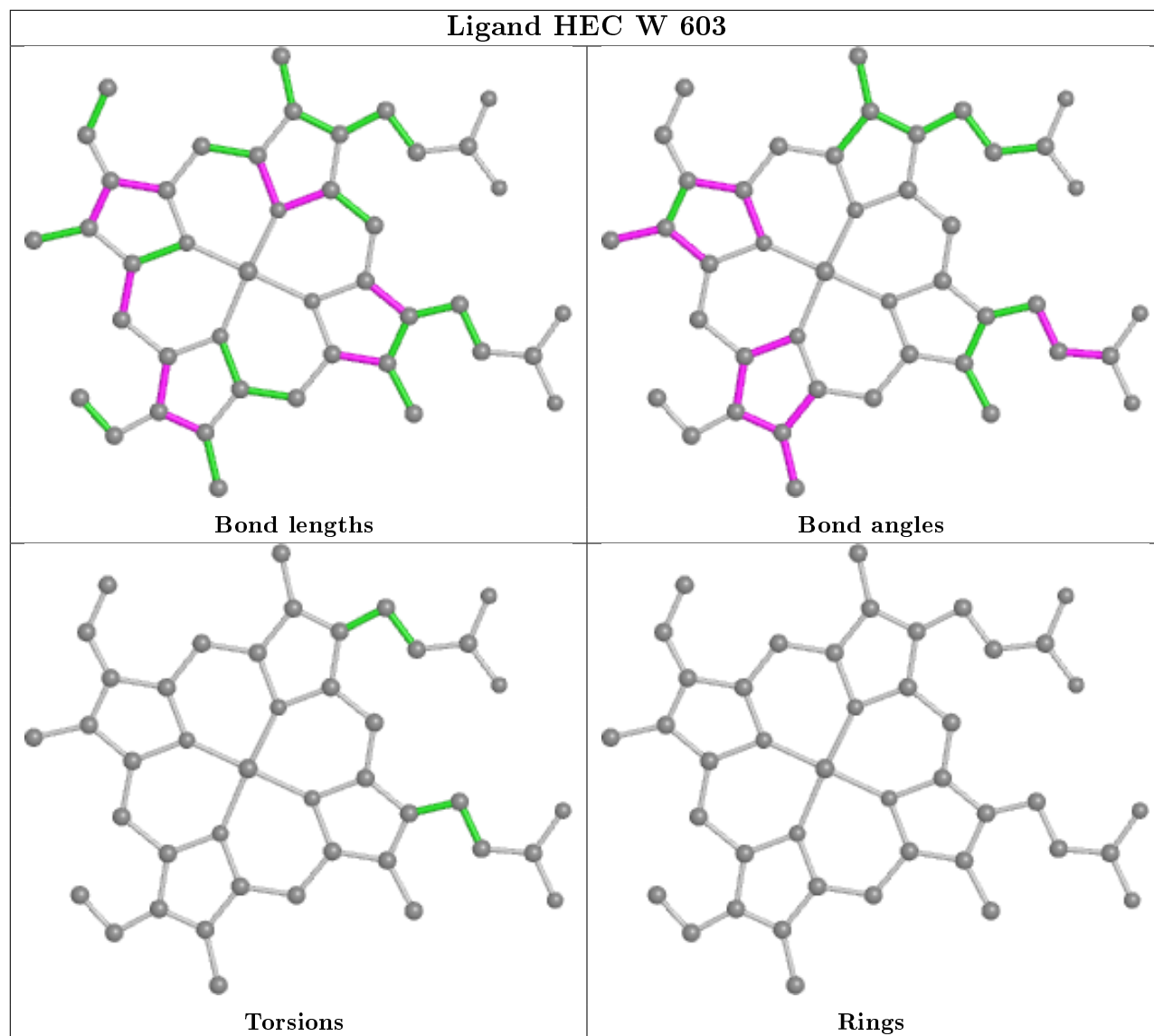


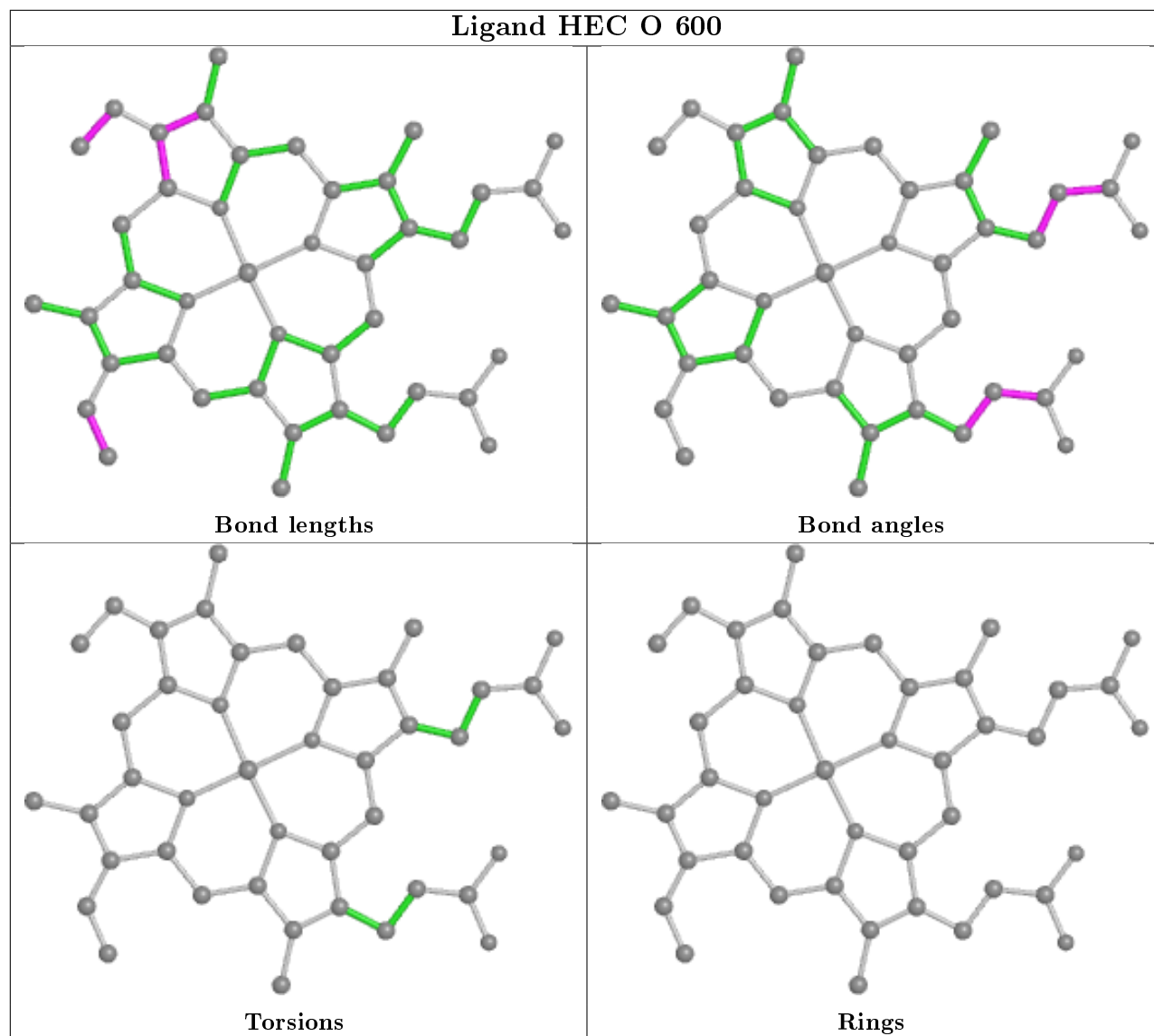
Torsions

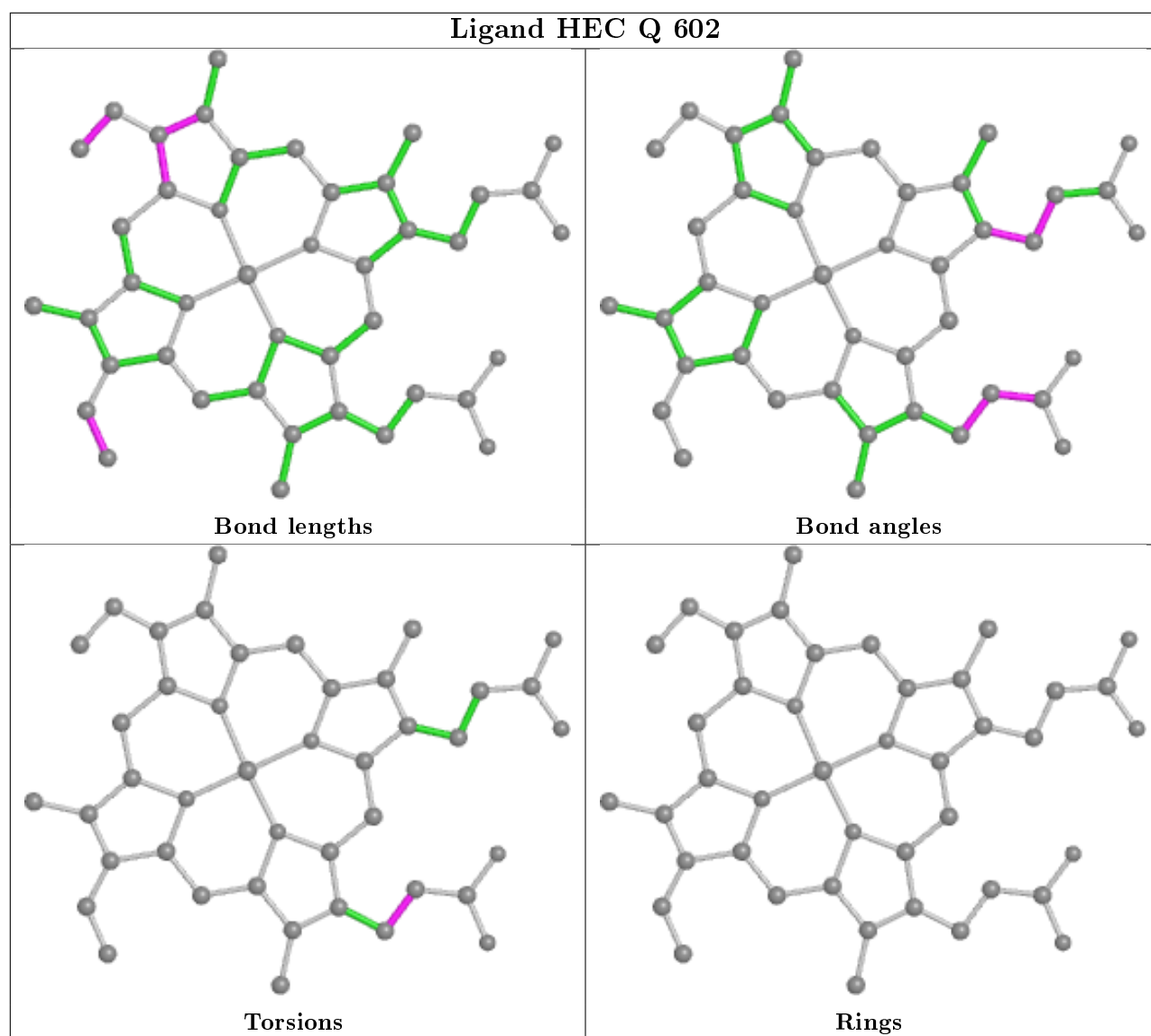


Rings

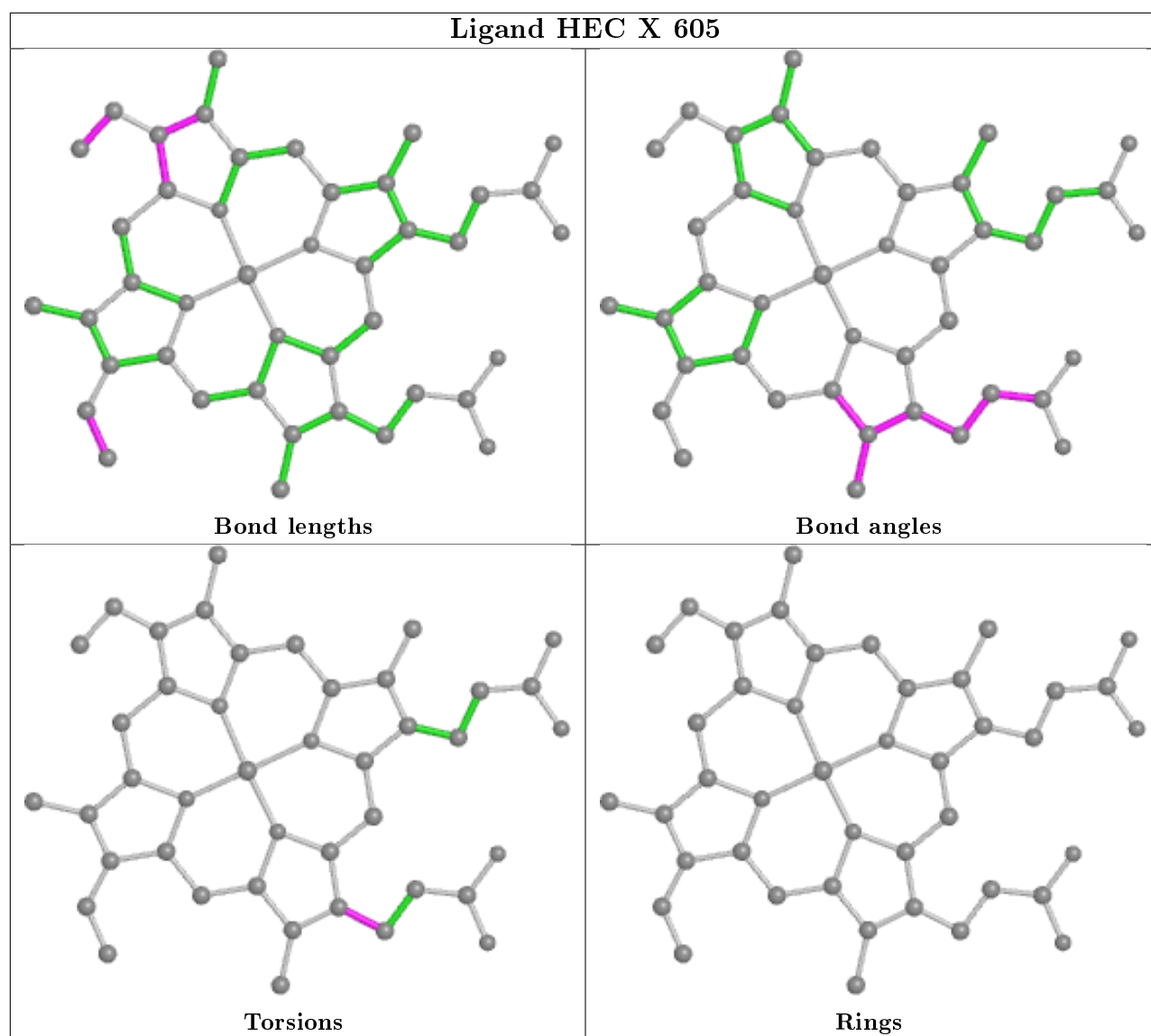


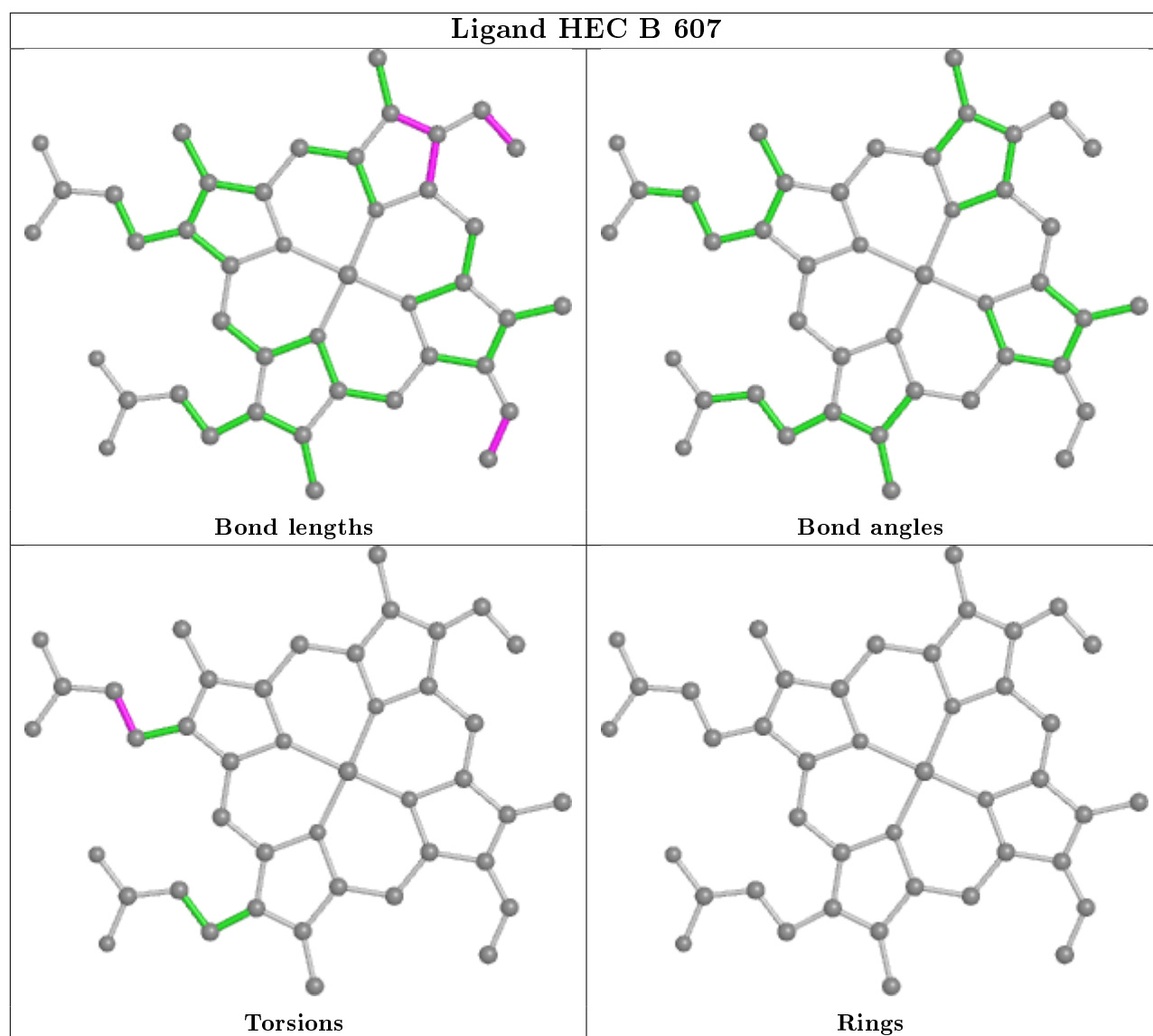


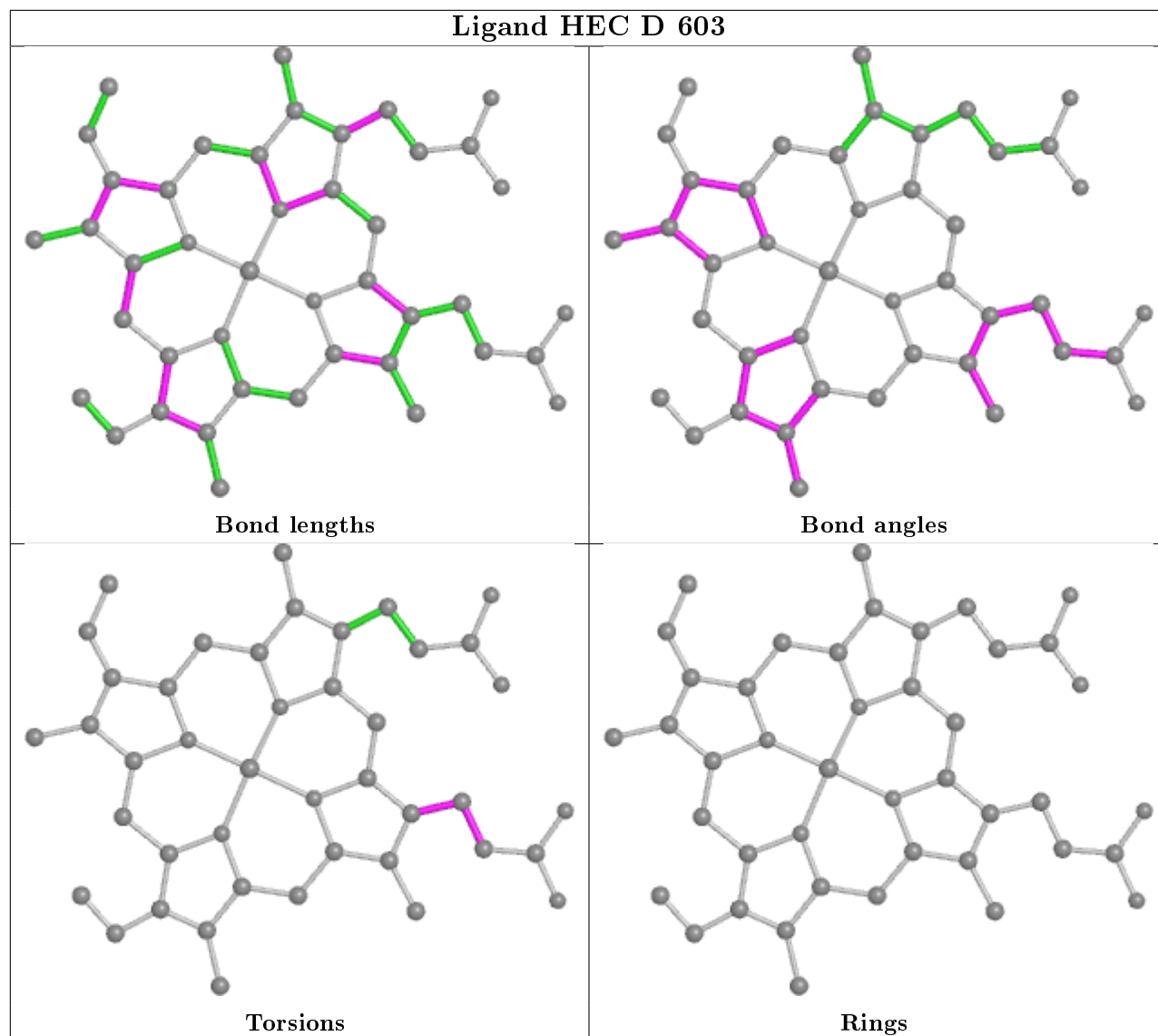




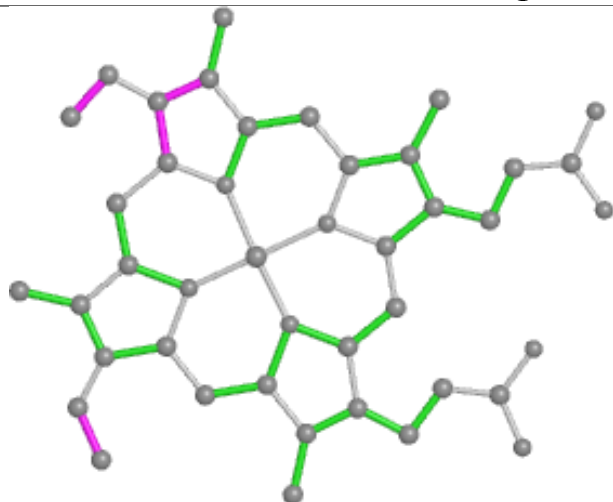




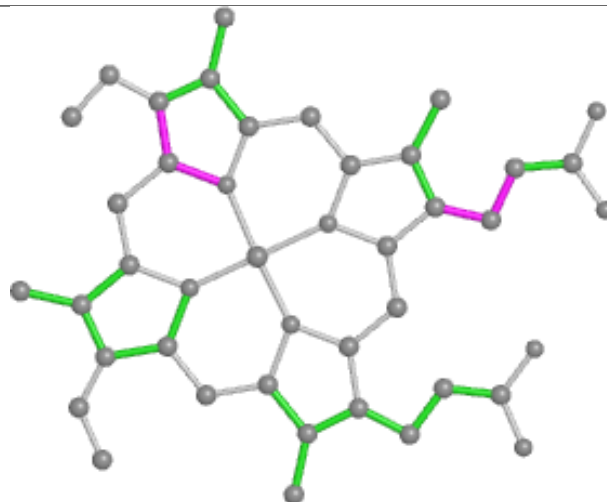




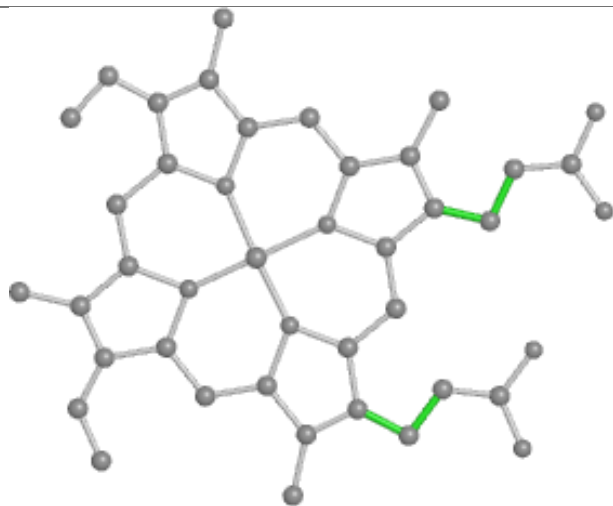
## Ligand HEC E 606



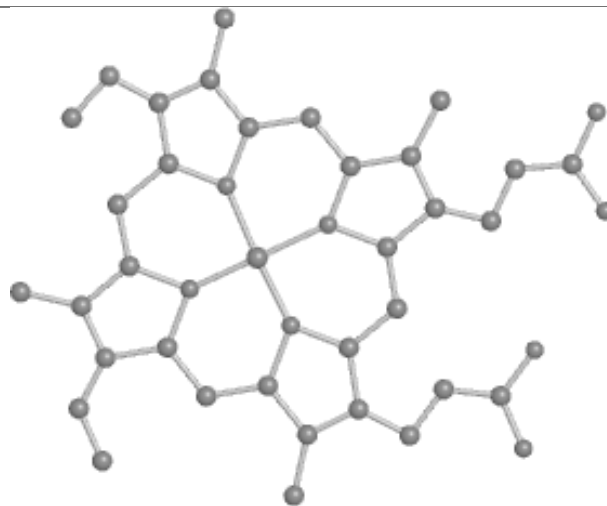
Bond lengths



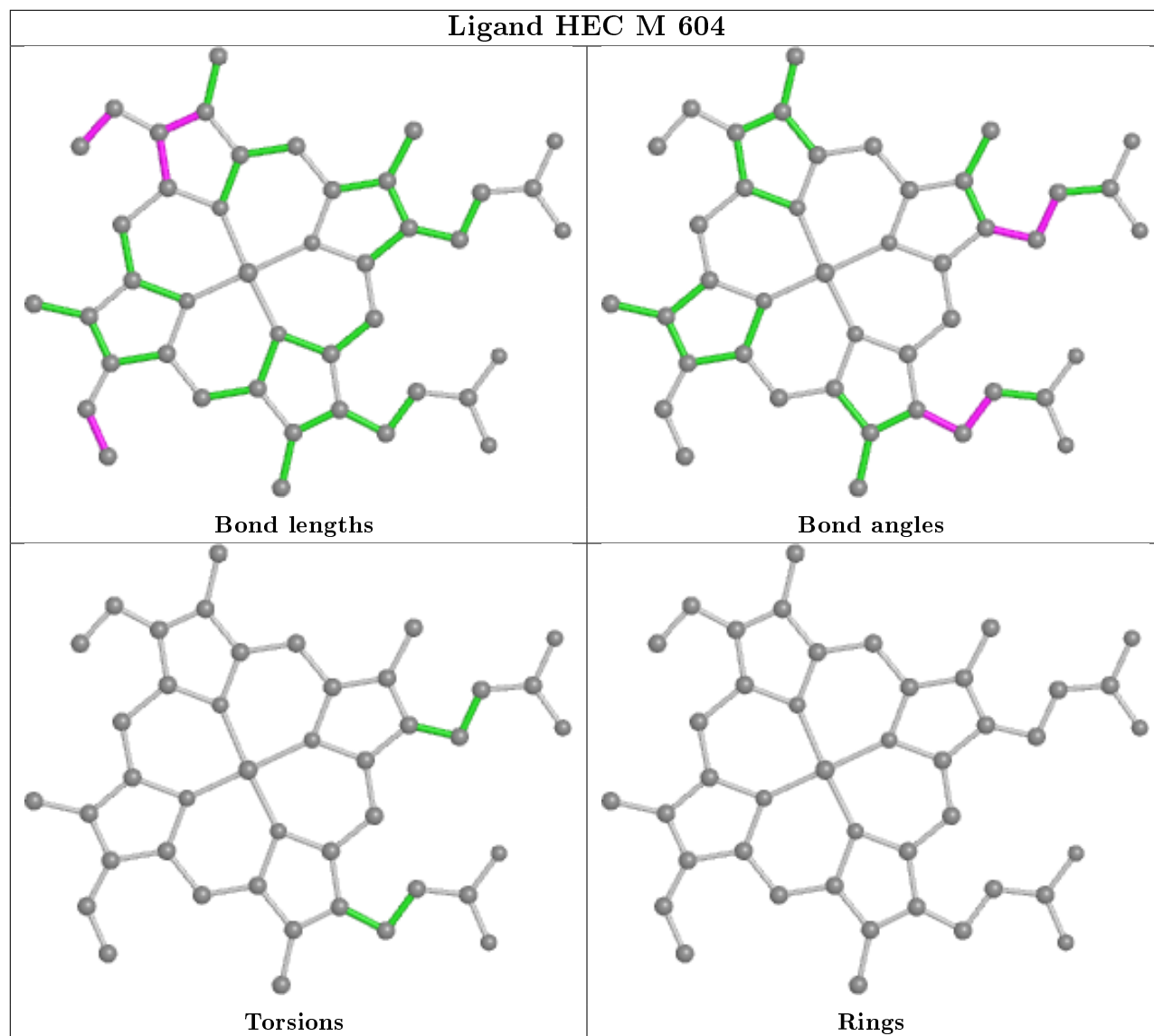
Bond angles



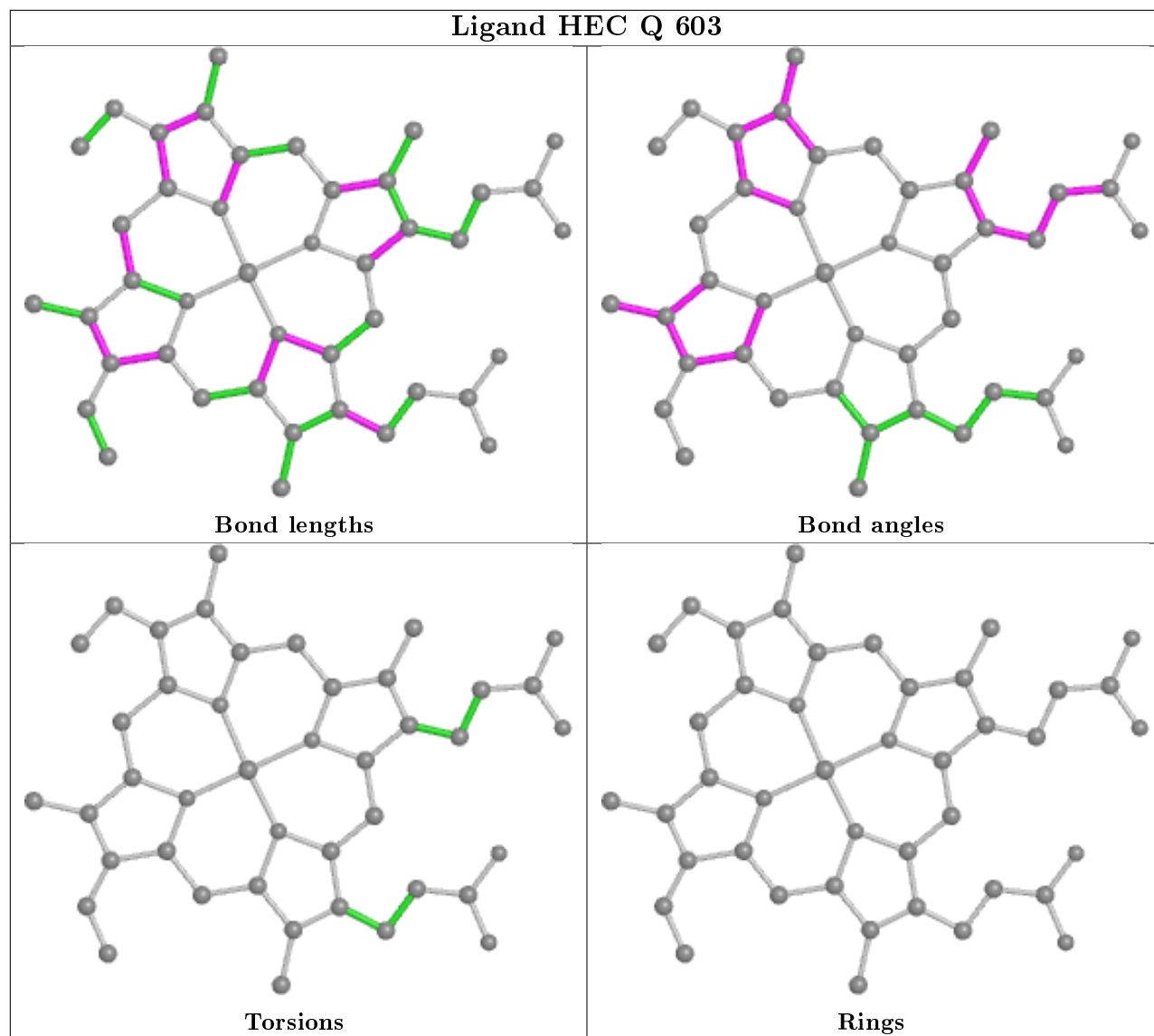
Torsions

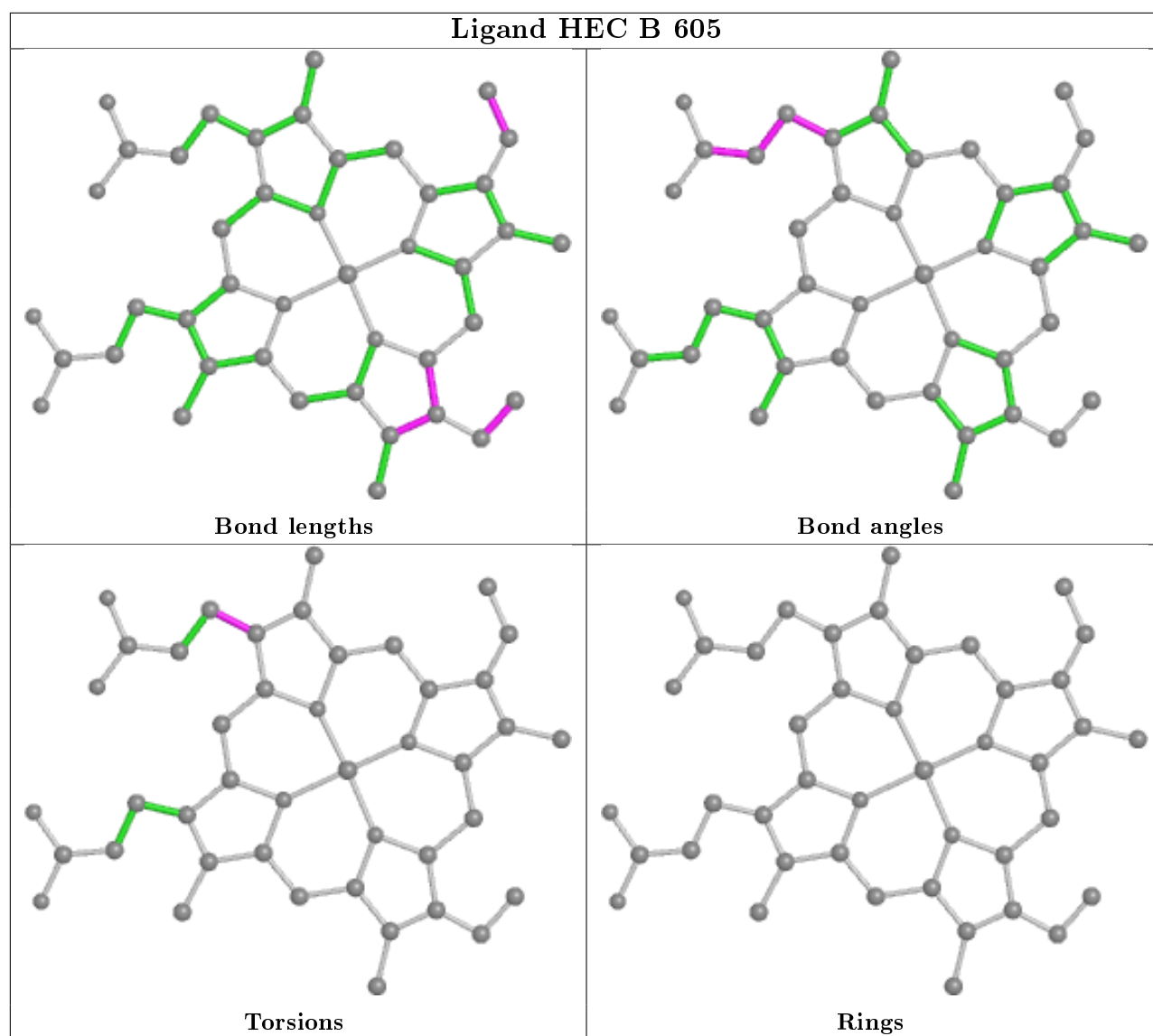


Rings

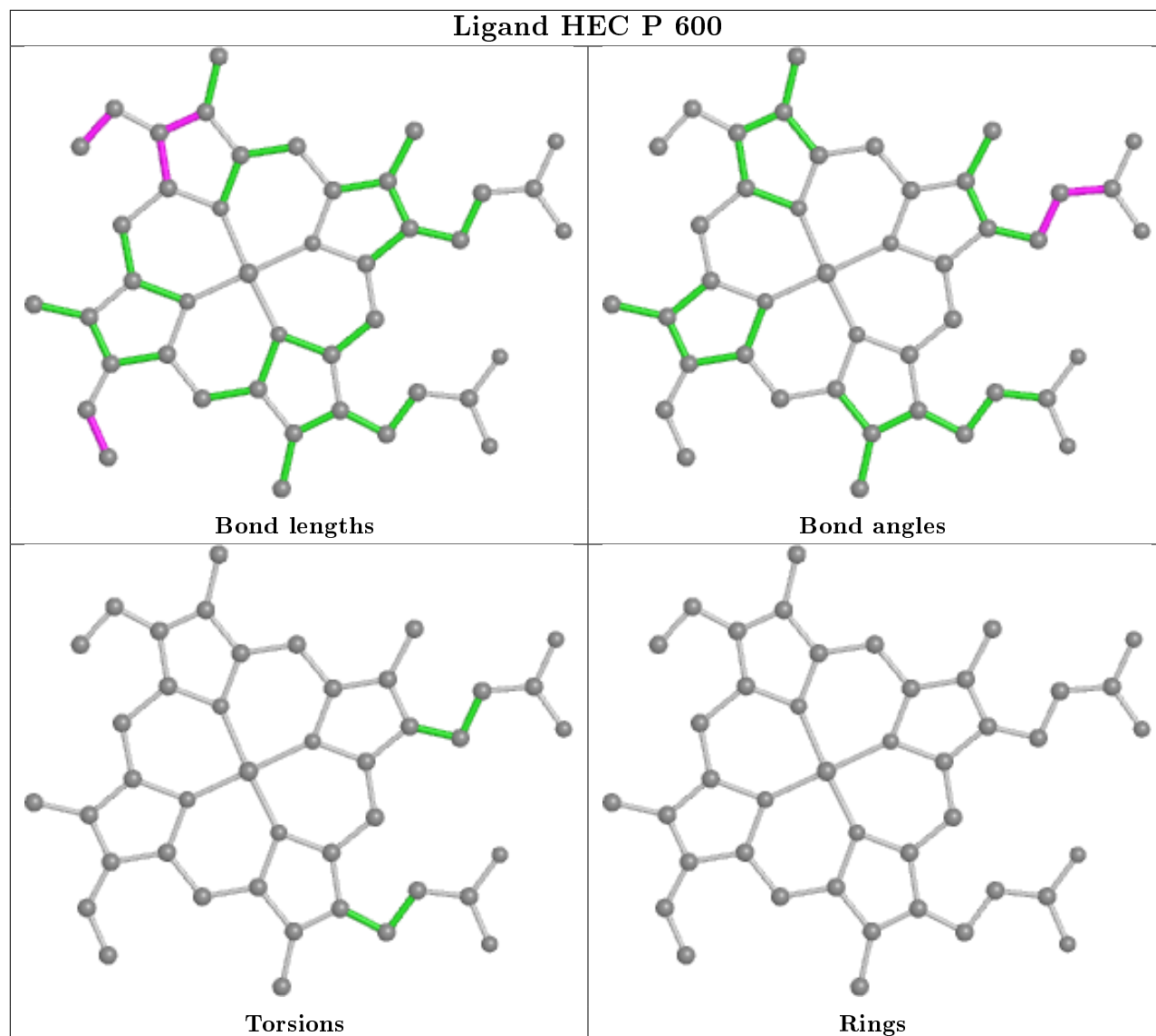


## Ligand HEC Q 603

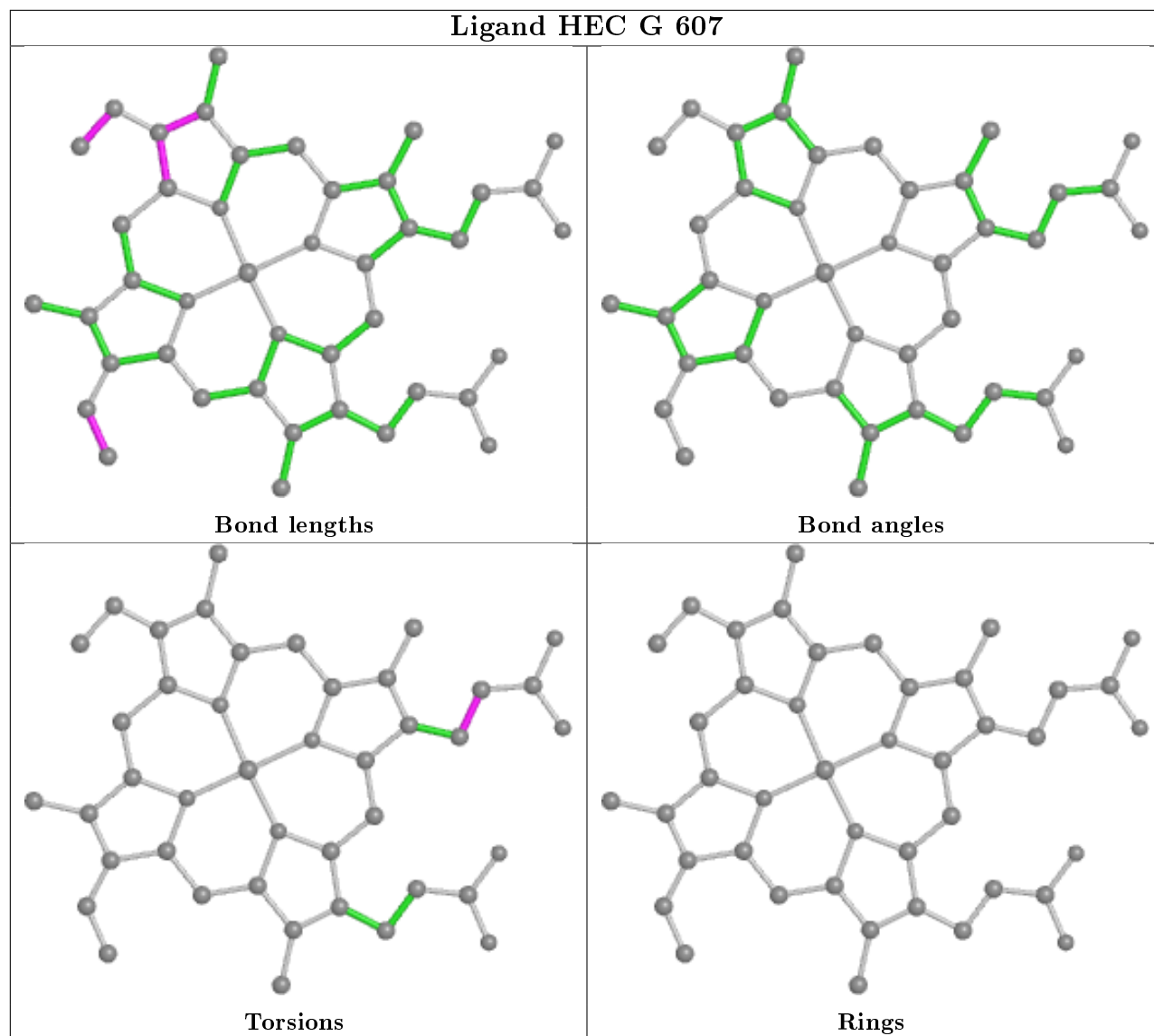




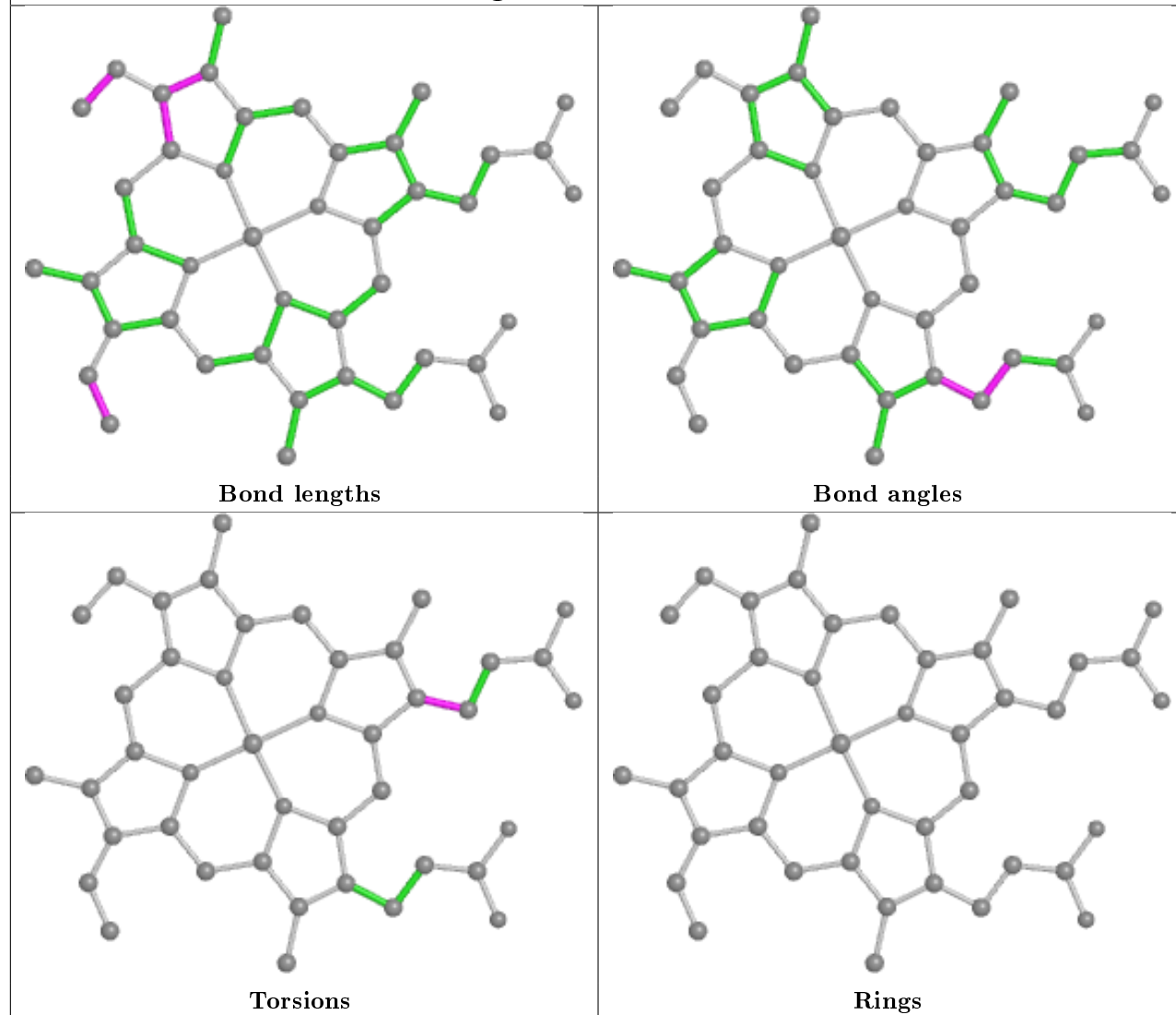
## Ligand HEC P 600

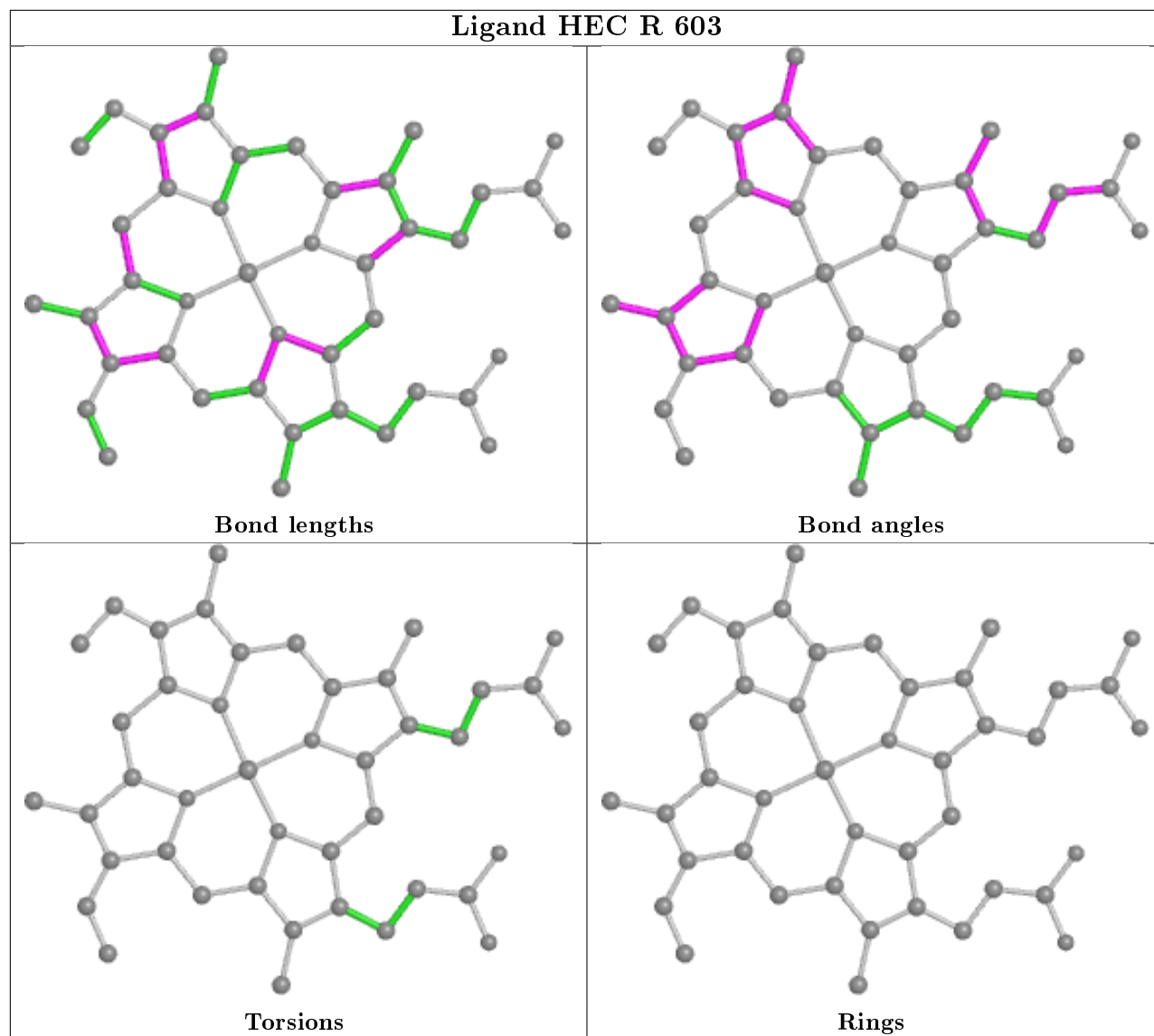


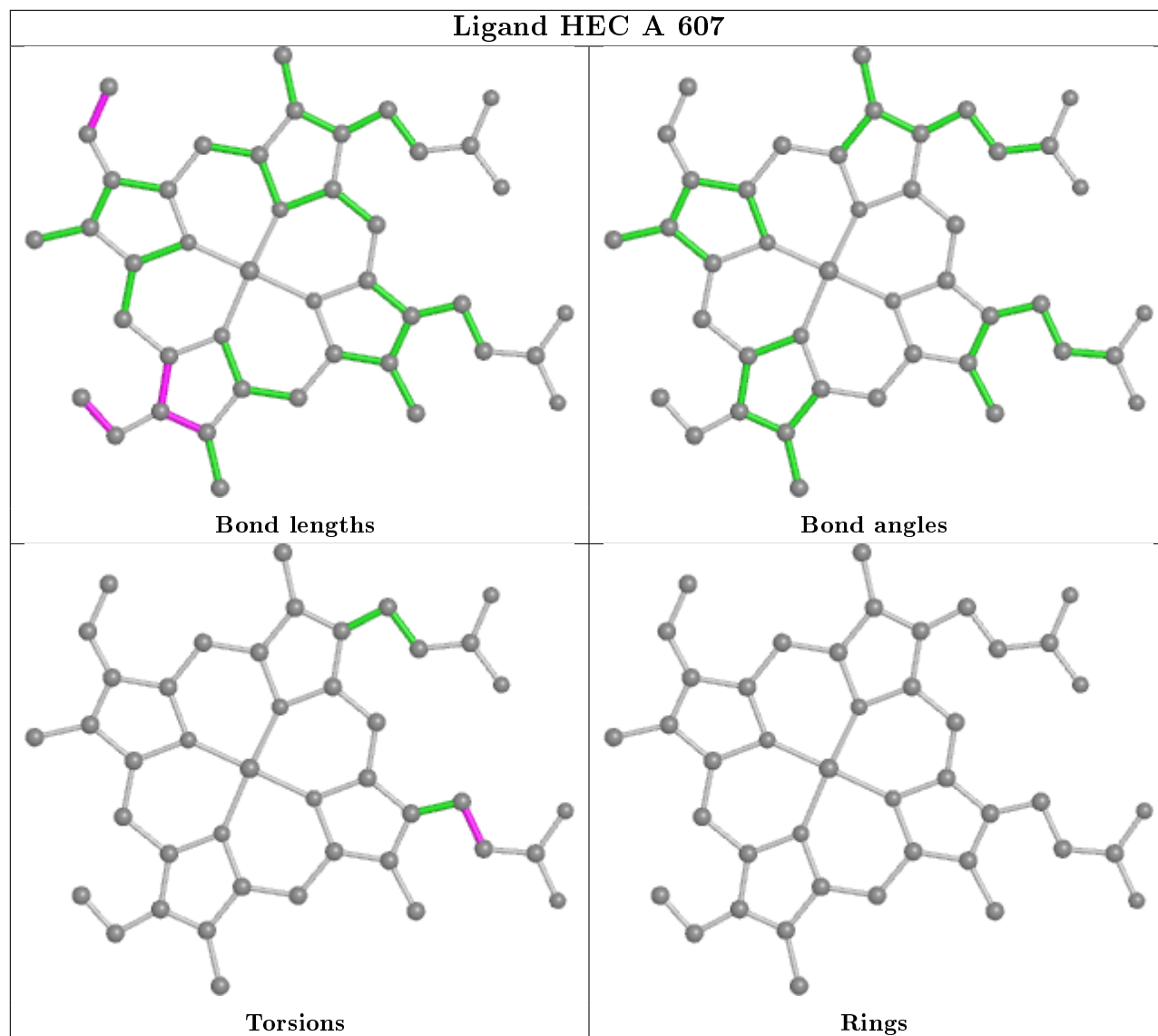




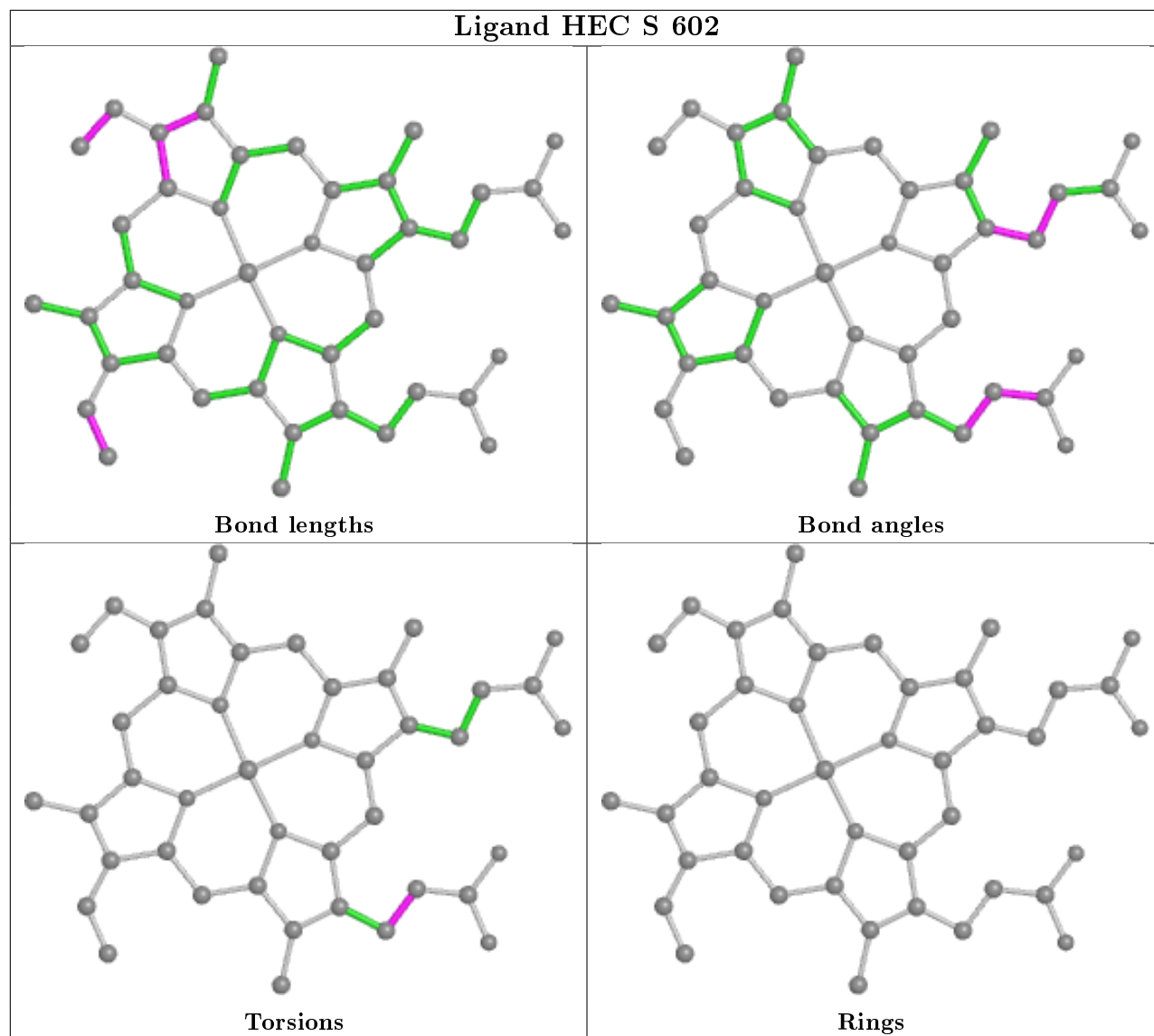
## Ligand HEC T 601



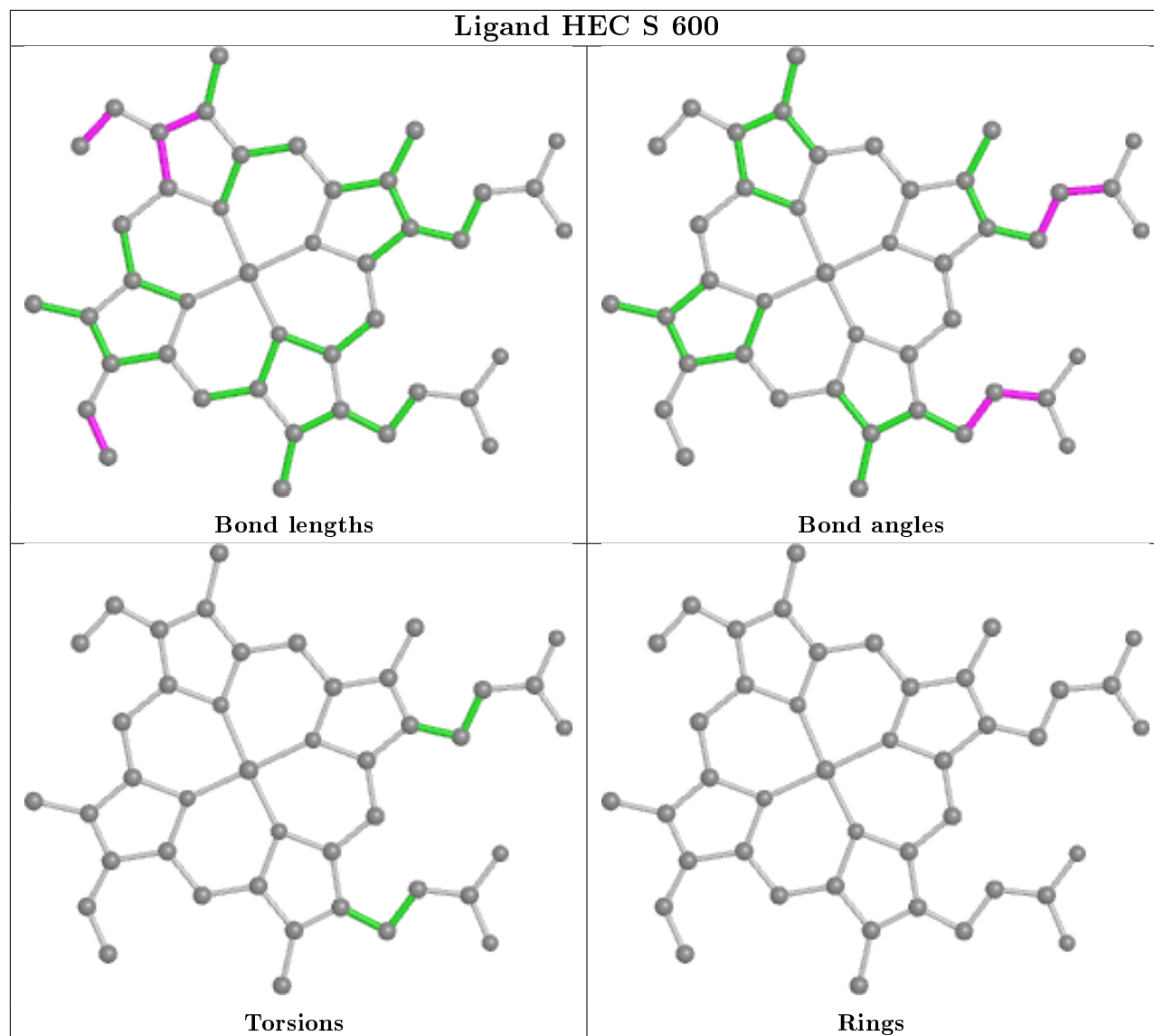




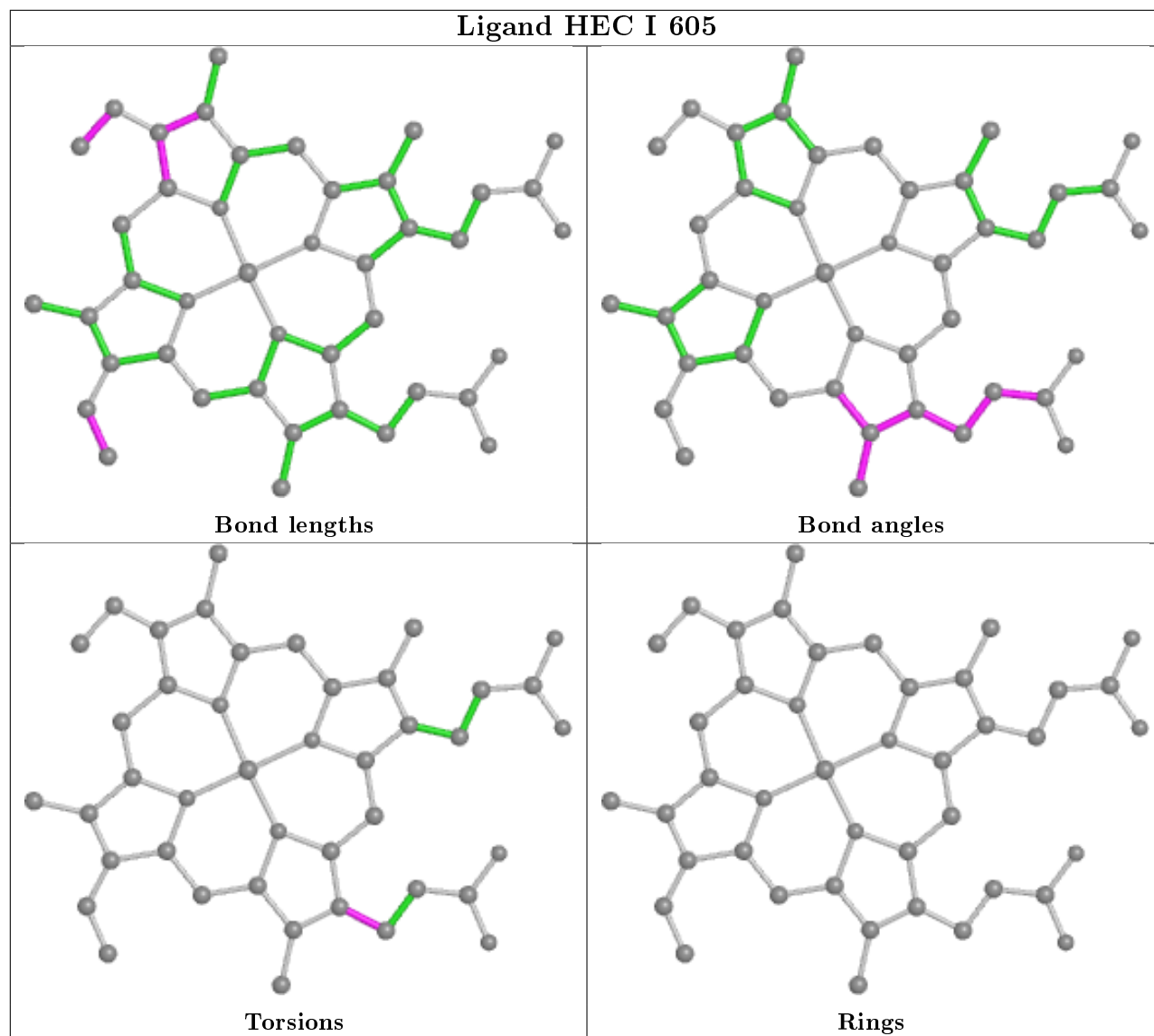
## Ligand HEC S 602

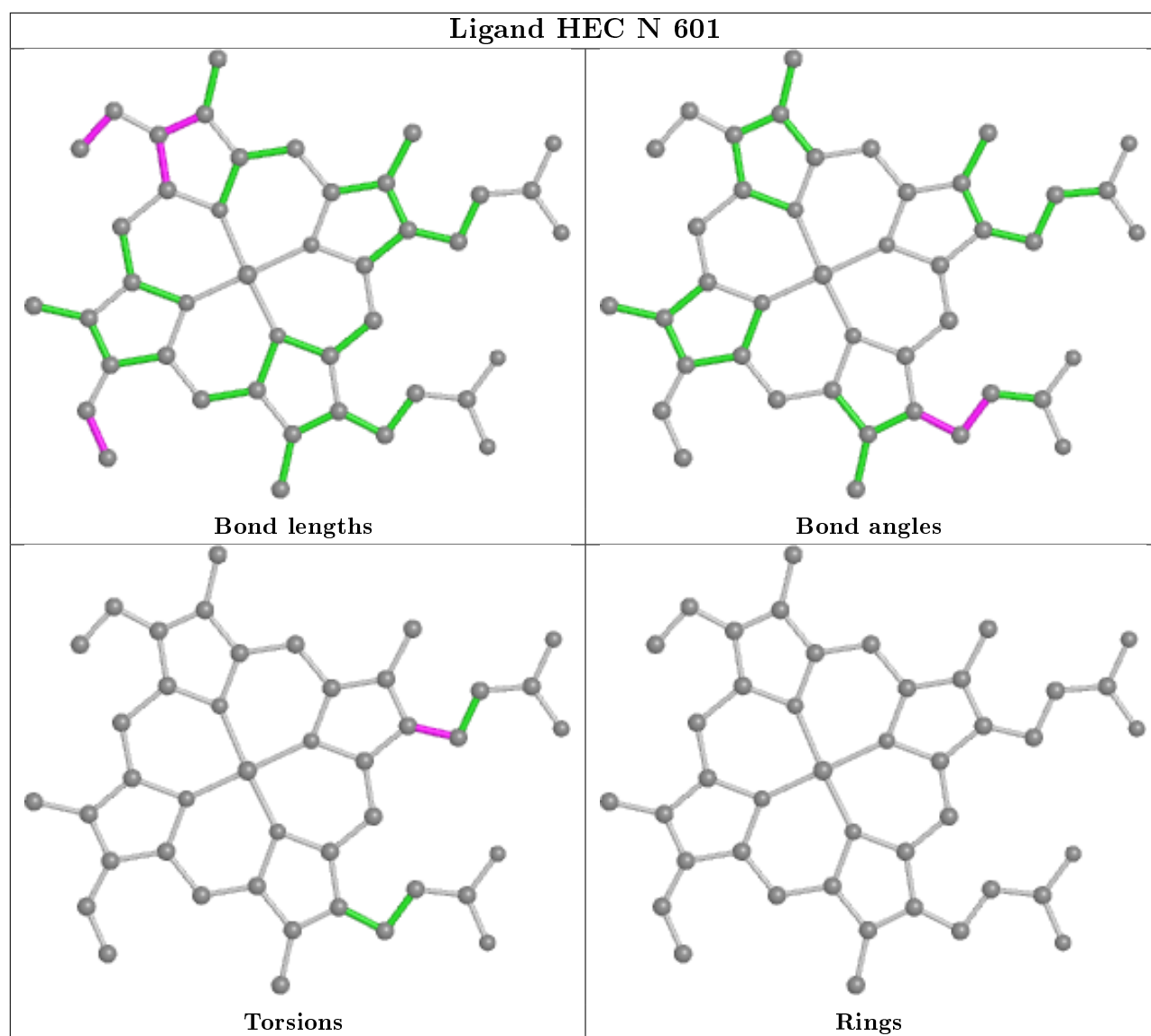


## Ligand HEC S 600

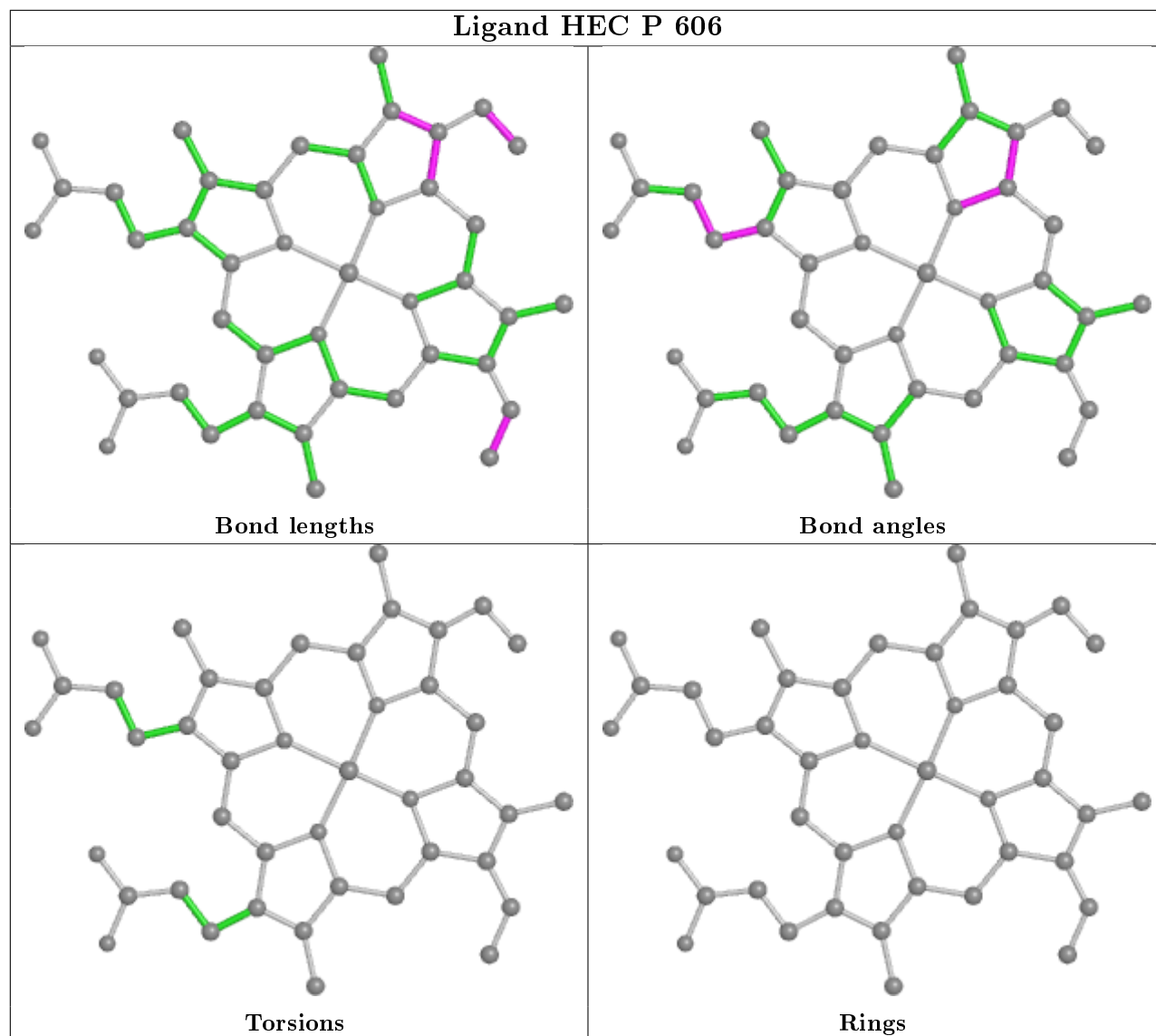


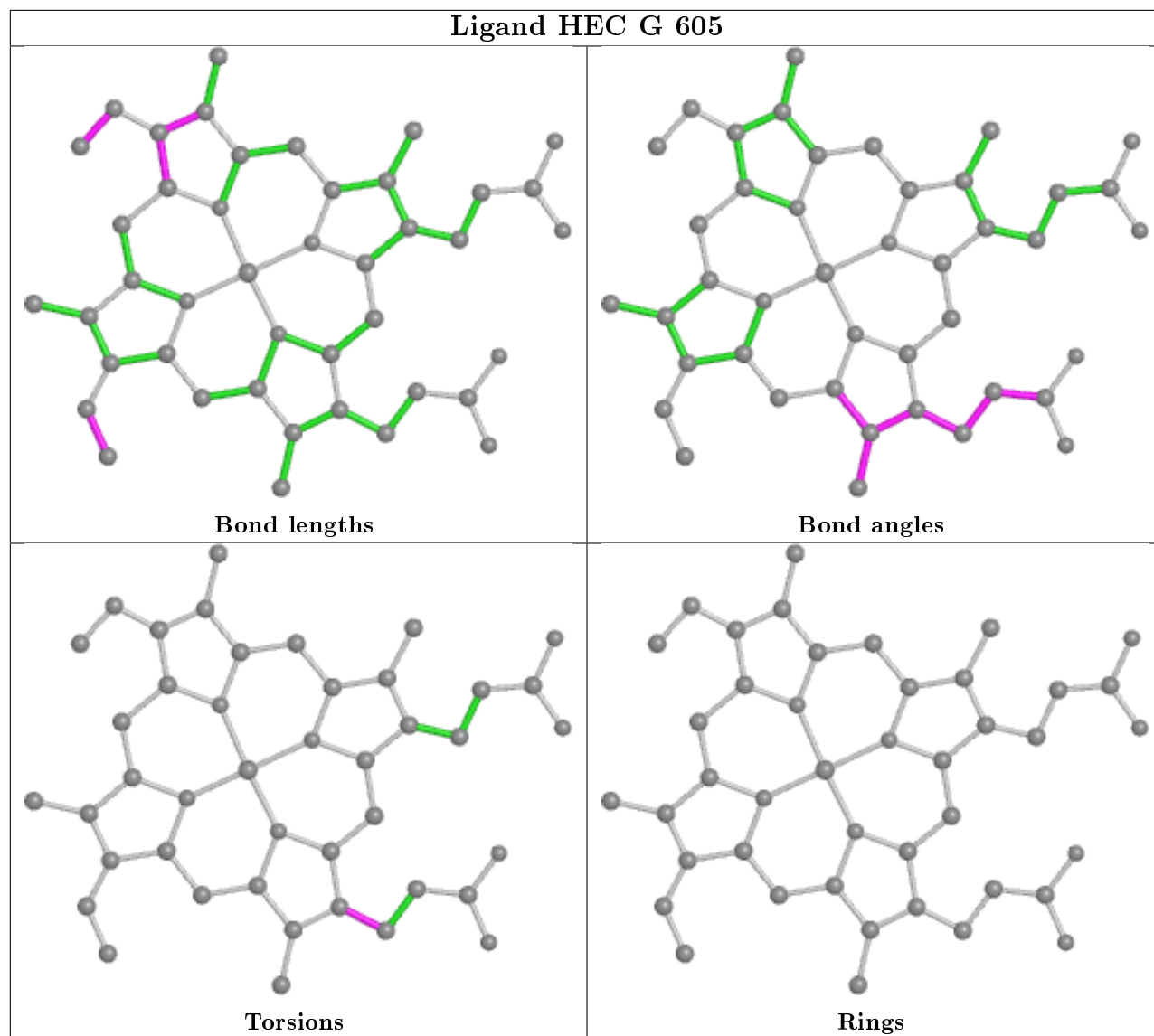
## Ligand HEC I 605

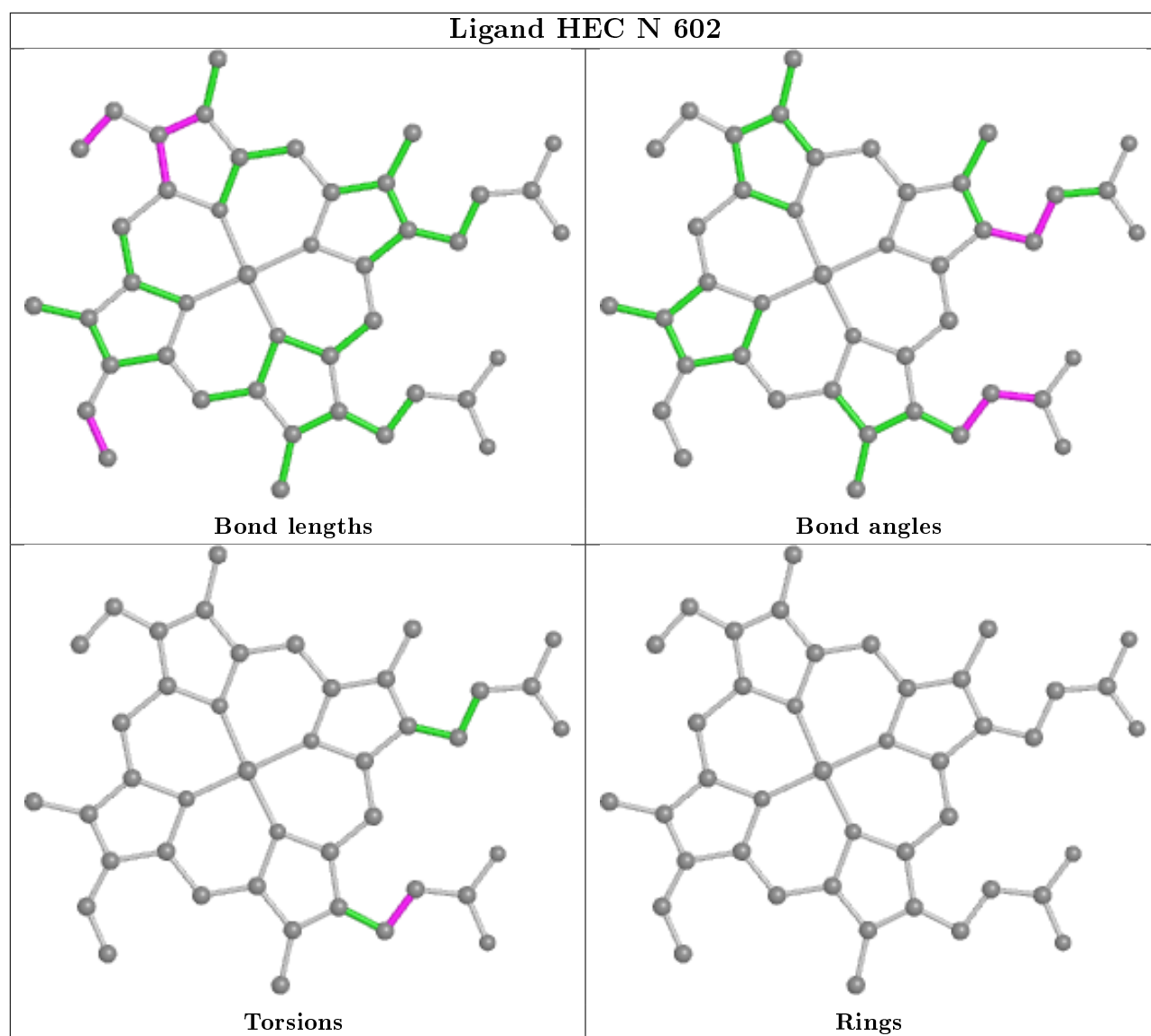


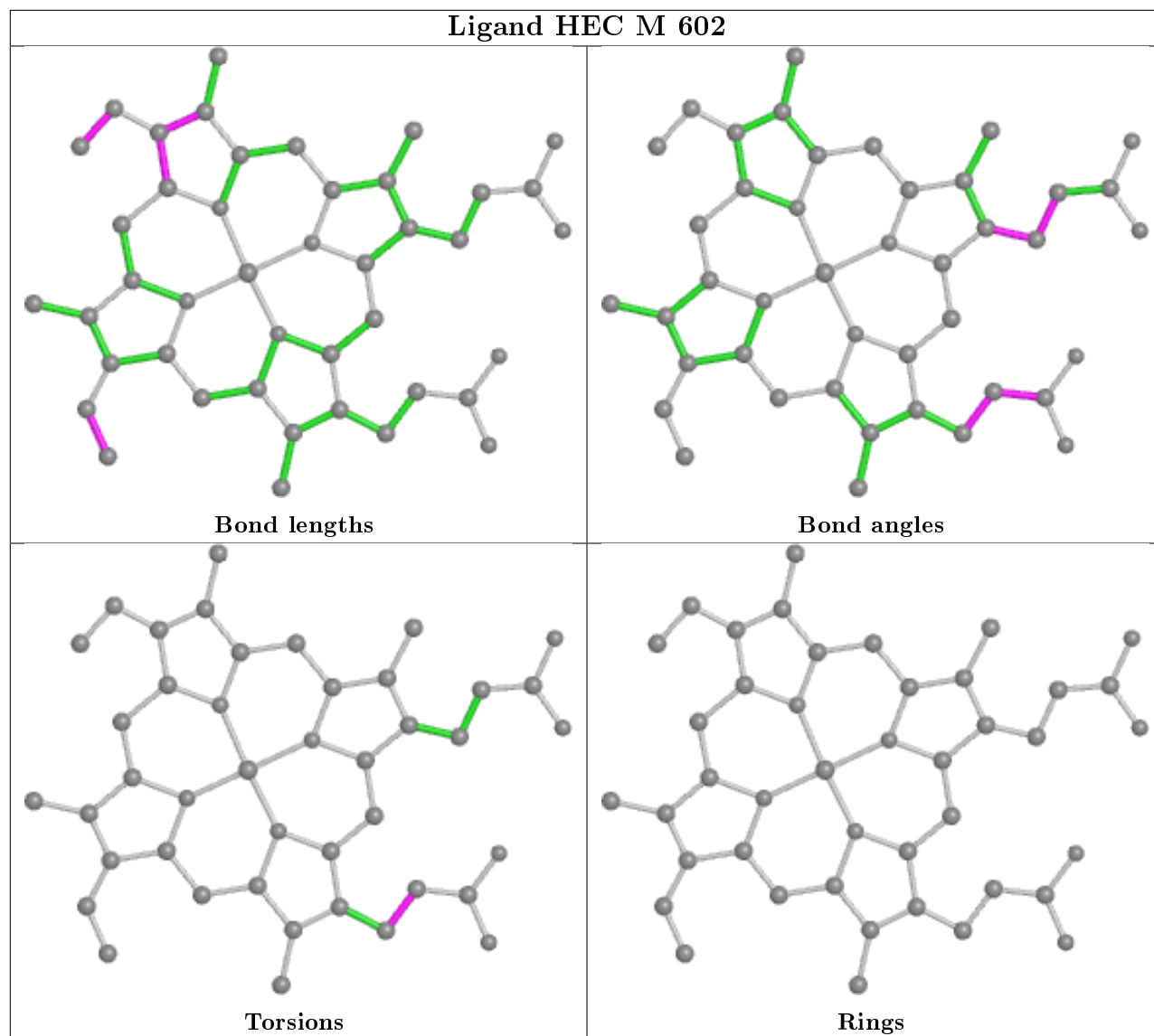


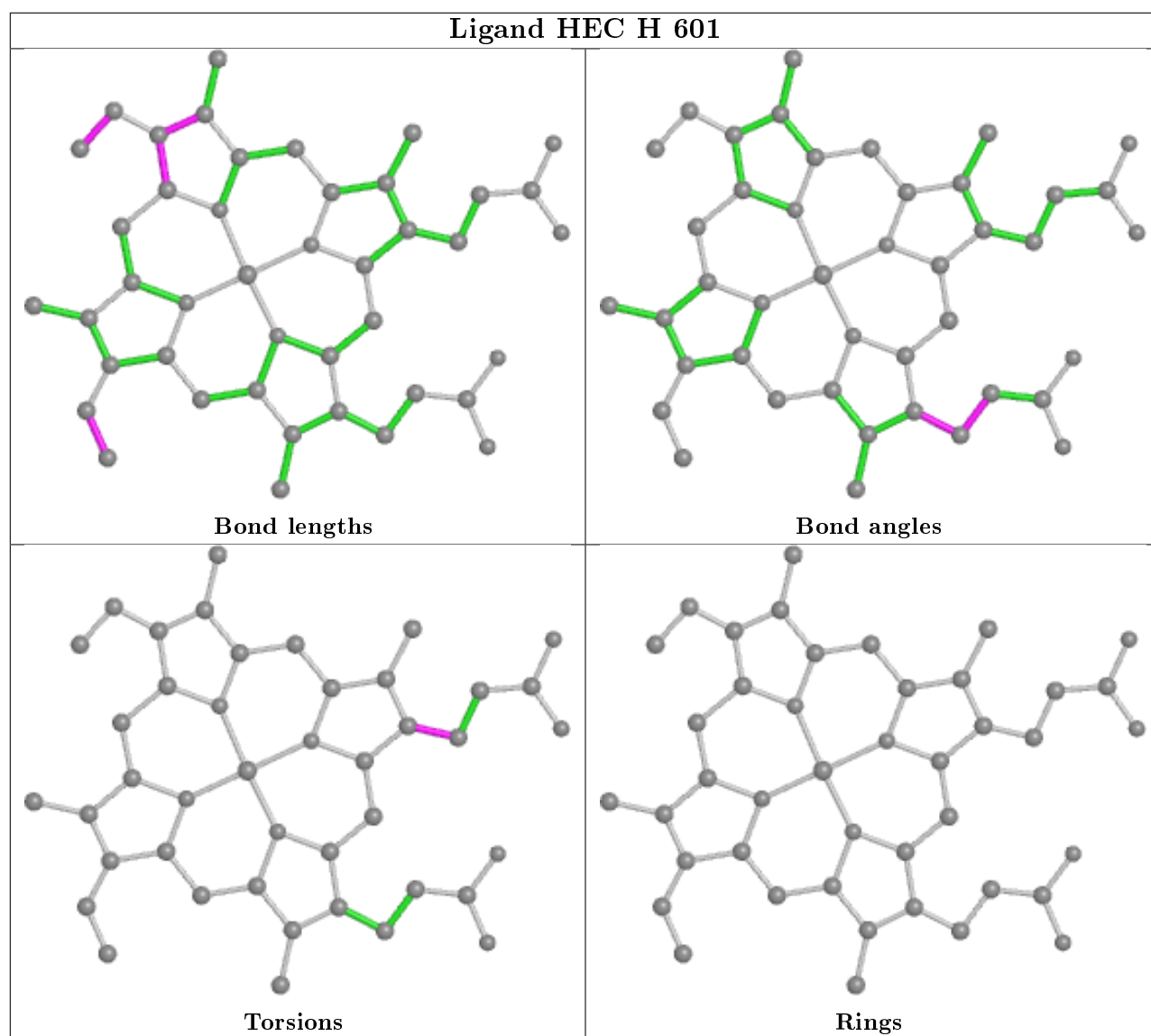




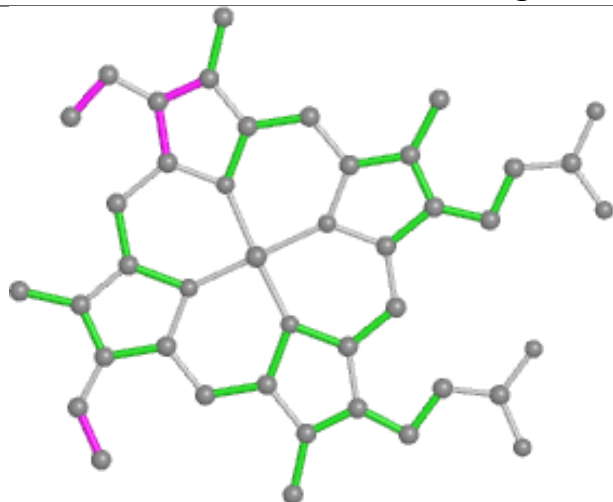




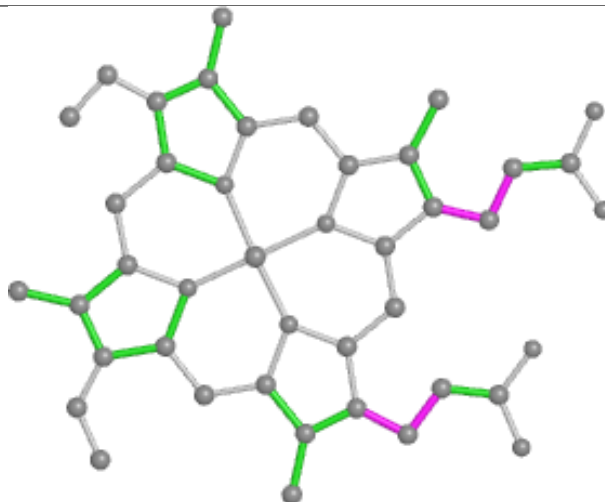




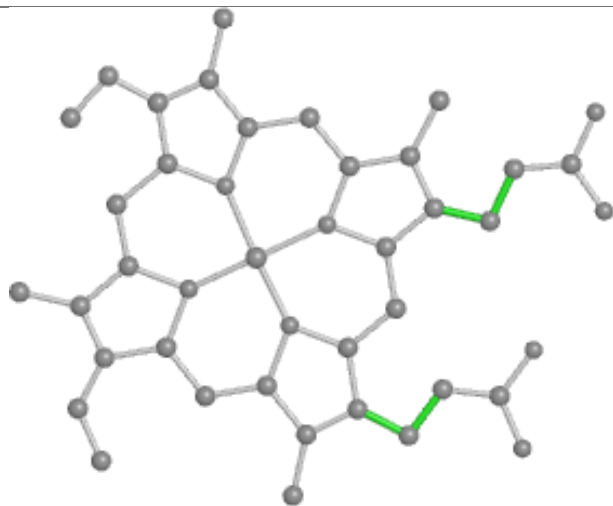
## Ligand HEC T 604



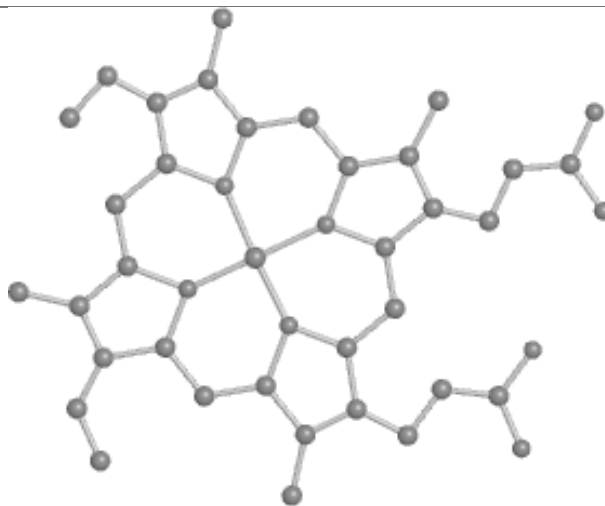
Bond lengths



Bond angles

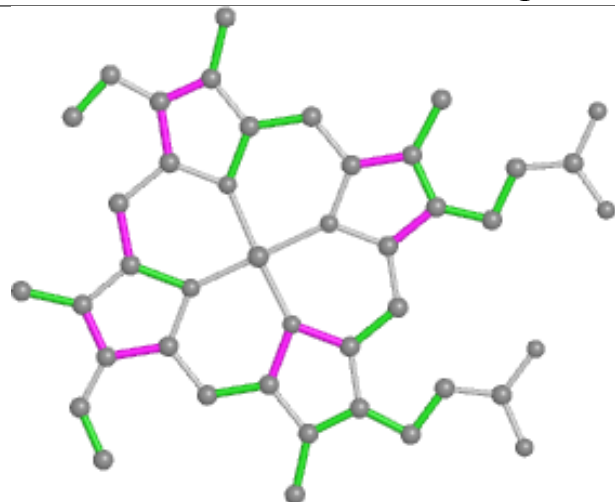


Torsions

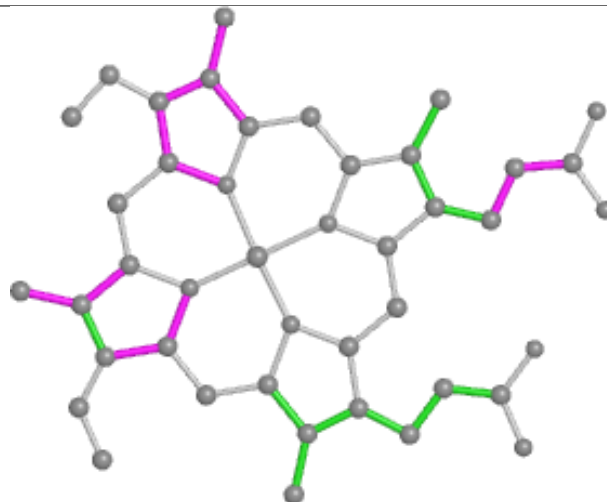


Rings

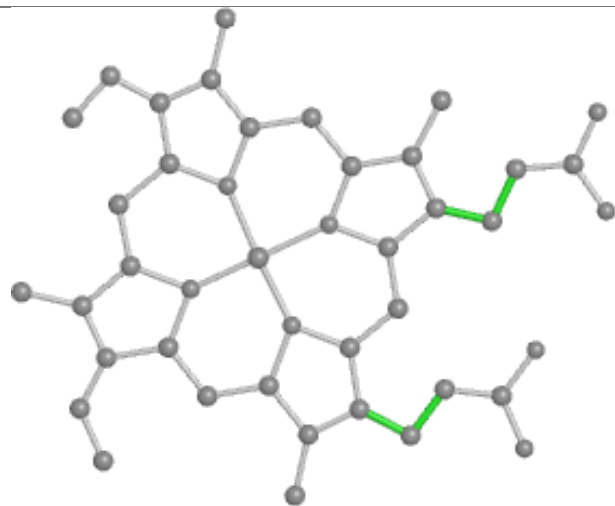
## Ligand HEC E 603



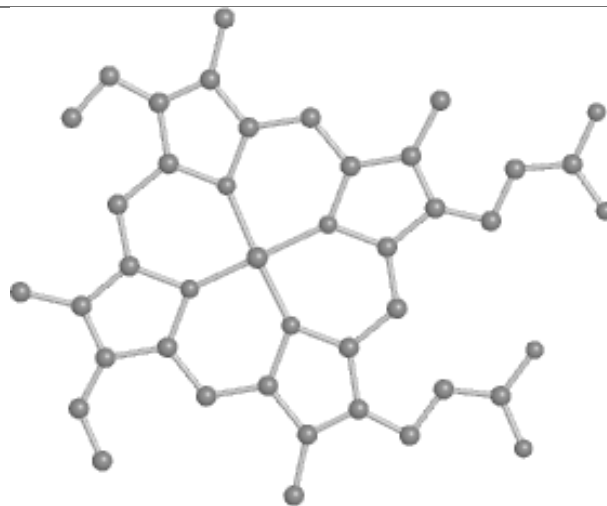
Bond lengths



Bond angles

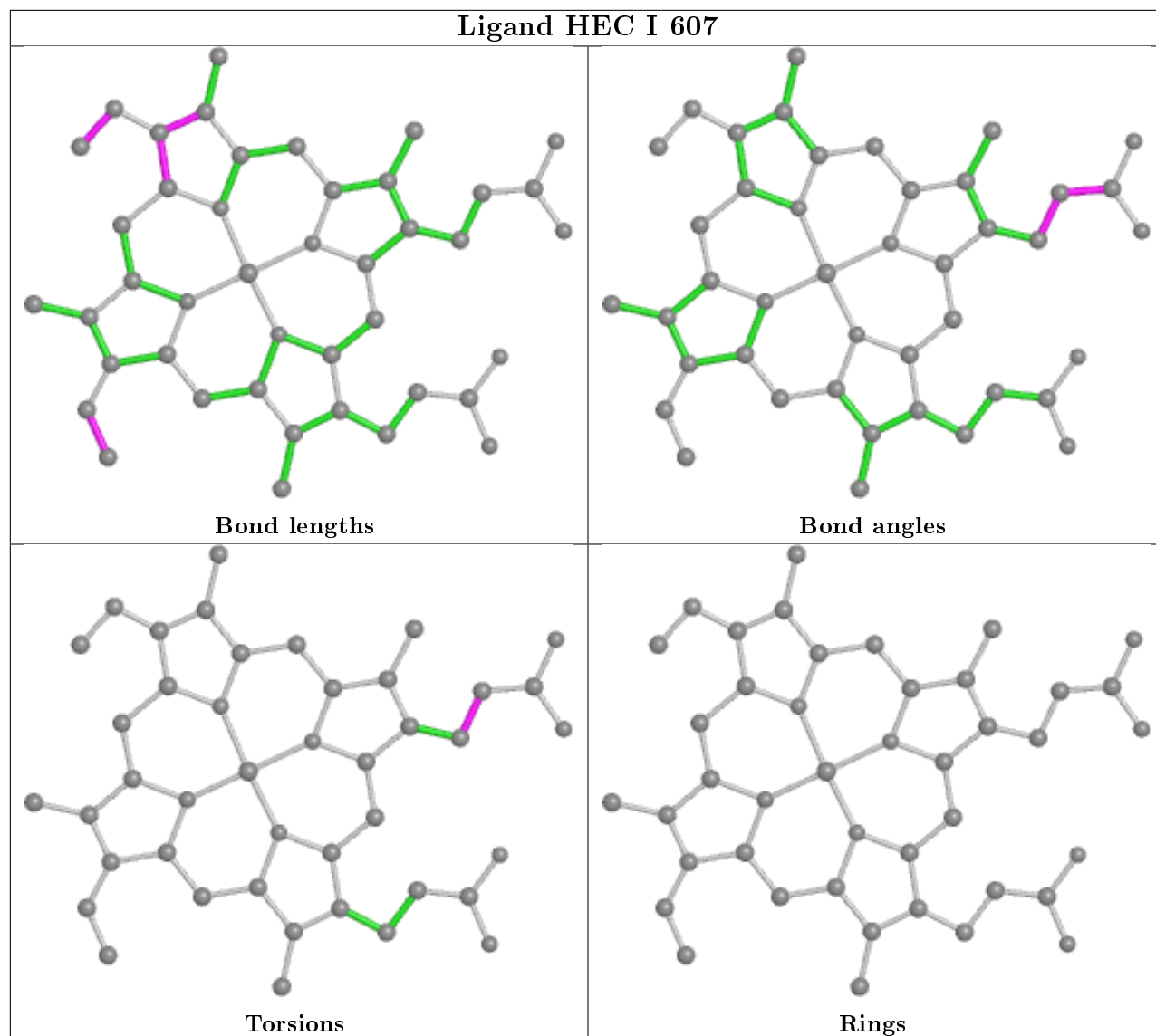


Torsions

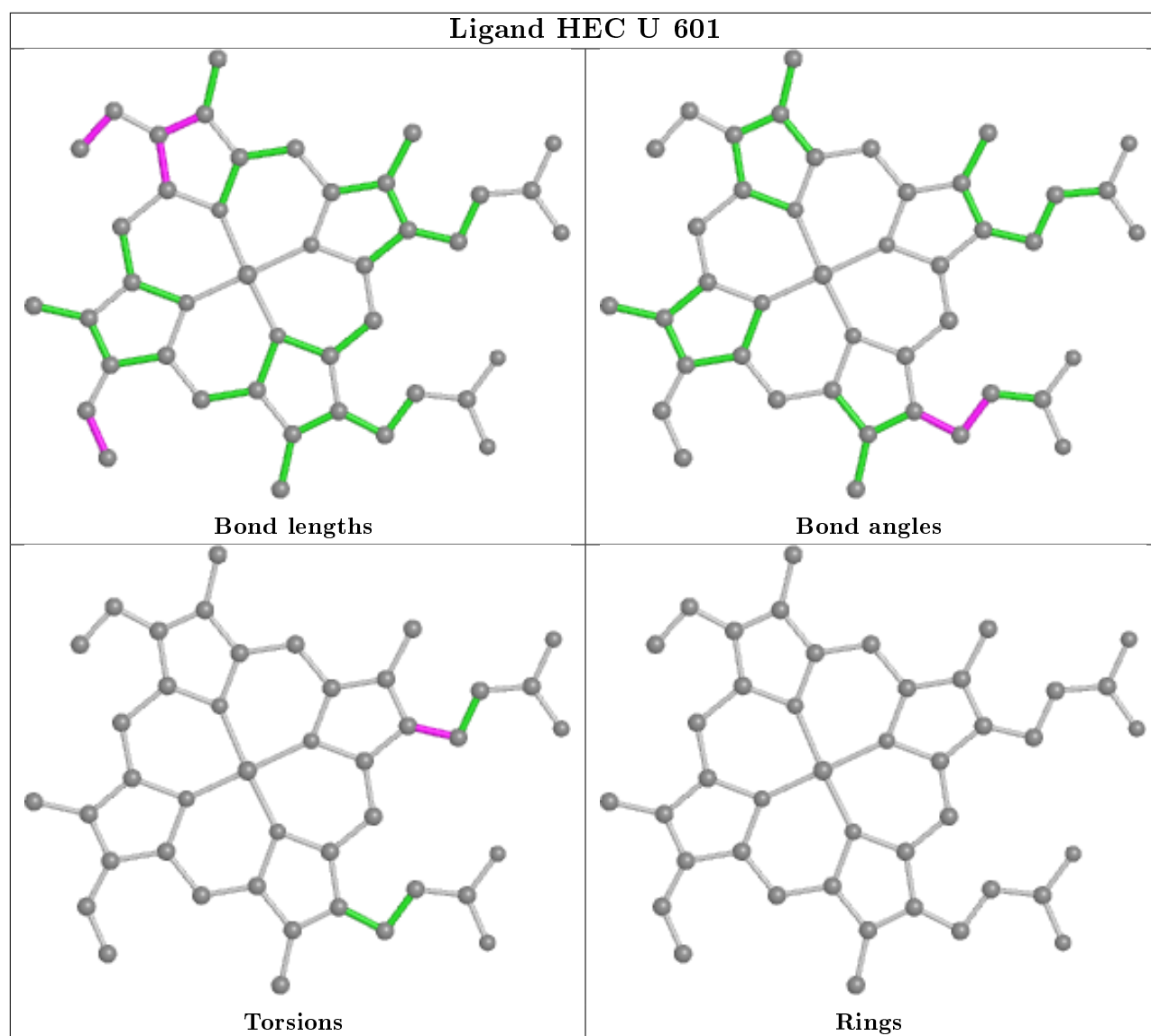


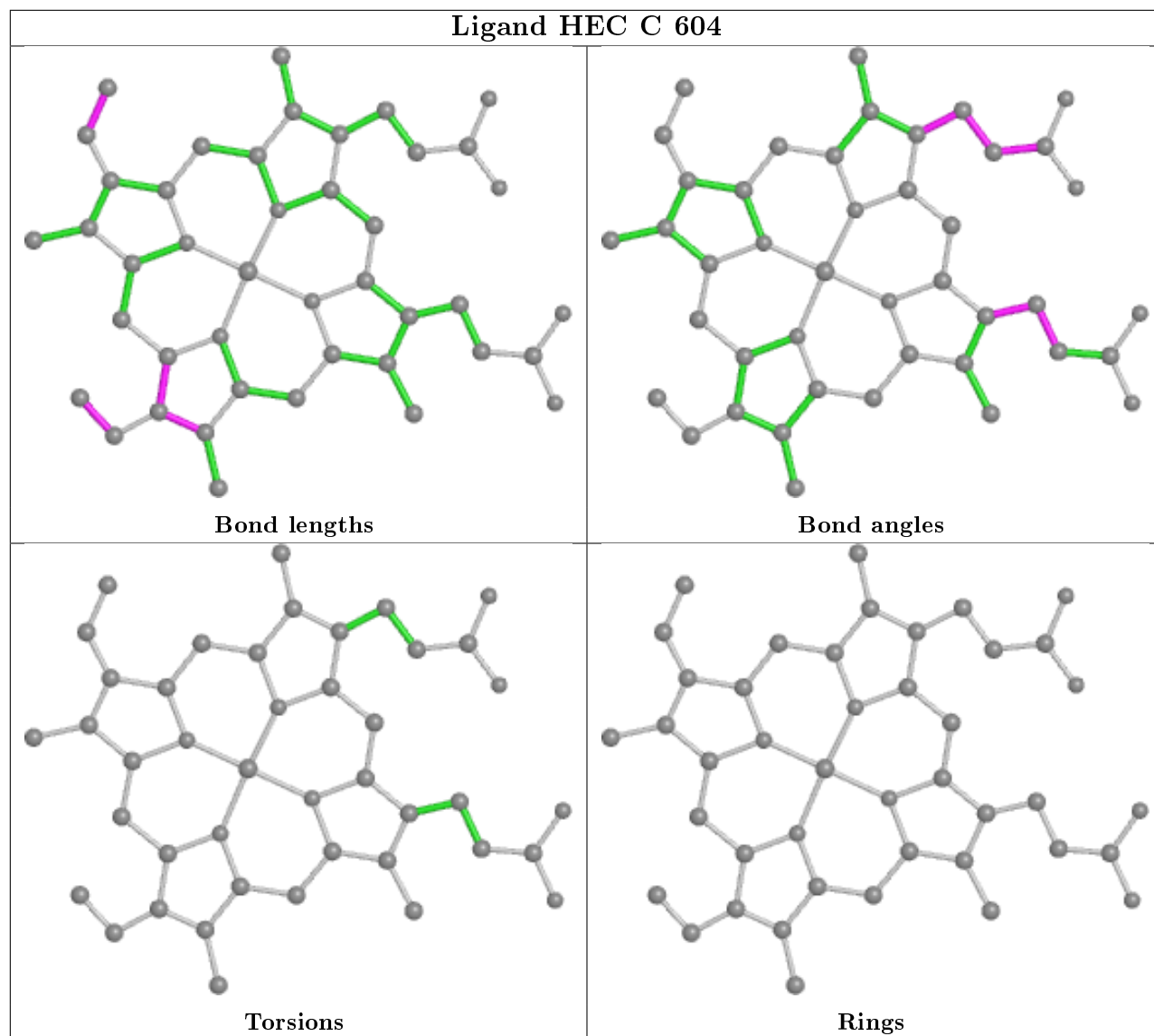
Rings

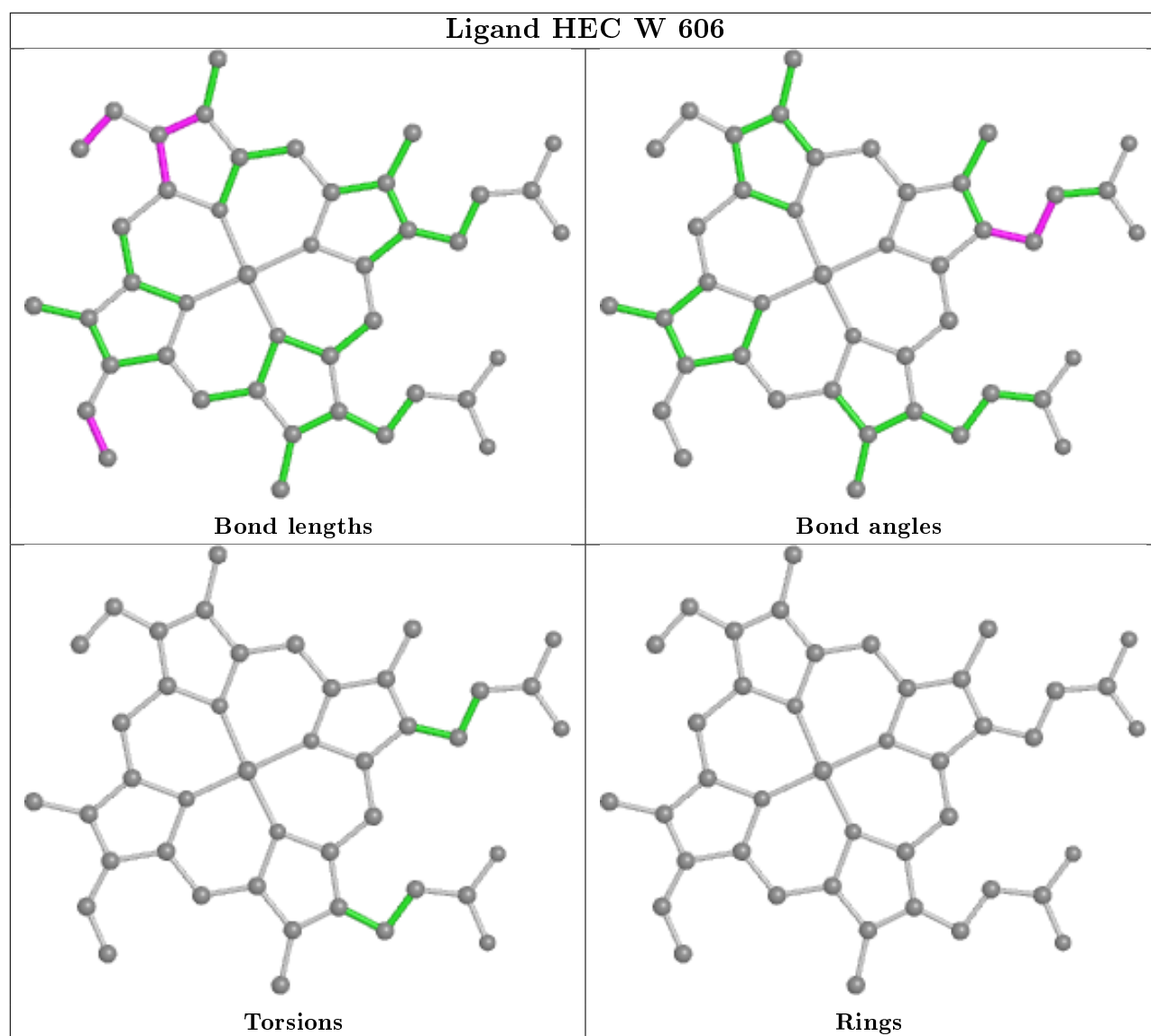
## Ligand HEC I 607

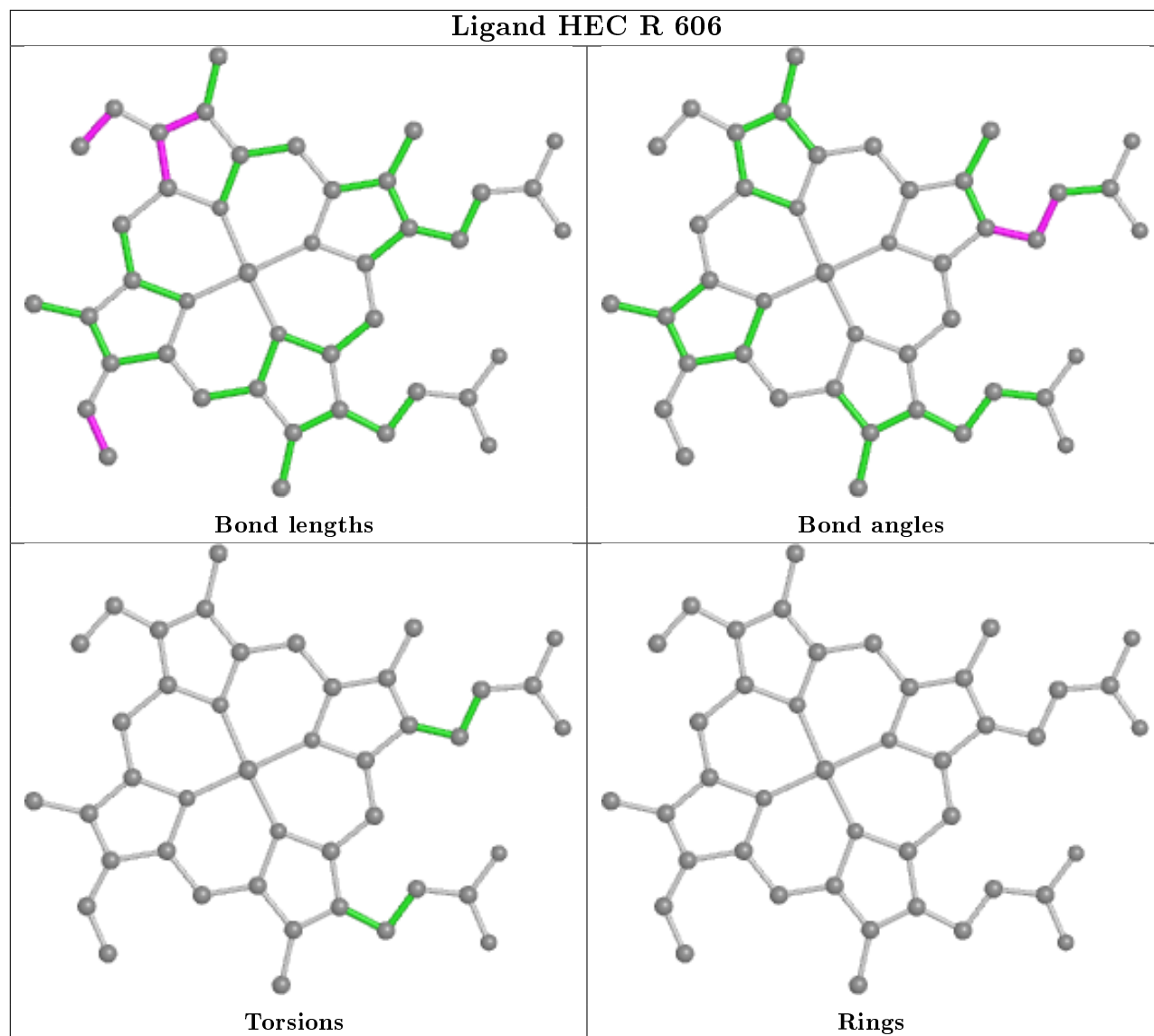




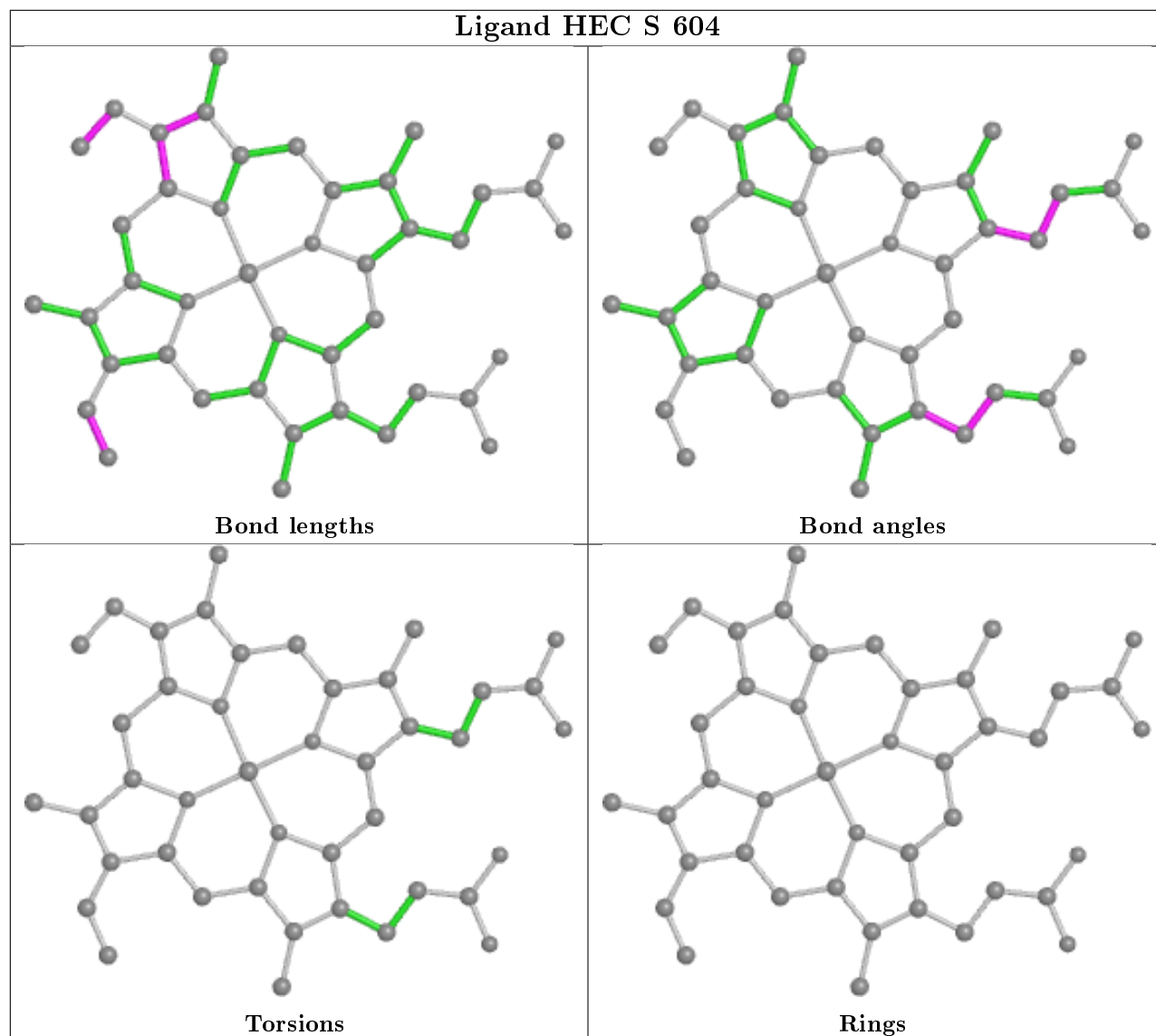


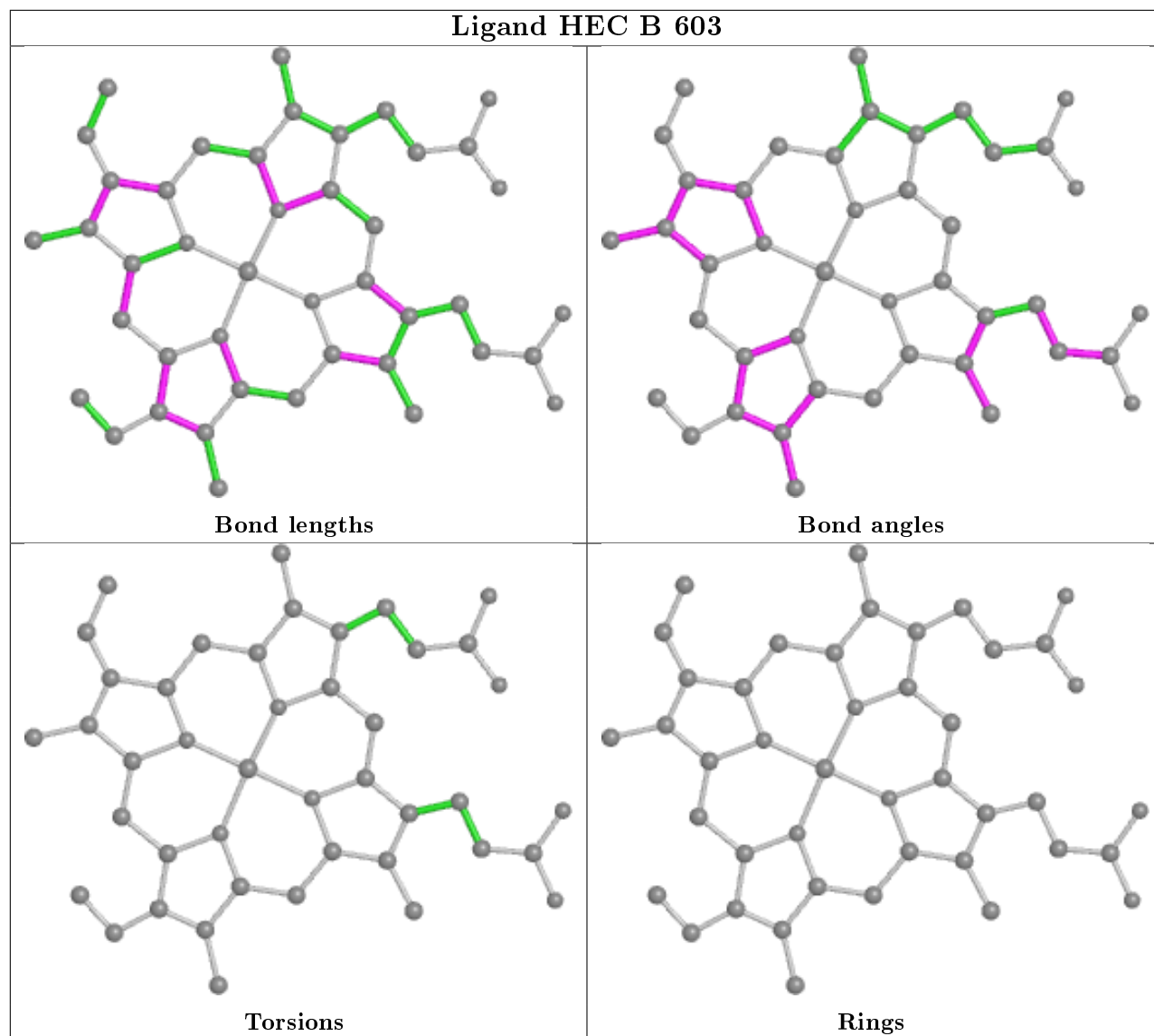


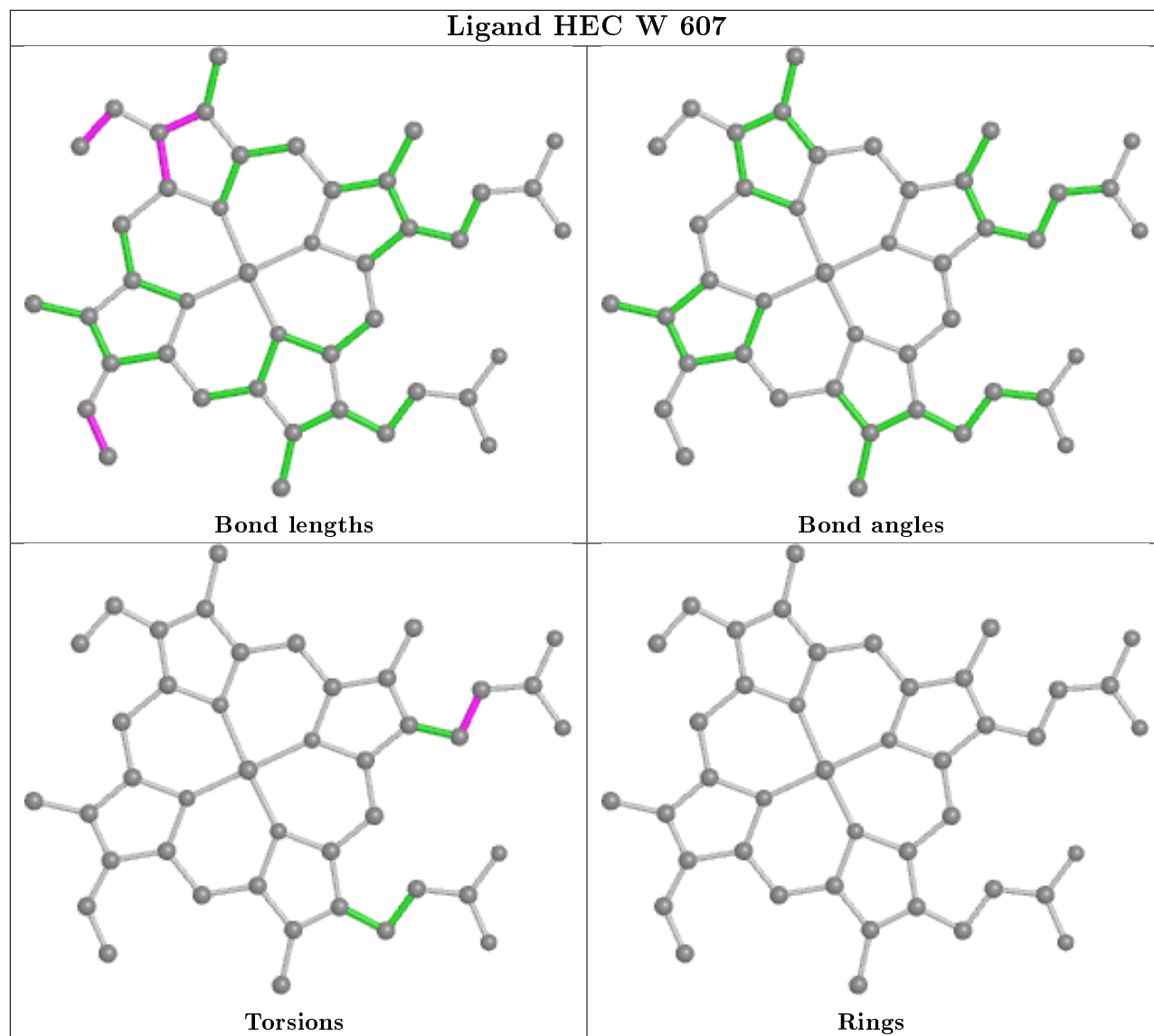


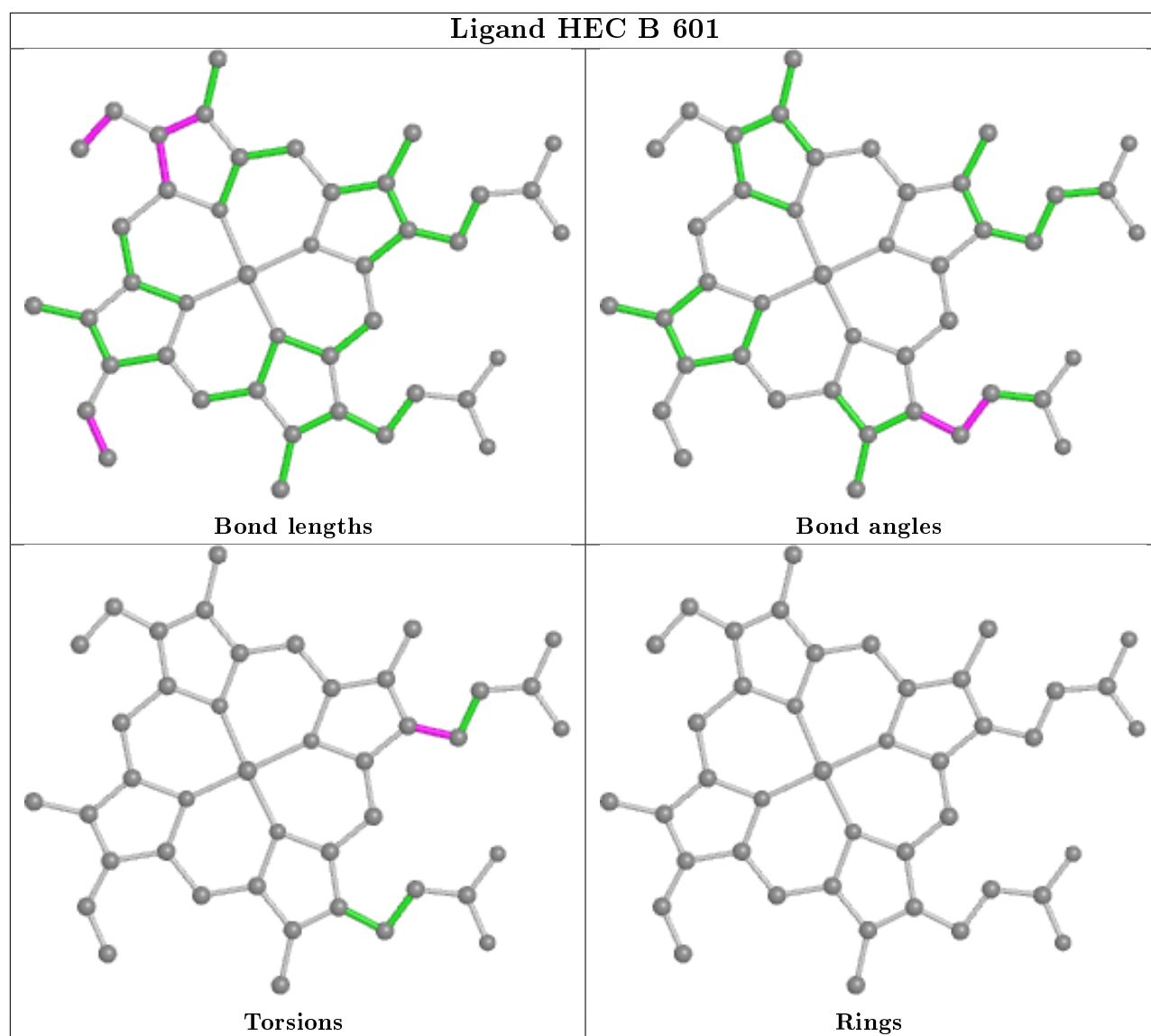


## Ligand HEC S 604

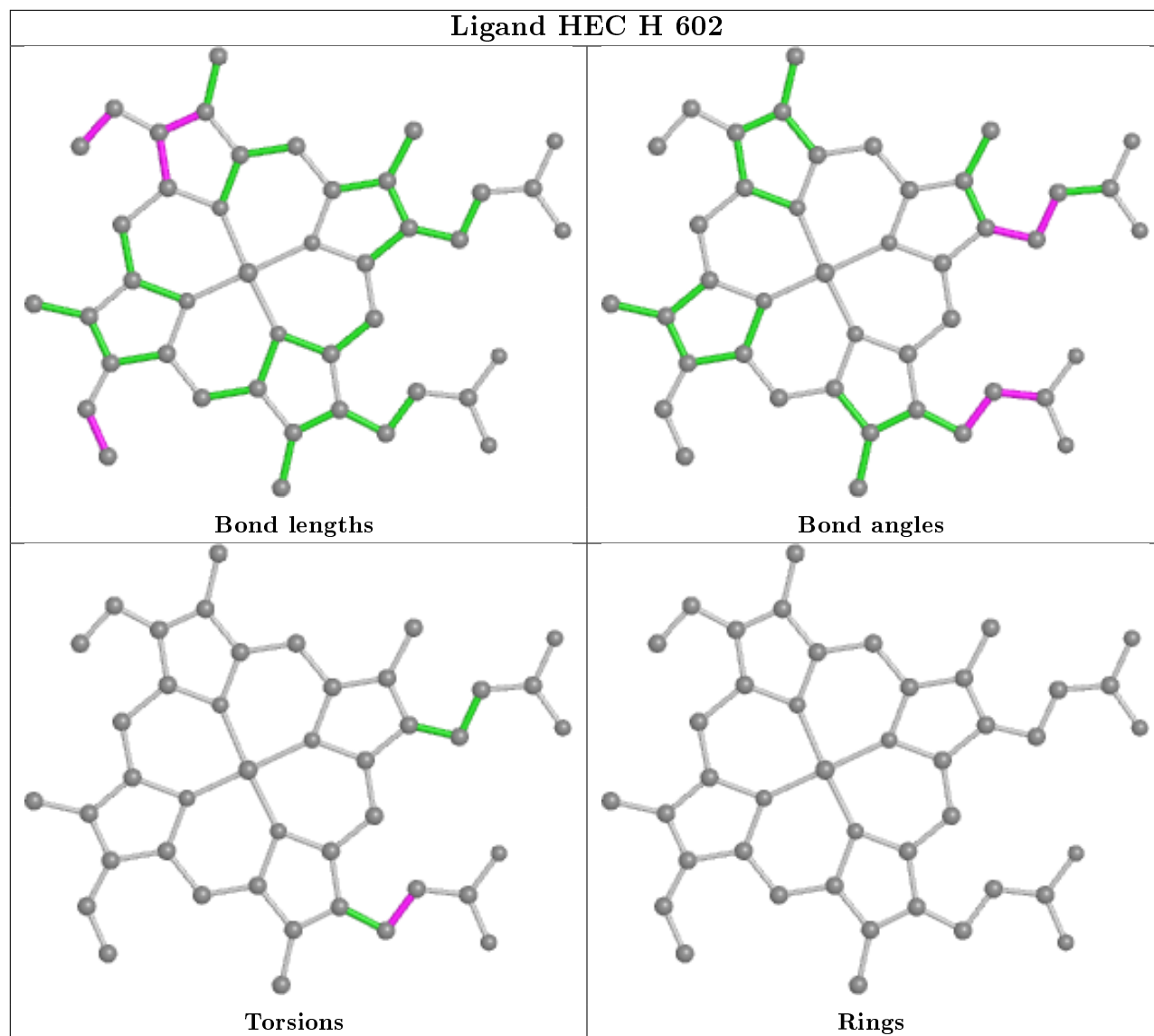


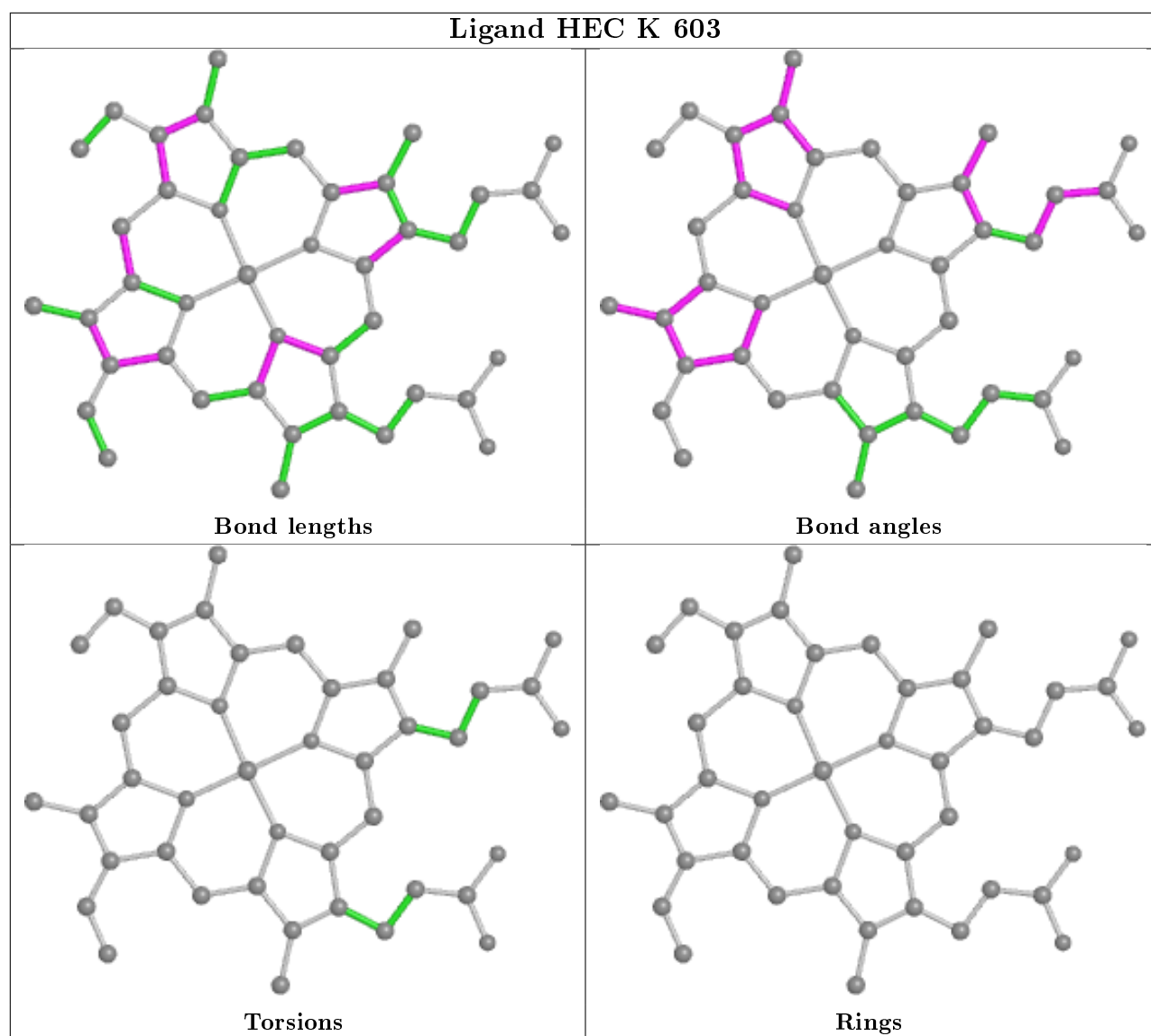


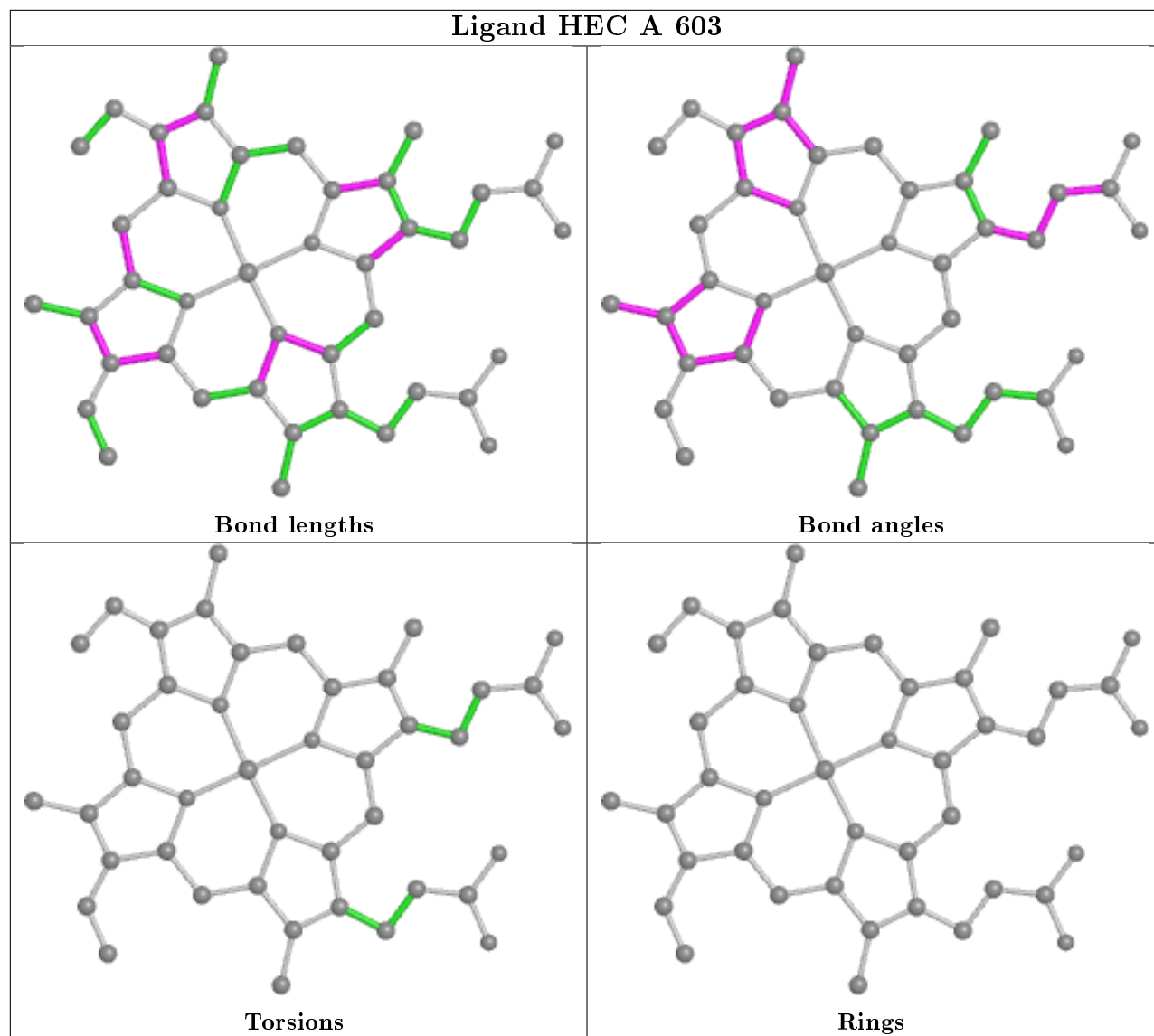


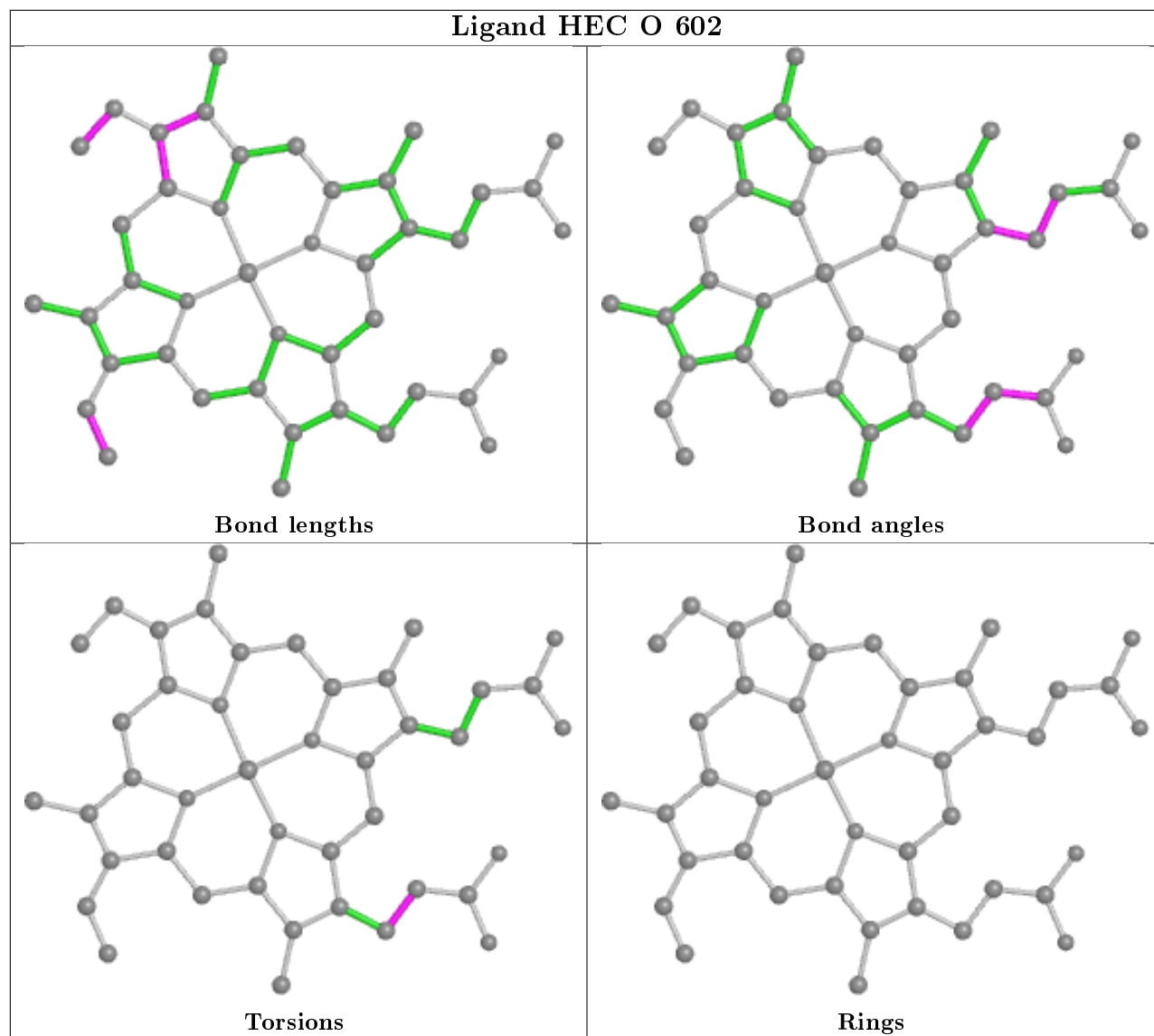




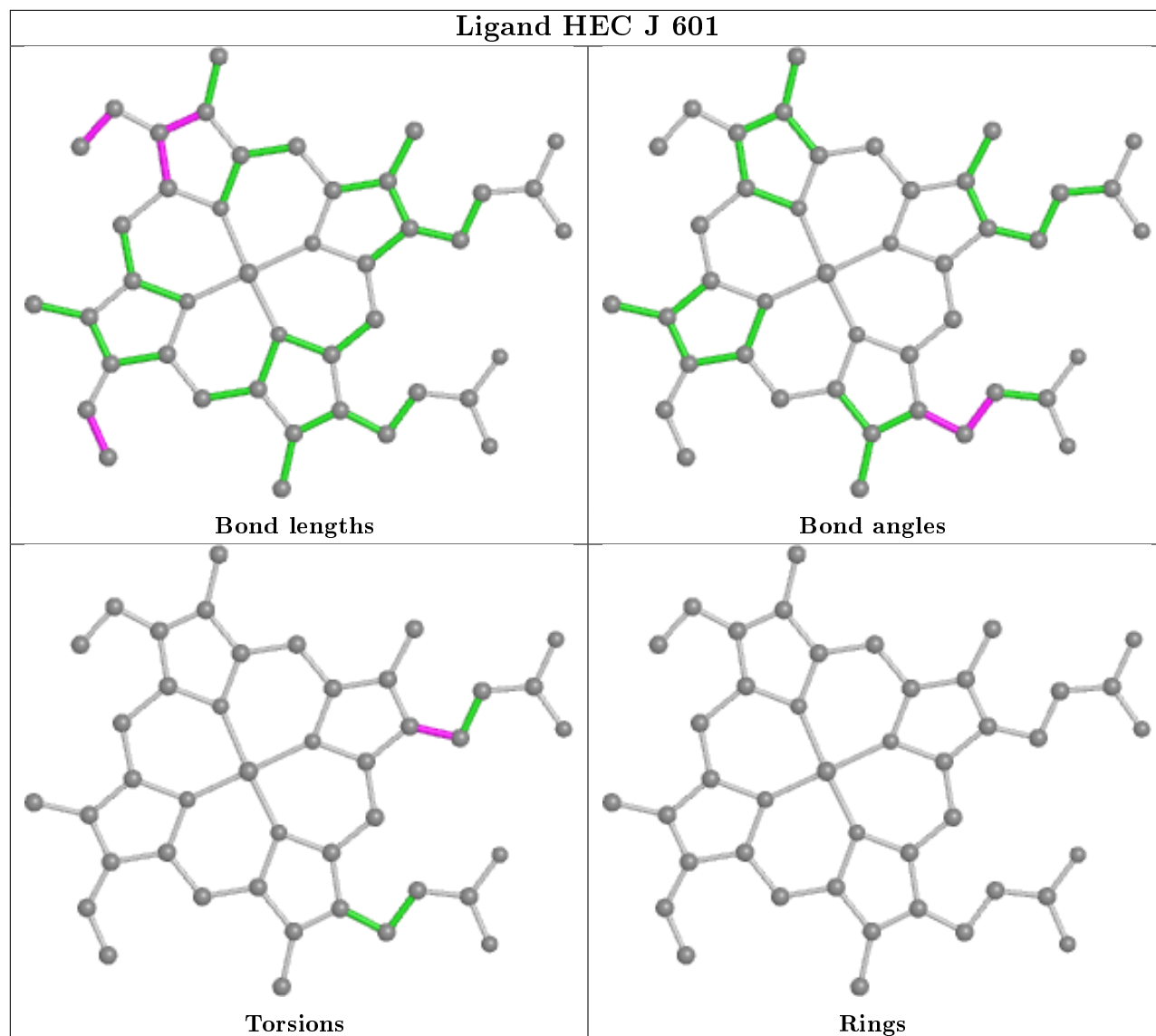


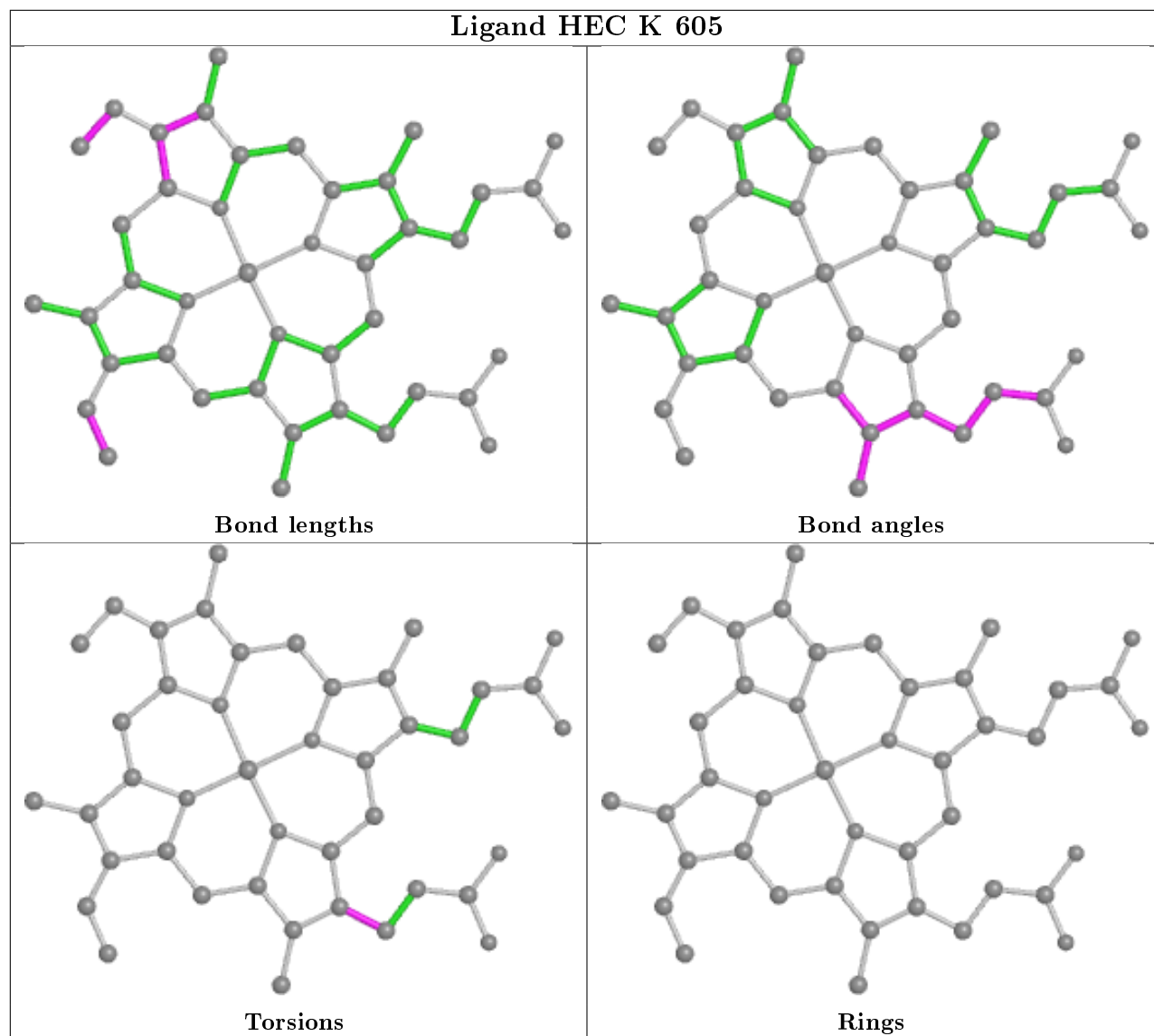




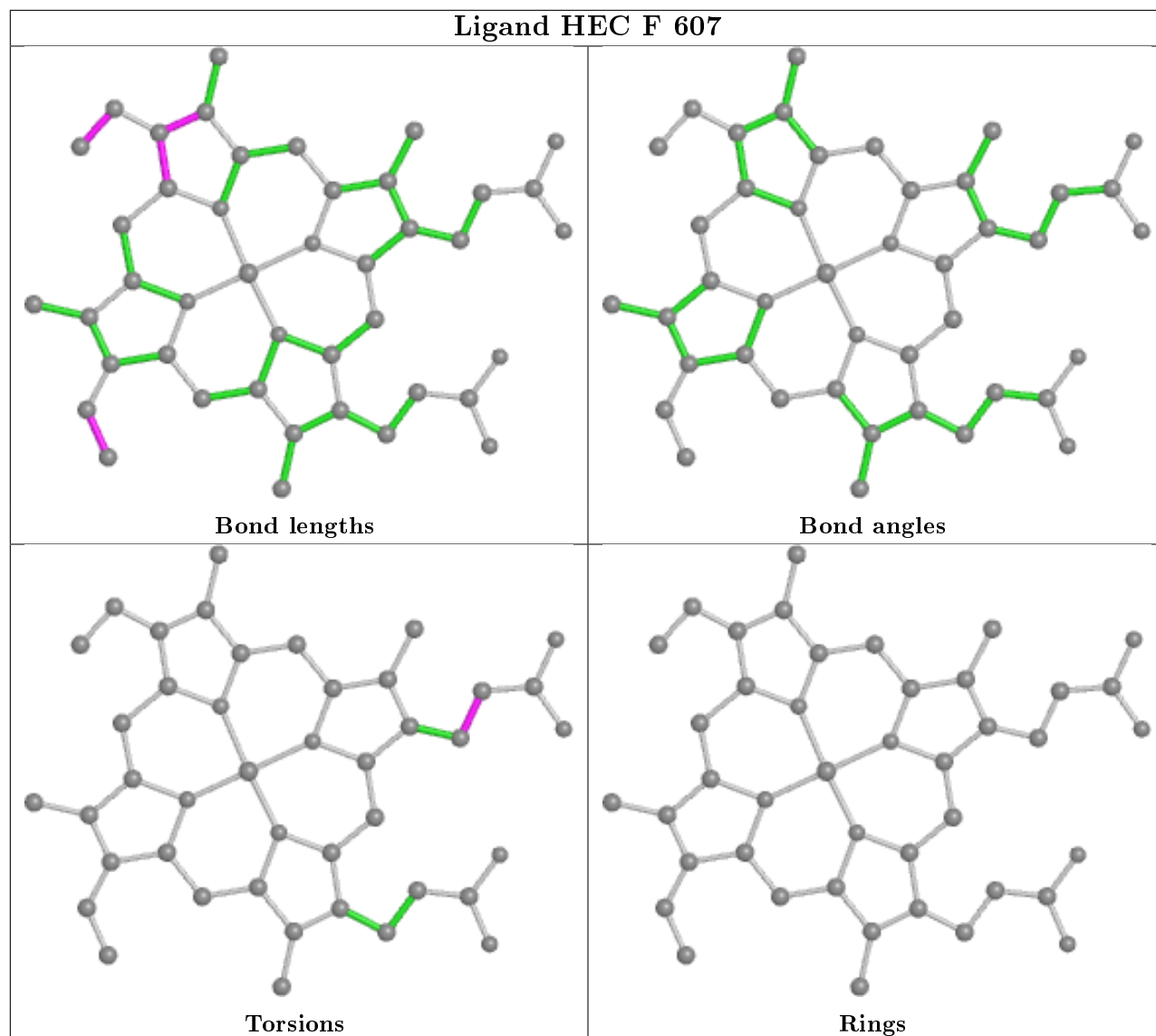


## Ligand HEC J 601

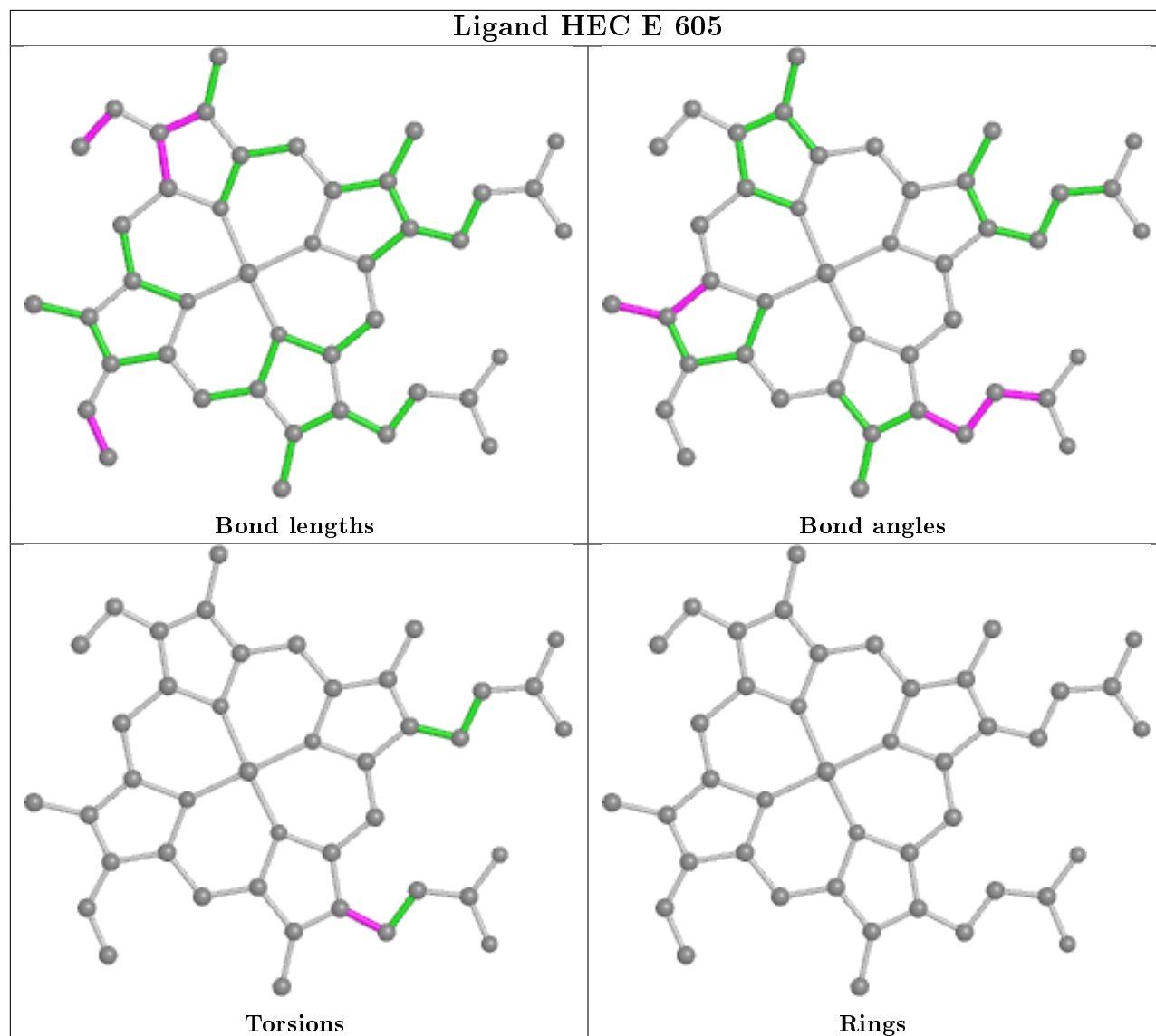




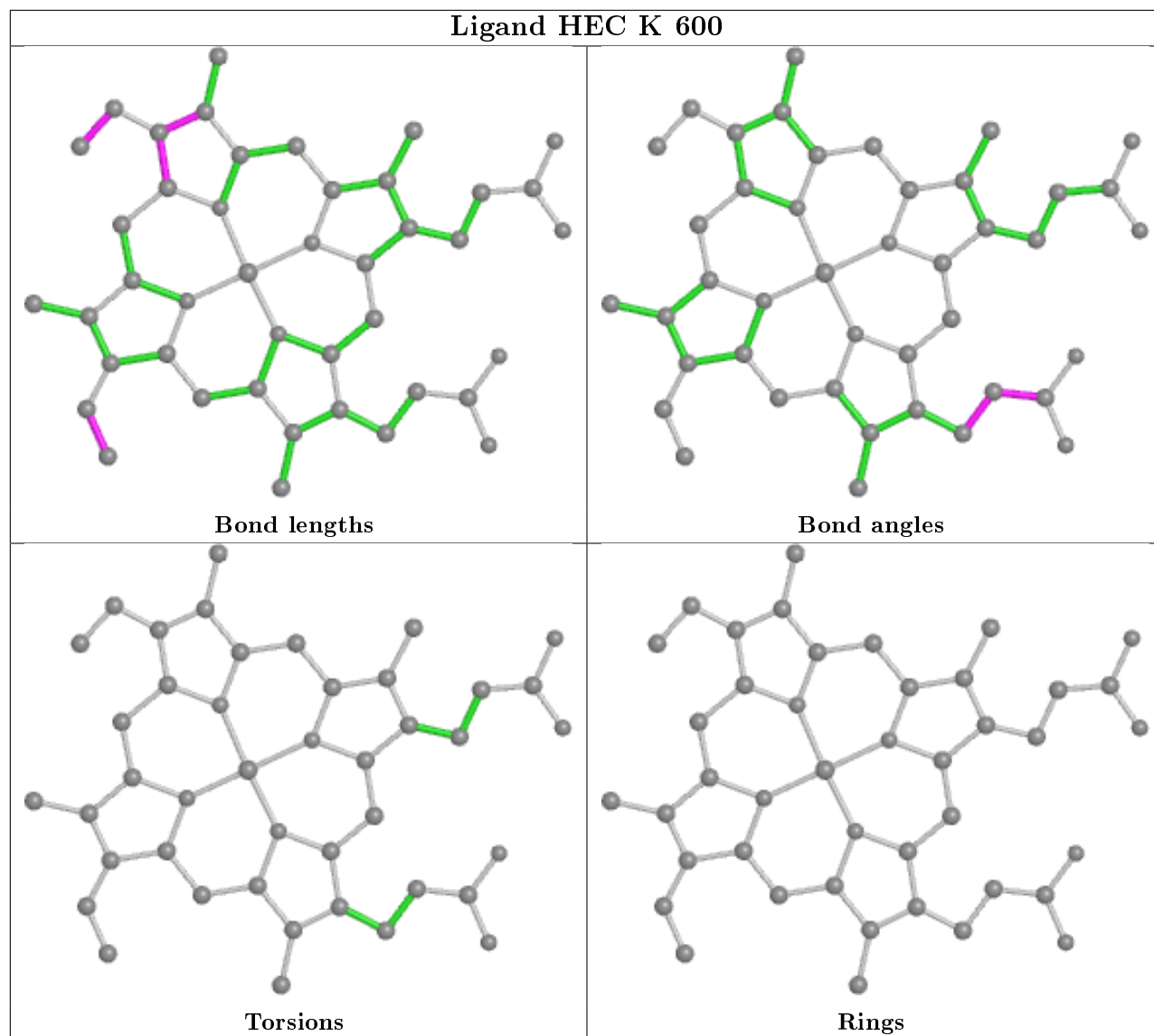
## Ligand HEC F 607



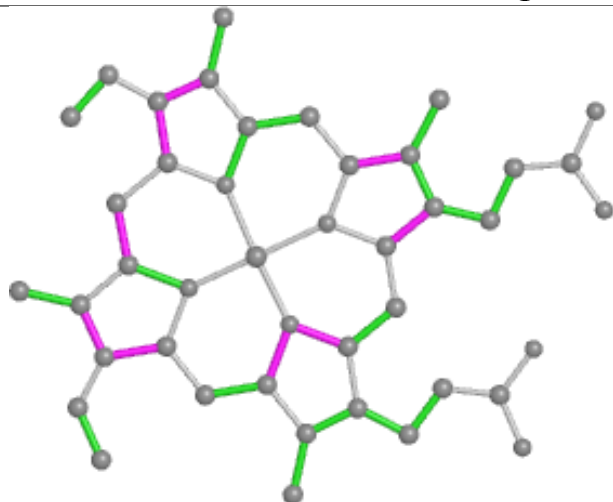
## Ligand HEC E 605



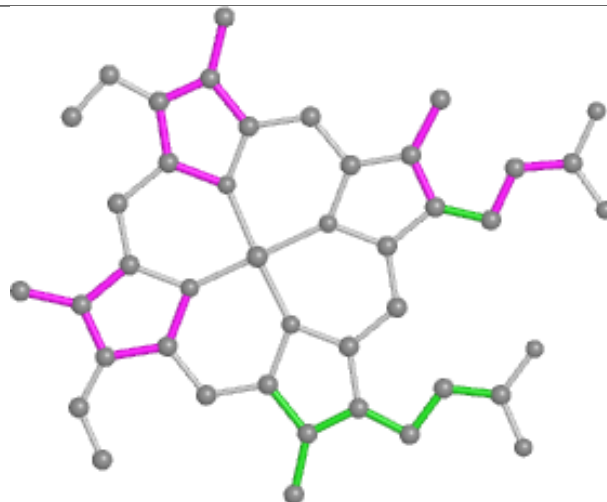




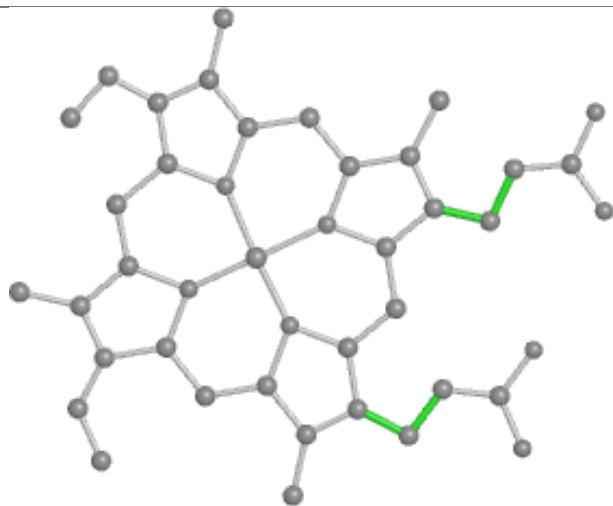
## Ligand HEC J 603



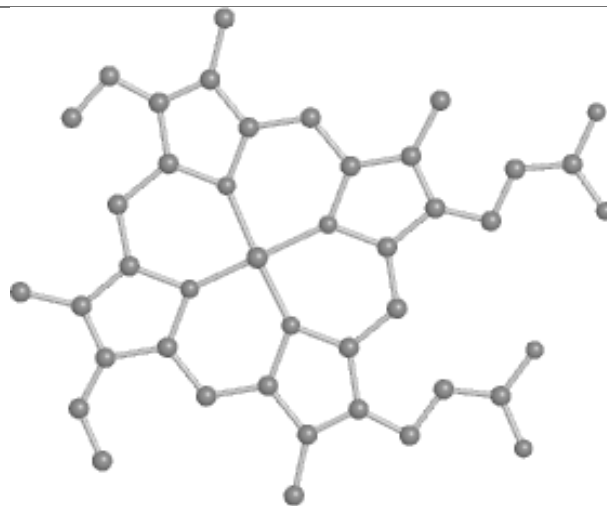
Bond lengths



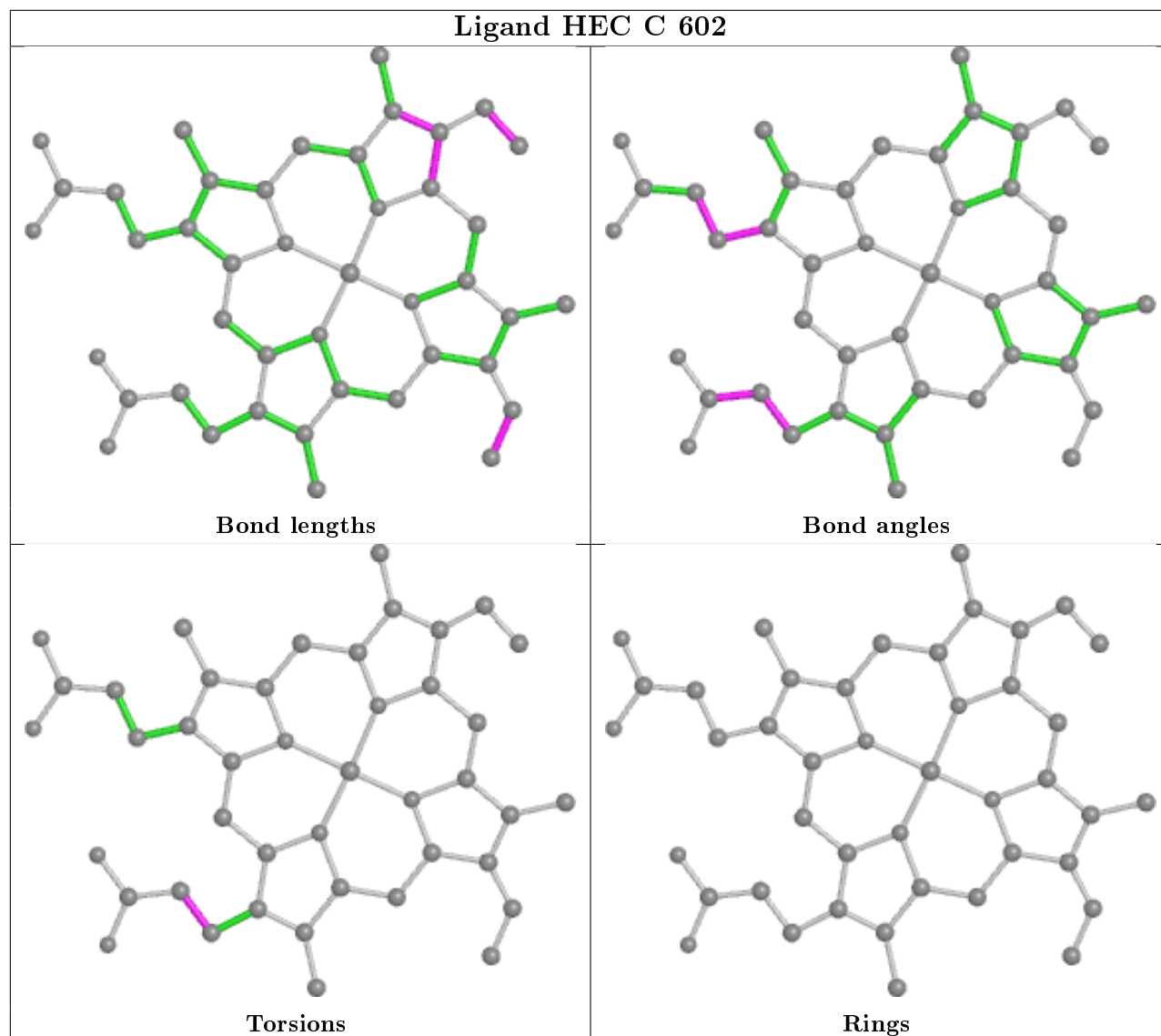
Bond angles

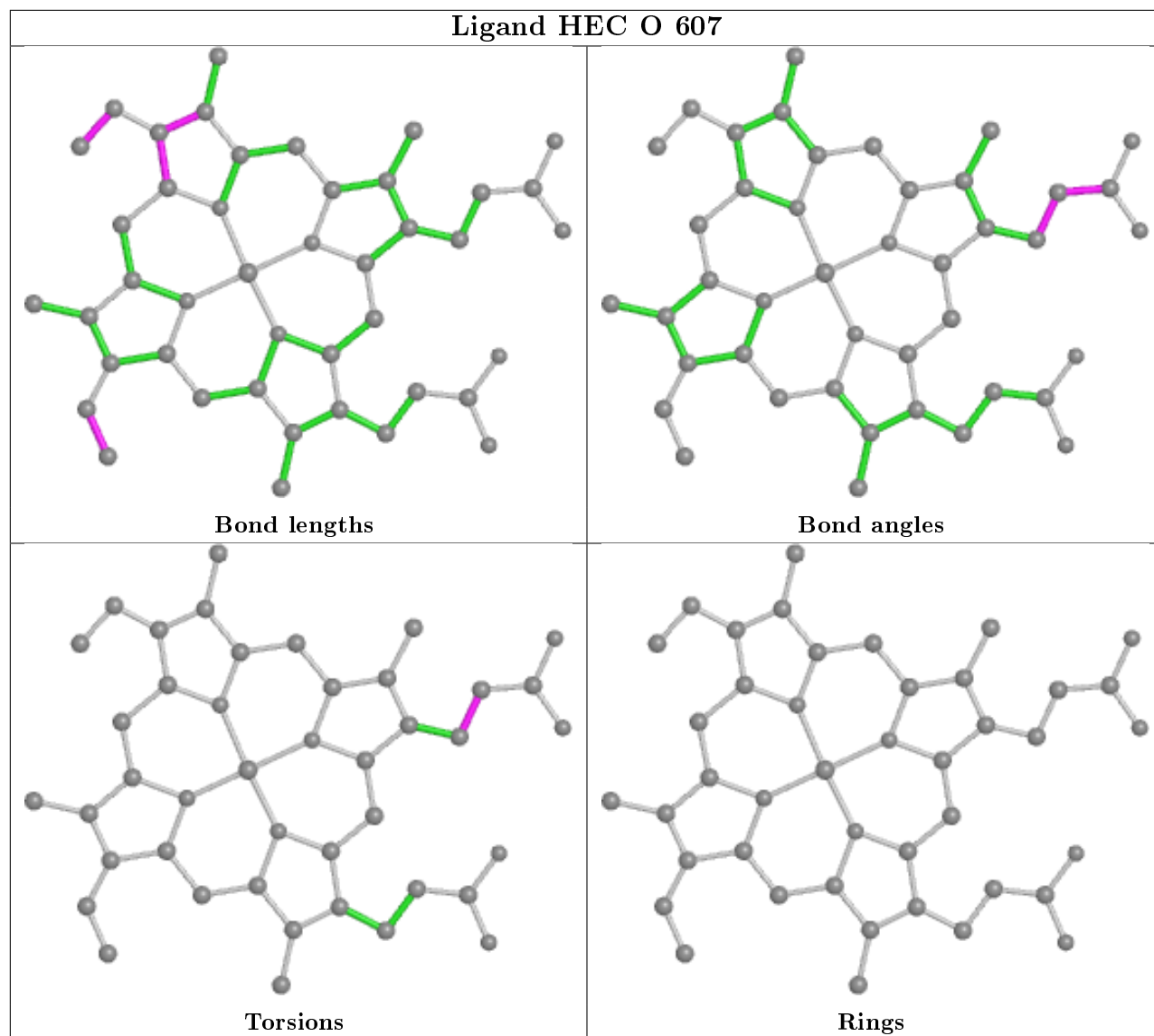


Torsions

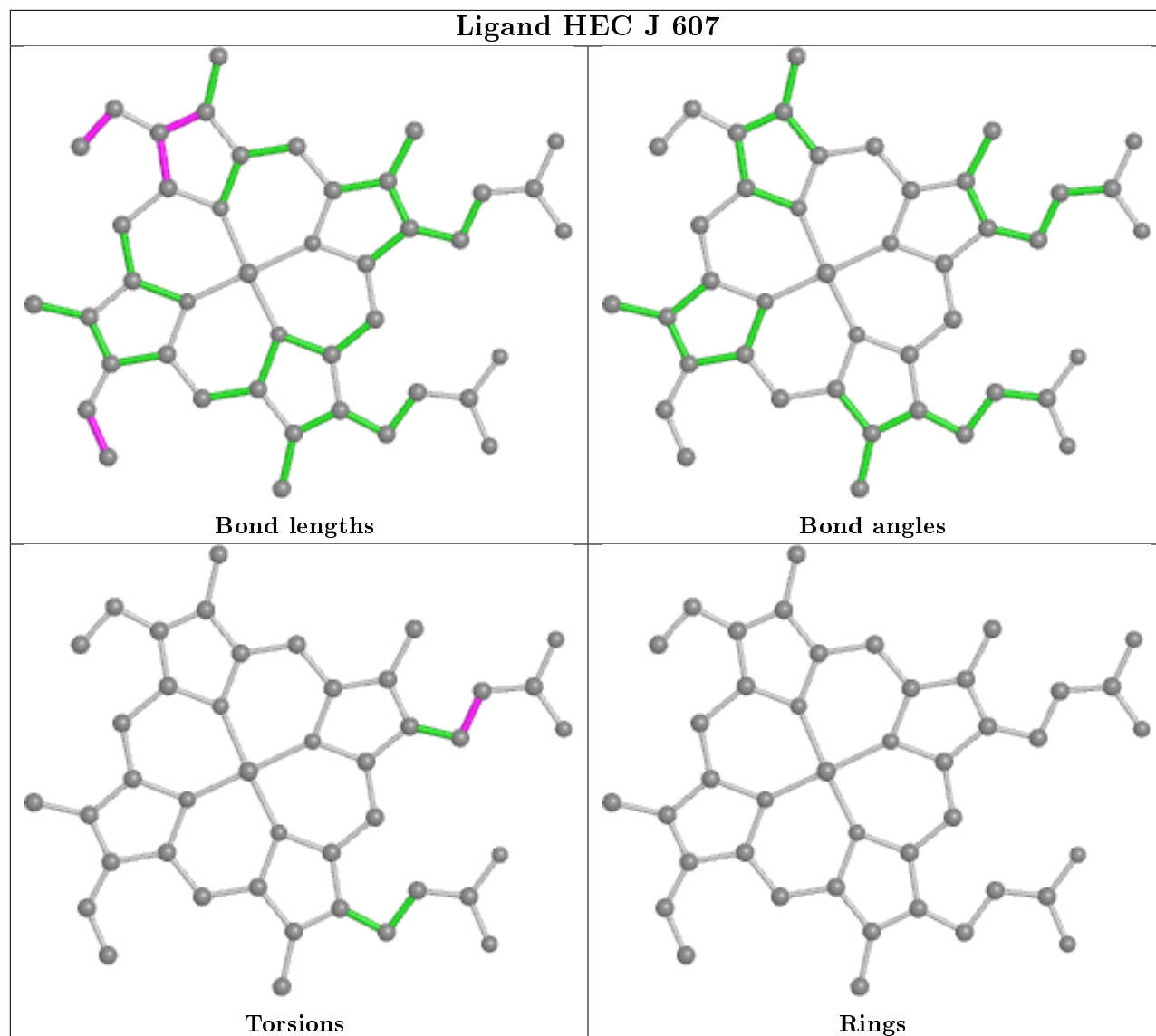


Rings

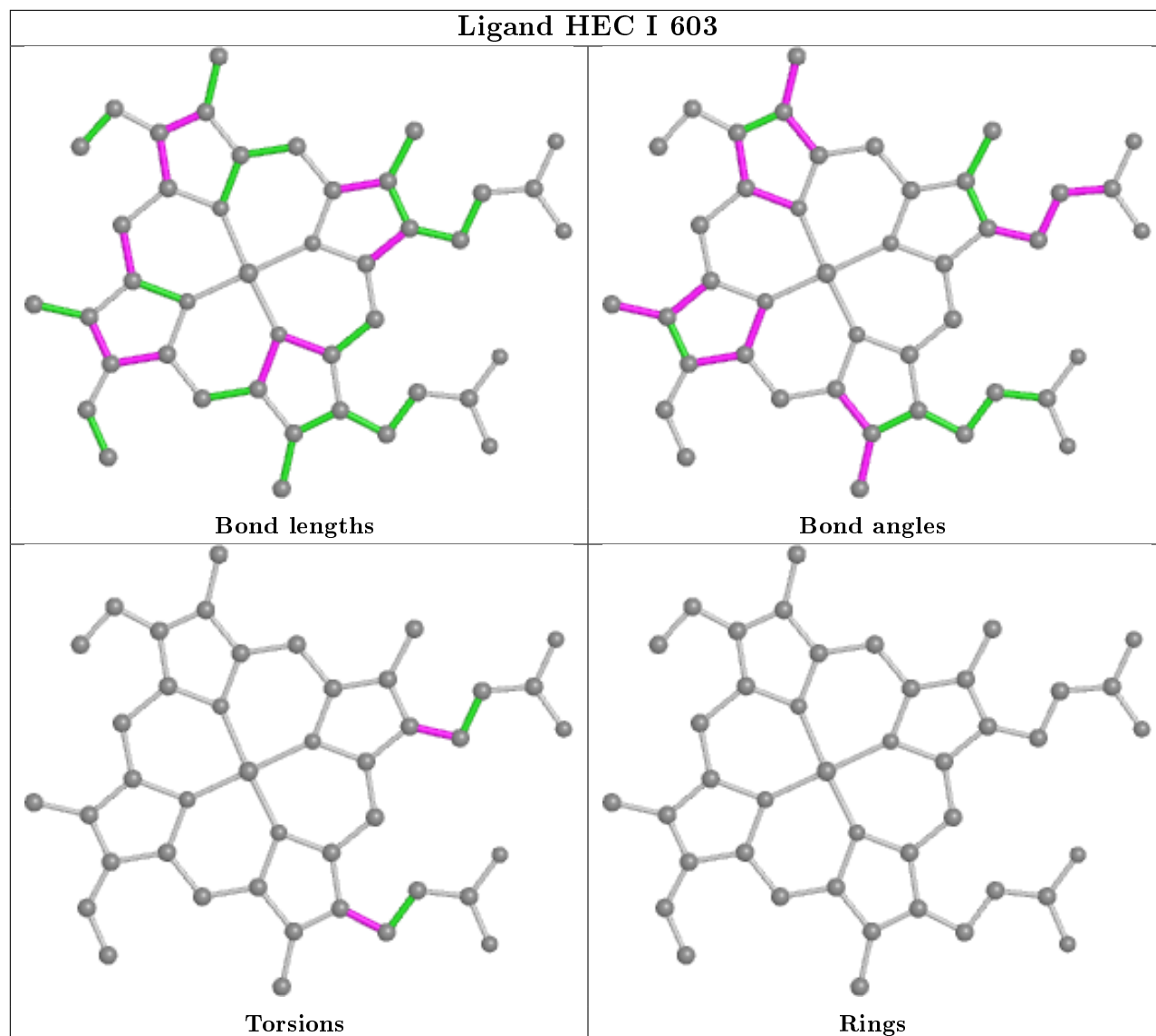


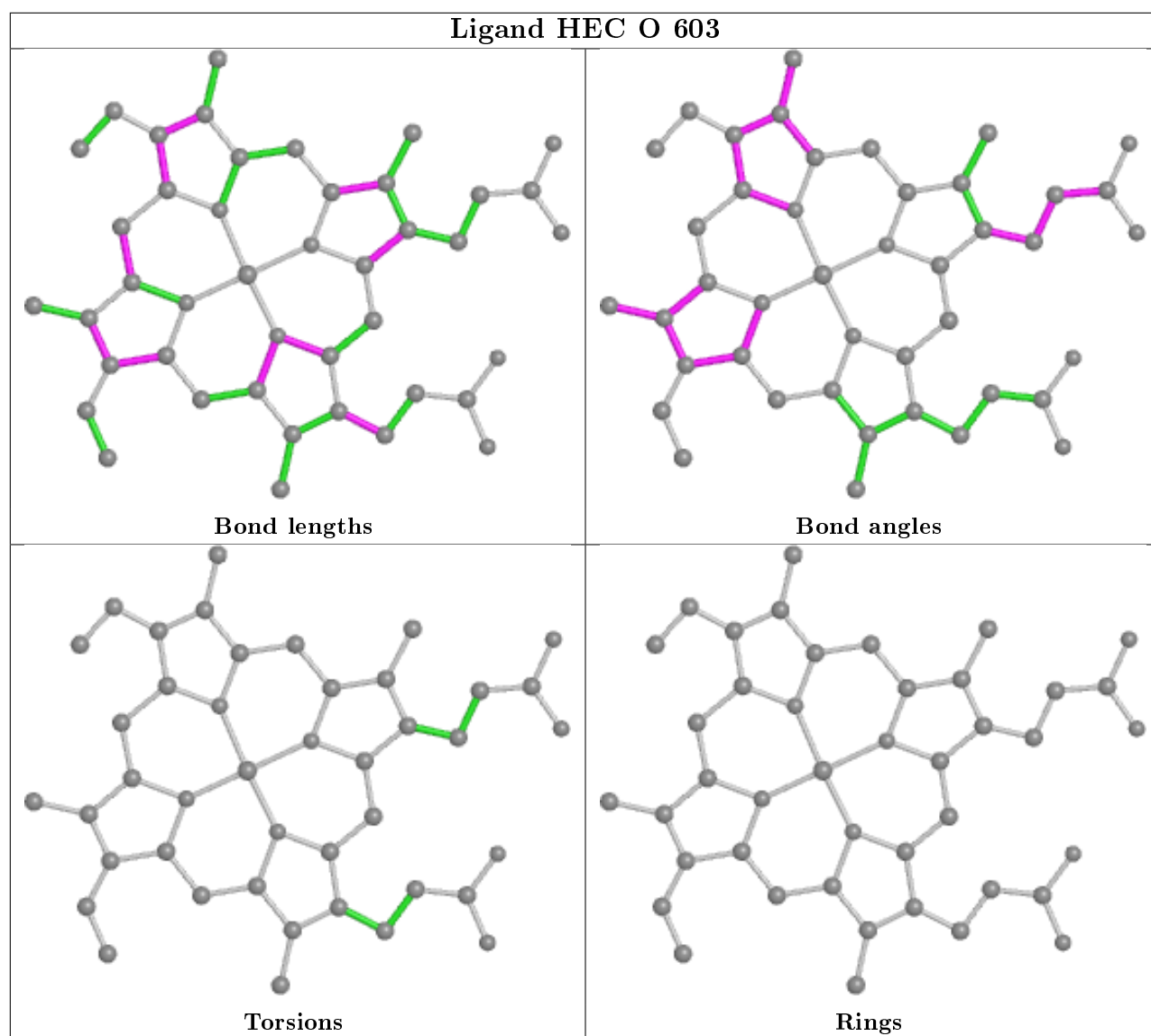


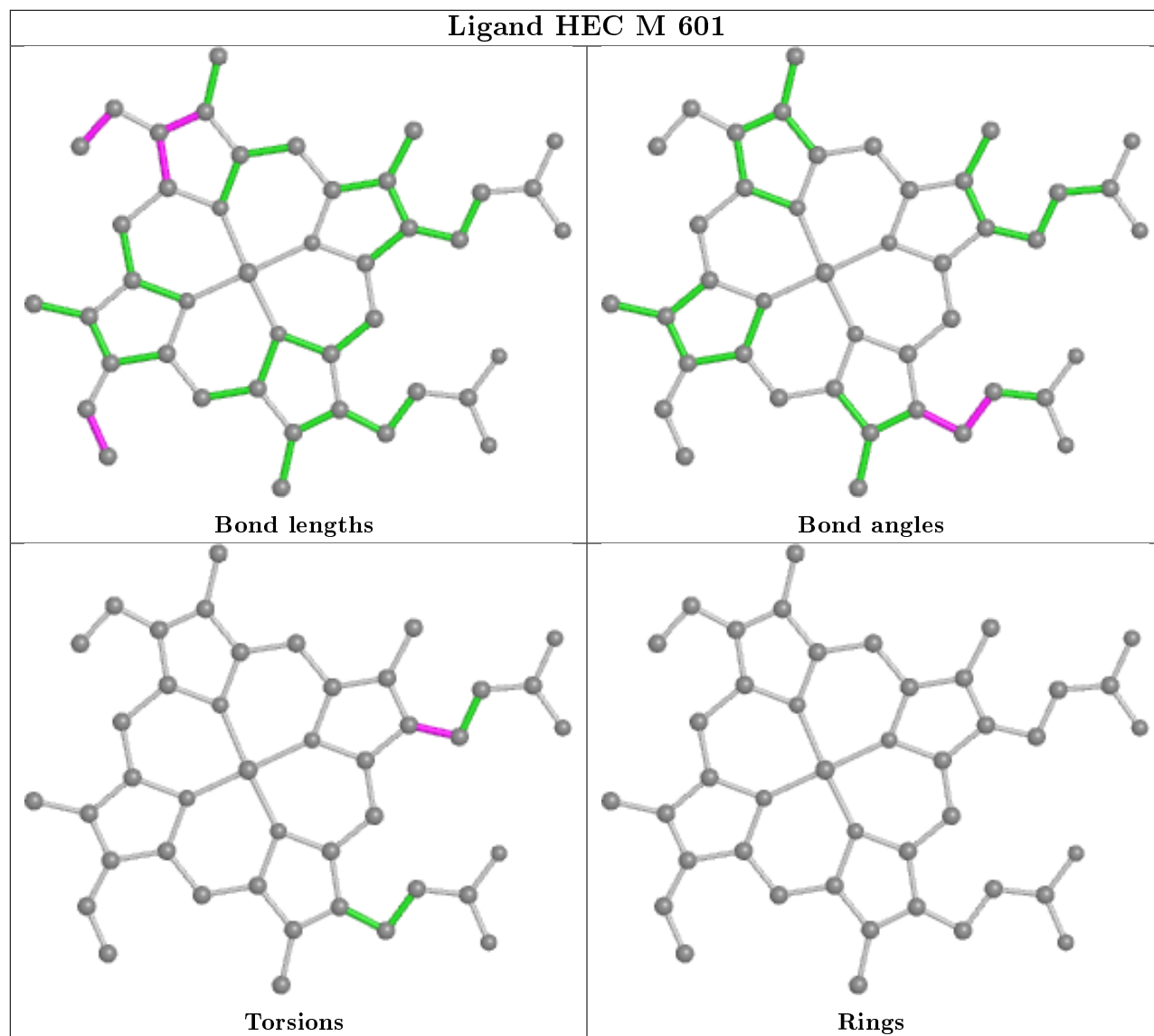
## Ligand HEC J 607



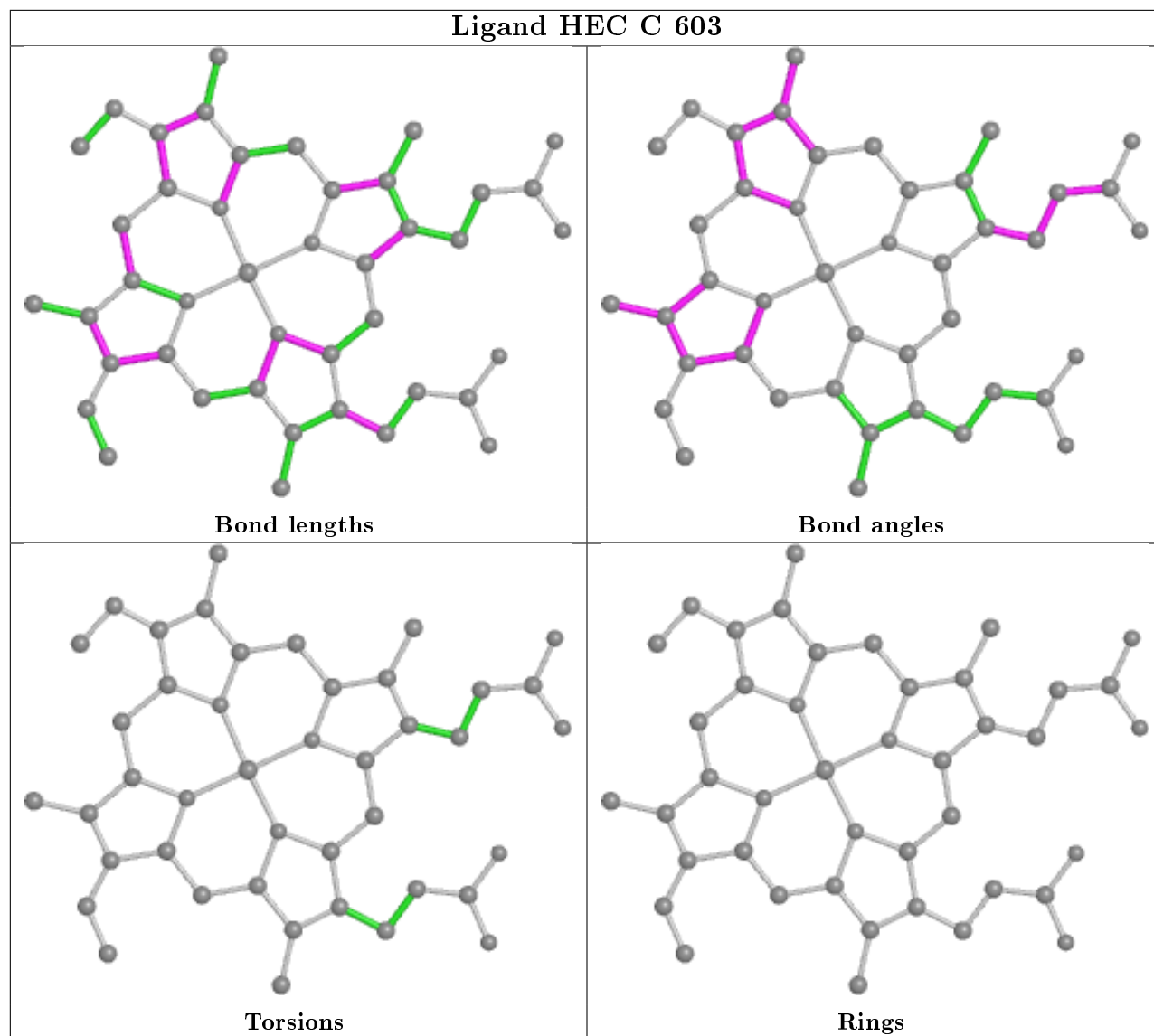
## Ligand HEC I 603



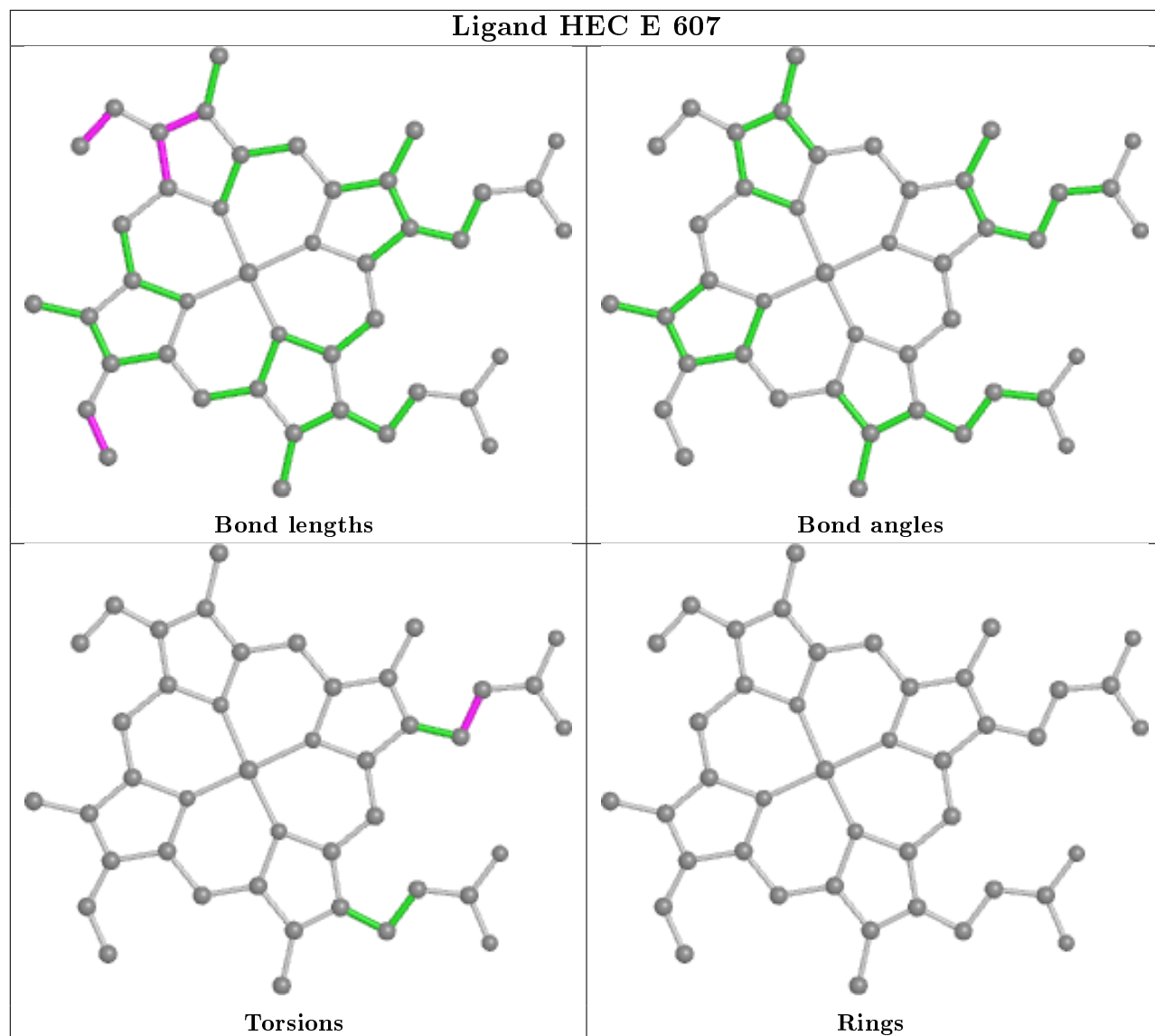




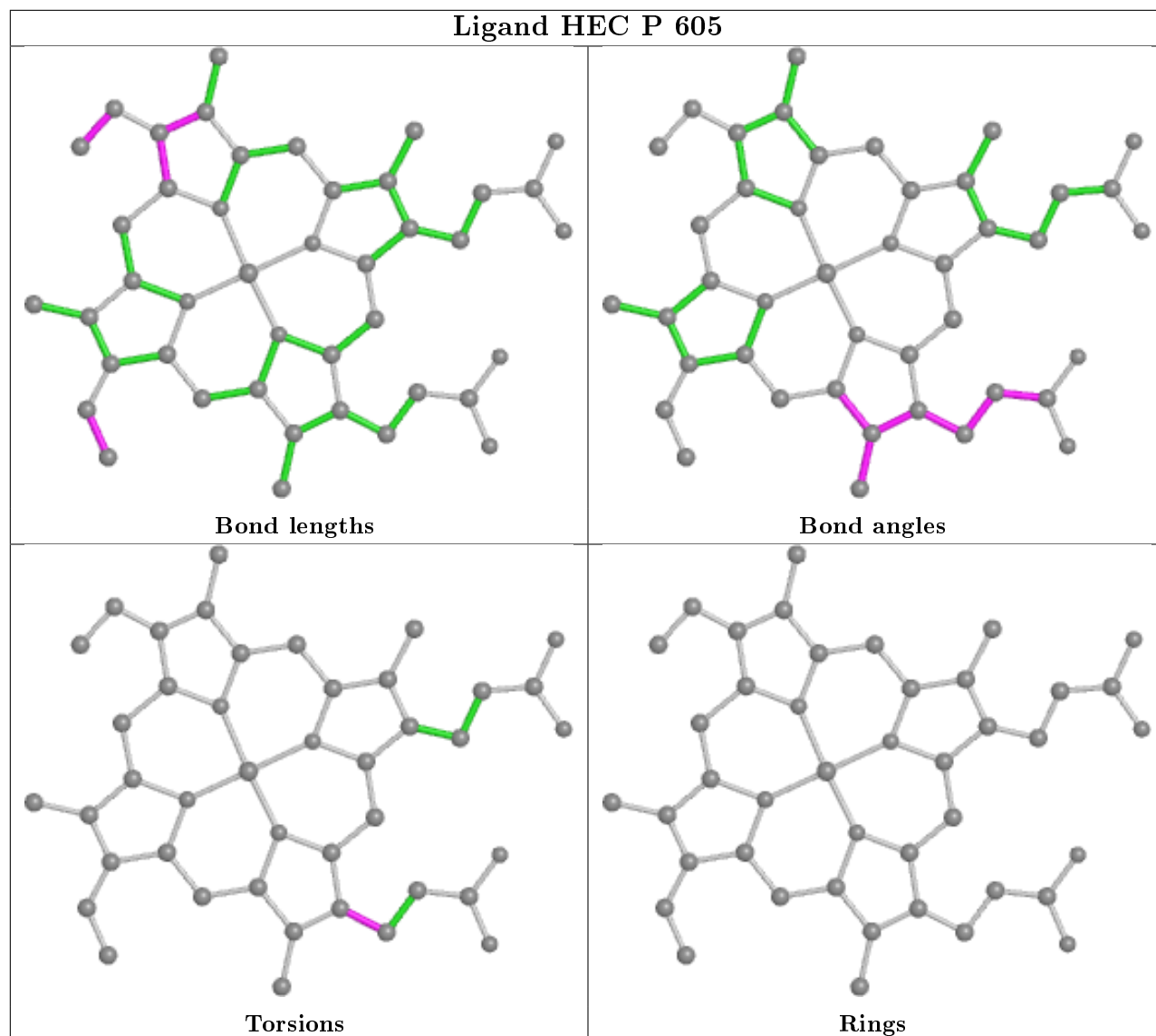




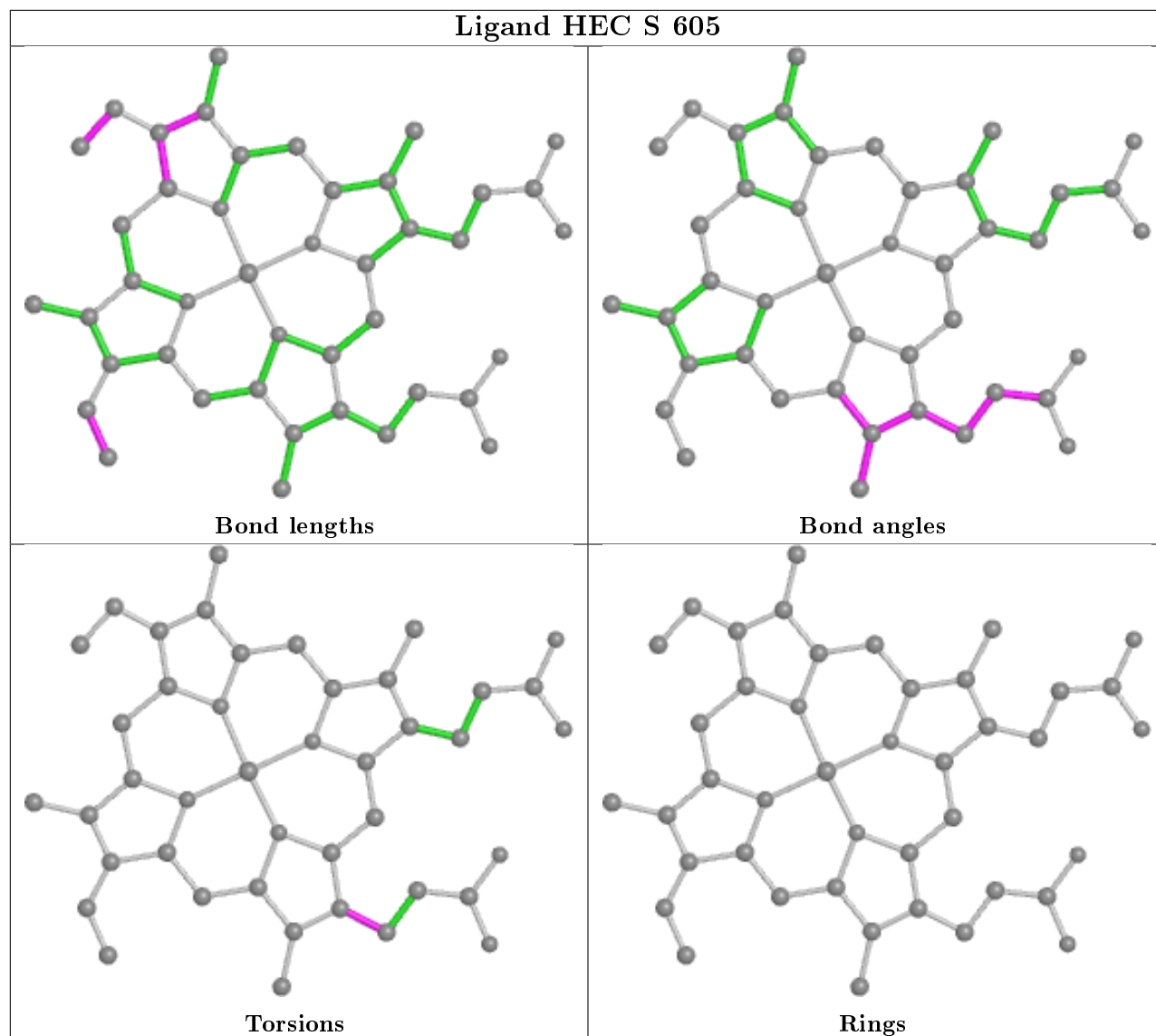
## Ligand HEC E 607

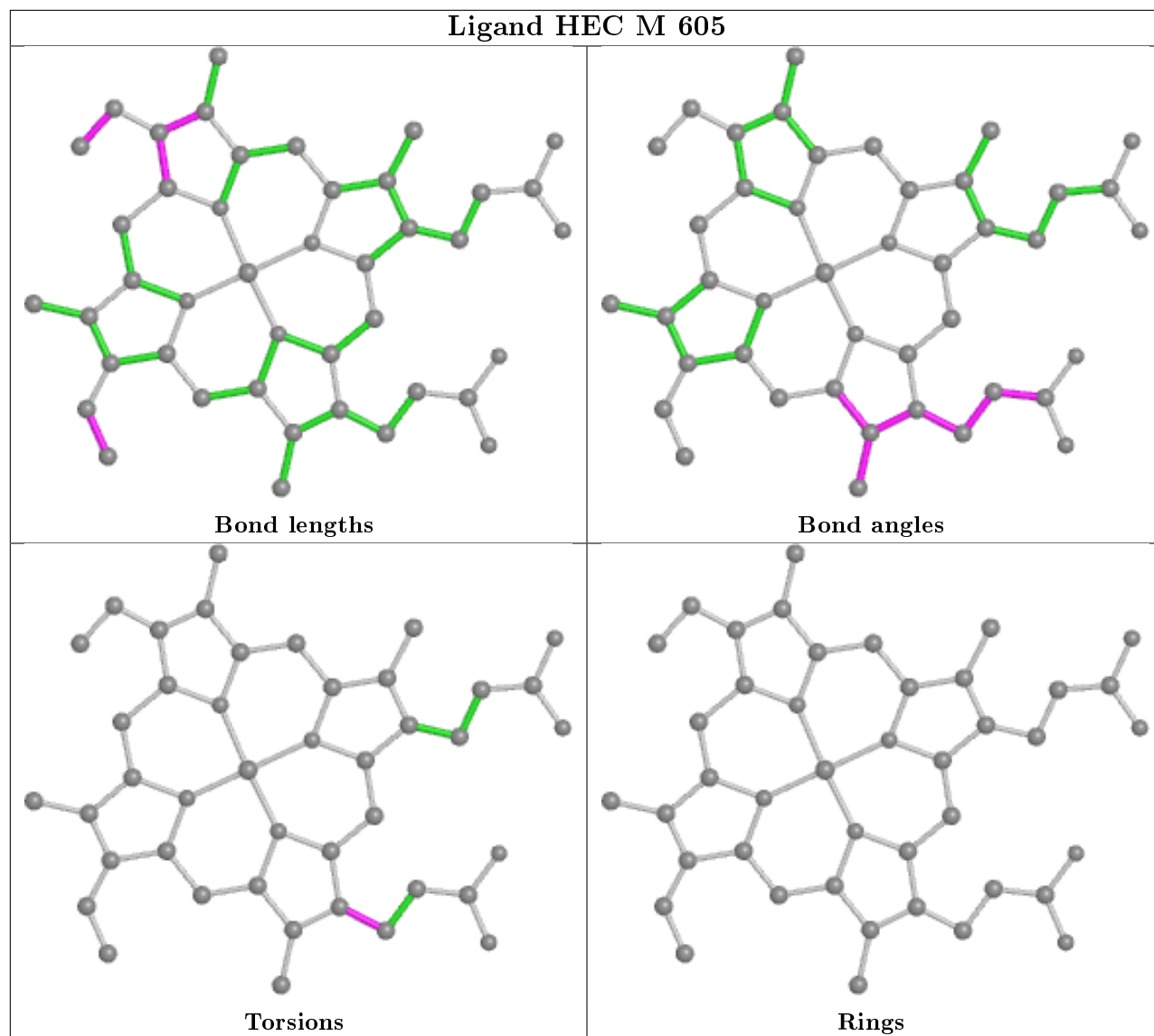


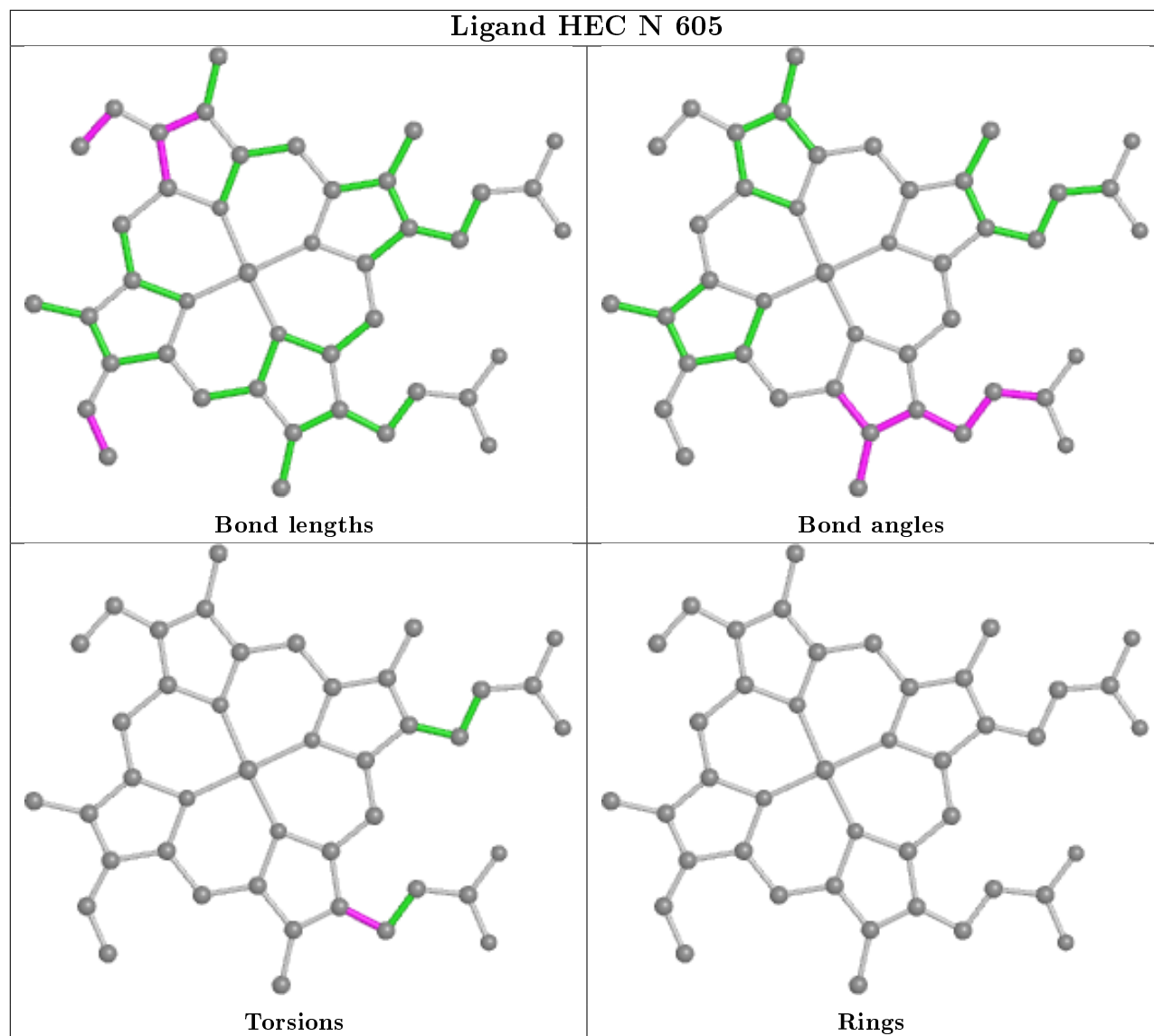
## Ligand HEC P 605

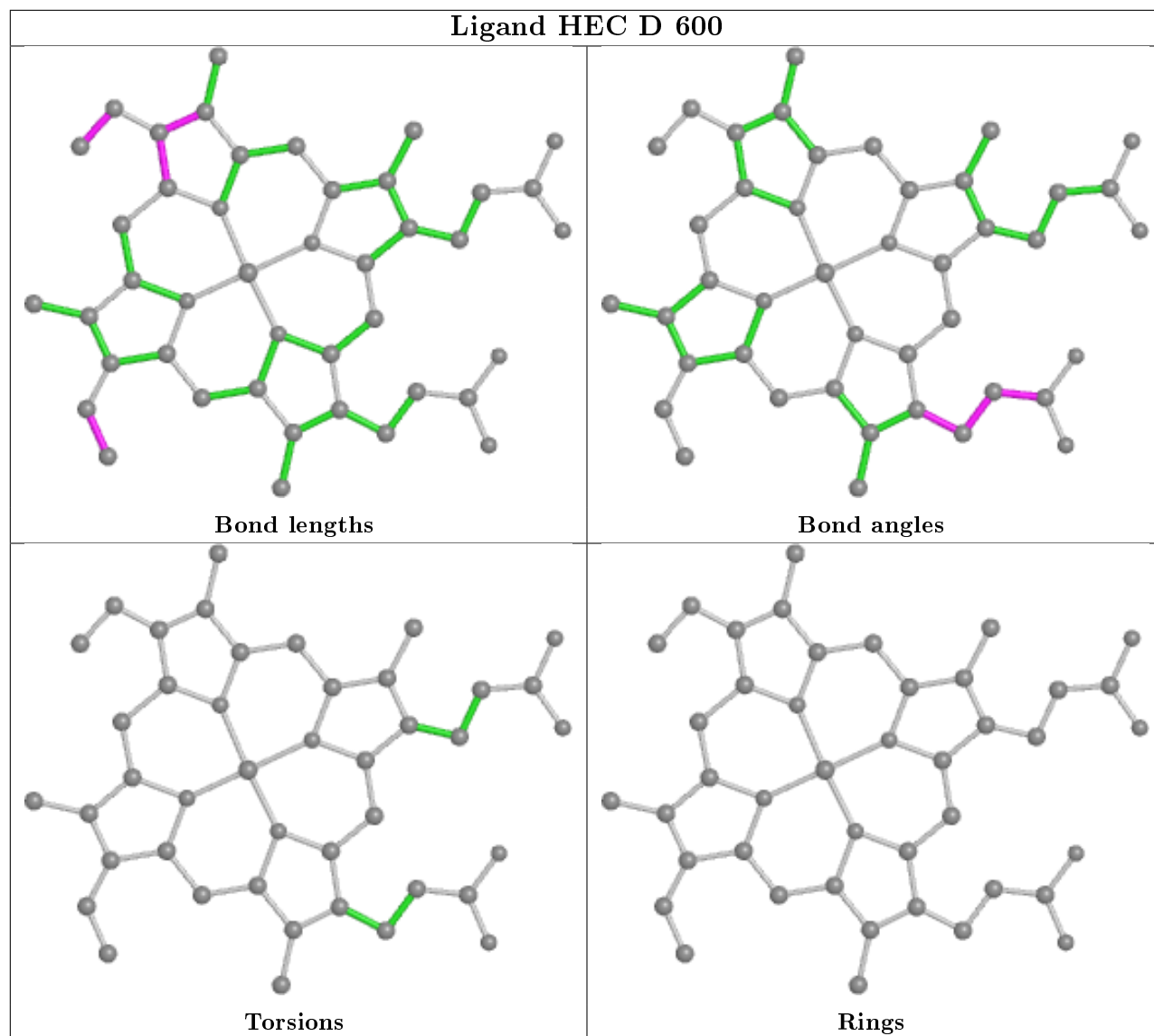


## Ligand HEC S 605

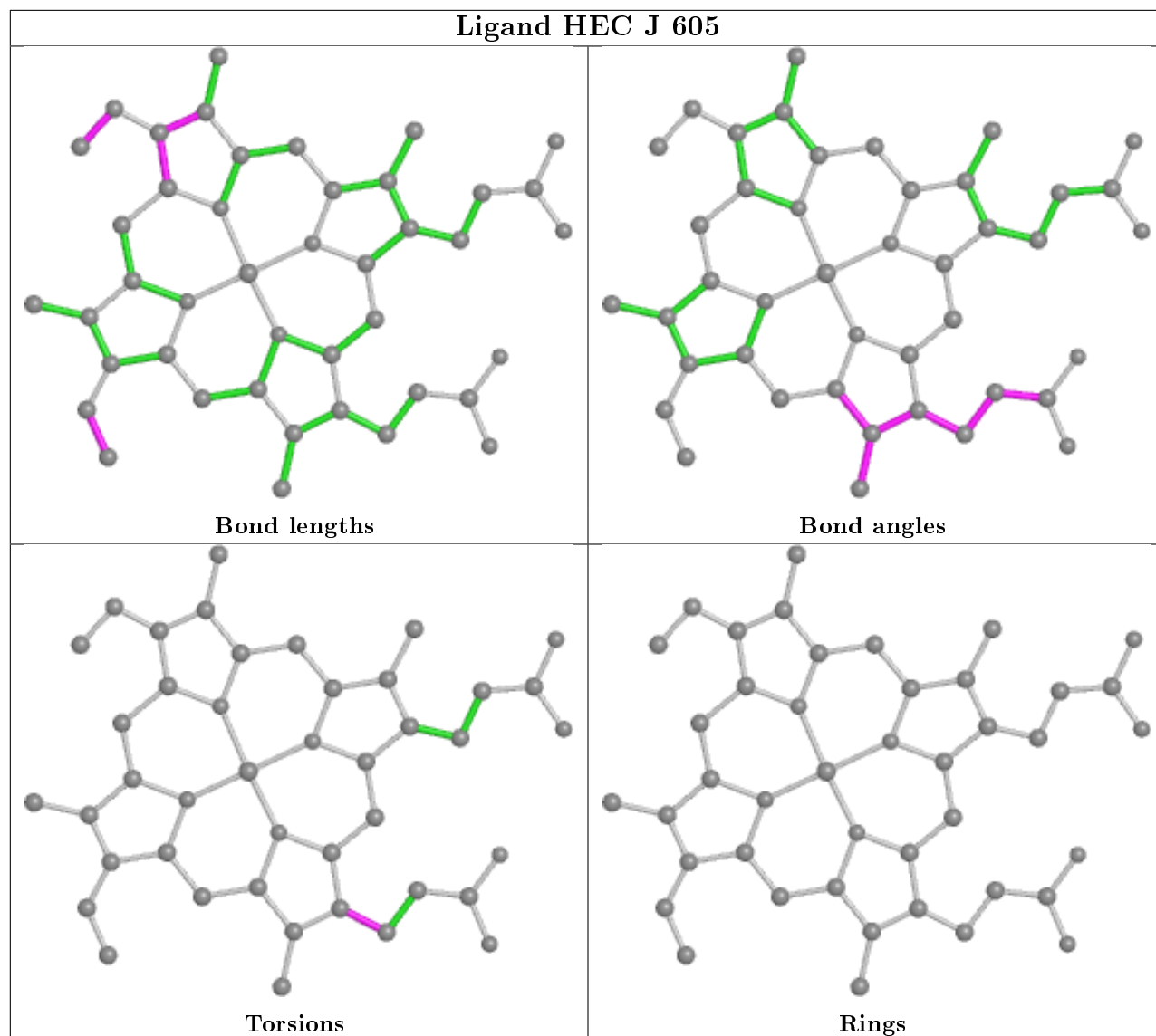




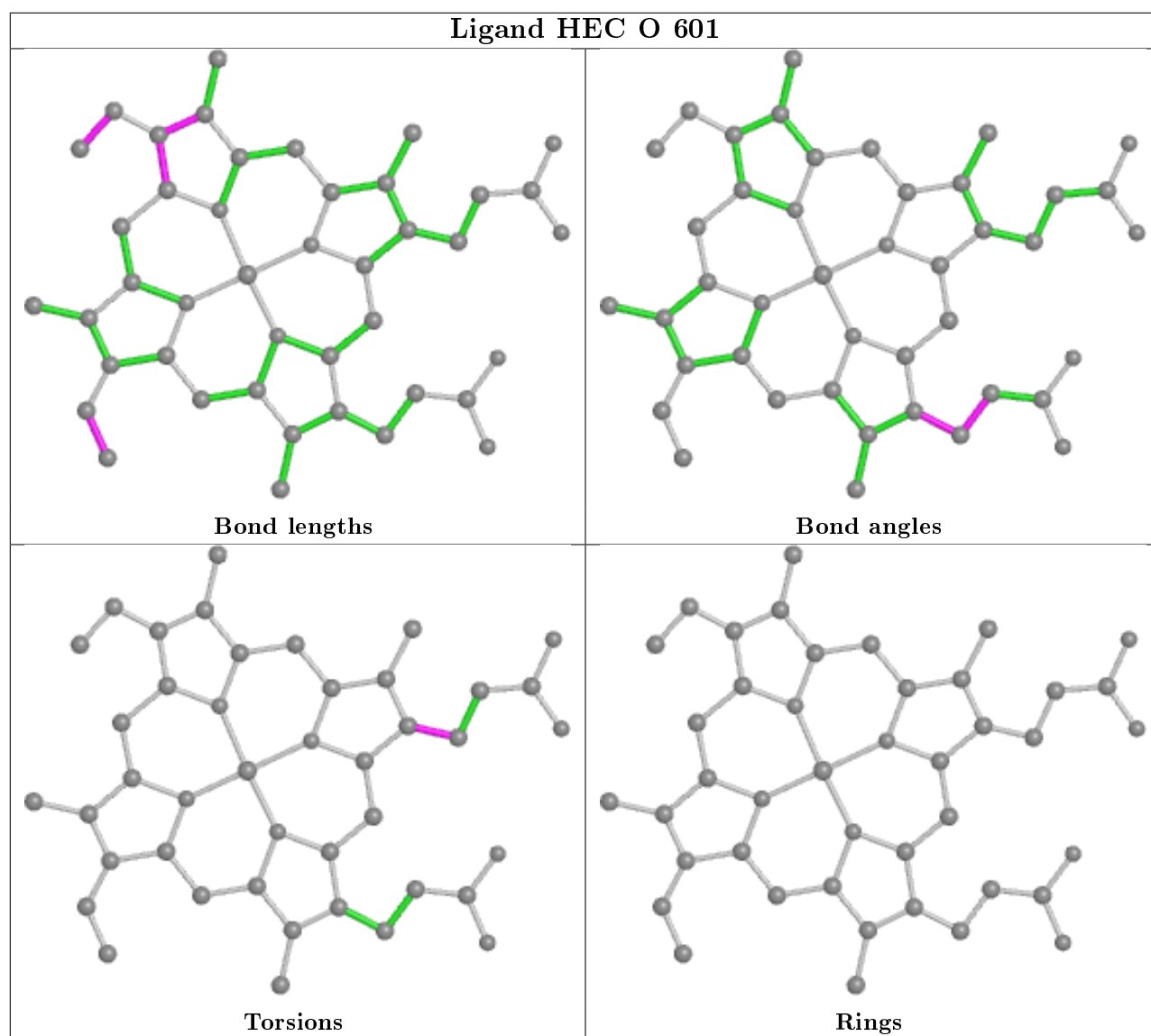




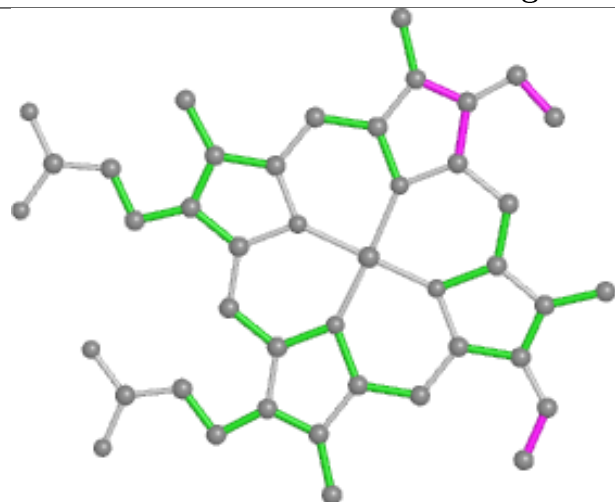
## Ligand HEC J 605



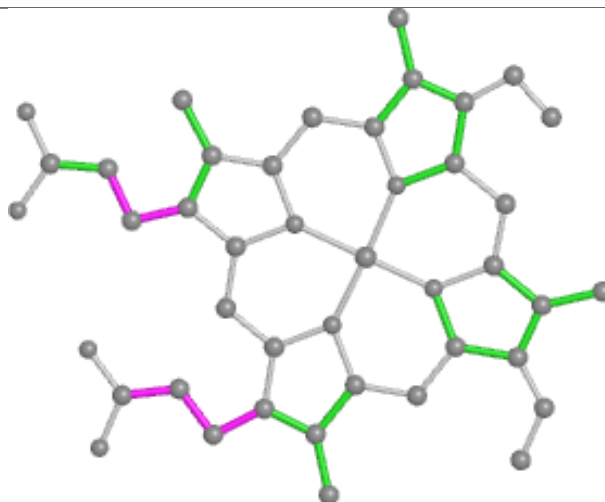




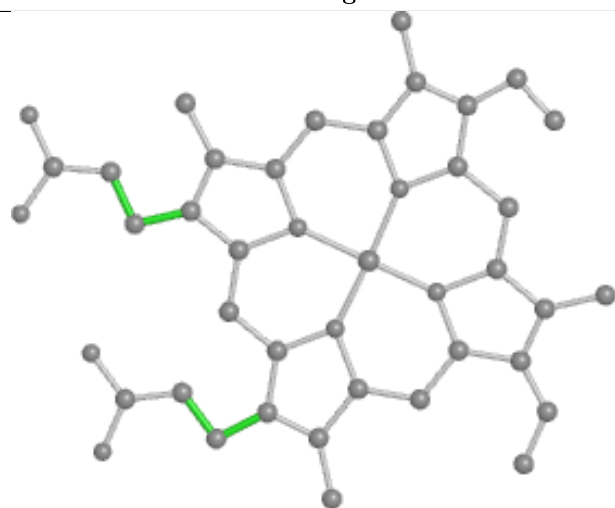
## Ligand HEC I 604



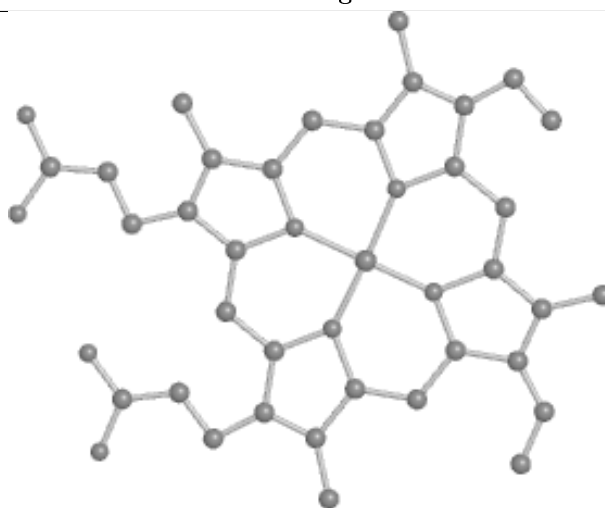
Bond lengths



Bond angles

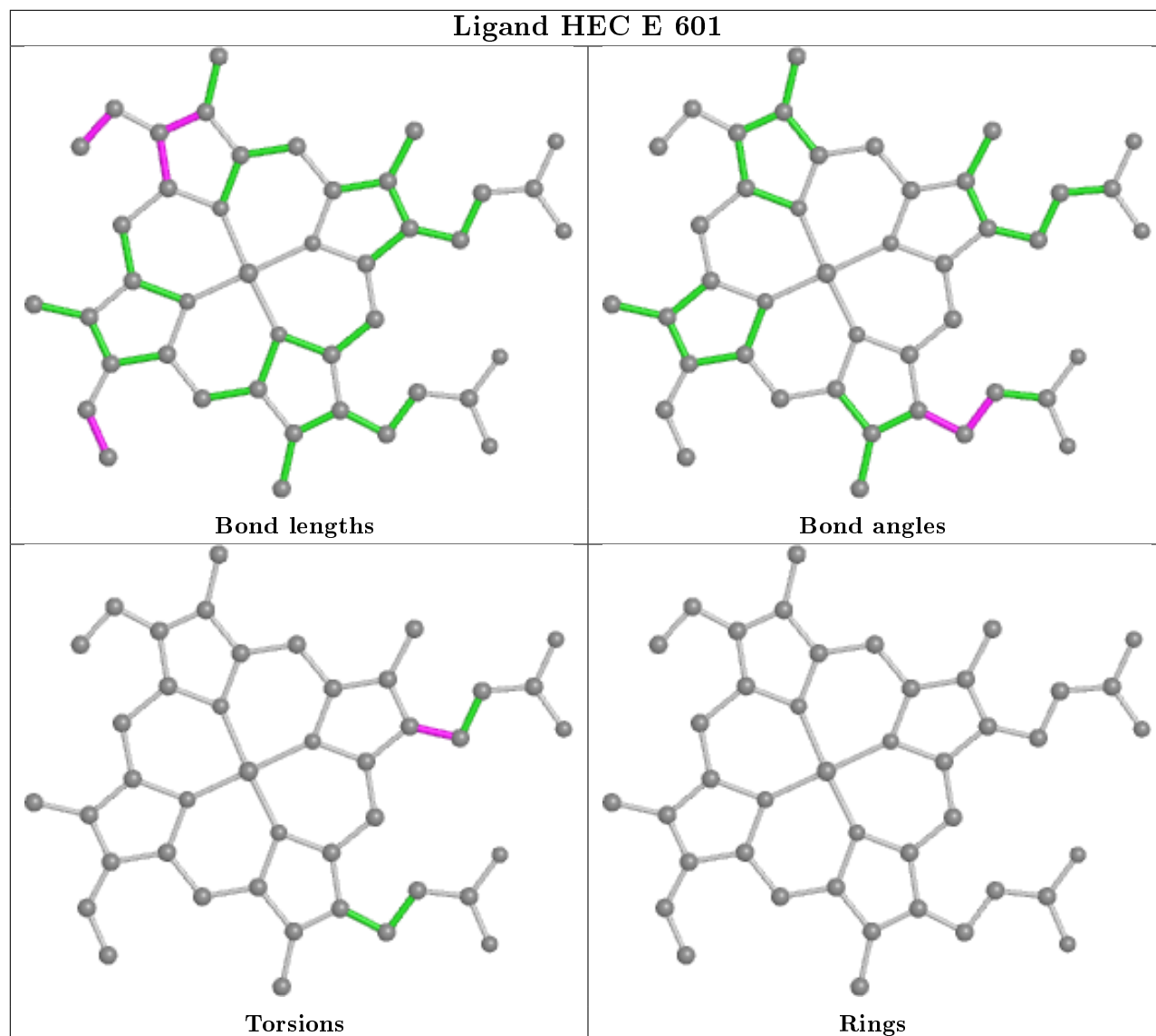


Torsions

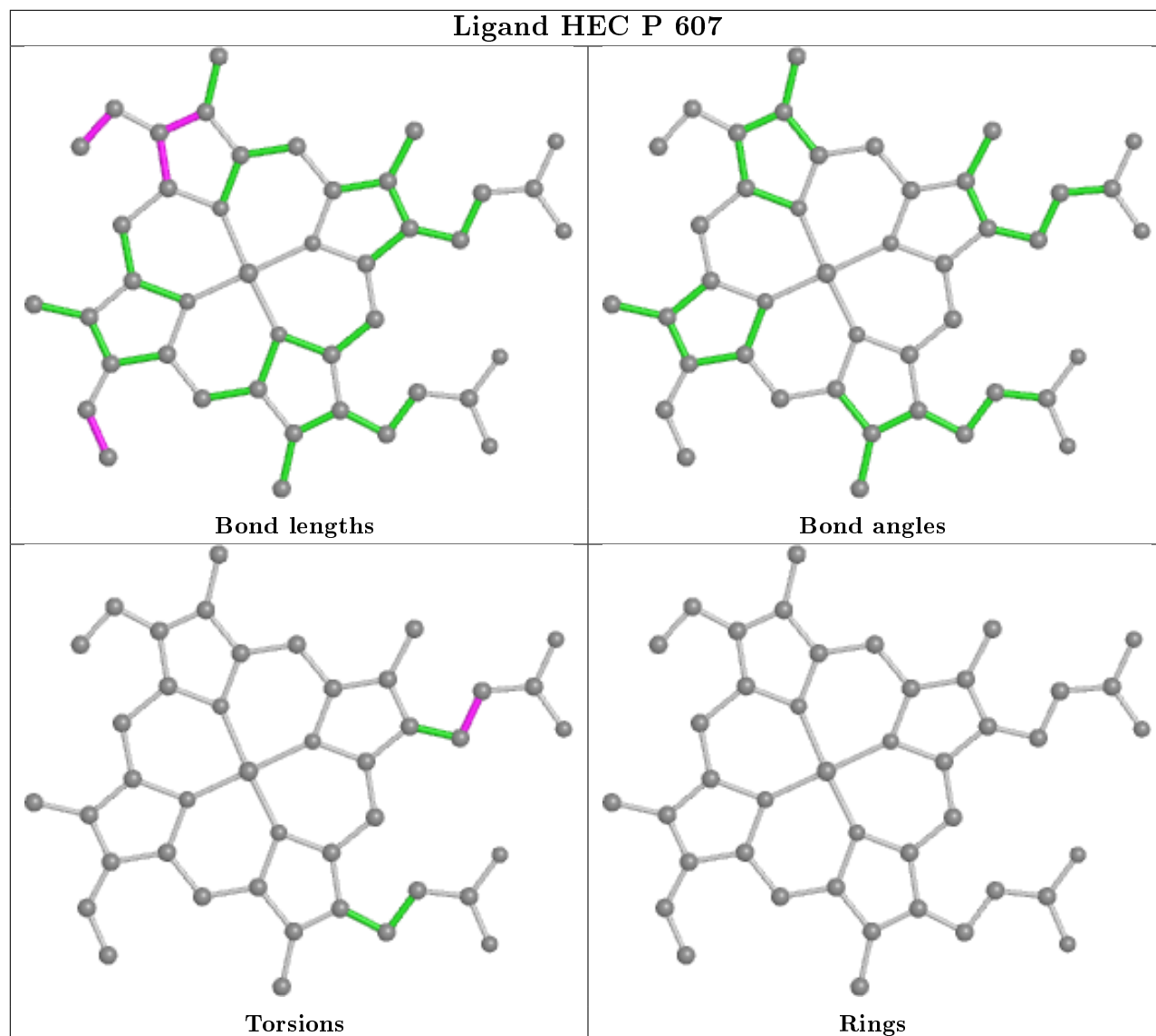


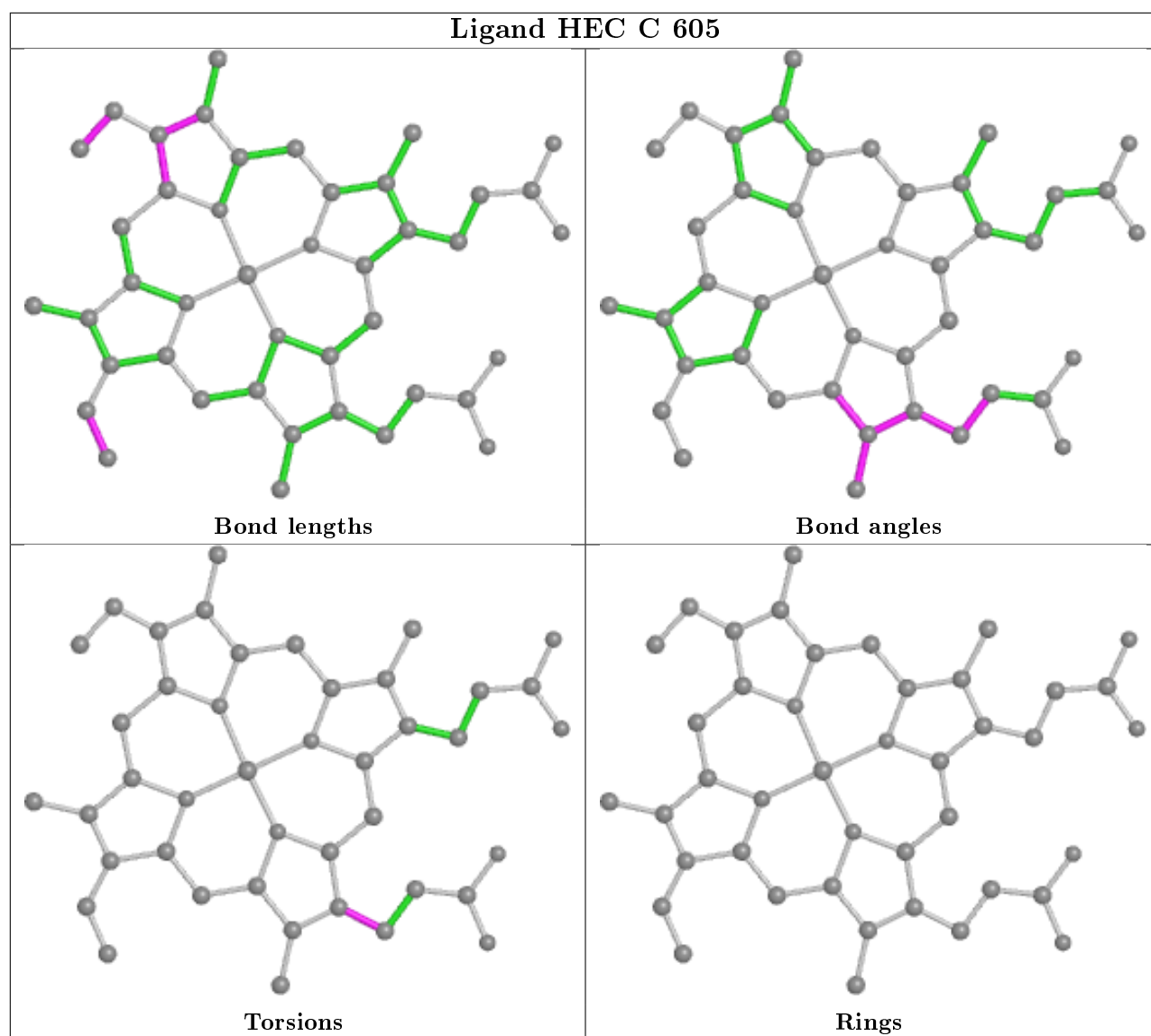
Rings

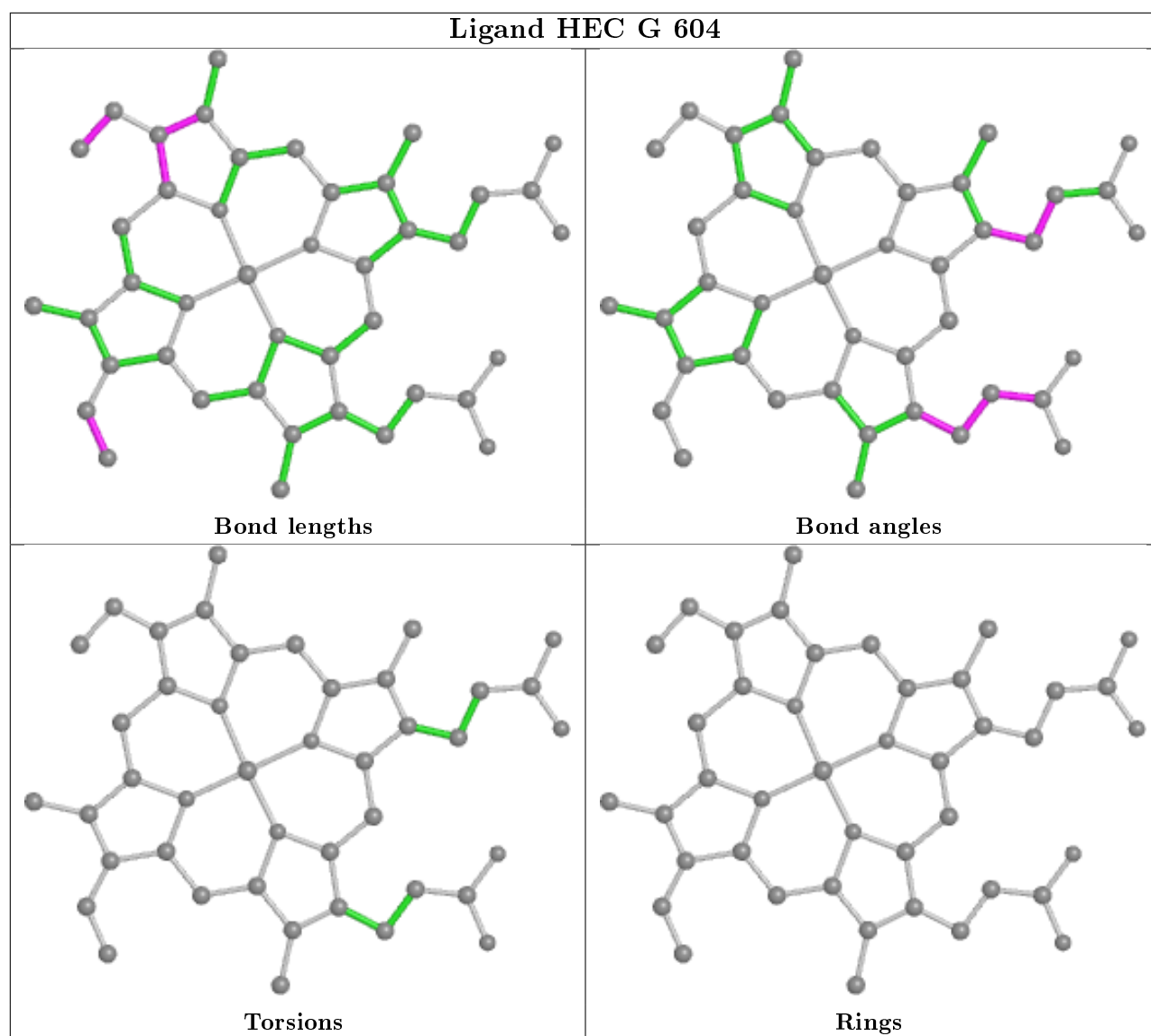
## Ligand HEC E 601

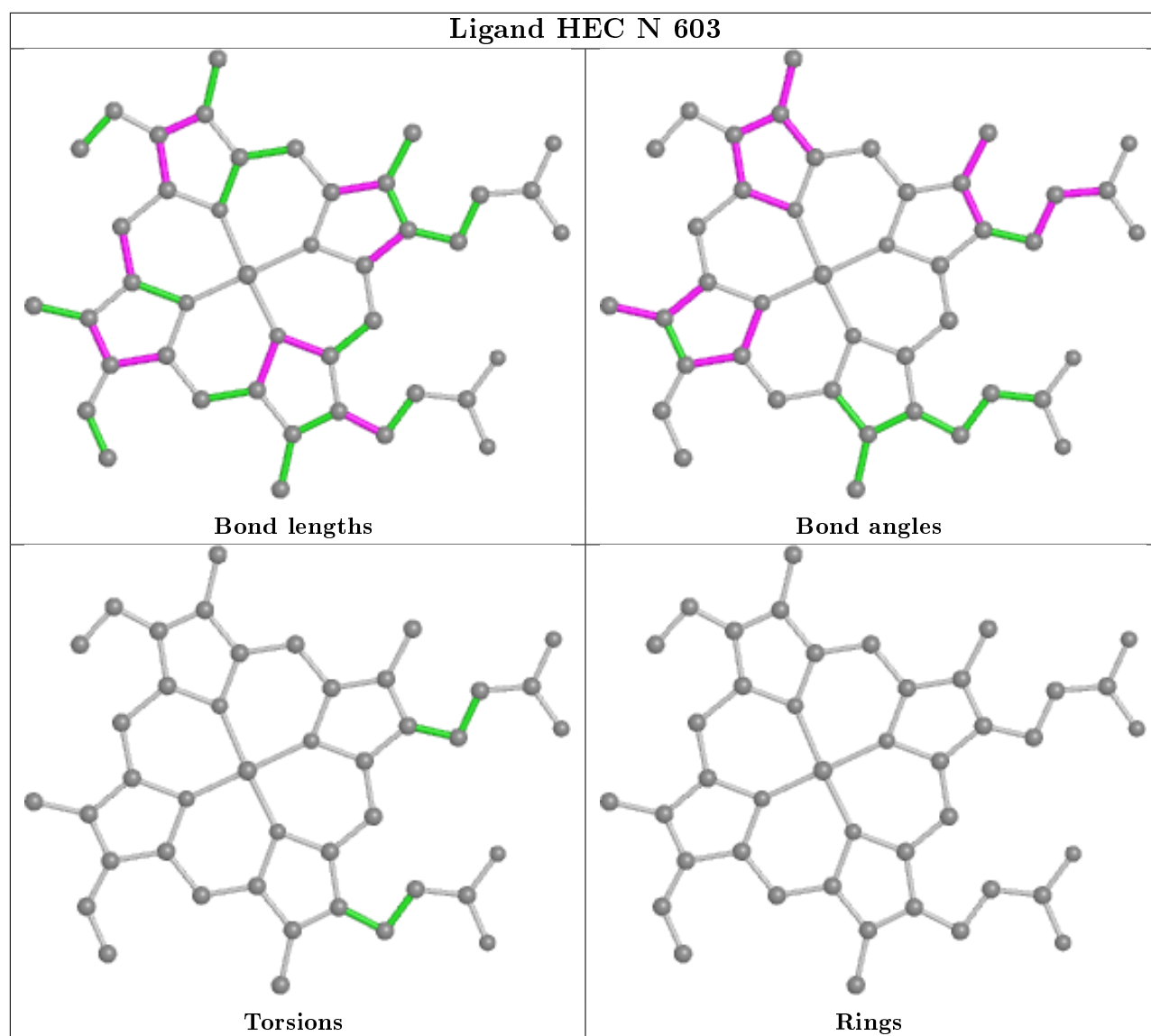


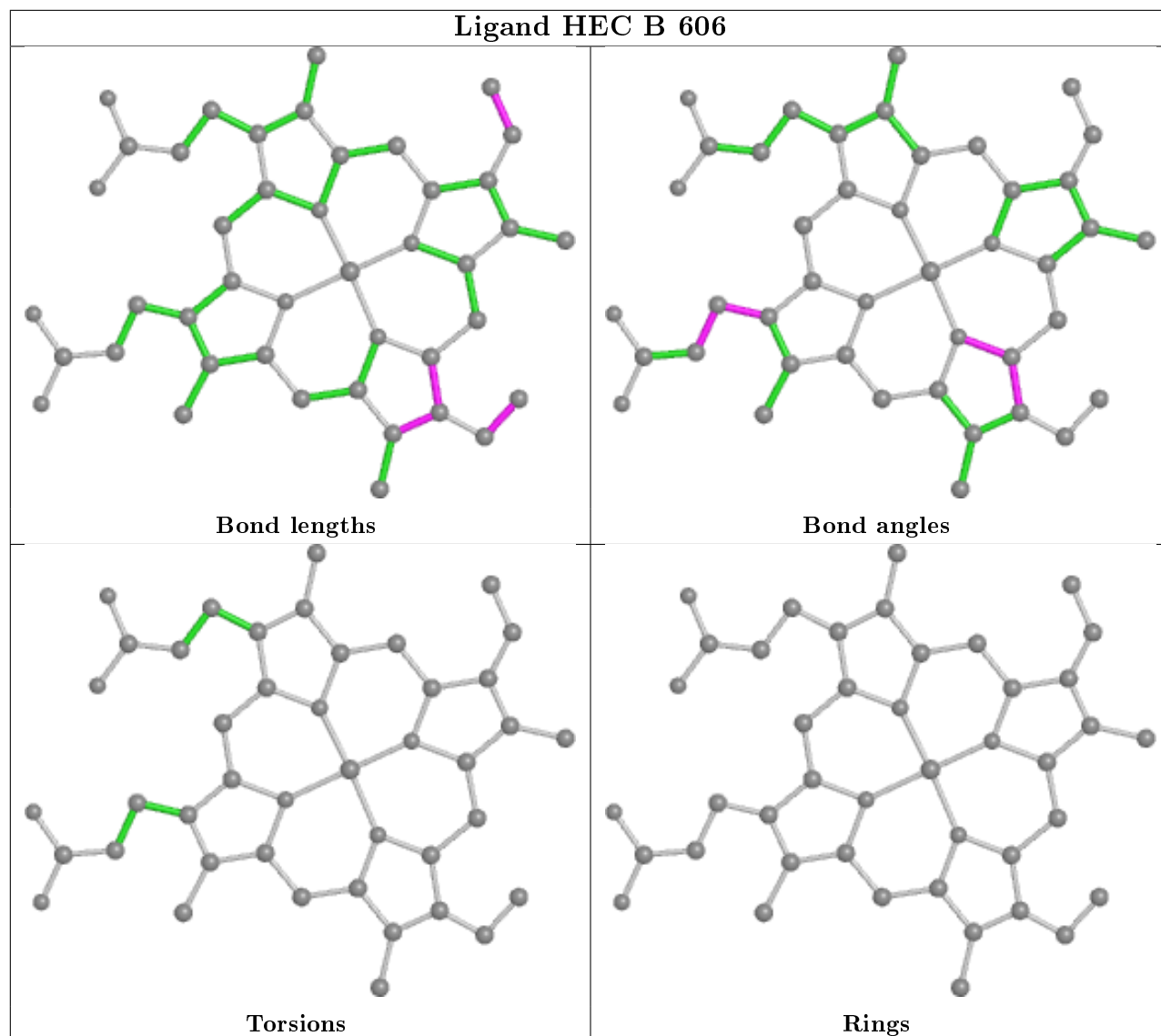
## Ligand HEC P 607



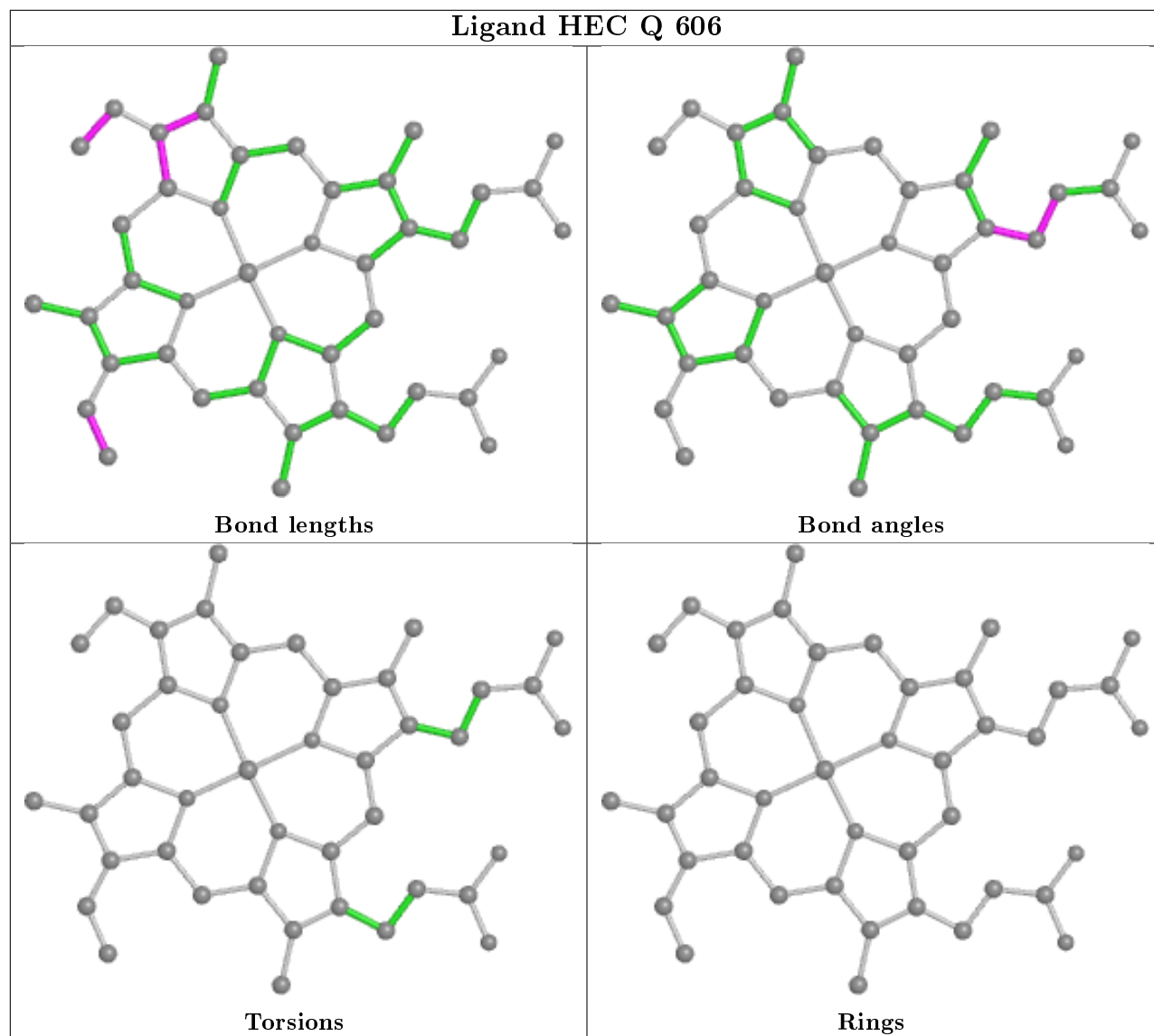


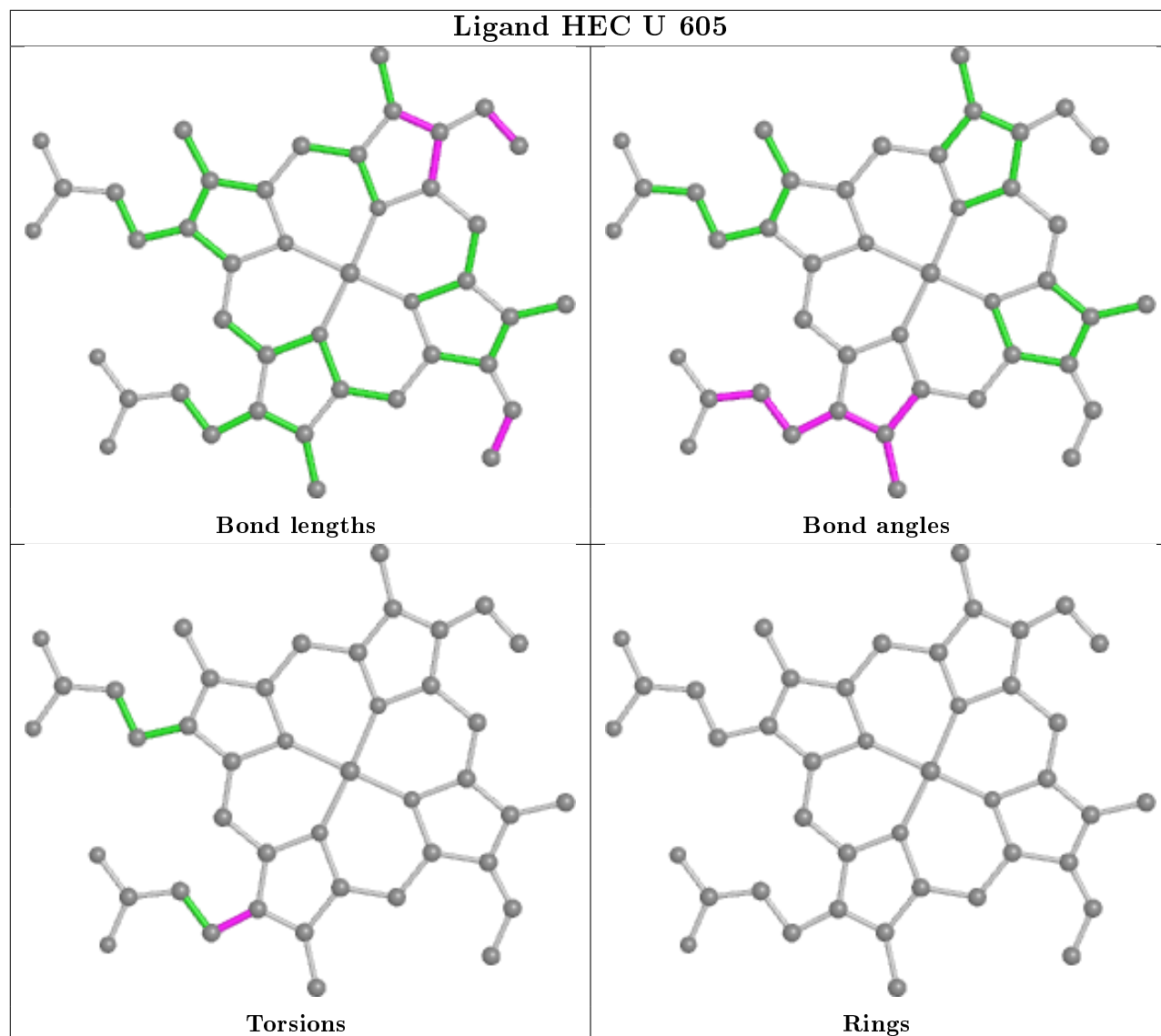




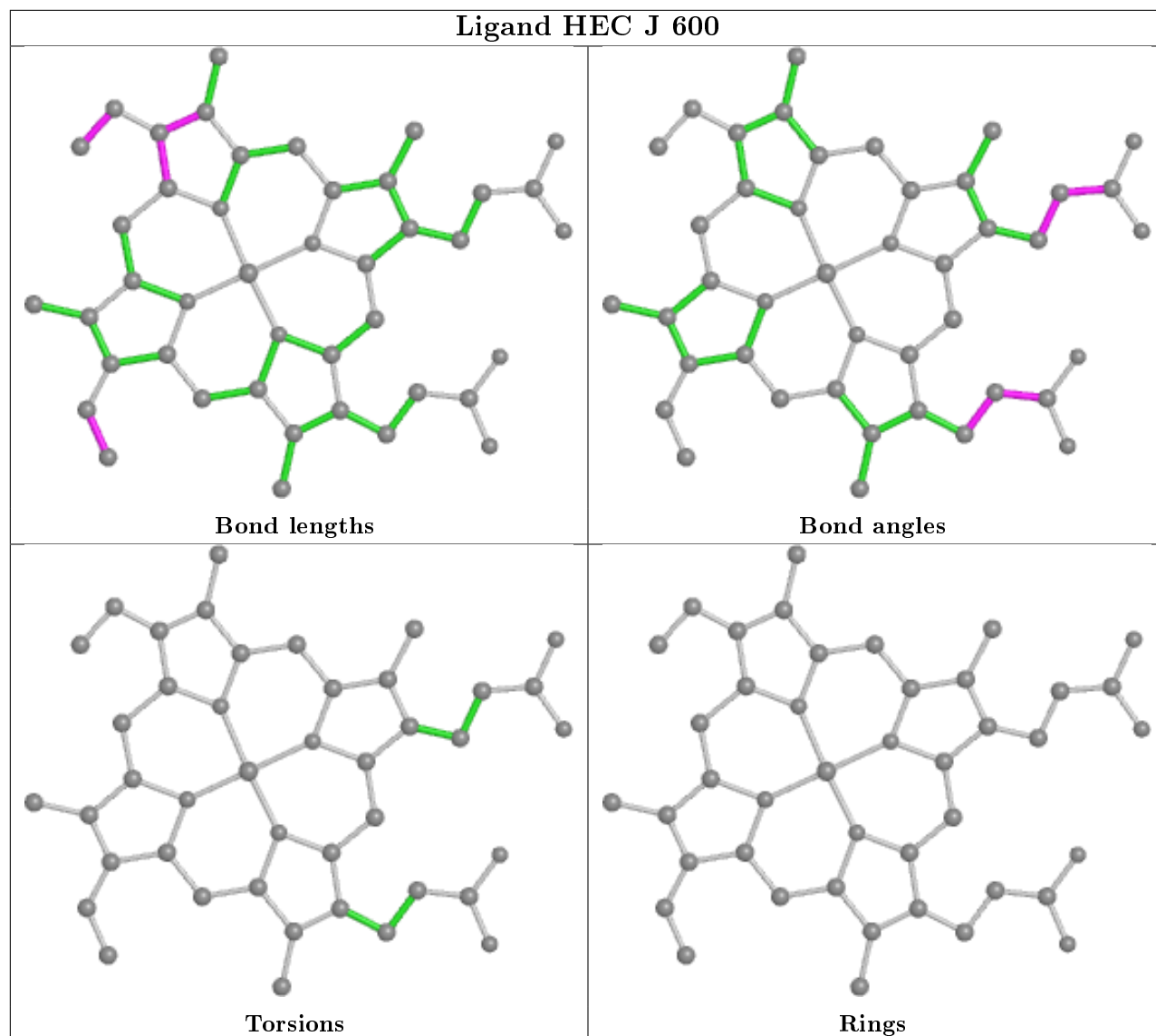




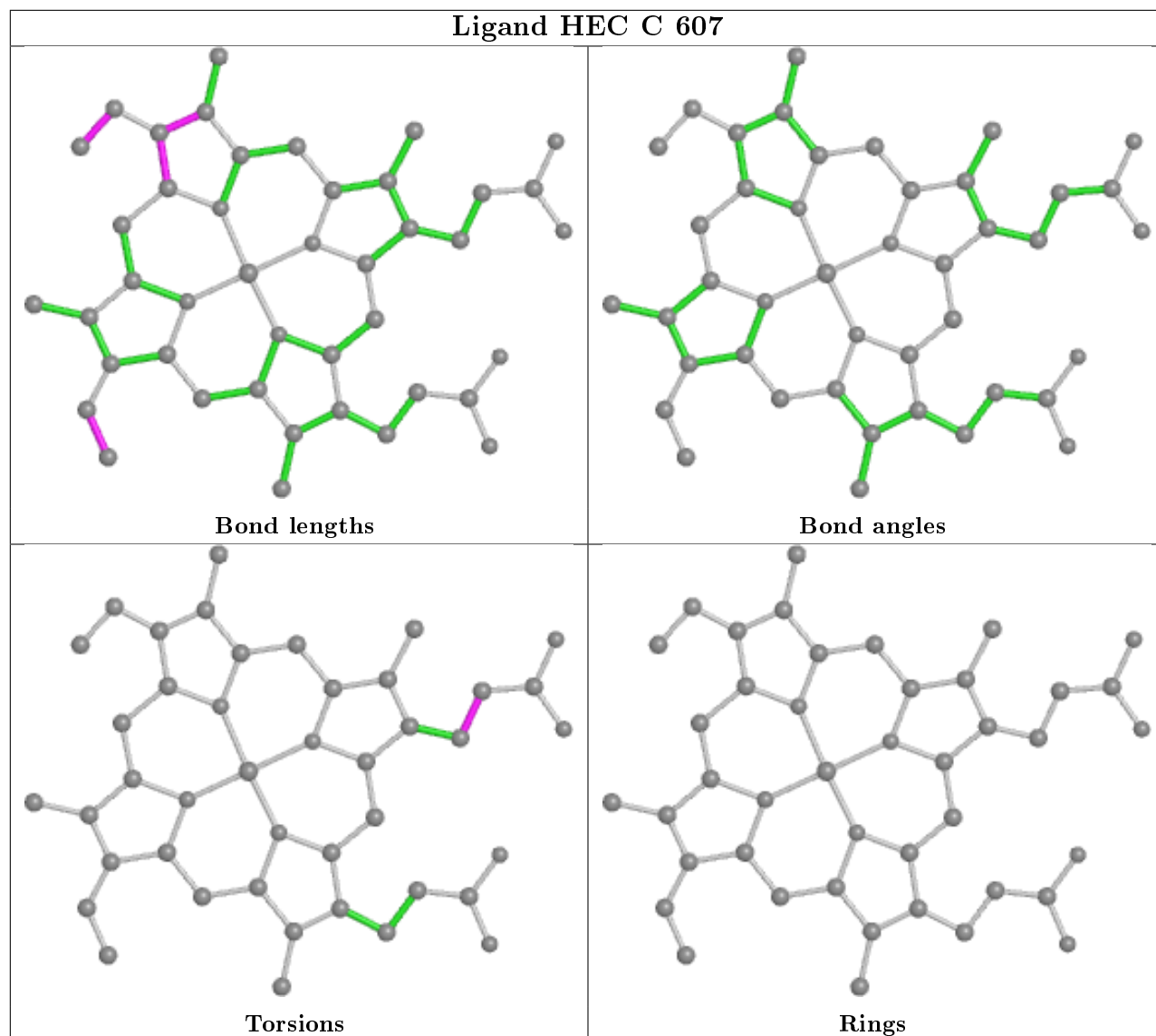




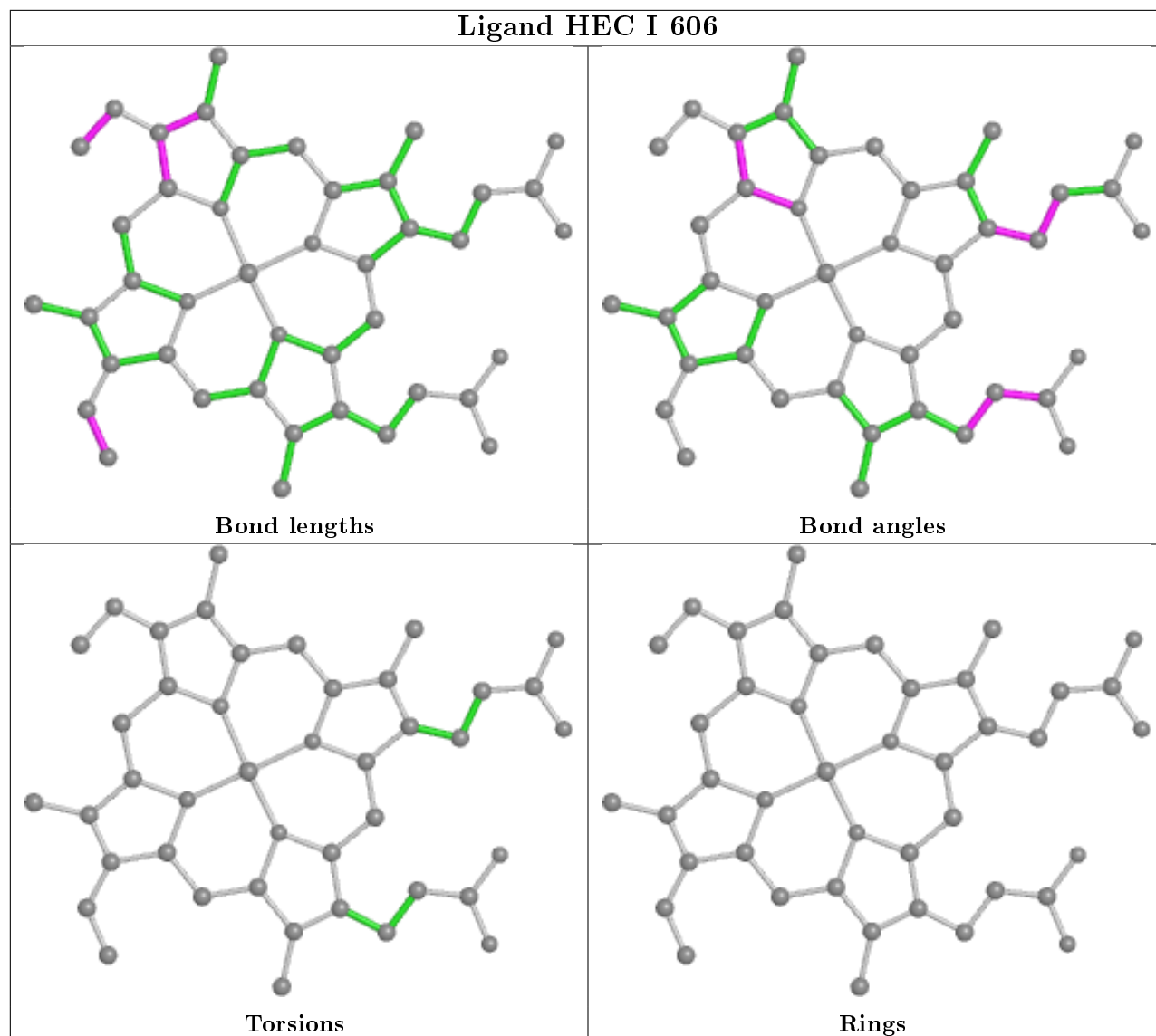
## Ligand HEC J 600

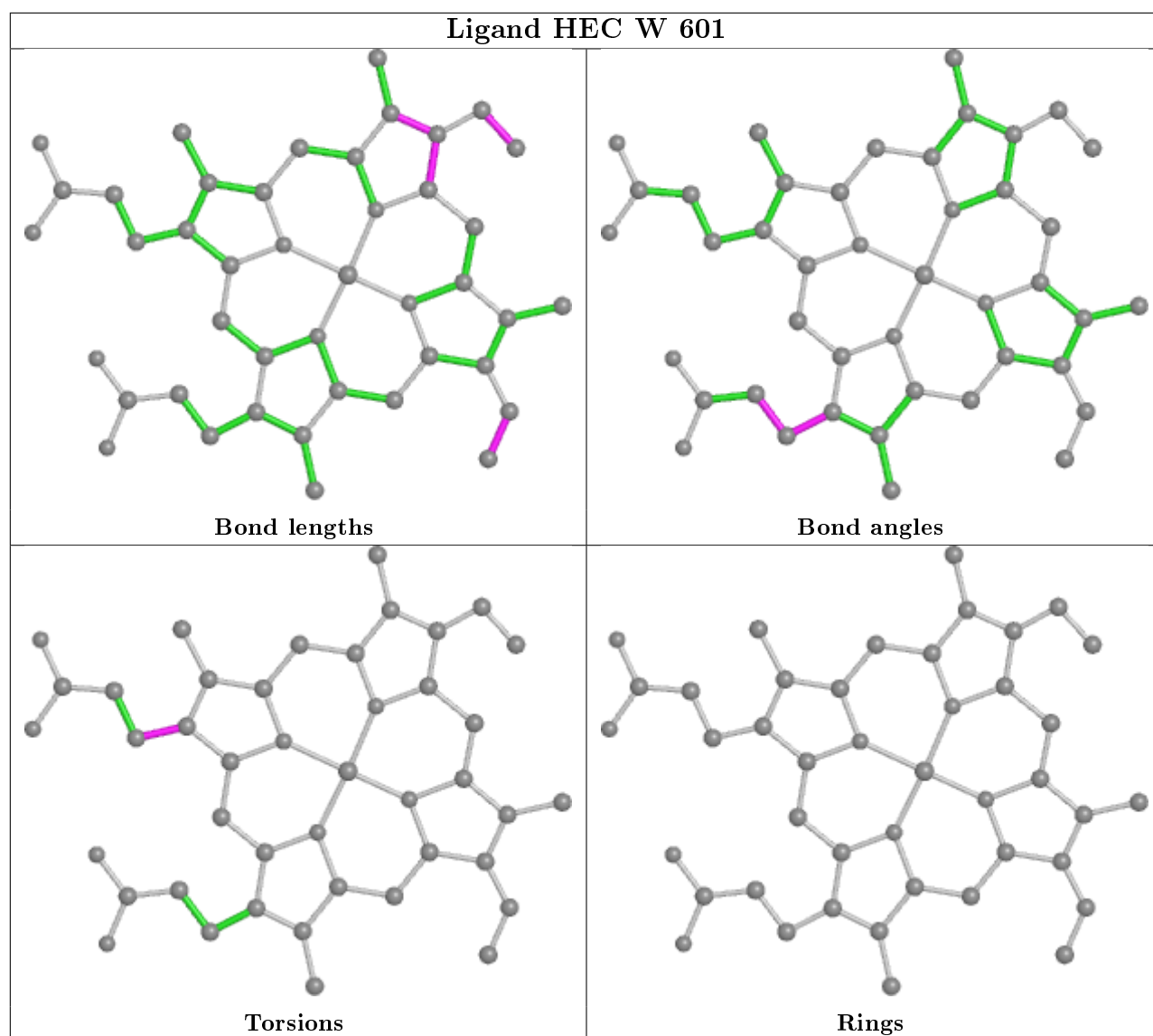


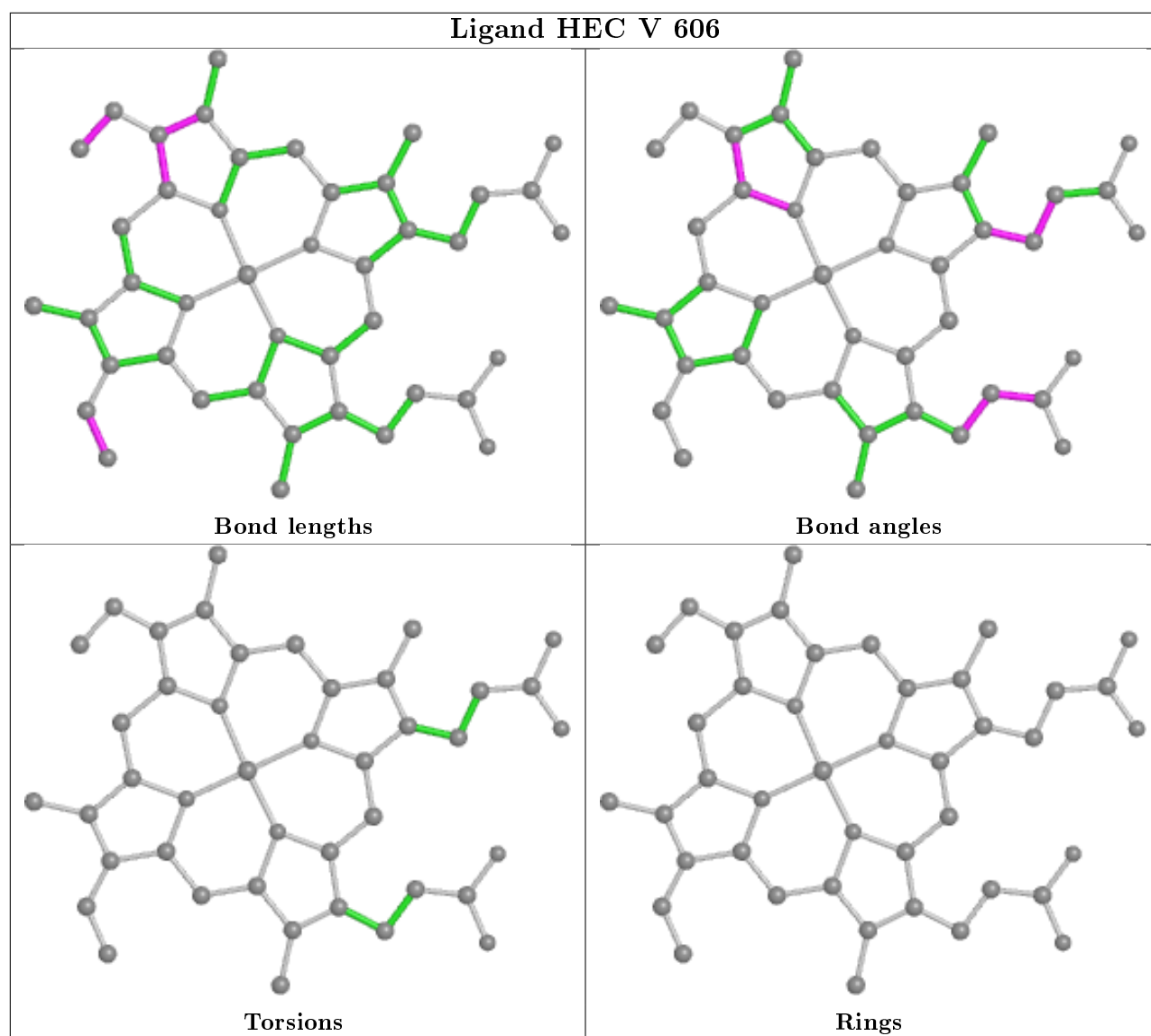
## Ligand HEC C 607

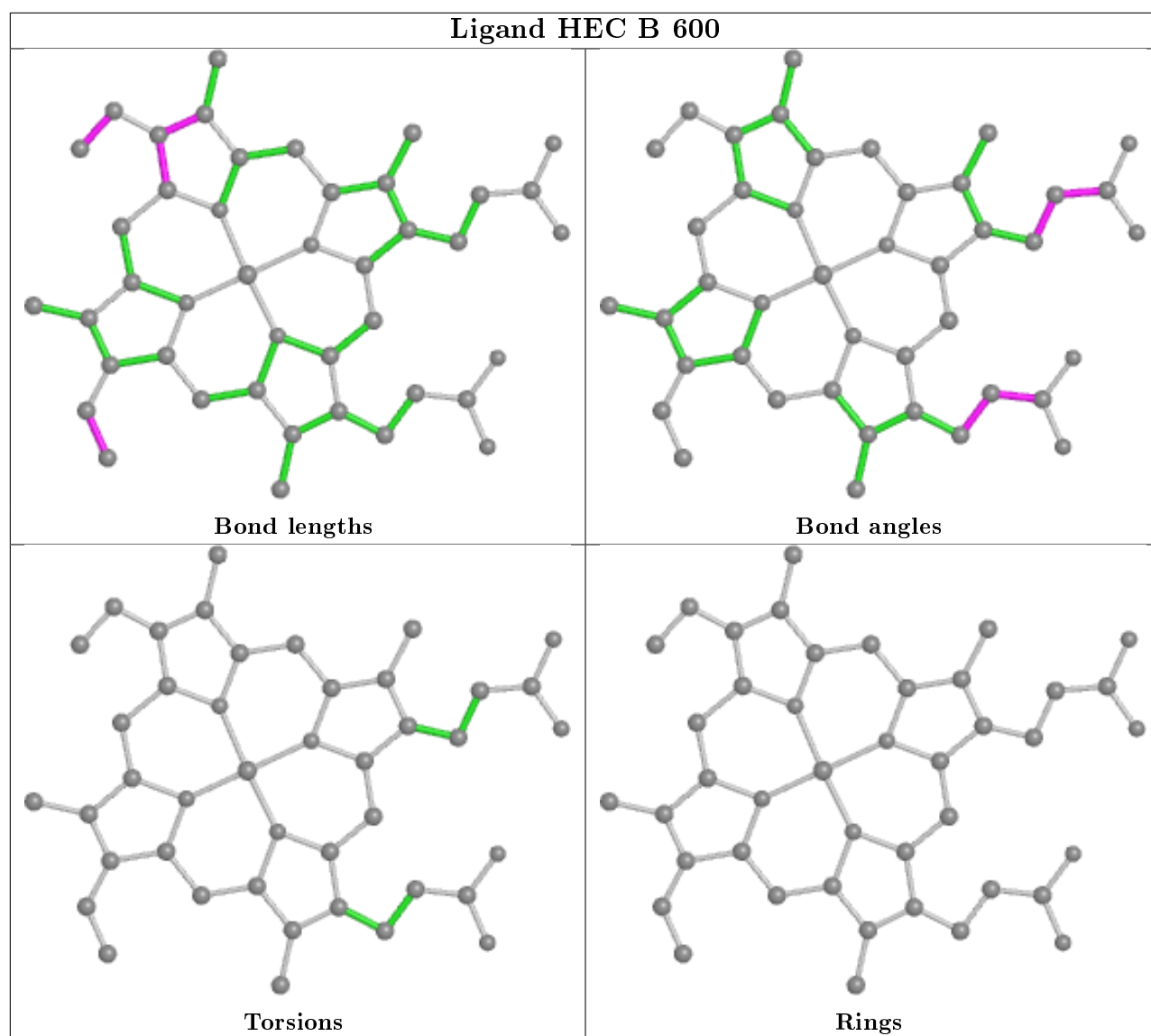


## Ligand HEC I 606

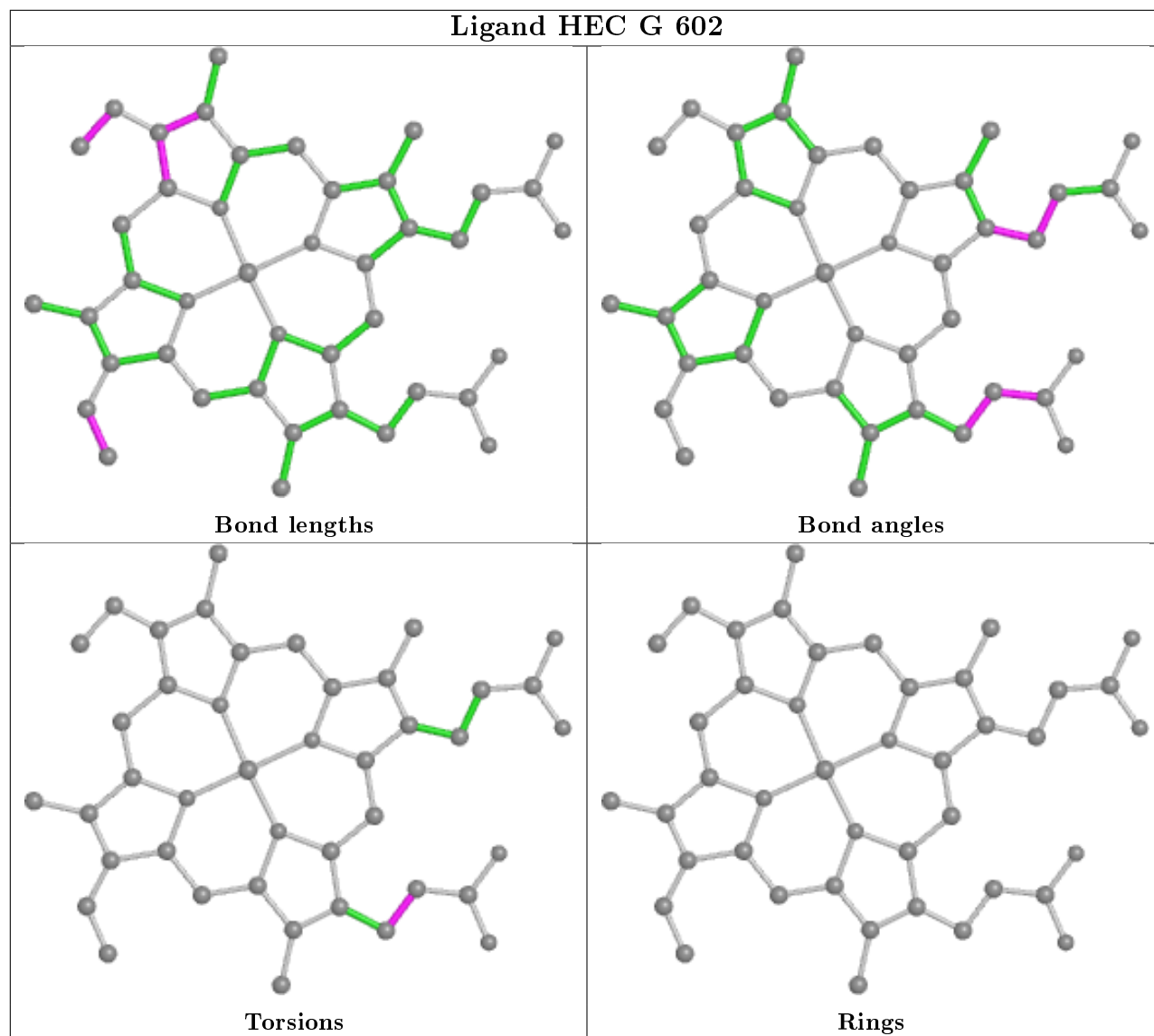


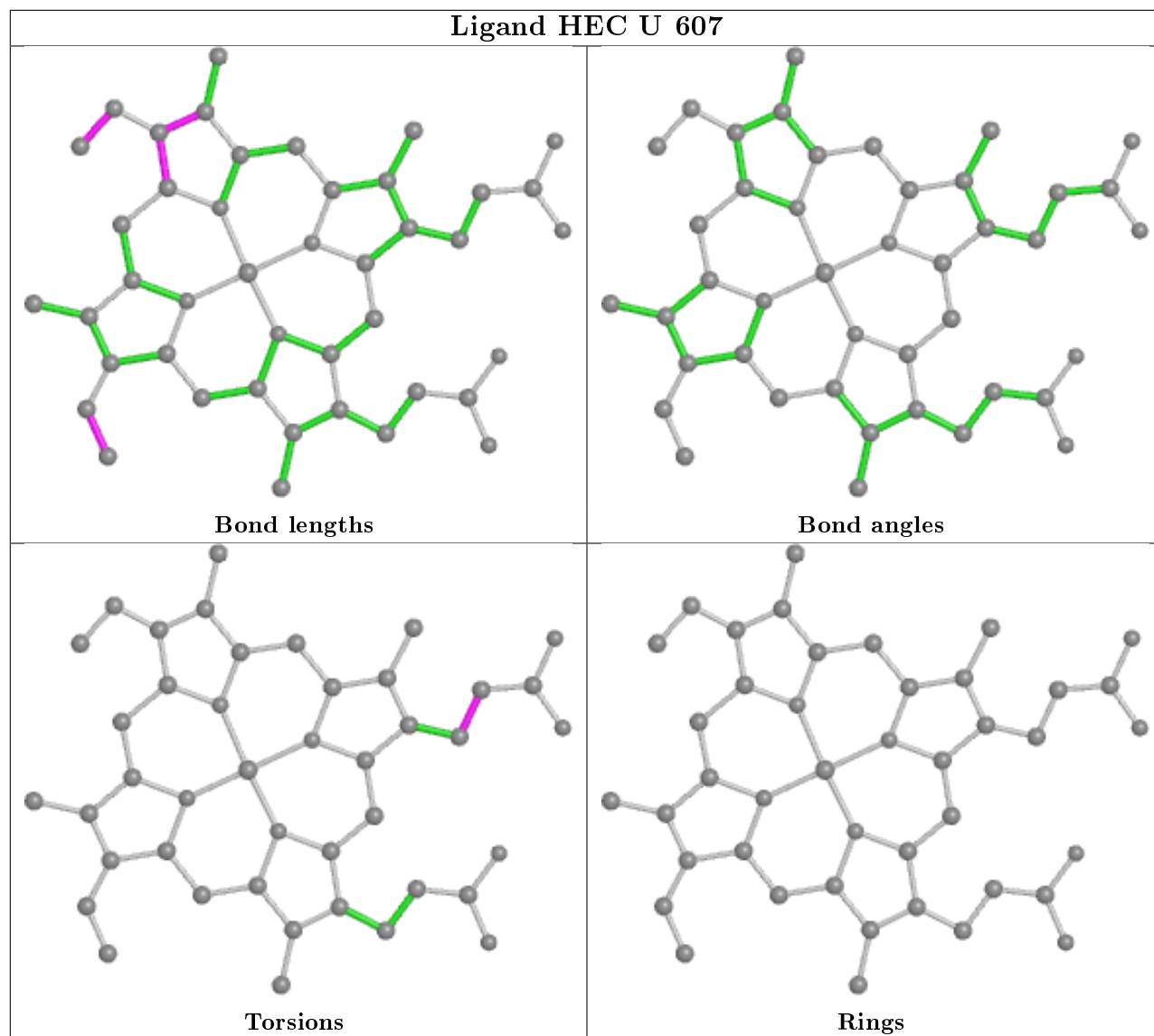


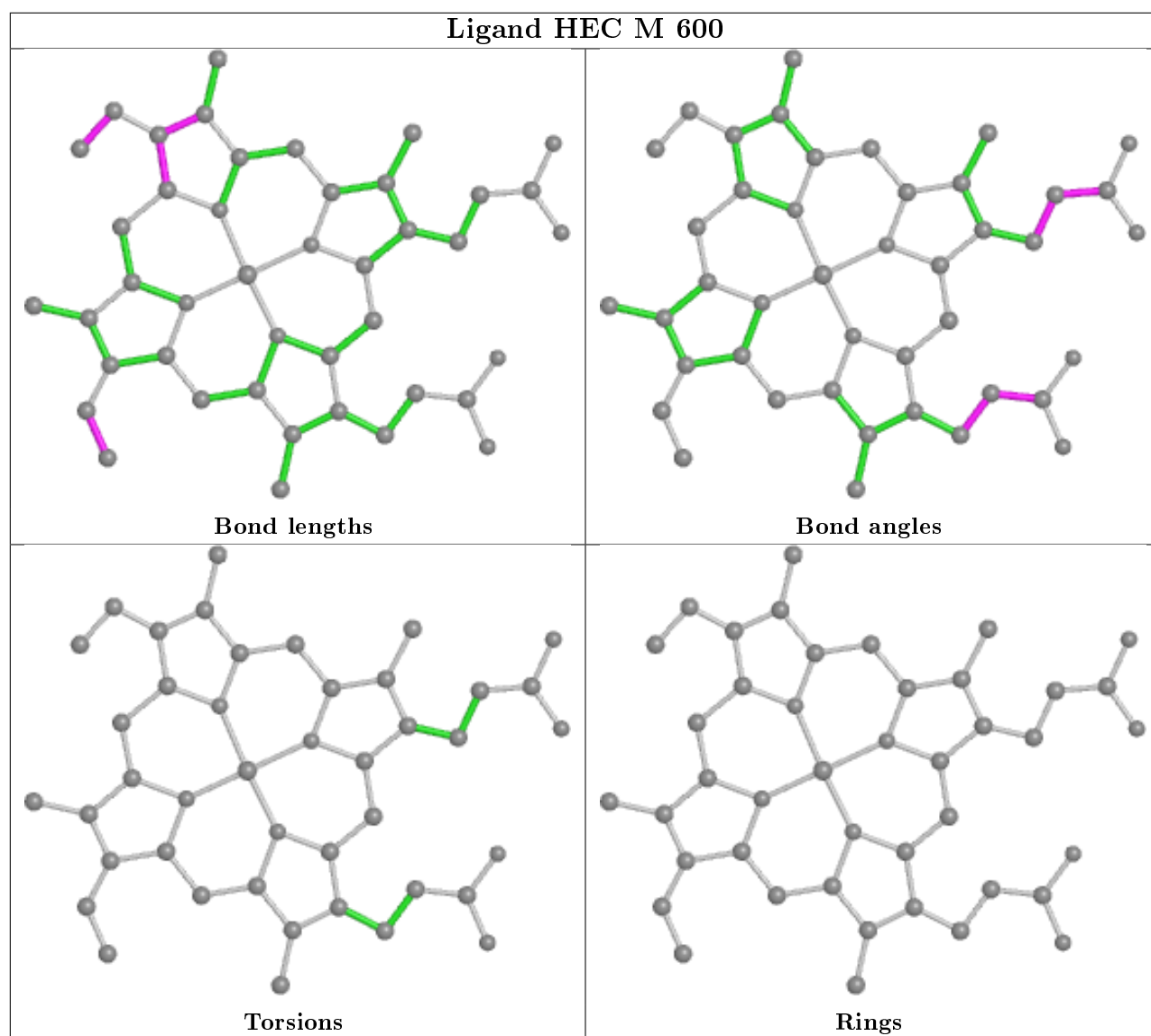




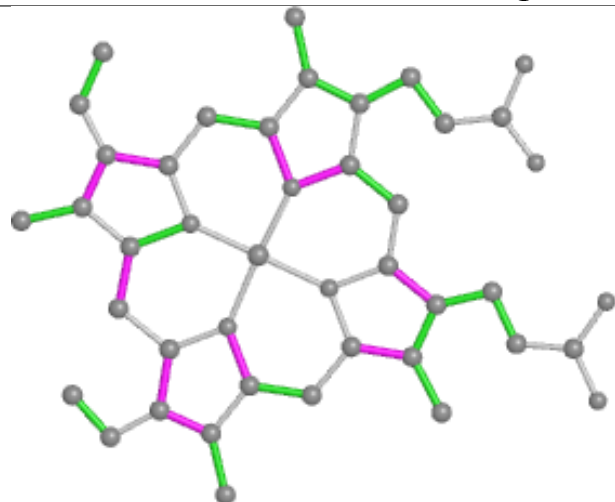




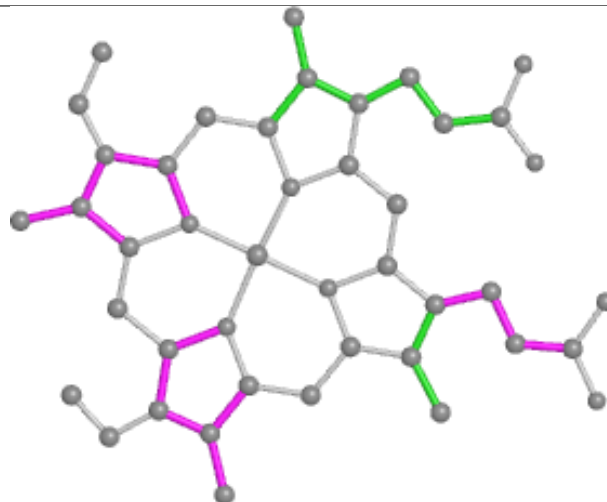




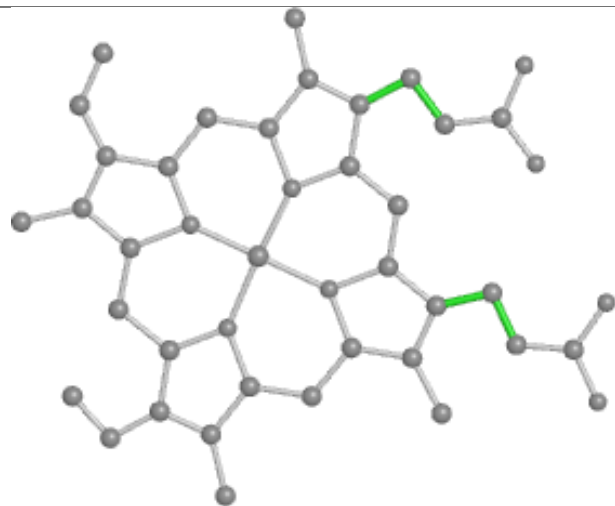
## Ligand HEC T 603



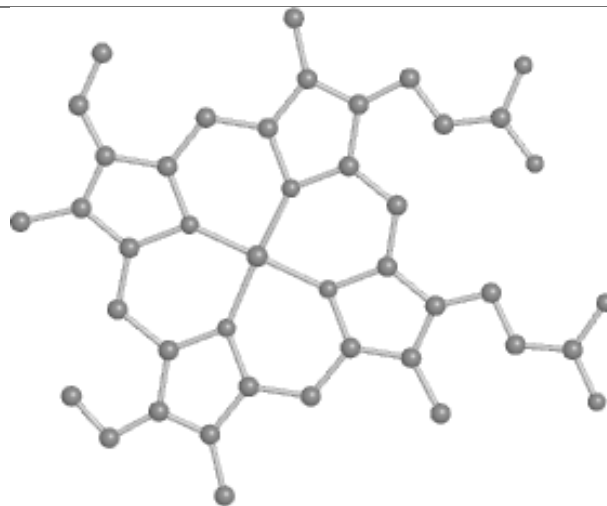
Bond lengths



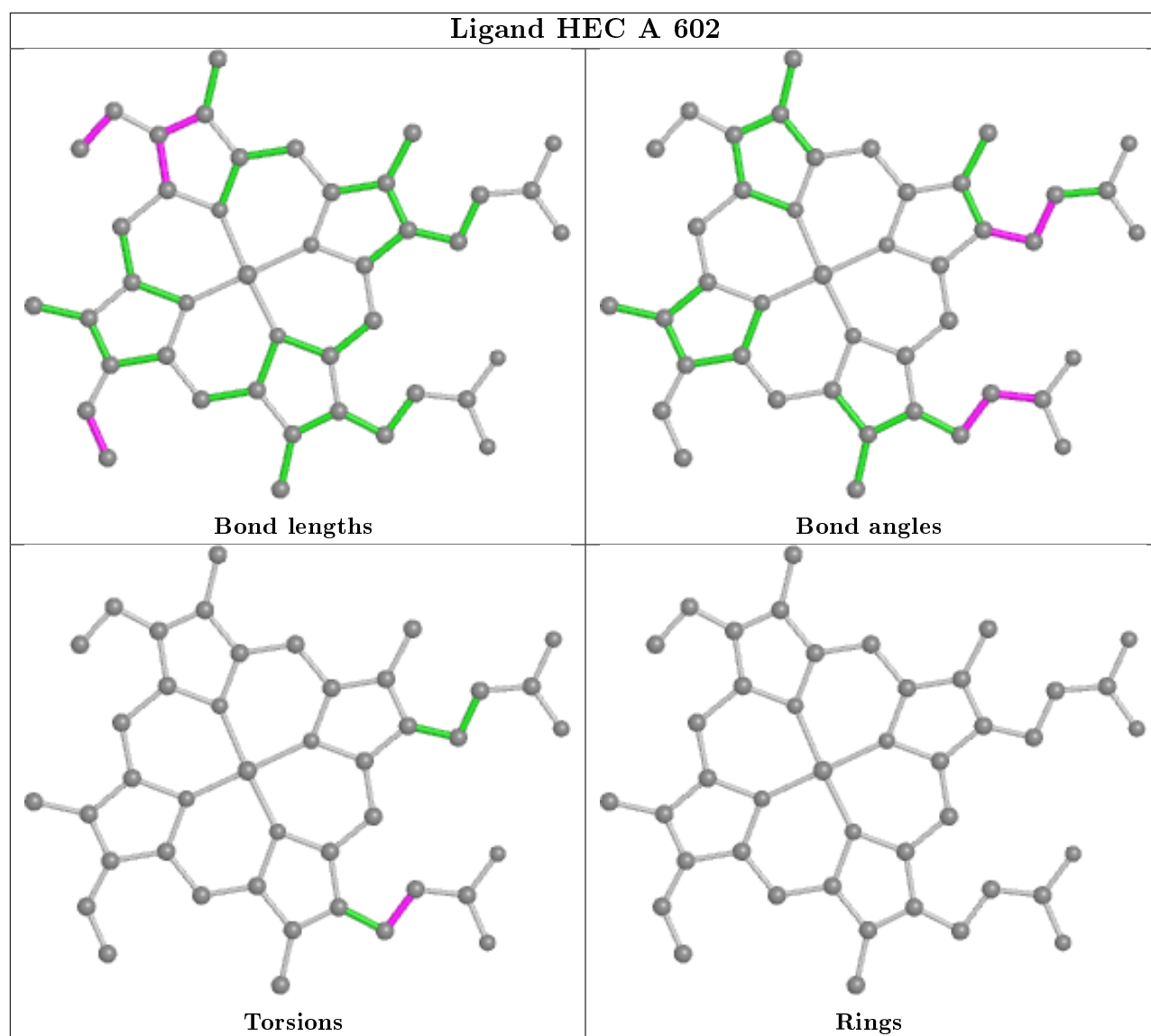
Bond angles



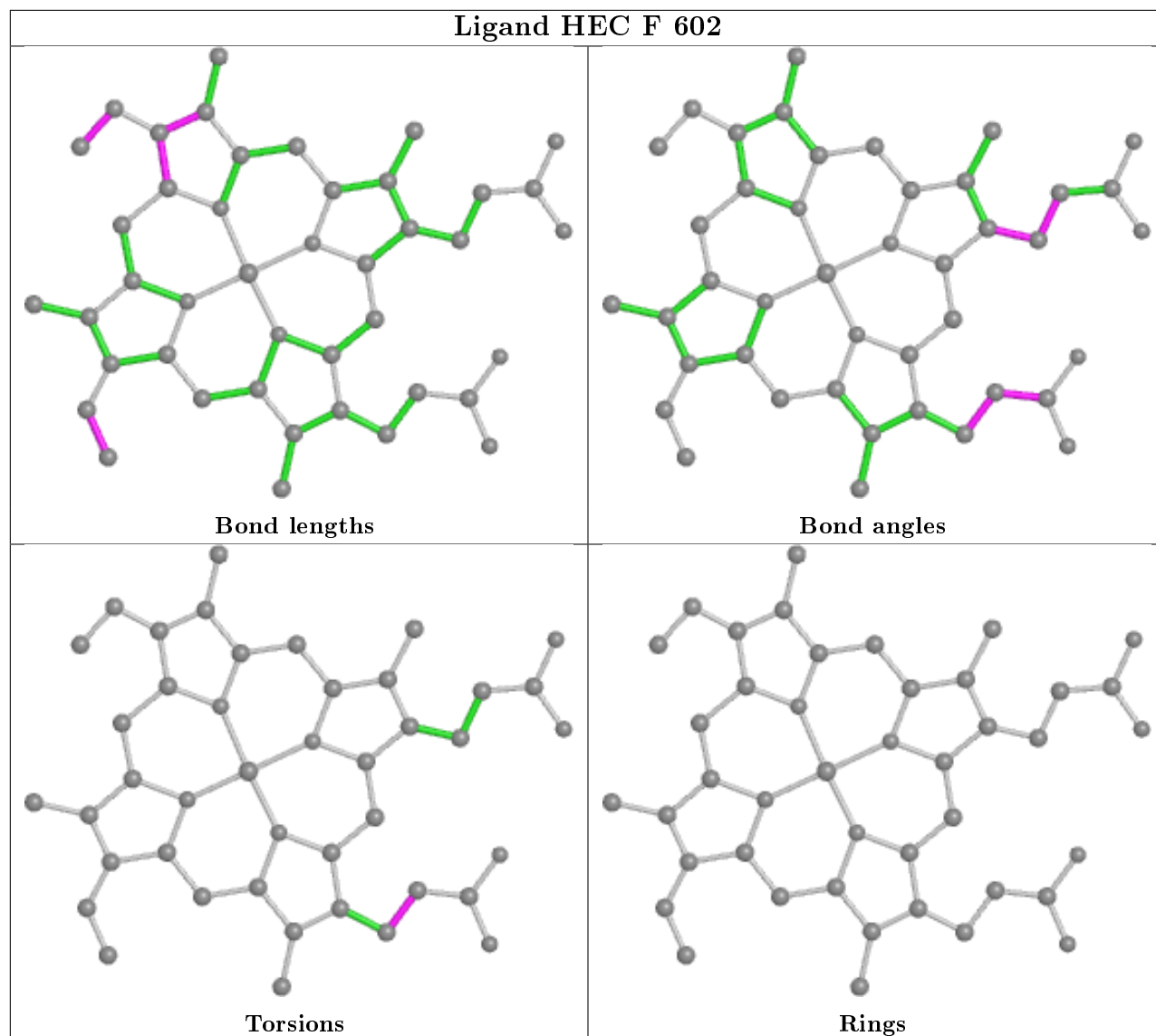
Torsions

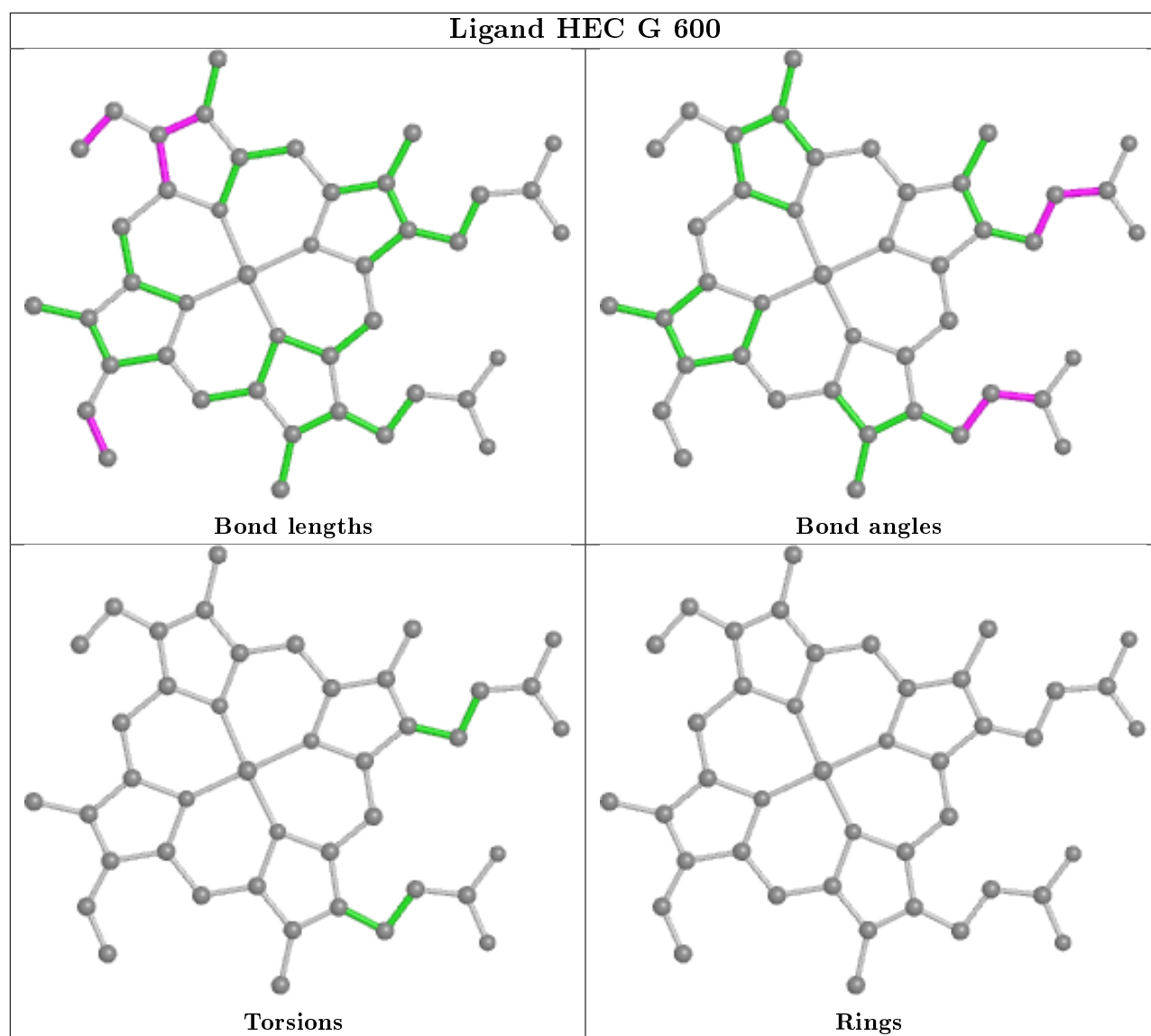


Rings

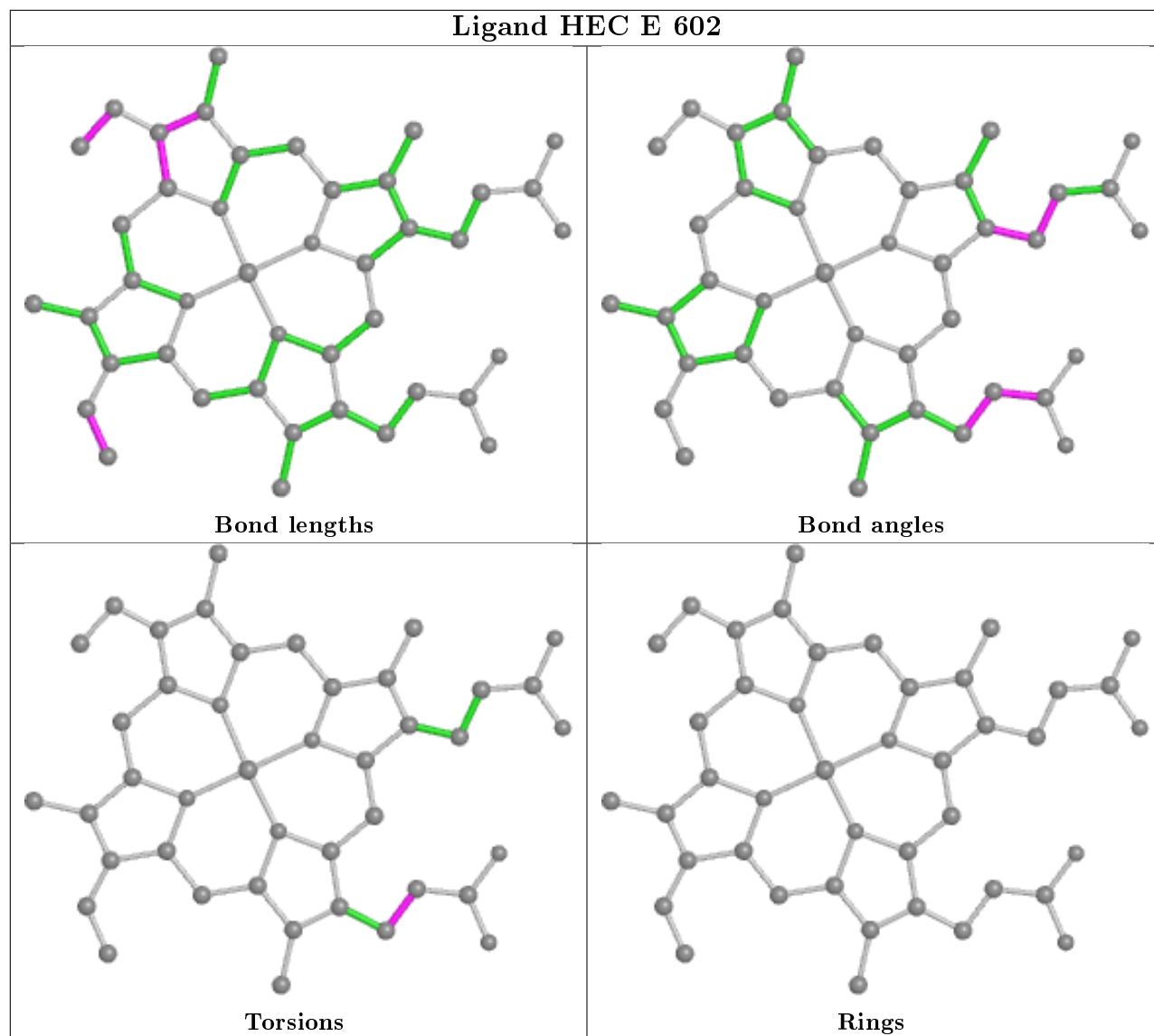


## Ligand HEC F 602



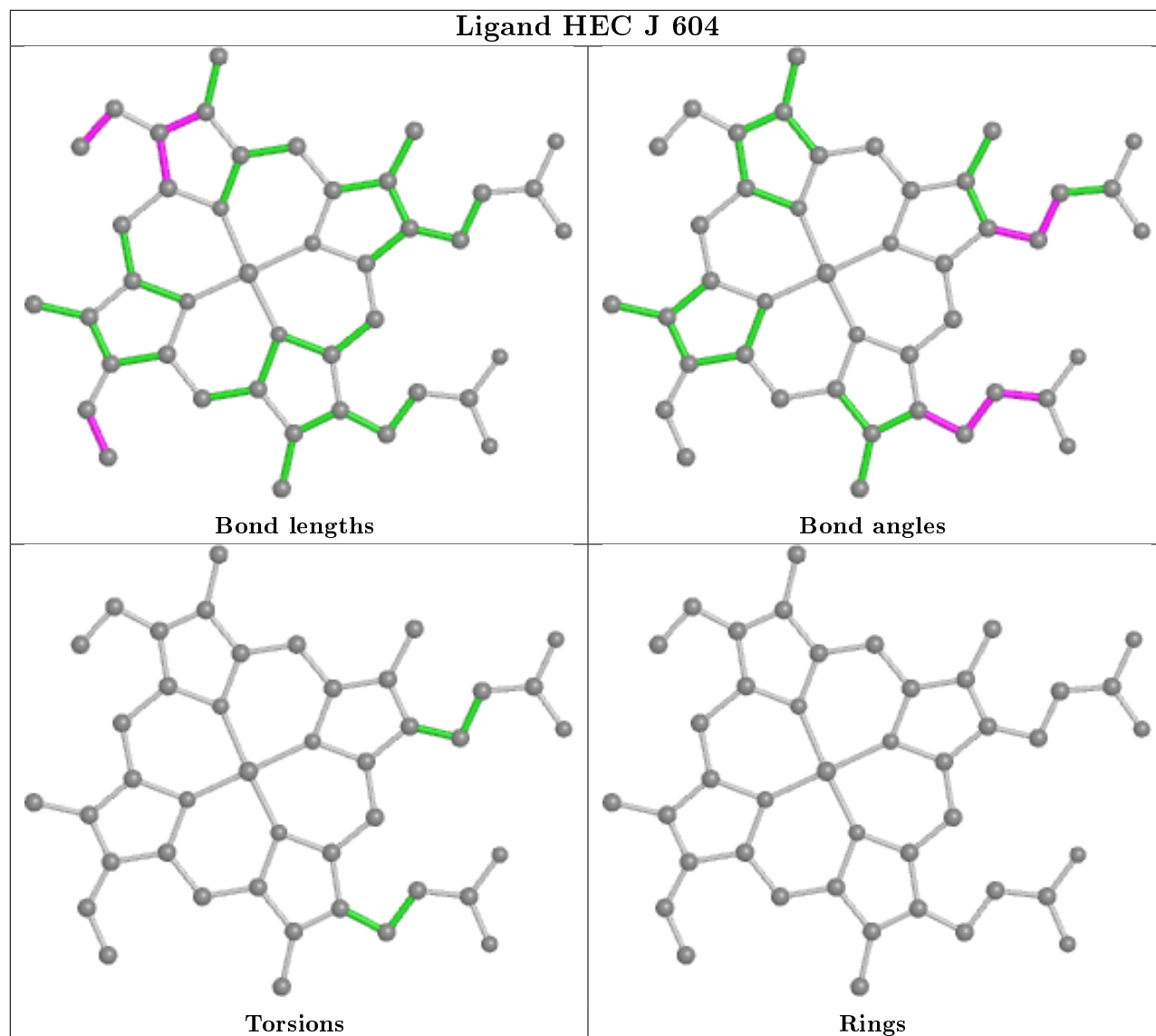


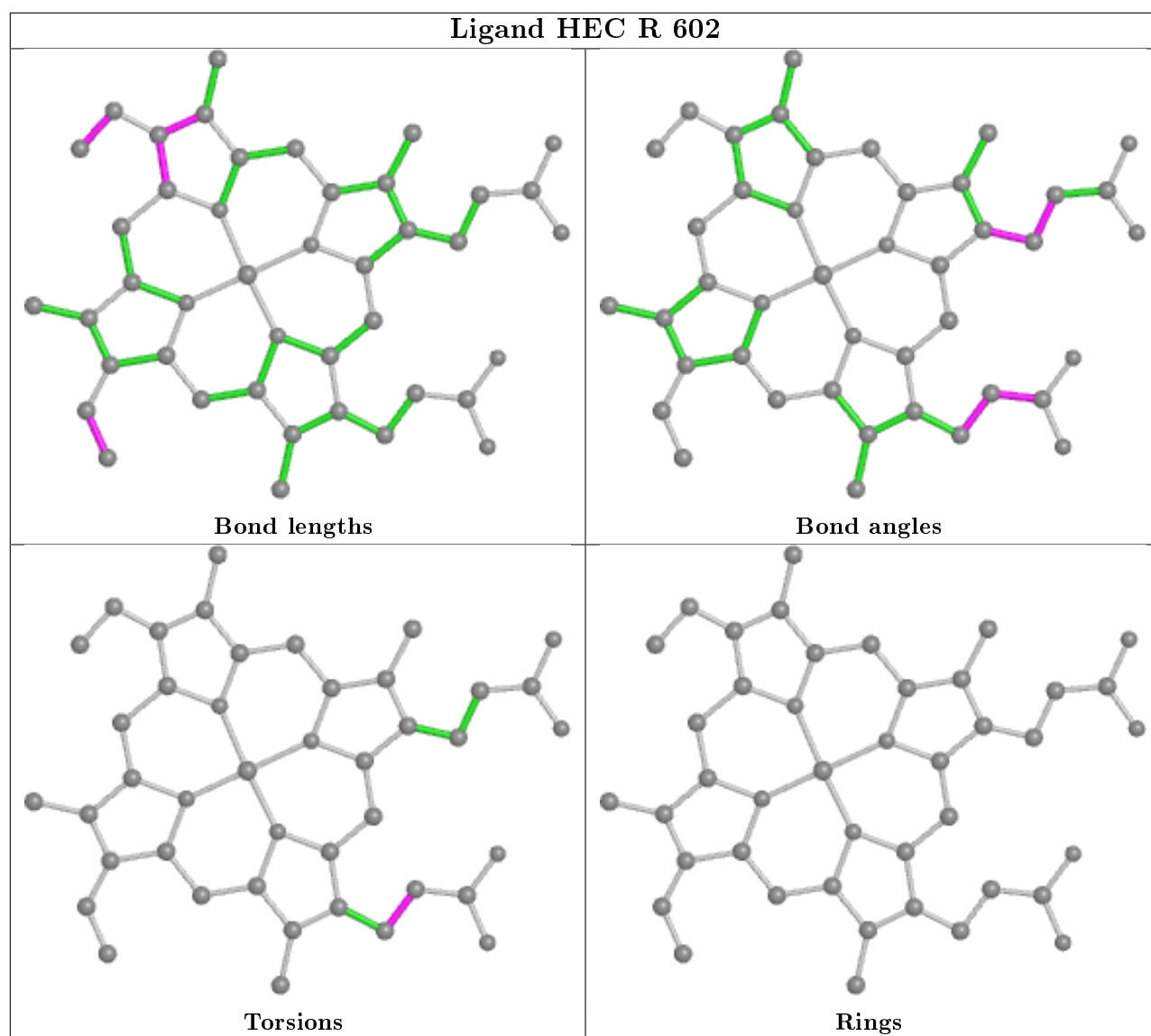
## Ligand HEC E 602

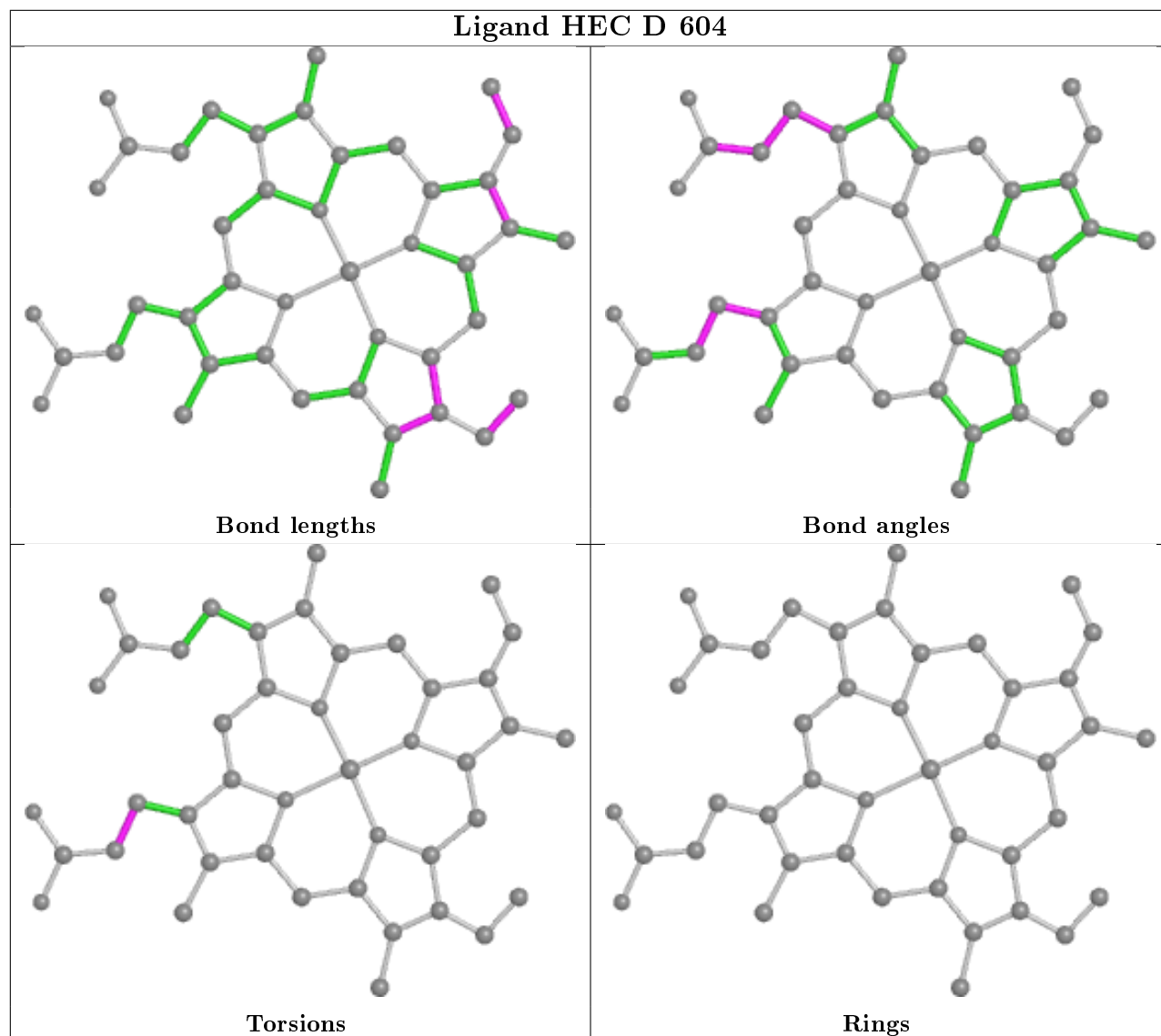




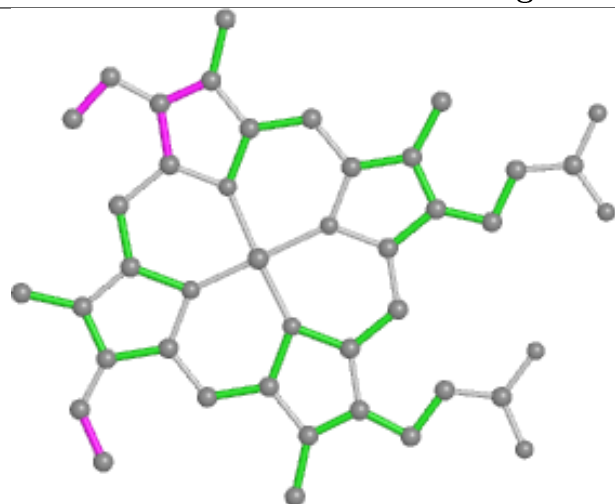
## Ligand HEC J 604



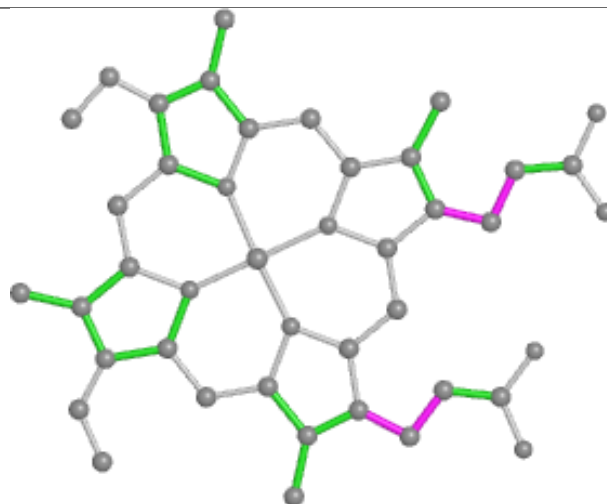




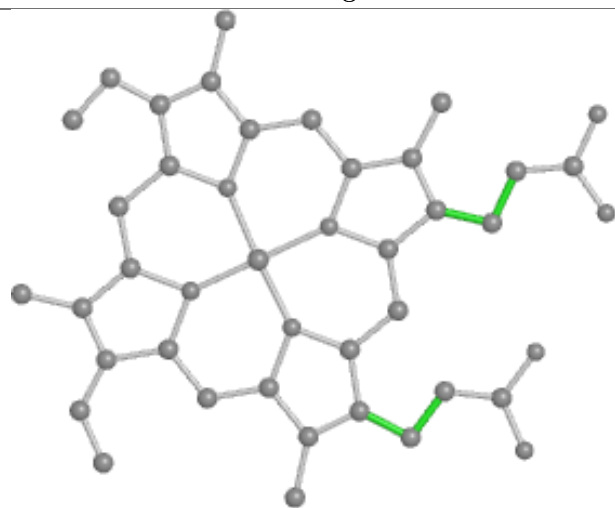
## Ligand HEC F 604



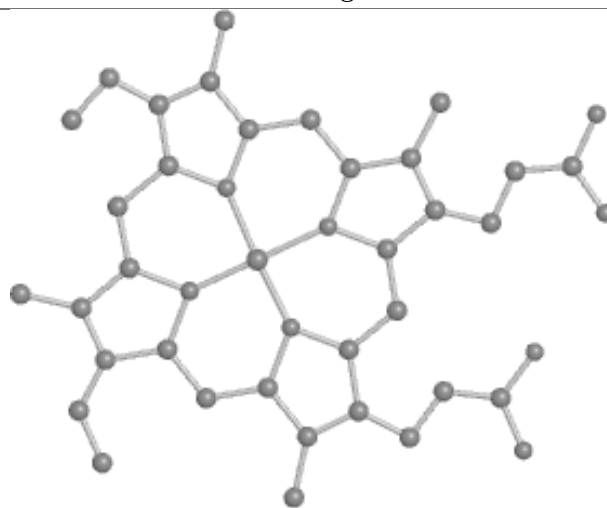
Bond lengths



Bond angles

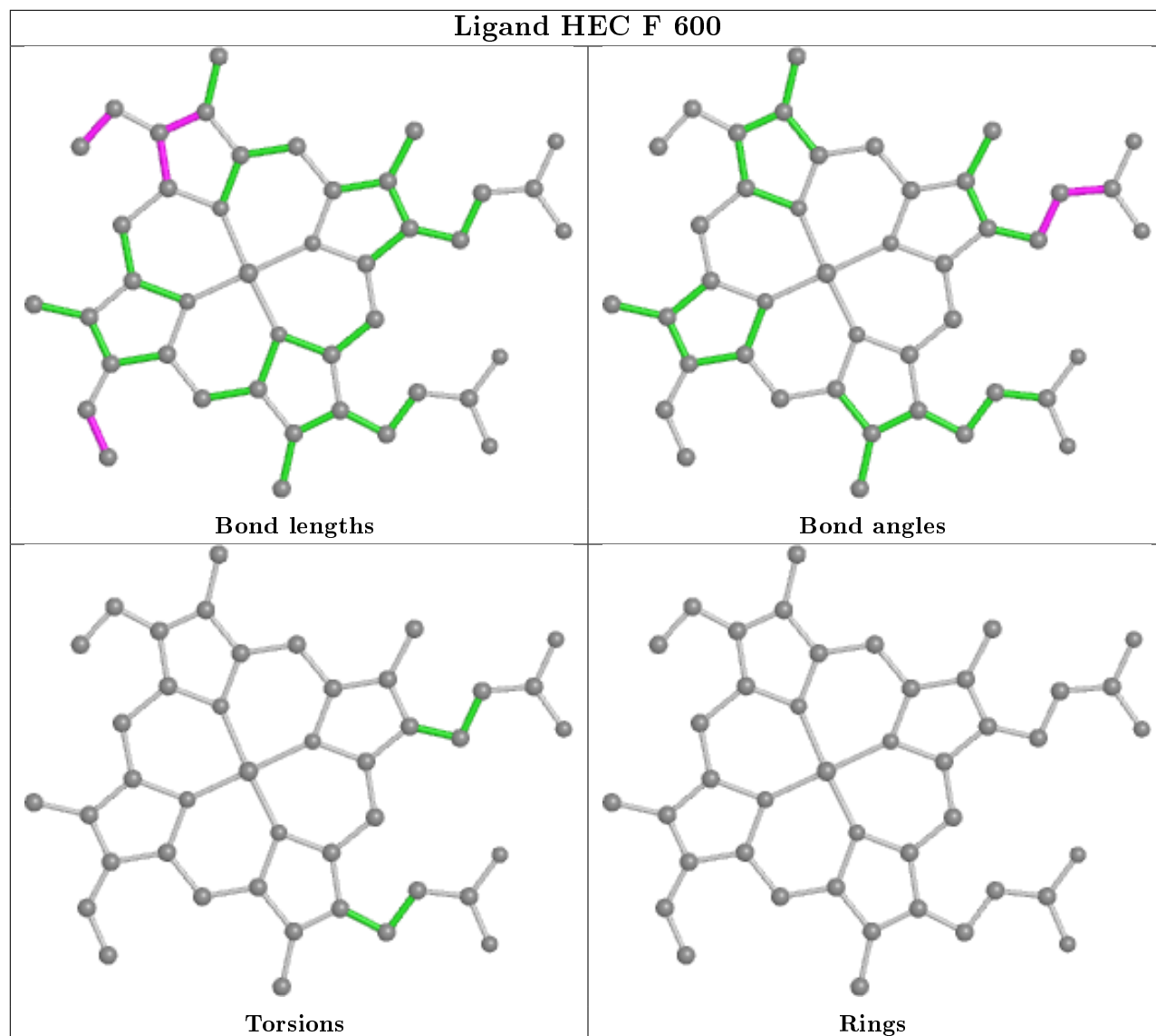


Torsions

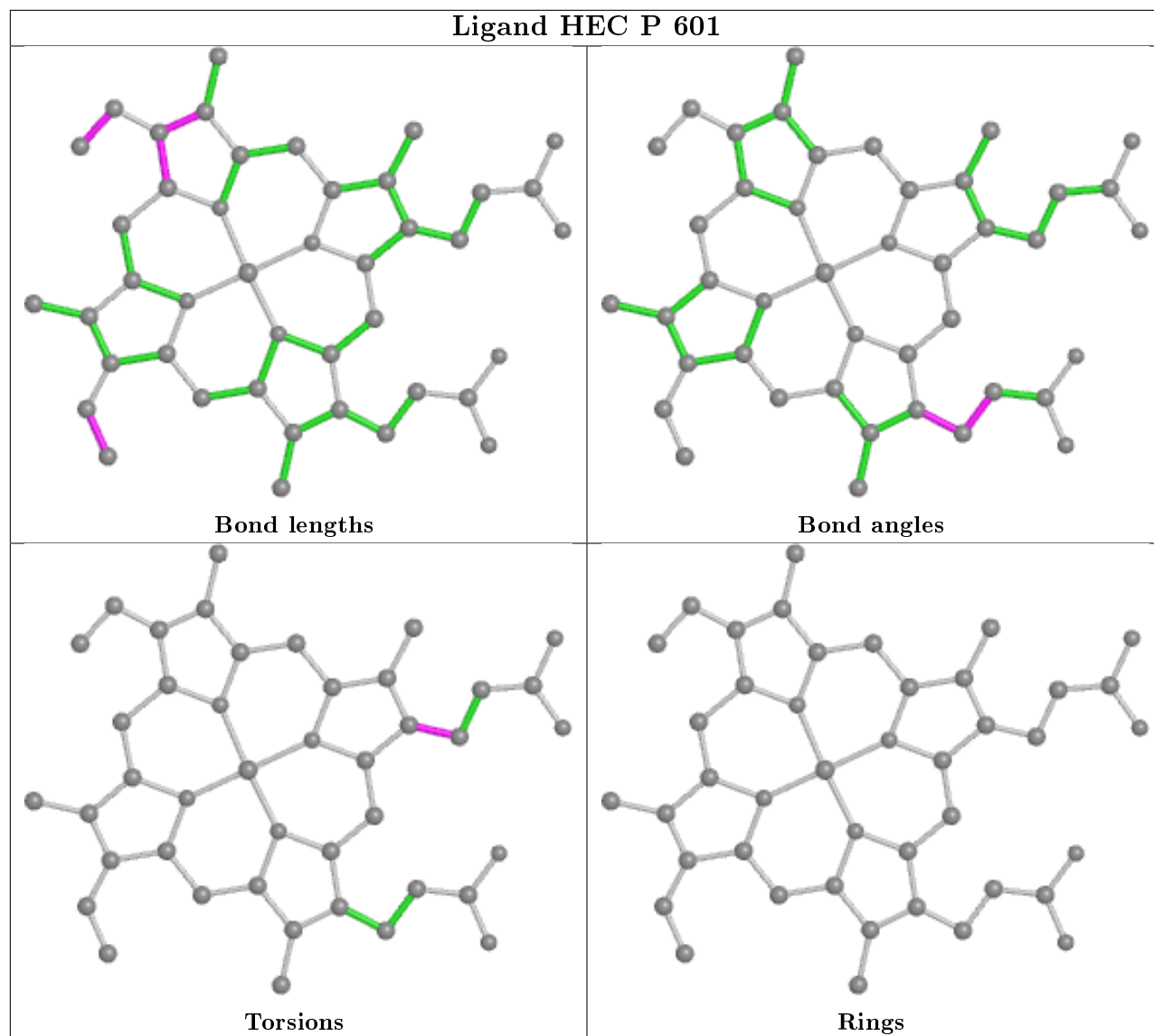


Rings

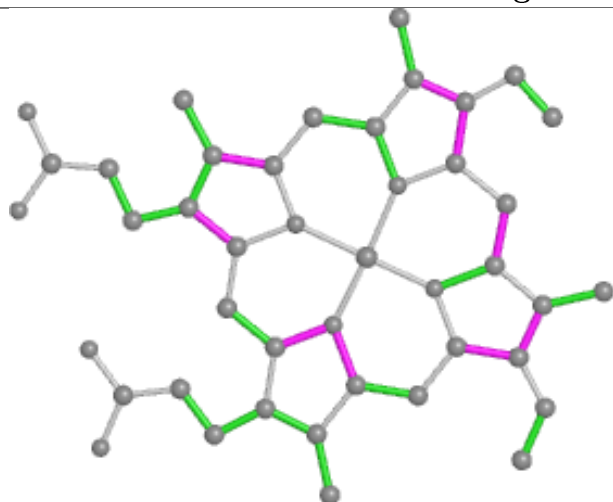
## Ligand HEC F 600



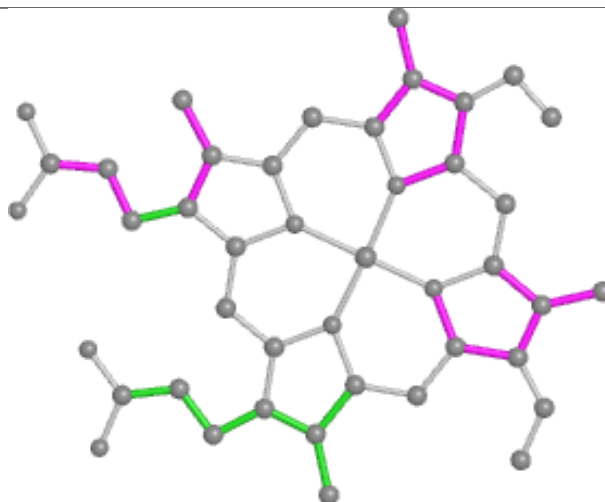
## Ligand HEC P 601



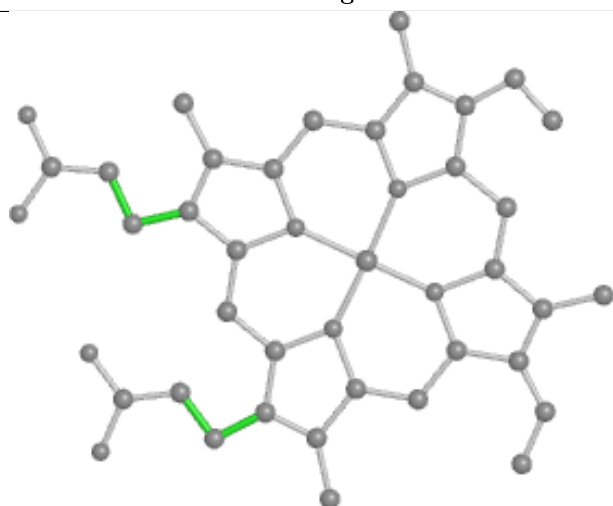
## Ligand HEC P 603



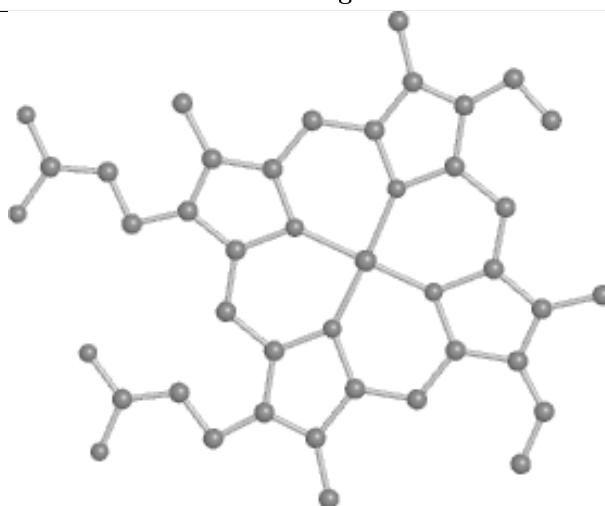
Bond lengths



Bond angles

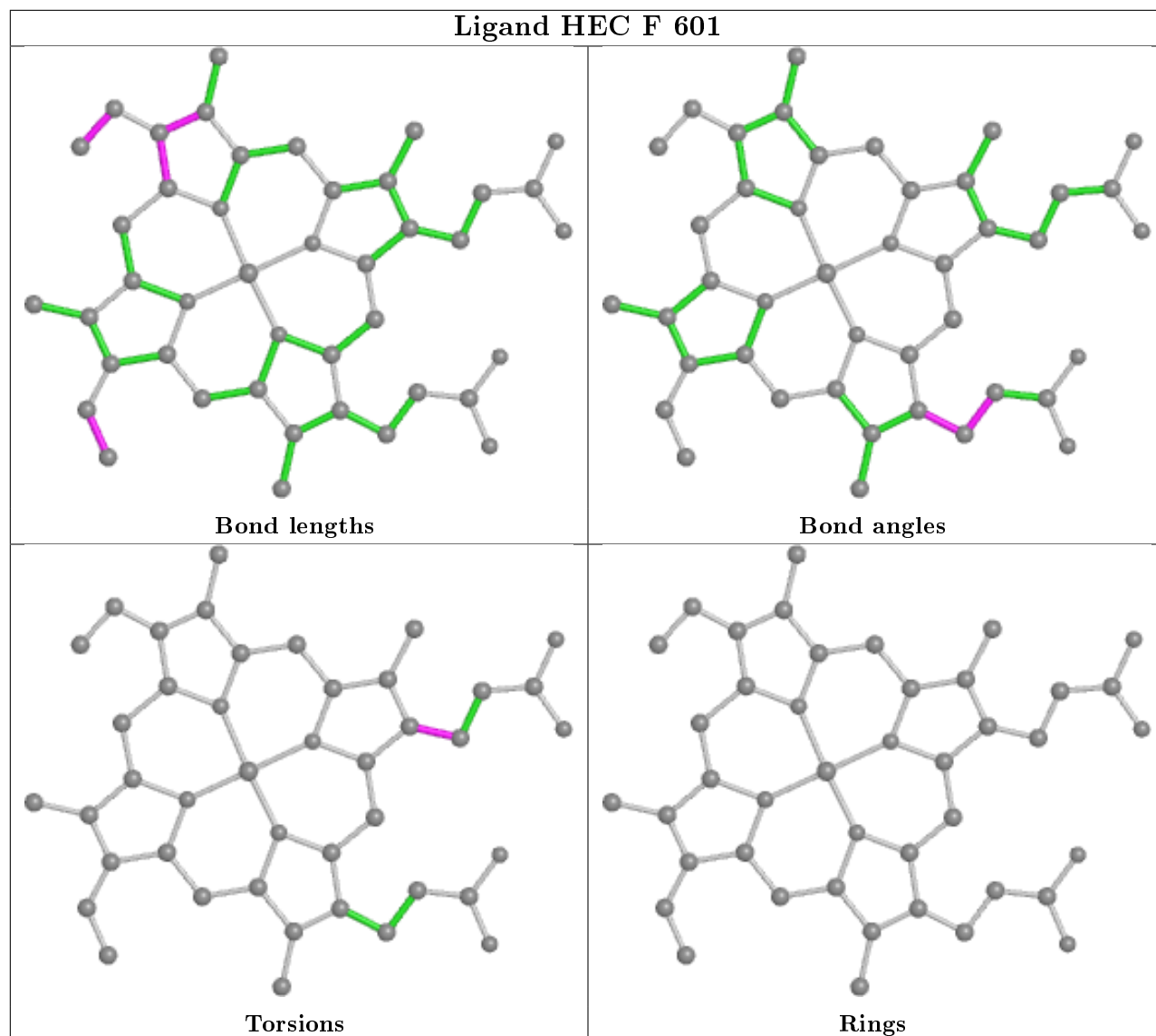


Torsions

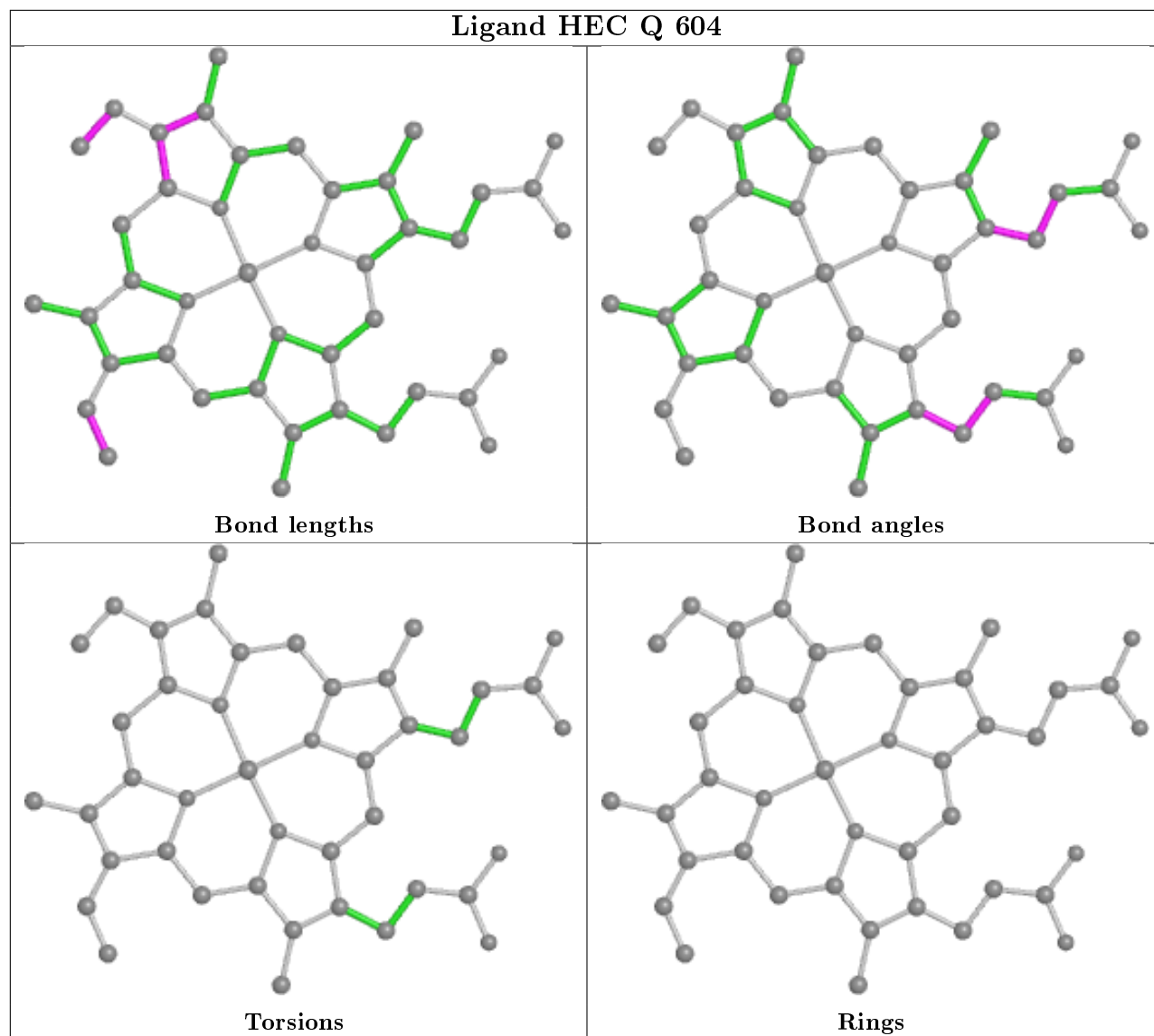


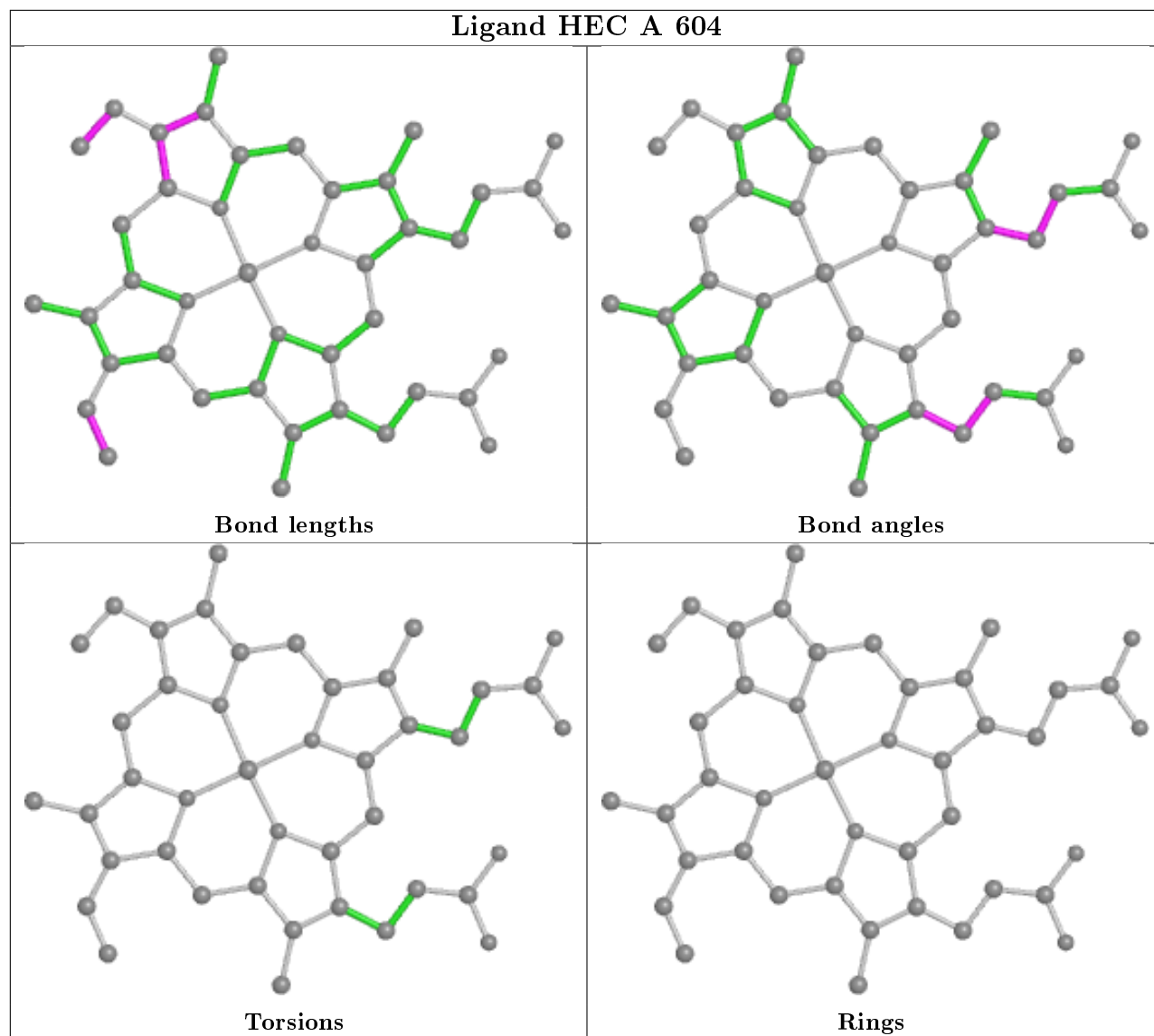
Rings

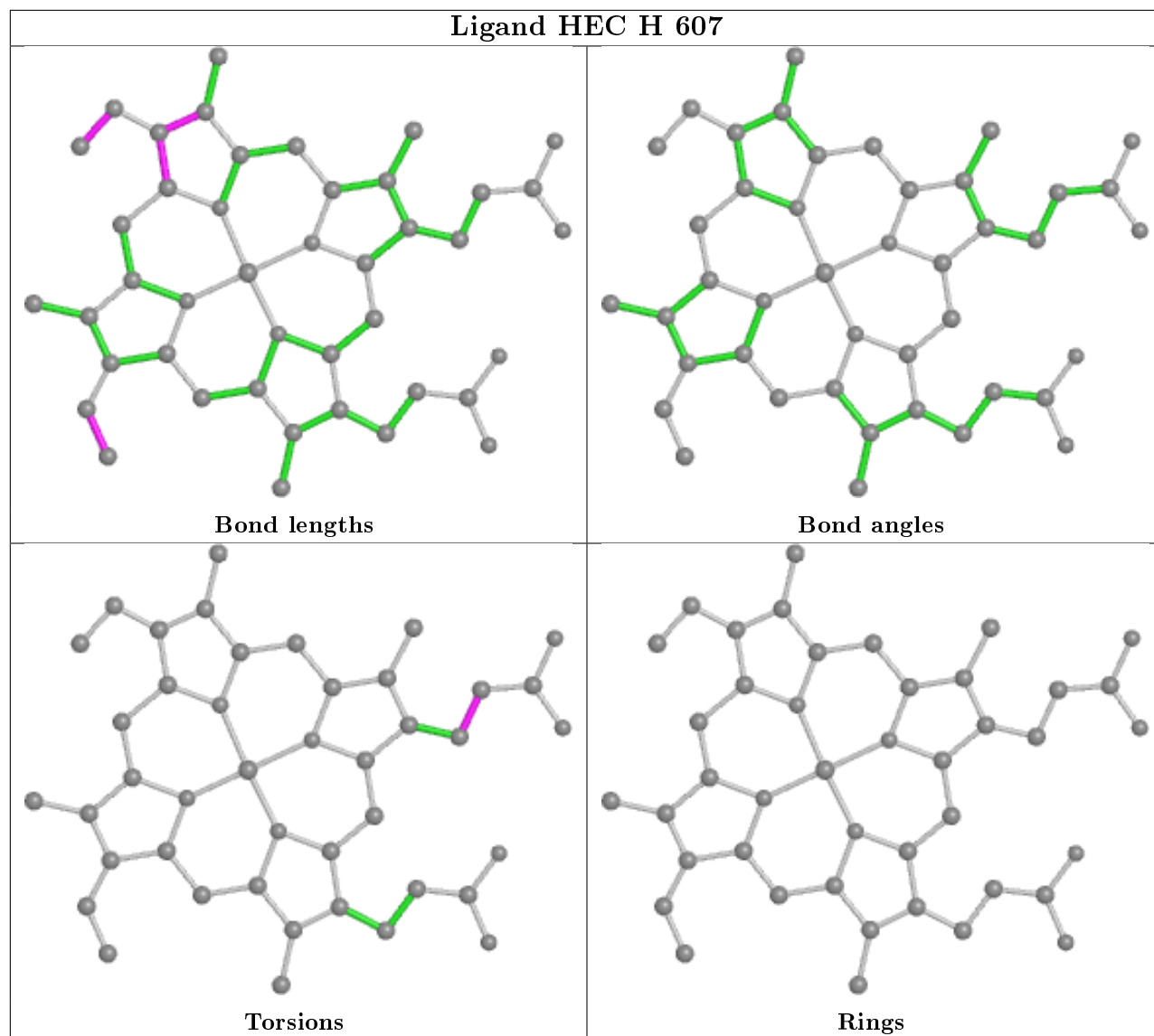
## Ligand HEC F 601



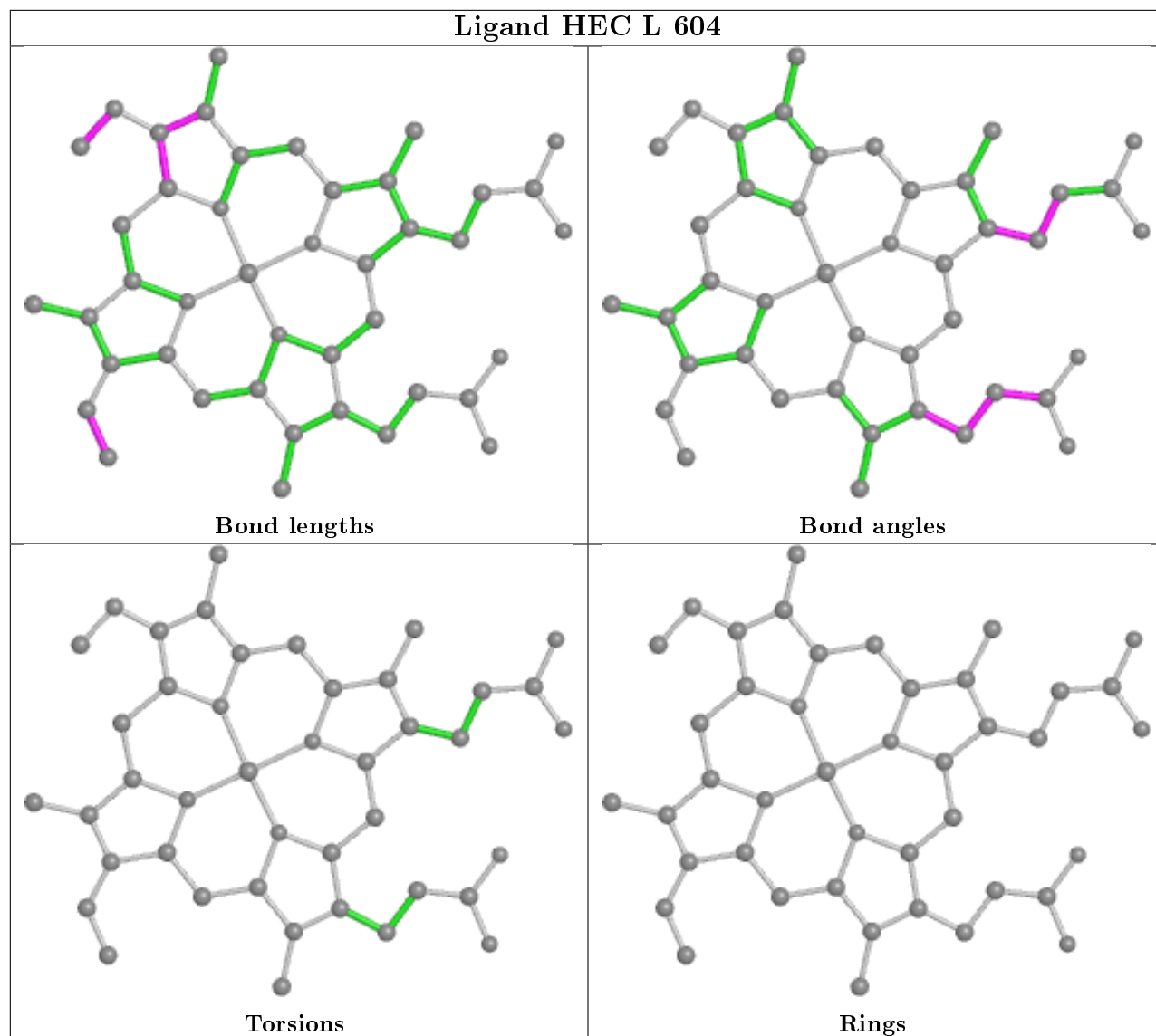


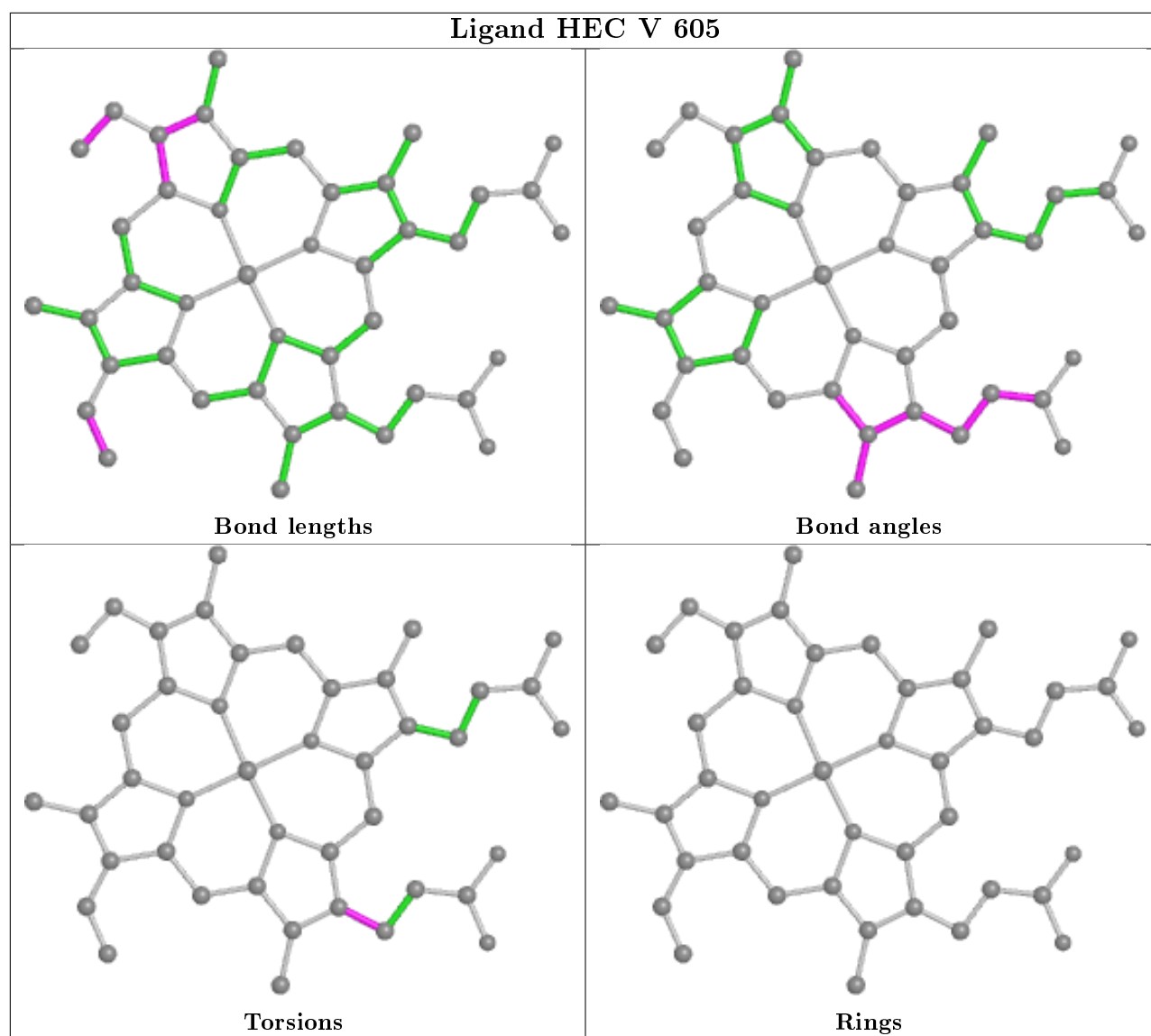






## Ligand HEC L 604





## 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     | 531/582 (91%) | 0.30   | 4 (0%) 86 81  | 39, 59, 87, 153       | 0     |
| 1   | B     | 531/582 (91%) | 0.31   | 4 (0%) 86 81  | 39, 57, 81, 173       | 0     |
| 1   | C     | 531/582 (91%) | 0.23   | 1 (0%) 95 94  | 40, 54, 84, 123       | 0     |
| 1   | D     | 531/582 (91%) | 0.30   | 1 (0%) 95 94  | 42, 68, 100, 140      | 0     |
| 1   | E     | 531/582 (91%) | 0.51   | 9 (1%) 70 63  | 39, 69, 104, 165      | 0     |
| 1   | F     | 531/582 (91%) | 0.58   | 14 (2%) 56 46 | 43, 76, 108, 158      | 0     |
| 1   | G     | 531/582 (91%) | 0.19   | 2 (0%) 92 91  | 29, 41, 64, 139       | 0     |
| 1   | H     | 531/582 (91%) | 0.22   | 1 (0%) 95 94  | 29, 39, 63, 156       | 0     |
| 1   | I     | 527/582 (90%) | 0.11   | 0 100 100     | 27, 38, 57, 104       | 0     |
| 1   | J     | 531/582 (91%) | 0.20   | 2 (0%) 92 91  | 29, 42, 66, 166       | 0     |
| 1   | K     | 531/582 (91%) | 0.28   | 6 (1%) 80 75  | 32, 44, 70, 159       | 0     |
| 1   | L     | 531/582 (91%) | 0.28   | 3 (0%) 89 86  | 32, 45, 73, 157       | 0     |
| 1   | M     | 531/582 (91%) | 0.34   | 3 (0%) 89 86  | 37, 54, 84, 150       | 0     |
| 1   | N     | 531/582 (91%) | 0.39   | 9 (1%) 70 63  | 37, 58, 85, 157       | 0     |
| 1   | O     | 531/582 (91%) | 0.24   | 5 (0%) 84 80  | 37, 51, 77, 133       | 0     |
| 1   | P     | 531/582 (91%) | 0.21   | 4 (0%) 86 81  | 37, 51, 72, 124       | 0     |
| 1   | Q     | 531/582 (91%) | 0.30   | 4 (0%) 86 81  | 34, 57, 82, 124       | 0     |
| 1   | R     | 531/582 (91%) | 0.23   | 1 (0%) 95 94  | 34, 52, 78, 142       | 0     |
| 1   | S     | 531/582 (91%) | 0.80   | 44 (8%) 11 6  | 51, 80, 111, 158      | 0     |
| 1   | T     | 531/582 (91%) | 0.60   | 21 (3%) 38 28 | 50, 74, 107, 184      | 0     |
| 1   | U     | 531/582 (91%) | 0.73   | 37 (6%) 16 9  | 50, 80, 111, 150      | 0     |
| 1   | V     | 531/582 (91%) | 0.83   | 47 (8%) 9 5   | 52, 79, 108, 161      | 0     |
| 1   | W     | 531/582 (91%) | 0.78   | 29 (5%) 25 16 | 50, 80, 105, 163      | 0     |
| 1   | X     | 531/582 (91%) | 0.76   | 33 (6%) 20 13 | 56, 83, 111, 160      | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 2   | Y     | 86/114 (75%)      | 0.41   | 3 (3%) 44 34   | 38, 54, 76, 105       | 0     |
| 2   | Z     | 86/114 (75%)      | 1.63   | 22 (25%) 0 0   | 76, 96, 128, 192      | 0     |
| 2   | a     | 86/114 (75%)      | 0.82   | 8 (9%) 8 4     | 64, 87, 116, 166      | 0     |
| 2   | b     | 86/114 (75%)      | 0.82   | 4 (4%) 31 22   | 61, 83, 118, 167      | 0     |
| 2   | c     | 86/114 (75%)      | 0.63   | 5 (5%) 23 15   | 58, 76, 101, 166      | 0     |
| 2   | d     | 86/114 (75%)      | 0.55   | 4 (4%) 31 22   | 54, 68, 107, 152      | 0     |
| 2   | e     | 86/114 (75%)      | 0.88   | 4 (4%) 31 22   | 57, 76, 109, 155      | 0     |
| 2   | f     | 86/114 (75%)      | 1.24   | 16 (18%) 1 1   | 71, 96, 131, 168      | 0     |
| 2   | g     | 86/114 (75%)      | 0.78   | 6 (6%) 16 9    | 68, 82, 114, 179      | 0     |
| 2   | h     | 86/114 (75%)      | 0.99   | 10 (11%) 4 2   | 82, 96, 130, 166      | 0     |
| 2   | i     | 86/114 (75%)      | 1.60   | 26 (30%) 0 0   | 85, 107, 137, 185     | 0     |
| 2   | j     | 86/114 (75%)      | 1.10   | 15 (17%) 1 1   | 96, 109, 147, 178     | 0     |
| All | All   | 13772/15336 (89%) | 0.45   | 407 (2%) 50 40 | 27, 60, 104, 192      | 0     |

The worst 5 of 407 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | Z     | 111 | SER  | 18.0 |
| 1   | T     | 563 | HIS  | 12.2 |
| 1   | B     | 563 | HIS  | 9.7  |
| 2   | a     | 111 | SER  | 9.5  |
| 1   | W     | 563 | HIS  | 9.4  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6   | K    | X     | 612 | 1/1   | 0.33 | 0.16 | 93,93,93,93                | 0     |
| 4   | SO4  | H     | 613 | 5/5   | 0.55 | 0.26 | 116,120,125,127            | 0     |
| 5   | GOL  | A     | 614 | 6/6   | 0.56 | 0.29 | 82,89,90,91                | 0     |
| 4   | SO4  | X     | 610 | 5/5   | 0.61 | 0.23 | 158,161,161,162            | 0     |
| 6   | K    | H     | 616 | 1/1   | 0.62 | 0.14 | 82,82,82,82                | 0     |
| 4   | SO4  | M     | 611 | 5/5   | 0.64 | 0.27 | 129,131,136,137            | 0     |
| 6   | K    | Q     | 612 | 1/1   | 0.67 | 0.15 | 96,96,96,96                | 0     |
| 4   | SO4  | S     | 609 | 5/5   | 0.69 | 0.18 | 129,133,135,135            | 0     |
| 5   | GOL  | J     | 612 | 6/6   | 0.69 | 0.28 | 58,64,67,67                | 0     |
| 6   | K    | K     | 616 | 1/1   | 0.69 | 0.11 | 85,85,85,85                | 0     |
| 4   | SO4  | V     | 611 | 5/5   | 0.70 | 0.18 | 131,133,134,135            | 0     |
| 4   | SO4  | G     | 612 | 5/5   | 0.71 | 0.28 | 120,124,126,126            | 0     |
| 5   | GOL  | A     | 612 | 6/6   | 0.71 | 0.25 | 76,78,79,81                | 0     |
| 4   | SO4  | L     | 610 | 5/5   | 0.71 | 0.24 | 142,143,145,150            | 0     |
| 5   | GOL  | H     | 615 | 6/6   | 0.76 | 0.68 | 78,86,90,100               | 0     |
| 4   | SO4  | G     | 611 | 5/5   | 0.76 | 0.41 | 139,139,143,149            | 0     |
| 4   | SO4  | H     | 612 | 5/5   | 0.77 | 0.23 | 110,113,116,118            | 0     |
| 5   | GOL  | A     | 613 | 6/6   | 0.78 | 0.27 | 74,77,78,79                | 0     |
| 4   | SO4  | H     | 610 | 5/5   | 0.79 | 0.17 | 106,111,113,114            | 0     |
| 4   | SO4  | U     | 611 | 5/5   | 0.80 | 0.19 | 127,130,131,133            | 0     |
| 4   | SO4  | X     | 611 | 5/5   | 0.80 | 0.33 | 139,139,141,144            | 0     |
| 4   | SO4  | Q     | 611 | 5/5   | 0.80 | 0.16 | 112,118,119,119            | 0     |
| 4   | SO4  | c     | 201 | 5/5   | 0.81 | 0.15 | 132,133,135,135            | 0     |
| 4   | SO4  | F     | 610 | 5/5   | 0.81 | 0.21 | 135,136,139,139            | 0     |
| 5   | GOL  | G     | 615 | 6/6   | 0.81 | 0.23 | 61,67,68,68                | 0     |
| 4   | SO4  | Y     | 201 | 5/5   | 0.82 | 0.22 | 136,136,137,141            | 0     |
| 4   | SO4  | C     | 610 | 5/5   | 0.82 | 0.40 | 143,145,147,149            | 0     |
| 4   | SO4  | I     | 611 | 5/5   | 0.82 | 0.17 | 115,115,116,117            | 0     |
| 4   | SO4  | a     | 201 | 5/5   | 0.83 | 0.23 | 139,139,140,140            | 0     |
| 5   | GOL  | I     | 614 | 6/6   | 0.83 | 0.71 | 67,78,80,83                | 0     |
| 4   | SO4  | M     | 612 | 5/5   | 0.83 | 0.18 | 121,122,123,125            | 0     |
| 5   | GOL  | K     | 612 | 6/6   | 0.83 | 0.36 | 76,80,86,90                | 0     |
| 4   | SO4  | N     | 611 | 5/5   | 0.83 | 0.18 | 123,126,127,129            | 0     |
| 4   | SO4  | L     | 611 | 5/5   | 0.84 | 0.14 | 116,119,121,122            | 0     |
| 4   | SO4  | Y     | 202 | 5/5   | 0.84 | 0.17 | 130,130,132,136            | 0     |
| 4   | SO4  | O     | 610 | 5/5   | 0.84 | 0.21 | 109,111,112,112            | 0     |
| 4   | SO4  | M     | 610 | 5/5   | 0.84 | 0.49 | 134,135,138,139            | 0     |
| 4   | SO4  | I     | 612 | 5/5   | 0.85 | 0.20 | 120,121,124,125            | 0     |
| 4   | SO4  | C     | 611 | 5/5   | 0.85 | 0.31 | 111,111,114,116            | 0     |
| 4   | SO4  | L     | 612 | 5/5   | 0.85 | 0.18 | 110,112,115,115            | 0     |
| 4   | SO4  | A     | 611 | 5/5   | 0.86 | 0.15 | 117,118,119,120            | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | GOL  | D     | 610 | 6/6   | 0.86 | 0.25 | 86,88,88,89                 | 0     |
| 4   | SO4  | Q     | 610 | 5/5   | 0.87 | 0.34 | 133,136,137,137             | 0     |
| 4   | SO4  | O     | 611 | 5/5   | 0.87 | 0.13 | 114,114,119,120             | 0     |
| 4   | SO4  | G     | 614 | 5/5   | 0.87 | 0.17 | 91,94,95,95                 | 0     |
| 4   | SO4  | J     | 611 | 5/5   | 0.87 | 0.49 | 118,118,120,123             | 0     |
| 4   | SO4  | J     | 610 | 5/5   | 0.88 | 0.20 | 99,100,101,103              | 0     |
| 5   | GOL  | I     | 615 | 6/6   | 0.88 | 0.20 | 51,55,56,57                 | 0     |
| 4   | SO4  | W     | 609 | 5/5   | 0.88 | 0.16 | 114,118,119,124             | 0     |
| 4   | SO4  | X     | 609 | 5/5   | 0.88 | 0.17 | 107,108,110,112             | 0     |
| 4   | SO4  | R     | 611 | 5/5   | 0.89 | 0.52 | 142,143,145,147             | 0     |
| 4   | SO4  | E     | 610 | 5/5   | 0.90 | 0.14 | 103,105,106,109             | 0     |
| 5   | GOL  | I     | 613 | 6/6   | 0.91 | 0.23 | 59,64,66,73                 | 0     |
| 5   | GOL  | H     | 614 | 6/6   | 0.91 | 0.74 | 56,63,64,68                 | 0     |
| 4   | SO4  | F     | 609 | 5/5   | 0.91 | 0.12 | 95,99,102,104               | 0     |
| 4   | SO4  | K     | 611 | 5/5   | 0.91 | 0.22 | 102,104,105,105             | 0     |
| 4   | SO4  | U     | 610 | 5/5   | 0.91 | 0.19 | 99,101,103,104              | 0     |
| 5   | GOL  | J     | 613 | 6/6   | 0.91 | 0.27 | 58,61,62,63                 | 0     |
| 4   | SO4  | B     | 609 | 5/5   | 0.92 | 0.46 | 116,117,119,124             | 0     |
| 4   | SO4  | B     | 610 | 5/5   | 0.93 | 0.15 | 88,89,91,91                 | 0     |
| 4   | SO4  | C     | 609 | 5/5   | 0.93 | 0.16 | 96,102,106,108              | 0     |
| 4   | SO4  | V     | 610 | 5/5   | 0.93 | 0.16 | 94,97,98,99                 | 0     |
| 5   | GOL  | K     | 613 | 6/6   | 0.93 | 0.23 | 45,51,52,53                 | 0     |
| 4   | SO4  | H     | 609 | 5/5   | 0.93 | 0.15 | 78,81,82,83                 | 0     |
| 4   | SO4  | N     | 610 | 5/5   | 0.93 | 0.16 | 101,105,107,109             | 0     |
| 4   | SO4  | P     | 609 | 5/5   | 0.93 | 0.17 | 95,95,96,98                 | 0     |
| 5   | GOL  | L     | 613 | 6/6   | 0.94 | 0.31 | 56,59,60,61                 | 0     |
| 4   | SO4  | H     | 611 | 5/5   | 0.94 | 0.15 | 97,100,101,105              | 0     |
| 4   | SO4  | T     | 609 | 5/5   | 0.94 | 0.10 | 98,100,102,102              | 0     |
| 5   | GOL  | K     | 615 | 6/6   | 0.94 | 0.65 | 53,55,58,59                 | 0     |
| 4   | SO4  | L     | 609 | 5/5   | 0.94 | 0.13 | 91,94,94,97                 | 0     |
| 4   | SO4  | O     | 609 | 5/5   | 0.94 | 0.13 | 77,78,80,82                 | 0     |
| 4   | SO4  | Q     | 609 | 5/5   | 0.94 | 0.09 | 84,87,88,89                 | 0     |
| 4   | SO4  | A     | 610 | 5/5   | 0.94 | 0.14 | 73,77,79,80                 | 0     |
| 4   | SO4  | G     | 610 | 5/5   | 0.94 | 0.42 | 104,106,107,108             | 0     |
| 4   | SO4  | D     | 609 | 5/5   | 0.95 | 0.11 | 82,82,84,87                 | 0     |
| 4   | SO4  | K     | 610 | 5/5   | 0.95 | 0.16 | 84,84,86,88                 | 0     |
| 3   | HEC  | X     | 606 | 43/43 | 0.95 | 0.25 | 69,83,87,90                 | 0     |
| 4   | SO4  | R     | 610 | 5/5   | 0.95 | 0.12 | 75,77,79,79                 | 0     |
| 3   | HEC  | X     | 605 | 43/43 | 0.95 | 0.31 | 79,86,97,100                | 0     |
| 3   | HEC  | V     | 602 | 43/43 | 0.95 | 0.24 | 68,73,87,100                | 0     |
| 5   | GOL  | G     | 616 | 6/6   | 0.95 | 0.19 | 37,40,41,41                 | 0     |
| 5   | GOL  | K     | 614 | 6/6   | 0.95 | 0.65 | 49,56,57,59                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | HEC  | A     | 606 | 43/43 | 0.96 | 0.26 | 45,60,73,78                 | 0     |
| 3   | HEC  | U     | 602 | 43/43 | 0.96 | 0.27 | 60,69,94,116                | 0     |
| 3   | HEC  | S     | 604 | 43/43 | 0.96 | 0.23 | 59,66,75,86                 | 0     |
| 3   | HEC  | H     | 602 | 43/43 | 0.96 | 0.23 | 35,44,64,77                 | 0     |
| 3   | HEC  | T     | 607 | 43/43 | 0.96 | 0.26 | 49,57,60,62                 | 0     |
| 3   | HEC  | U     | 606 | 43/43 | 0.96 | 0.29 | 65,72,88,96                 | 0     |
| 3   | HEC  | W     | 605 | 43/43 | 0.96 | 0.28 | 74,81,87,89                 | 0     |
| 3   | HEC  | X     | 602 | 43/43 | 0.96 | 0.24 | 69,75,91,106                | 0     |
| 3   | HEC  | P     | 602 | 43/43 | 0.96 | 0.20 | 41,45,63,76                 | 0     |
| 3   | HEC  | T     | 602 | 43/43 | 0.96 | 0.23 | 59,68,83,97                 | 0     |
| 3   | HEC  | Q     | 604 | 43/43 | 0.96 | 0.25 | 54,60,68,76                 | 0     |
| 3   | HEC  | E     | 605 | 43/43 | 0.96 | 0.23 | 53,63,75,82                 | 0     |
| 3   | HEC  | W     | 603 | 43/43 | 0.96 | 0.27 | 67,77,85,89                 | 0     |
| 3   | HEC  | U     | 600 | 43/43 | 0.96 | 0.18 | 58,64,71,72                 | 0     |
| 3   | HEC  | Q     | 602 | 43/43 | 0.96 | 0.23 | 64,68,88,97                 | 0     |
| 3   | HEC  | N     | 606 | 43/43 | 0.96 | 0.22 | 47,51,60,64                 | 0     |
| 3   | HEC  | S     | 605 | 43/43 | 0.96 | 0.30 | 63,72,82,83                 | 0     |
| 3   | HEC  | V     | 603 | 43/43 | 0.96 | 0.25 | 51,65,82,86                 | 0     |
| 3   | HEC  | U     | 604 | 43/43 | 0.96 | 0.23 | 52,60,72,81                 | 0     |
| 3   | HEC  | B     | 602 | 43/43 | 0.96 | 0.22 | 49,56,80,99                 | 0     |
| 4   | SO4  | S     | 610 | 5/5   | 0.96 | 0.09 | 92,93,94,95                 | 0     |
| 3   | HEC  | F     | 603 | 43/43 | 0.96 | 0.22 | 62,70,74,79                 | 0     |
| 3   | HEC  | E     | 606 | 43/43 | 0.96 | 0.26 | 55,60,68,75                 | 0     |
| 4   | SO4  | J     | 609 | 5/5   | 0.96 | 0.19 | 77,79,80,80                 | 0     |
| 3   | HEC  | S     | 603 | 43/43 | 0.96 | 0.25 | 72,77,88,94                 | 0     |
| 3   | HEC  | F     | 602 | 43/43 | 0.96 | 0.23 | 64,75,85,96                 | 0     |
| 4   | SO4  | M     | 609 | 5/5   | 0.96 | 0.11 | 89,90,91,92                 | 0     |
| 4   | SO4  | G     | 609 | 5/5   | 0.96 | 0.12 | 72,72,74,74                 | 0     |
| 3   | HEC  | S     | 602 | 43/43 | 0.96 | 0.23 | 63,71,86,104                | 0     |
| 3   | HEC  | W     | 602 | 43/43 | 0.96 | 0.23 | 54,58,83,99                 | 0     |
| 3   | HEC  | E     | 602 | 43/43 | 0.96 | 0.24 | 48,53,73,94                 | 0     |
| 3   | HEC  | X     | 604 | 43/43 | 0.96 | 0.21 | 63,73,78,80                 | 0     |
| 3   | HEC  | V     | 604 | 43/43 | 0.96 | 0.28 | 59,71,81,85                 | 0     |
| 3   | HEC  | A     | 604 | 43/43 | 0.96 | 0.22 | 47,50,61,73                 | 0     |
| 3   | HEC  | C     | 600 | 43/43 | 0.97 | 0.22 | 49,52,56,58                 | 0     |
| 3   | HEC  | E     | 600 | 43/43 | 0.97 | 0.21 | 39,41,53,55                 | 0     |
| 3   | HEC  | T     | 600 | 43/43 | 0.97 | 0.20 | 53,60,68,69                 | 0     |
| 3   | HEC  | L     | 600 | 43/43 | 0.97 | 0.22 | 41,44,50,51                 | 0     |
| 3   | HEC  | F     | 605 | 43/43 | 0.97 | 0.25 | 54,60,69,78                 | 0     |
| 3   | HEC  | S     | 601 | 43/43 | 0.97 | 0.25 | 67,70,81,85                 | 0     |
| 3   | HEC  | X     | 603 | 43/43 | 0.97 | 0.24 | 70,80,103,109               | 0     |
| 3   | HEC  | K     | 600 | 43/43 | 0.97 | 0.22 | 38,40,46,55                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | HEC  | C     | 604 | 43/43 | 0.97 | 0.22 | 42,47,53,60                 | 0     |
| 3   | HEC  | Q     | 607 | 43/43 | 0.97 | 0.20 | 36,40,44,46                 | 0     |
| 3   | HEC  | R     | 603 | 43/43 | 0.97 | 0.19 | 37,43,48,52                 | 0     |
| 3   | HEC  | W     | 604 | 43/43 | 0.97 | 0.21 | 50,57,67,74                 | 0     |
| 3   | HEC  | A     | 607 | 43/43 | 0.97 | 0.21 | 41,45,50,53                 | 0     |
| 3   | HEC  | T     | 606 | 43/43 | 0.97 | 0.27 | 52,56,65,74                 | 0     |
| 3   | HEC  | S     | 600 | 43/43 | 0.97 | 0.22 | 60,65,73,75                 | 0     |
| 3   | HEC  | N     | 600 | 43/43 | 0.97 | 0.25 | 46,49,57,63                 | 0     |
| 3   | HEC  | N     | 601 | 43/43 | 0.97 | 0.23 | 41,44,55,65                 | 0     |
| 3   | HEC  | P     | 606 | 43/43 | 0.97 | 0.23 | 43,47,48,49                 | 0     |
| 3   | HEC  | L     | 602 | 43/43 | 0.97 | 0.22 | 42,45,57,72                 | 0     |
| 3   | HEC  | M     | 607 | 43/43 | 0.97 | 0.23 | 36,39,52,62                 | 0     |
| 3   | HEC  | N     | 602 | 43/43 | 0.97 | 0.23 | 48,52,75,92                 | 0     |
| 3   | HEC  | F     | 601 | 43/43 | 0.97 | 0.25 | 51,55,68,70                 | 0     |
| 3   | HEC  | P     | 604 | 43/43 | 0.97 | 0.22 | 36,40,52,63                 | 0     |
| 3   | HEC  | T     | 604 | 43/43 | 0.97 | 0.23 | 59,65,70,80                 | 0     |
| 3   | HEC  | E     | 603 | 43/43 | 0.97 | 0.23 | 56,66,92,96                 | 0     |
| 3   | HEC  | D     | 602 | 43/43 | 0.97 | 0.19 | 45,48,65,79                 | 0     |
| 3   | HEC  | U     | 601 | 43/43 | 0.97 | 0.23 | 54,57,67,73                 | 0     |
| 3   | HEC  | W     | 606 | 43/43 | 0.97 | 0.31 | 64,76,88,96                 | 0     |
| 3   | HEC  | Q     | 600 | 43/43 | 0.97 | 0.23 | 47,52,59,65                 | 0     |
| 3   | HEC  | S     | 607 | 43/43 | 0.97 | 0.24 | 51,57,59,60                 | 0     |
| 3   | HEC  | W     | 607 | 43/43 | 0.97 | 0.25 | 63,68,71,71                 | 0     |
| 3   | HEC  | I     | 602 | 43/43 | 0.97 | 0.21 | 37,42,59,70                 | 0     |
| 3   | HEC  | B     | 604 | 43/43 | 0.97 | 0.21 | 44,51,62,67                 | 0     |
| 3   | HEC  | O     | 604 | 43/43 | 0.97 | 0.21 | 34,41,50,60                 | 0     |
| 3   | HEC  | U     | 603 | 43/43 | 0.97 | 0.24 | 61,72,83,85                 | 0     |
| 3   | HEC  | V     | 600 | 43/43 | 0.97 | 0.23 | 67,70,84,91                 | 0     |
| 3   | HEC  | A     | 603 | 43/43 | 0.97 | 0.22 | 54,66,71,73                 | 0     |
| 3   | HEC  | O     | 602 | 43/43 | 0.97 | 0.22 | 47,51,72,91                 | 0     |
| 3   | HEC  | F     | 606 | 43/43 | 0.97 | 0.24 | 50,56,67,76                 | 0     |
| 3   | HEC  | D     | 605 | 43/43 | 0.97 | 0.26 | 48,53,61,66                 | 0     |
| 3   | HEC  | Q     | 601 | 43/43 | 0.97 | 0.22 | 46,50,54,56                 | 0     |
| 3   | HEC  | F     | 607 | 43/43 | 0.97 | 0.27 | 49,56,57,60                 | 0     |
| 3   | HEC  | V     | 601 | 43/43 | 0.97 | 0.20 | 52,63,65,67                 | 0     |
| 3   | HEC  | M     | 604 | 43/43 | 0.97 | 0.24 | 40,43,51,62                 | 0     |
| 3   | HEC  | M     | 602 | 43/43 | 0.97 | 0.23 | 44,48,72,89                 | 0     |
| 3   | HEC  | A     | 600 | 43/43 | 0.97 | 0.22 | 47,49,56,59                 | 0     |
| 3   | HEC  | C     | 602 | 43/43 | 0.97 | 0.21 | 45,48,66,80                 | 0     |
| 3   | HEC  | O     | 603 | 43/43 | 0.97 | 0.20 | 40,44,49,51                 | 0     |
| 3   | HEC  | T     | 605 | 43/43 | 0.97 | 0.24 | 54,60,74,76                 | 0     |
| 3   | HEC  | C     | 603 | 43/43 | 0.97 | 0.22 | 44,48,58,63                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | HEC  | E     | 607 | 43/43 | 0.97 | 0.27 | 47,54,60,62                 | 0     |
| 3   | HEC  | E     | 604 | 43/43 | 0.97 | 0.21 | 40,45,53,63                 | 0     |
| 3   | HEC  | M     | 605 | 43/43 | 0.97 | 0.27 | 36,38,46,51                 | 0     |
| 3   | HEC  | D     | 600 | 43/43 | 0.97 | 0.22 | 54,60,68,74                 | 0     |
| 3   | HEC  | O     | 601 | 43/43 | 0.97 | 0.23 | 40,44,49,56                 | 0     |
| 3   | HEC  | V     | 607 | 43/43 | 0.97 | 0.29 | 54,66,69,70                 | 0     |
| 3   | HEC  | K     | 604 | 43/43 | 0.97 | 0.20 | 36,41,49,57                 | 0     |
| 3   | HEC  | P     | 607 | 43/43 | 0.97 | 0.22 | 38,48,52,54                 | 0     |
| 3   | HEC  | C     | 605 | 43/43 | 0.97 | 0.22 | 38,43,53,57                 | 0     |
| 3   | HEC  | G     | 604 | 43/43 | 0.97 | 0.23 | 31,34,49,57                 | 0     |
| 3   | HEC  | Q     | 606 | 43/43 | 0.97 | 0.23 | 44,55,65,69                 | 0     |
| 3   | HEC  | U     | 605 | 43/43 | 0.97 | 0.27 | 62,68,80,87                 | 0     |
| 3   | HEC  | J     | 602 | 43/43 | 0.97 | 0.22 | 38,41,67,86                 | 0     |
| 3   | HEC  | J     | 600 | 43/43 | 0.97 | 0.22 | 37,41,52,60                 | 0     |
| 3   | HEC  | C     | 607 | 43/43 | 0.97 | 0.22 | 44,48,49,52                 | 0     |
| 3   | HEC  | W     | 601 | 43/43 | 0.97 | 0.27 | 61,70,77,80                 | 0     |
| 3   | HEC  | M     | 603 | 43/43 | 0.97 | 0.24 | 42,46,49,50                 | 0     |
| 3   | HEC  | V     | 606 | 43/43 | 0.97 | 0.26 | 57,60,76,81                 | 0     |
| 3   | HEC  | X     | 600 | 43/43 | 0.97 | 0.19 | 57,63,75,81                 | 0     |
| 3   | HEC  | B     | 600 | 43/43 | 0.97 | 0.19 | 48,52,59,61                 | 0     |
| 3   | HEC  | G     | 602 | 43/43 | 0.97 | 0.22 | 34,38,59,77                 | 0     |
| 3   | HEC  | L     | 601 | 43/43 | 0.97 | 0.22 | 36,40,45,46                 | 0     |
| 4   | SO4  | E     | 609 | 5/5   | 0.97 | 0.15 | 50,51,53,53                 | 0     |
| 3   | HEC  | U     | 607 | 43/43 | 0.97 | 0.29 | 53,70,73,74                 | 0     |
| 3   | HEC  | M     | 600 | 43/43 | 0.97 | 0.21 | 44,48,56,62                 | 0     |
| 3   | HEC  | T     | 603 | 43/43 | 0.97 | 0.23 | 60,66,71,73                 | 0     |
| 4   | SO4  | I     | 610 | 5/5   | 0.97 | 0.11 | 67,67,69,69                 | 0     |
| 3   | HEC  | R     | 600 | 43/43 | 0.97 | 0.21 | 49,54,62,64                 | 0     |
| 4   | SO4  | G     | 613 | 5/5   | 0.97 | 0.18 | 63,63,64,66                 | 0     |
| 3   | HEC  | G     | 600 | 43/43 | 0.97 | 0.21 | 40,42,45,49                 | 0     |
| 3   | HEC  | X     | 601 | 43/43 | 0.97 | 0.23 | 62,69,78,82                 | 0     |
| 3   | HEC  | R     | 602 | 43/43 | 0.97 | 0.24 | 45,48,74,89                 | 0     |
| 3   | HEC  | A     | 602 | 43/43 | 0.97 | 0.23 | 51,56,79,99                 | 0     |
| 3   | HEC  | F     | 604 | 43/43 | 0.97 | 0.23 | 58,65,74,84                 | 0     |
| 3   | HEC  | R     | 604 | 43/43 | 0.97 | 0.21 | 38,43,53,61                 | 0     |
| 3   | HEC  | X     | 607 | 43/43 | 0.97 | 0.23 | 57,61,65,67                 | 0     |
| 3   | HEC  | F     | 600 | 43/43 | 0.97 | 0.21 | 46,52,62,68                 | 0     |
| 3   | HEC  | P     | 601 | 43/43 | 0.97 | 0.22 | 39,44,46,47                 | 0     |
| 3   | HEC  | G     | 601 | 43/43 | 0.97 | 0.21 | 37,41,43,48                 | 0     |
| 3   | HEC  | P     | 603 | 43/43 | 0.97 | 0.23 | 40,49,56,62                 | 0     |
| 3   | HEC  | W     | 600 | 43/43 | 0.97 | 0.23 | 61,68,74,77                 | 0     |
| 3   | HEC  | K     | 602 | 43/43 | 0.97 | 0.22 | 44,47,65,81                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | HEC  | E     | 601 | 43/43 | 0.97 | 0.22 | 39,43,47,55                 | 0     |
| 3   | HEC  | A     | 605 | 43/43 | 0.97 | 0.26 | 50,59,63,64                 | 0     |
| 3   | HEC  | S     | 606 | 43/43 | 0.97 | 0.26 | 61,69,74,79                 | 0     |
| 3   | HEC  | L     | 604 | 43/43 | 0.97 | 0.22 | 35,41,48,58                 | 0     |
| 3   | HEC  | V     | 605 | 43/43 | 0.97 | 0.26 | 56,65,73,76                 | 0     |
| 3   | HEC  | G     | 603 | 43/43 | 0.98 | 0.20 | 34,36,39,42                 | 0     |
| 3   | HEC  | H     | 604 | 43/43 | 0.98 | 0.21 | 38,43,53,64                 | 0     |
| 3   | HEC  | Q     | 603 | 43/43 | 0.98 | 0.23 | 52,55,58,59                 | 0     |
| 3   | HEC  | O     | 607 | 43/43 | 0.98 | 0.23 | 34,37,38,39                 | 0     |
| 3   | HEC  | J     | 607 | 43/43 | 0.98 | 0.22 | 28,30,33,37                 | 0     |
| 3   | HEC  | I     | 603 | 43/43 | 0.98 | 0.21 | 30,33,37,39                 | 0     |
| 3   | HEC  | B     | 605 | 43/43 | 0.98 | 0.22 | 42,45,53,59                 | 0     |
| 3   | HEC  | P     | 600 | 43/43 | 0.98 | 0.20 | 44,46,51,53                 | 0     |
| 3   | HEC  | R     | 605 | 43/43 | 0.98 | 0.19 | 35,40,45,46                 | 0     |
| 3   | HEC  | G     | 607 | 43/43 | 0.98 | 0.21 | 30,31,34,34                 | 0     |
| 3   | HEC  | P     | 605 | 43/43 | 0.98 | 0.23 | 43,46,49,50                 | 0     |
| 3   | HEC  | O     | 605 | 43/43 | 0.98 | 0.21 | 36,41,49,52                 | 0     |
| 3   | HEC  | T     | 601 | 43/43 | 0.98 | 0.22 | 55,58,61,63                 | 0     |
| 3   | HEC  | N     | 605 | 43/43 | 0.98 | 0.24 | 48,52,66,73                 | 0     |
| 3   | HEC  | R     | 607 | 43/43 | 0.98 | 0.22 | 37,38,43,48                 | 0     |
| 3   | HEC  | J     | 605 | 43/43 | 0.98 | 0.23 | 32,38,43,47                 | 0     |
| 3   | HEC  | N     | 604 | 43/43 | 0.98 | 0.23 | 42,47,56,59                 | 0     |
| 3   | HEC  | H     | 605 | 43/43 | 0.98 | 0.23 | 28,32,34,35                 | 0     |
| 3   | HEC  | A     | 601 | 43/43 | 0.98 | 0.23 | 44,47,53,54                 | 0     |
| 3   | HEC  | I     | 604 | 43/43 | 0.98 | 0.22 | 36,38,51,58                 | 0     |
| 3   | HEC  | J     | 606 | 43/43 | 0.98 | 0.23 | 33,39,41,46                 | 0     |
| 3   | HEC  | Q     | 605 | 43/43 | 0.98 | 0.24 | 45,51,57,60                 | 0     |
| 3   | HEC  | H     | 603 | 43/43 | 0.98 | 0.22 | 31,34,42,48                 | 0     |
| 3   | HEC  | I     | 605 | 43/43 | 0.98 | 0.23 | 29,33,38,40                 | 0     |
| 3   | HEC  | N     | 603 | 43/43 | 0.98 | 0.20 | 47,56,60,62                 | 0     |
| 3   | HEC  | B     | 606 | 43/43 | 0.98 | 0.23 | 39,42,50,57                 | 0     |
| 3   | HEC  | L     | 605 | 43/43 | 0.98 | 0.23 | 35,37,41,45                 | 0     |
| 3   | HEC  | D     | 601 | 43/43 | 0.98 | 0.23 | 51,59,61,62                 | 0     |
| 3   | HEC  | D     | 606 | 43/43 | 0.98 | 0.27 | 46,51,62,66                 | 0     |
| 3   | HEC  | G     | 605 | 43/43 | 0.98 | 0.22 | 33,36,41,43                 | 0     |
| 3   | HEC  | C     | 601 | 43/43 | 0.98 | 0.23 | 41,45,50,51                 | 0     |
| 3   | HEC  | I     | 606 | 43/43 | 0.98 | 0.22 | 34,35,44,47                 | 0     |
| 3   | HEC  | C     | 606 | 43/43 | 0.98 | 0.22 | 41,43,59,65                 | 0     |
| 3   | HEC  | K     | 601 | 43/43 | 0.98 | 0.20 | 33,34,38,43                 | 0     |
| 3   | HEC  | R     | 601 | 43/43 | 0.98 | 0.23 | 43,48,50,50                 | 0     |
| 3   | HEC  | H     | 601 | 43/43 | 0.98 | 0.21 | 34,36,41,47                 | 0     |
| 3   | HEC  | O     | 606 | 43/43 | 0.98 | 0.21 | 37,41,49,52                 | 0     |

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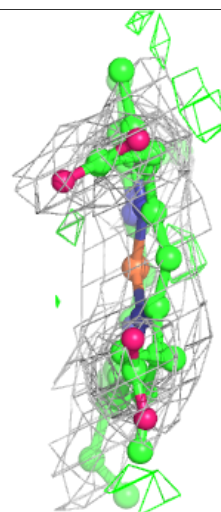
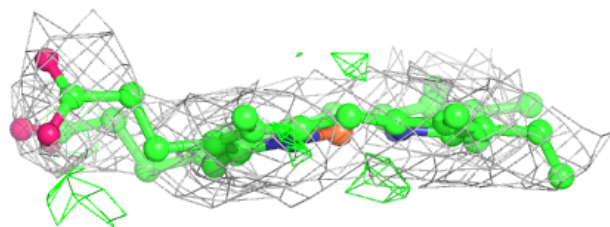
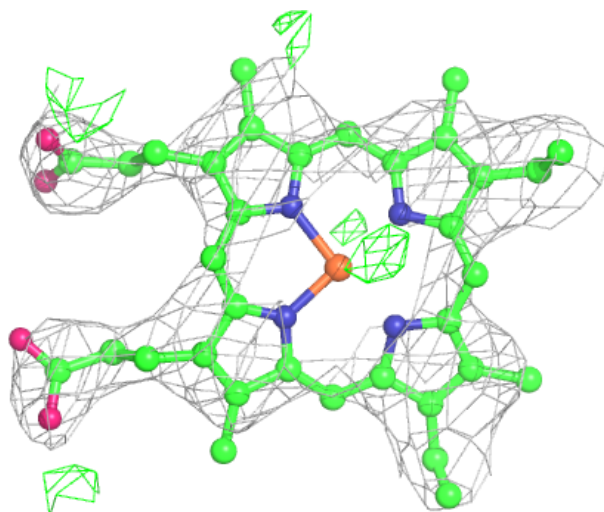
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | HEC  | I     | 600 | 43/43 | 0.98 | 0.21 | 39,43,50,52                 | 0     |
| 3   | HEC  | I     | 607 | 43/43 | 0.98 | 0.21 | 32,34,36,38                 | 0     |
| 3   | HEC  | H     | 600 | 43/43 | 0.98 | 0.20 | 32,37,42,44                 | 0     |
| 3   | HEC  | M     | 606 | 43/43 | 0.98 | 0.25 | 37,40,50,55                 | 0     |
| 3   | HEC  | H     | 606 | 43/43 | 0.98 | 0.22 | 32,34,39,44                 | 0     |
| 3   | HEC  | I     | 601 | 43/43 | 0.98 | 0.21 | 35,37,41,44                 | 0     |
| 3   | HEC  | M     | 601 | 43/43 | 0.98 | 0.23 | 41,44,47,51                 | 0     |
| 3   | HEC  | L     | 607 | 43/43 | 0.98 | 0.23 | 32,34,35,36                 | 0     |
| 3   | HEC  | B     | 603 | 43/43 | 0.98 | 0.20 | 45,49,53,54                 | 0     |
| 3   | HEC  | G     | 606 | 43/43 | 0.98 | 0.21 | 35,37,42,46                 | 0     |
| 3   | HEC  | B     | 601 | 43/43 | 0.98 | 0.21 | 43,47,56,68                 | 0     |
| 3   | HEC  | J     | 604 | 43/43 | 0.98 | 0.20 | 32,35,44,55                 | 0     |
| 3   | HEC  | O     | 600 | 43/43 | 0.98 | 0.21 | 44,48,58,60                 | 0     |
| 3   | HEC  | D     | 604 | 43/43 | 0.98 | 0.21 | 44,47,54,60                 | 0     |
| 3   | HEC  | K     | 607 | 43/43 | 0.98 | 0.21 | 30,32,34,36                 | 0     |
| 3   | HEC  | L     | 603 | 43/43 | 0.98 | 0.24 | 35,41,50,52                 | 0     |
| 3   | HEC  | K     | 603 | 43/43 | 0.98 | 0.20 | 37,39,42,44                 | 0     |
| 4   | SO4  | U     | 609 | 5/5   | 0.98 | 0.18 | 57,58,60,64                 | 0     |
| 3   | HEC  | D     | 607 | 43/43 | 0.98 | 0.23 | 40,45,55,61                 | 0     |
| 4   | SO4  | V     | 609 | 5/5   | 0.98 | 0.20 | 56,59,60,62                 | 0     |
| 3   | HEC  | R     | 606 | 43/43 | 0.98 | 0.22 | 37,43,59,63                 | 0     |
| 3   | HEC  | J     | 601 | 43/43 | 0.98 | 0.21 | 34,37,41,47                 | 0     |
| 3   | HEC  | L     | 606 | 43/43 | 0.98 | 0.21 | 35,37,43,47                 | 0     |
| 3   | HEC  | J     | 603 | 43/43 | 0.98 | 0.20 | 37,39,44,46                 | 0     |
| 3   | HEC  | B     | 607 | 43/43 | 0.98 | 0.23 | 37,40,45,47                 | 0     |
| 3   | HEC  | K     | 605 | 43/43 | 0.98 | 0.23 | 35,38,43,48                 | 0     |
| 3   | HEC  | D     | 603 | 43/43 | 0.98 | 0.22 | 54,66,69,72                 | 0     |
| 3   | HEC  | H     | 607 | 43/43 | 0.98 | 0.21 | 28,30,32,35                 | 0     |
| 3   | HEC  | N     | 607 | 43/43 | 0.98 | 0.20 | 37,41,44,46                 | 0     |
| 3   | HEC  | K     | 606 | 43/43 | 0.98 | 0.23 | 33,39,42,46                 | 0     |
| 4   | SO4  | I     | 609 | 5/5   | 0.99 | 0.22 | 28,28,29,30                 | 0     |
| 4   | SO4  | K     | 609 | 5/5   | 0.99 | 0.23 | 28,28,29,30                 | 0     |
| 4   | SO4  | N     | 609 | 5/5   | 0.99 | 0.20 | 40,40,41,42                 | 0     |
| 4   | SO4  | R     | 609 | 5/5   | 0.99 | 0.20 | 36,39,40,40                 | 0     |
| 4   | SO4  | A     | 609 | 5/5   | 0.99 | 0.21 | 47,49,49,52                 | 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.

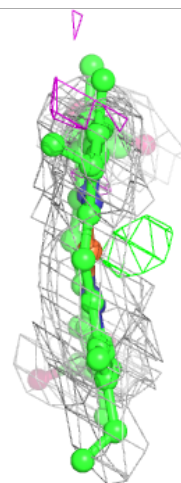
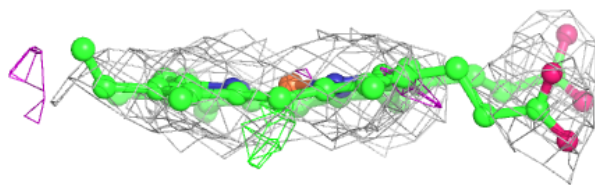
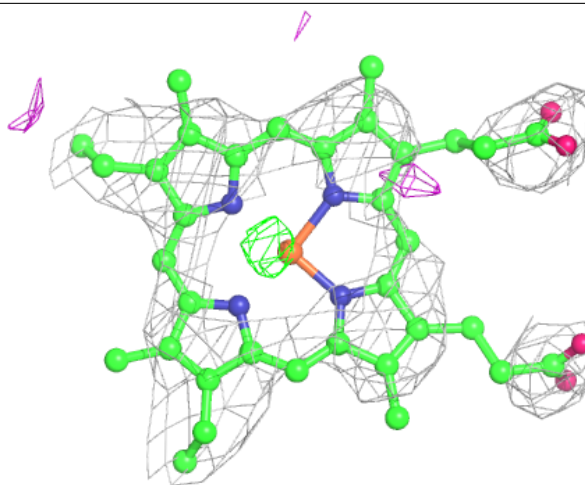
**Electron density around HEC X 606:**

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



**Electron density around HEC X 605:**

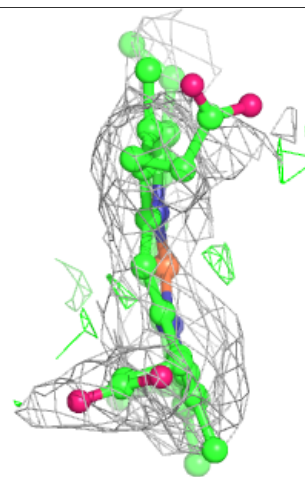
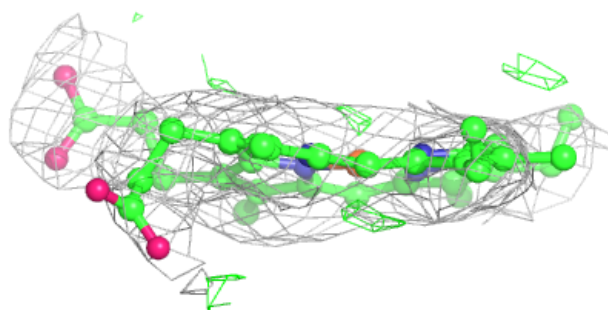
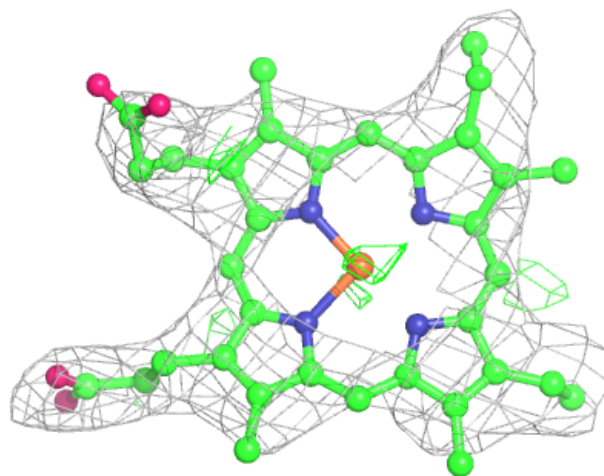
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





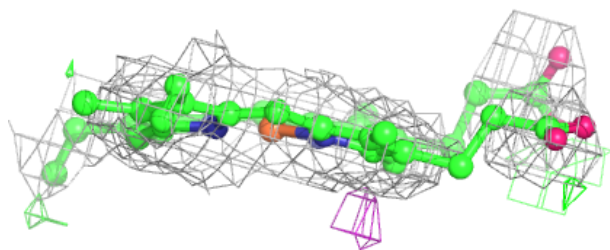
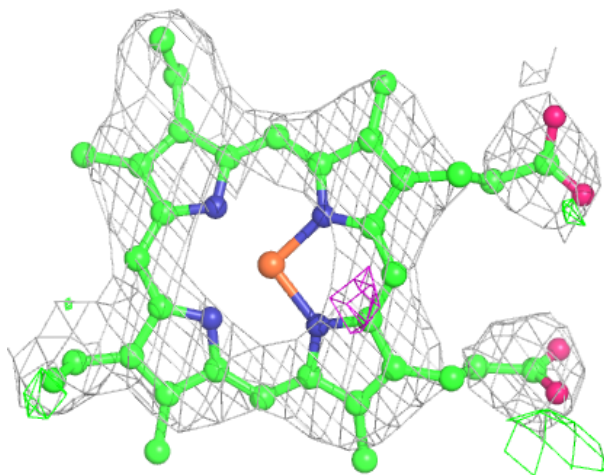
**Electron density around HEC V 602:**

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



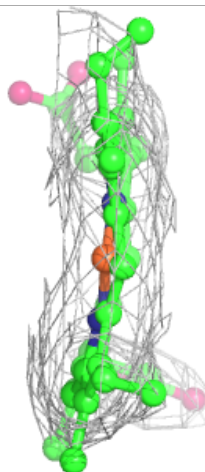
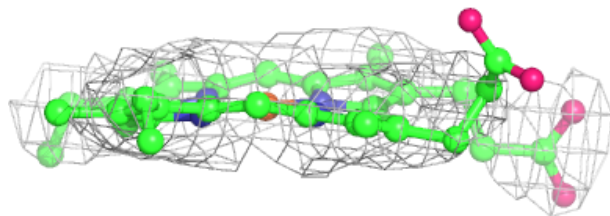
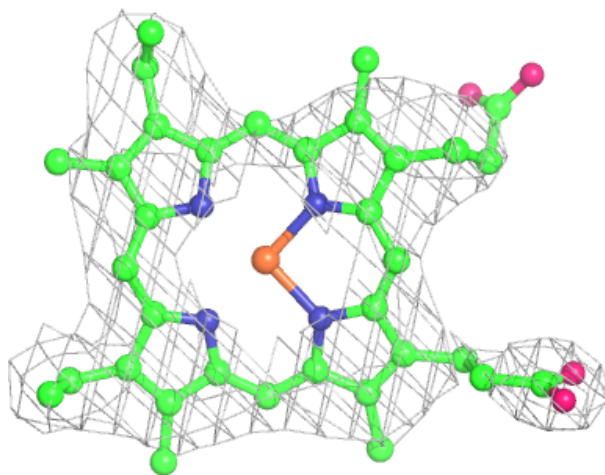
**Electron density around HEC A 606:**

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



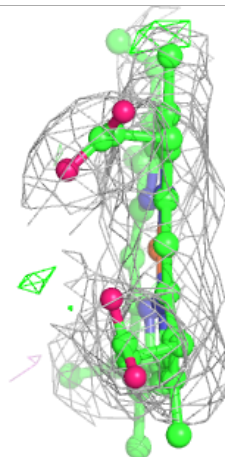
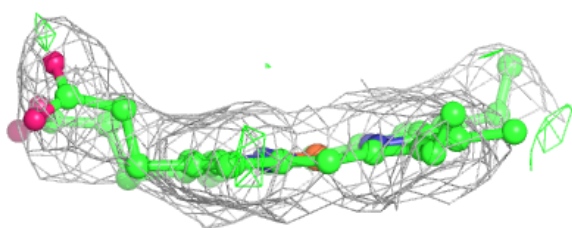
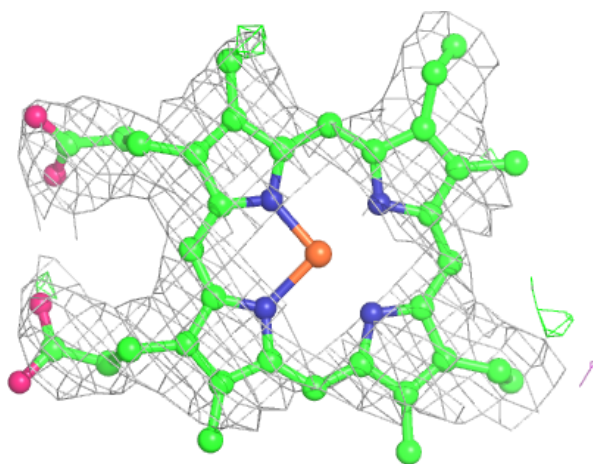
**Electron density around HEC U 602:**

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



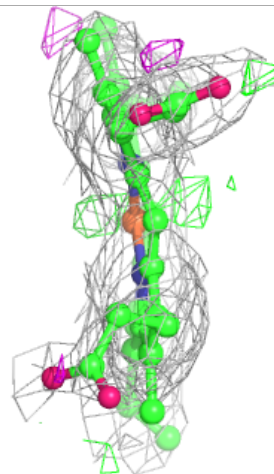
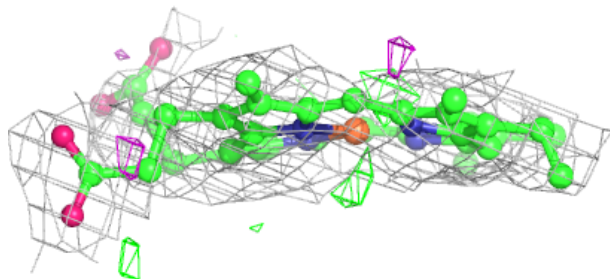
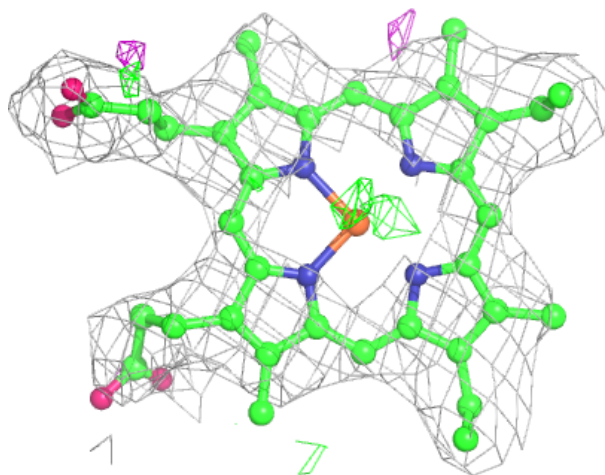
**Electron density around HEC S 604:**

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



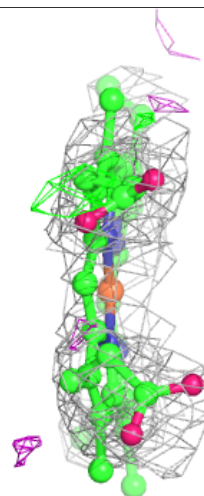
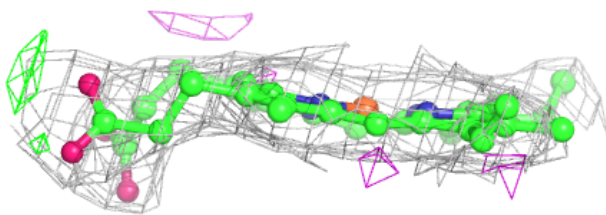
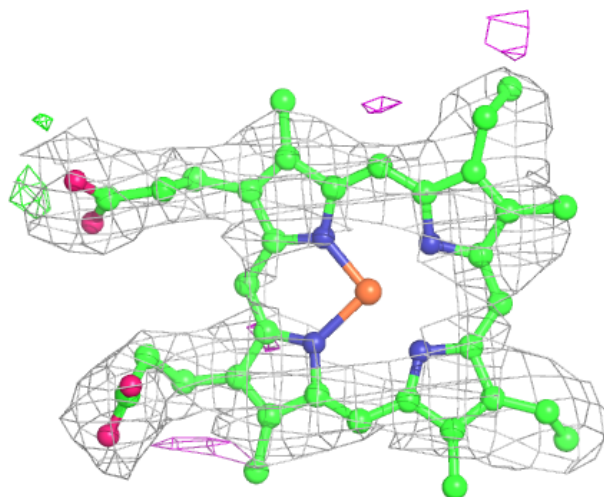
**Electron density around HEC H 602:**

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



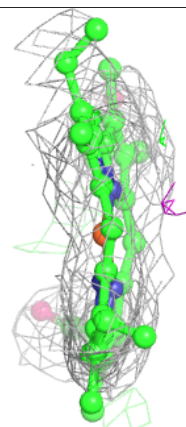
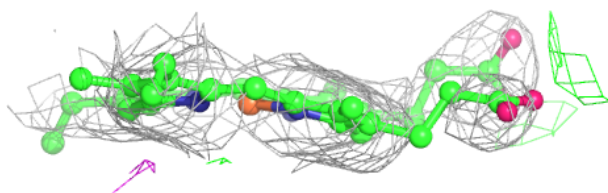
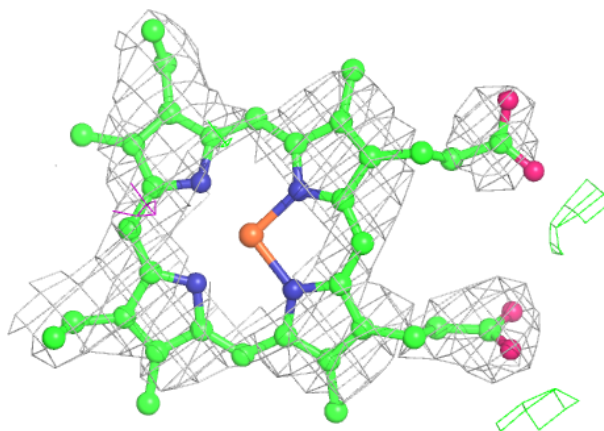
**Electron density around HEC T 607:**

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



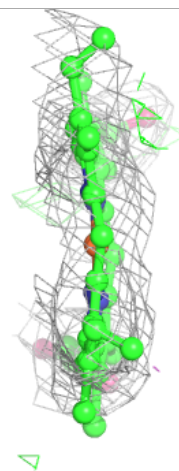
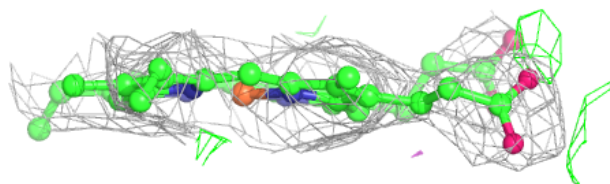
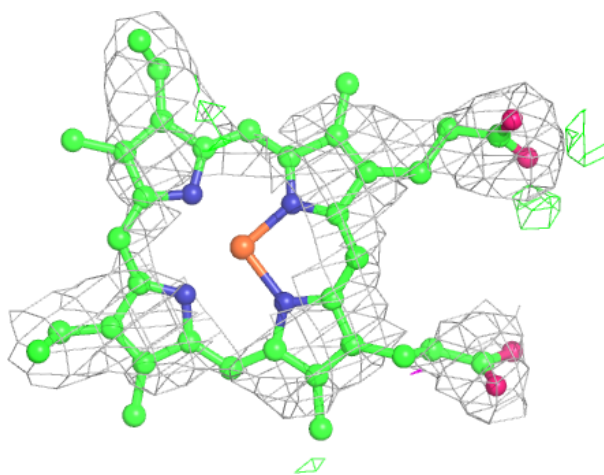
**Electron density around HEC U 606:**

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



**Electron density around HEC W 605:**

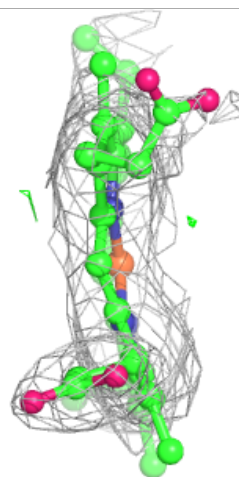
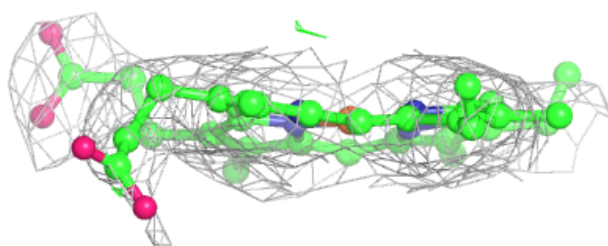
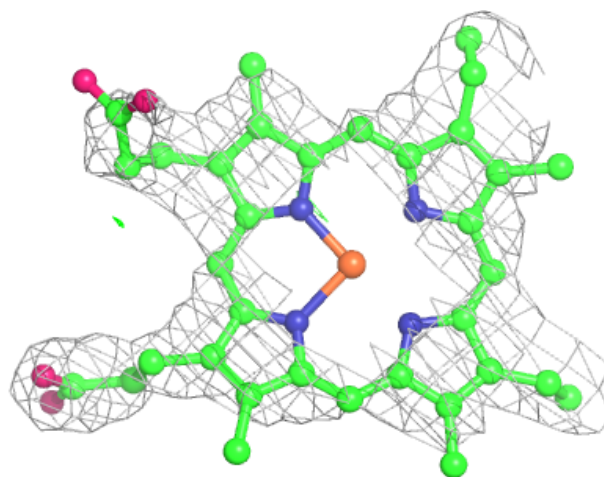
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





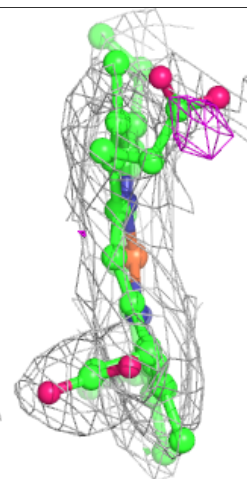
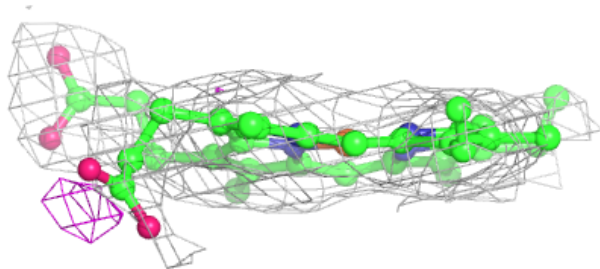
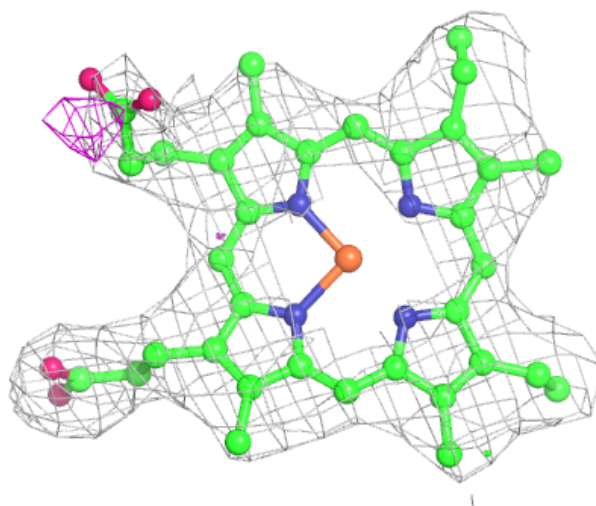
**Electron density around HEC X 602:**

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



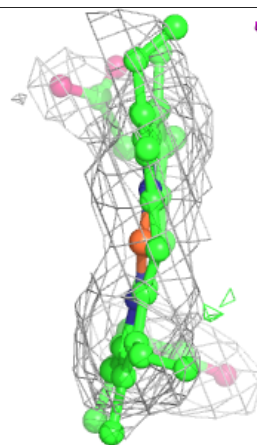
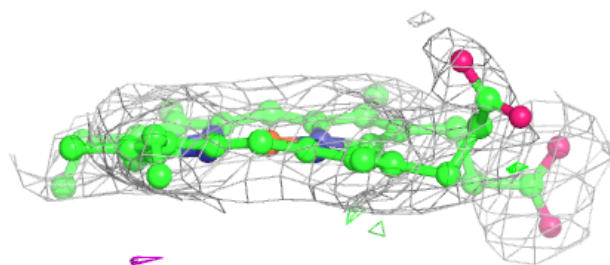
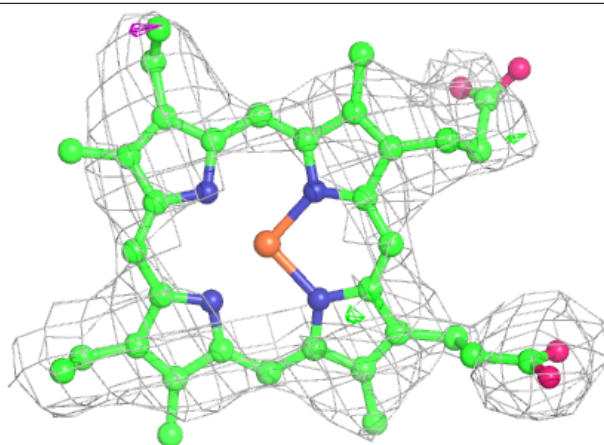
**Electron density around HEC P 602:**

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



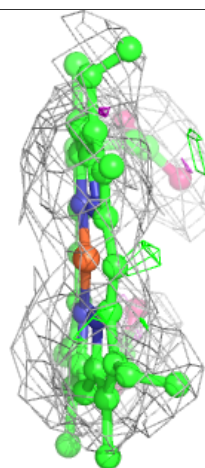
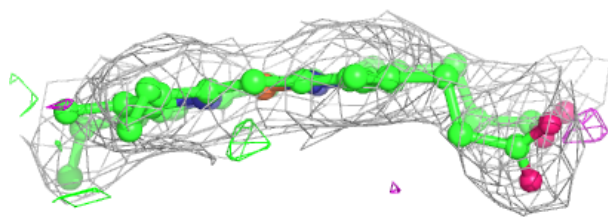
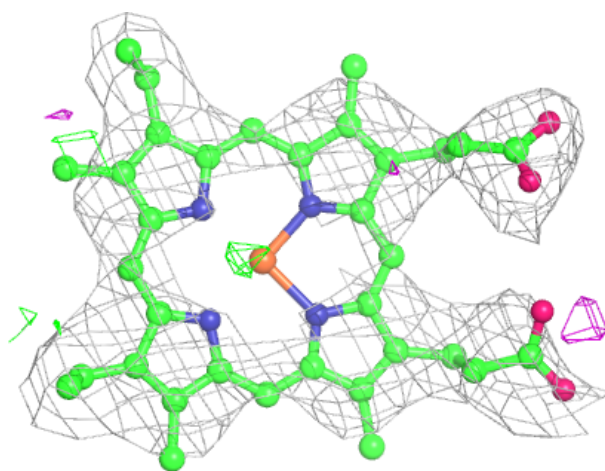
**Electron density around HEC T 602:**

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



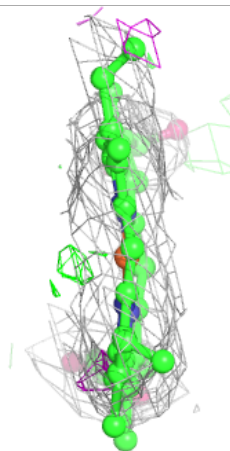
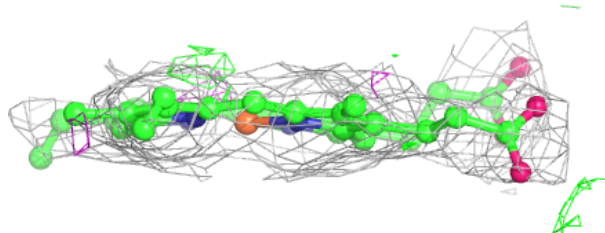
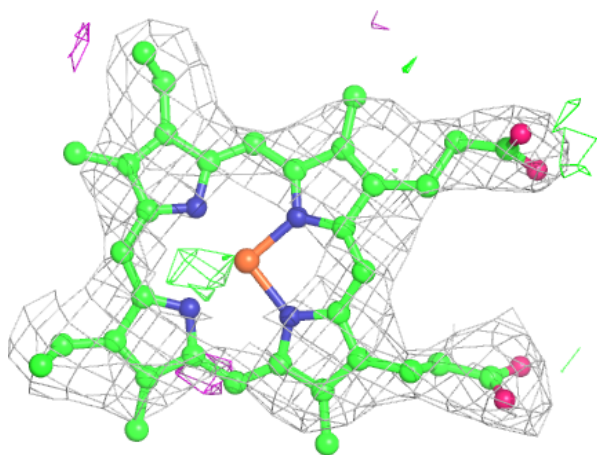
**Electron density around HEC Q 604:**

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



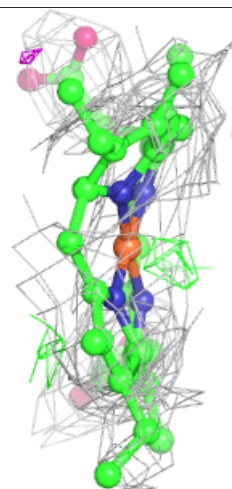
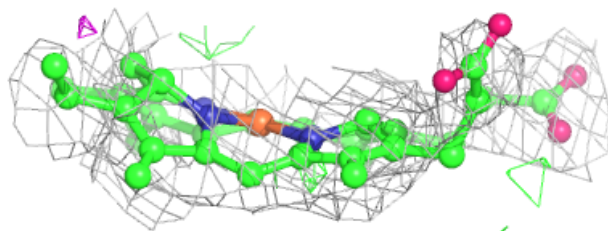
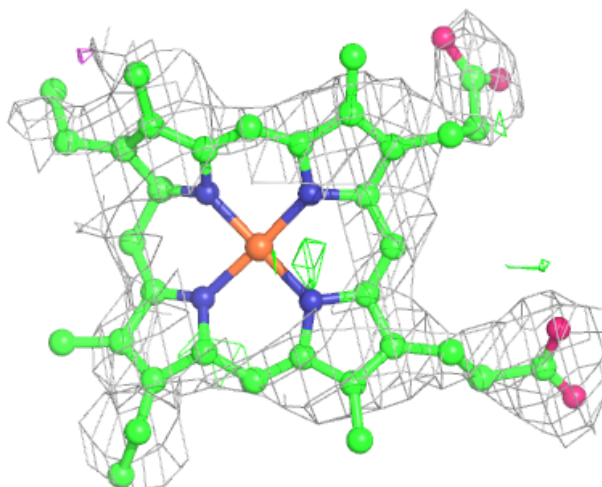
**Electron density around HEC E 605:**

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



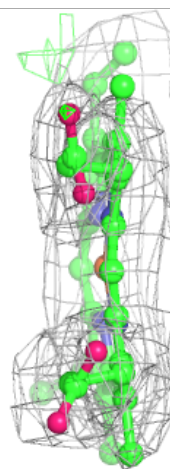
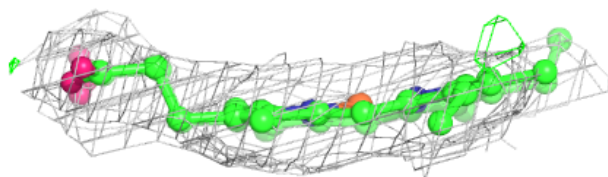
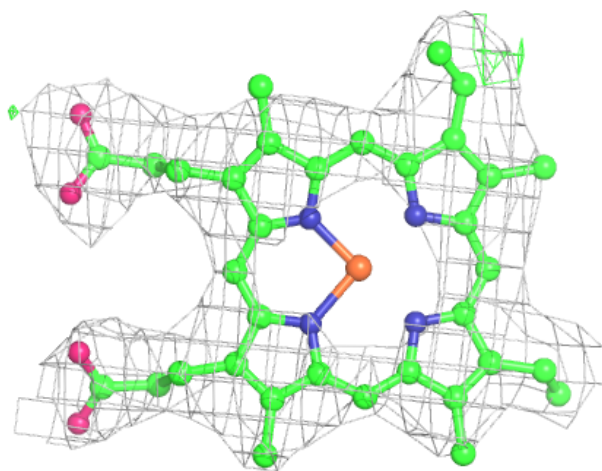
**Electron density around HEC W 603:**

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



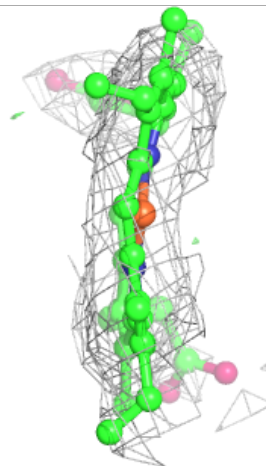
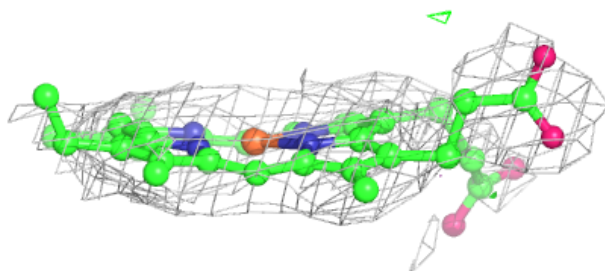
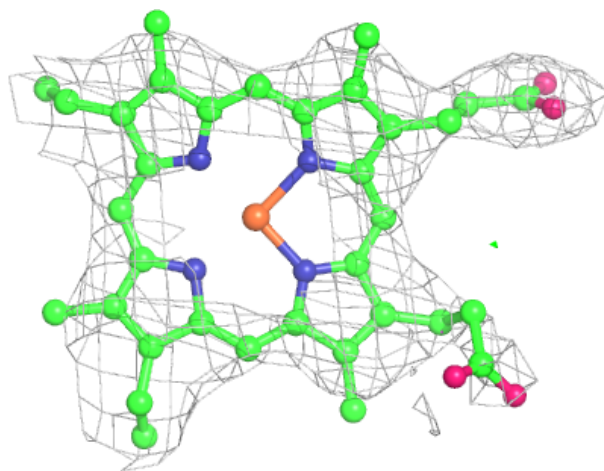
**Electron density around HEC U 600:**

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



**Electron density around HEC Q 602:**

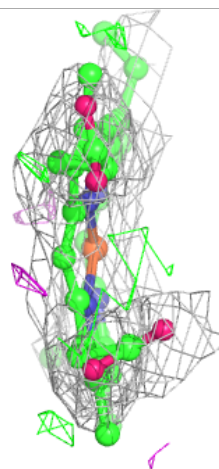
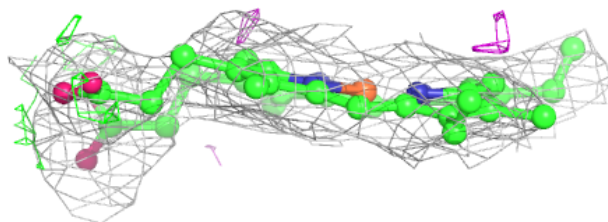
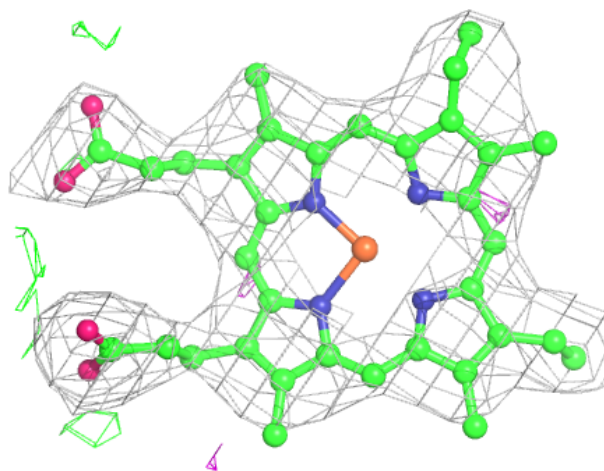
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





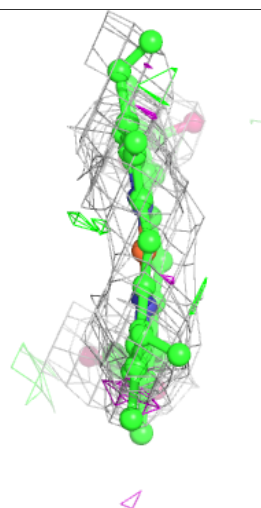
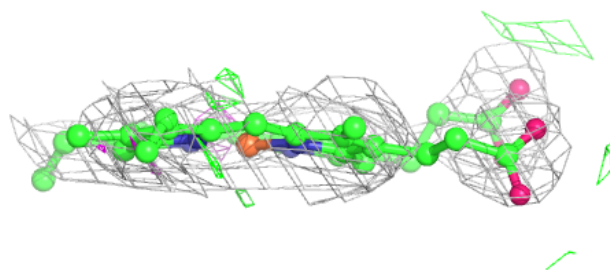
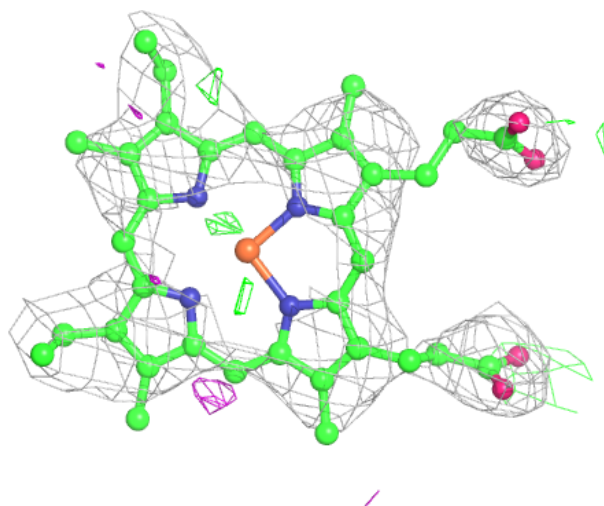
**Electron density around HEC N 606:**

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



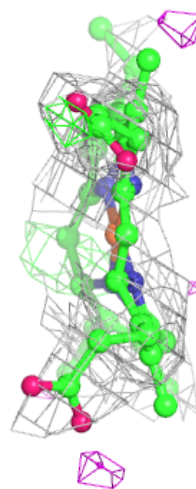
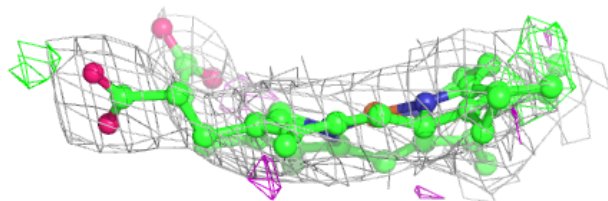
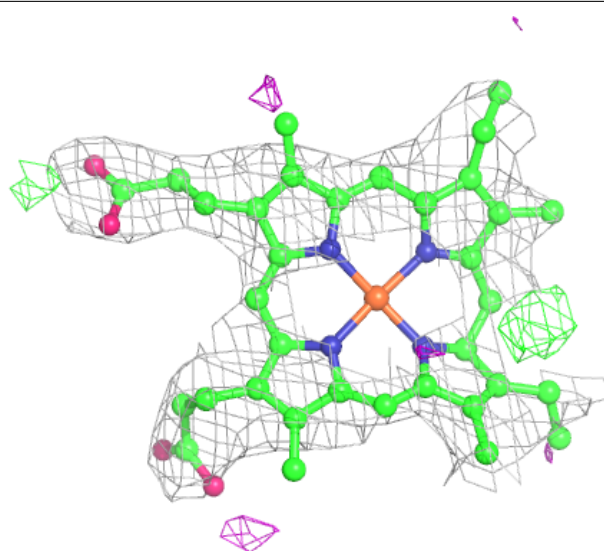
**Electron density around HEC S 605:**

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



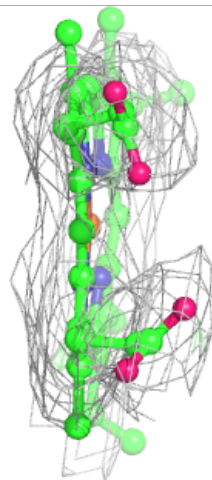
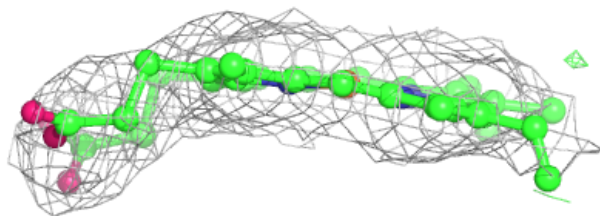
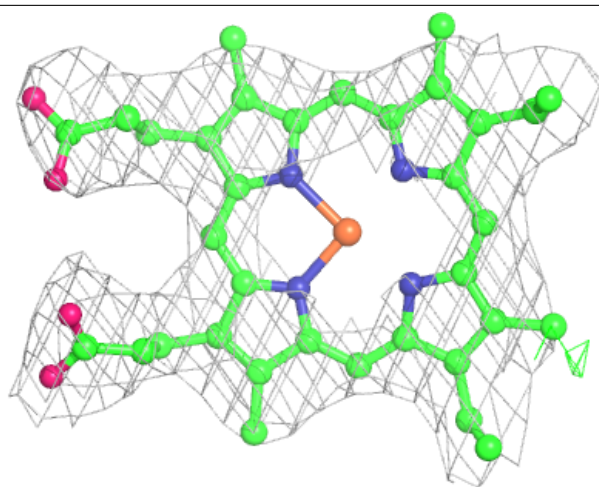
**Electron density around HEC V 603:**

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



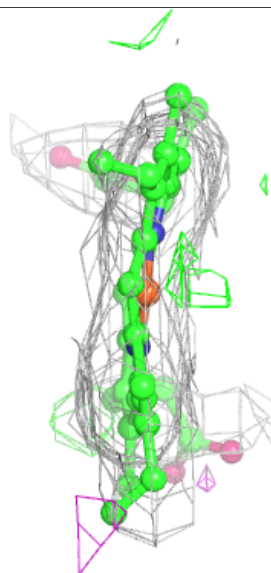
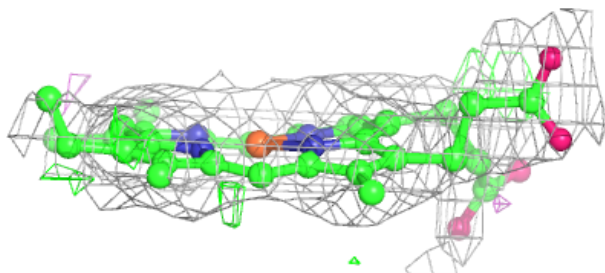
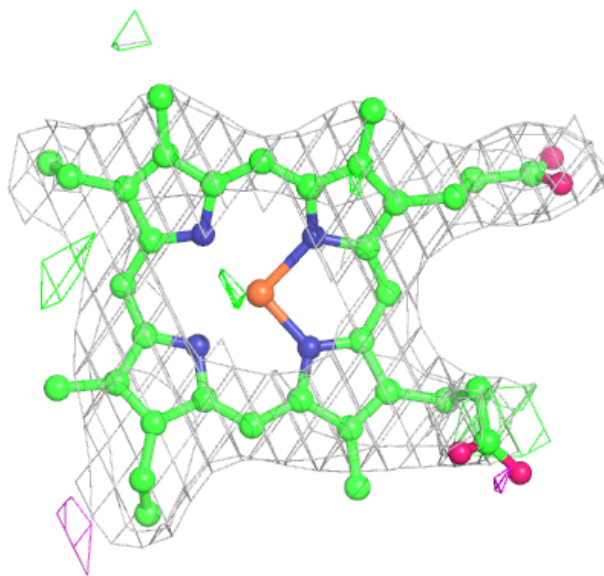
**Electron density around HEC U 604:**

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



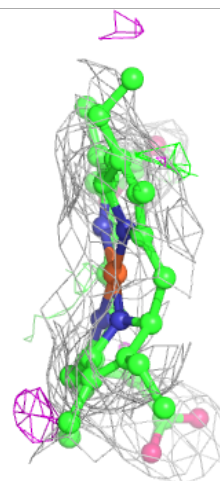
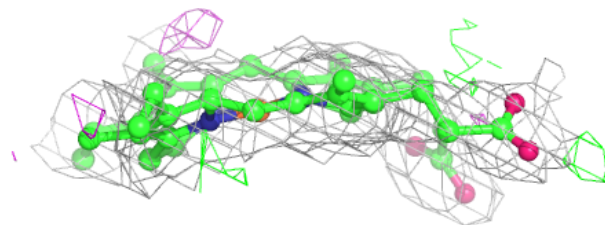
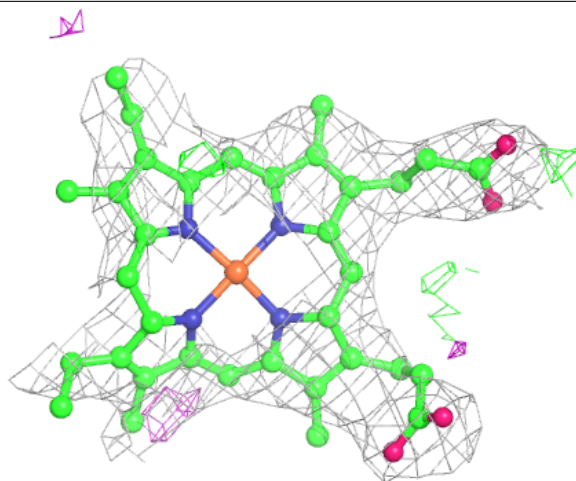
**Electron density around HEC B 602:**

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



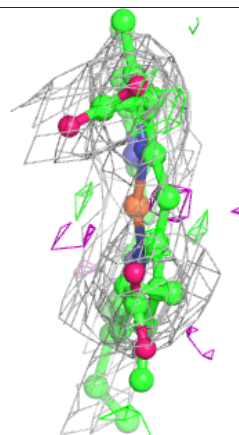
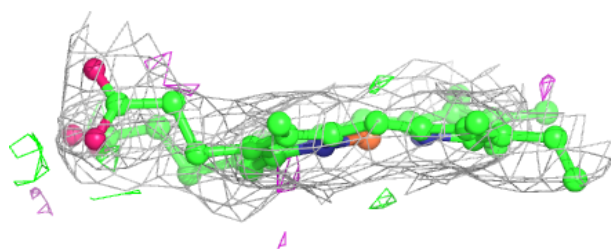
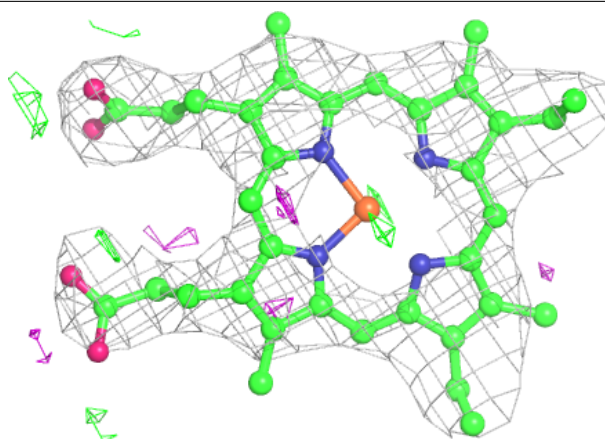
**Electron density around HEC F 603:**

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



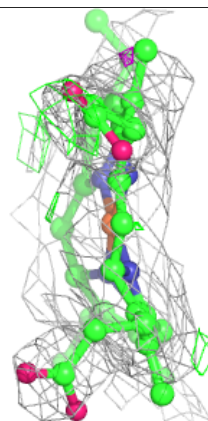
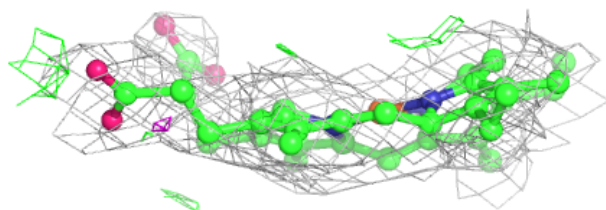
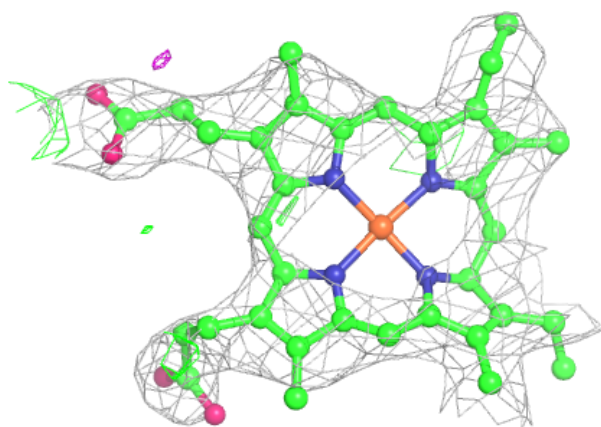
**Electron density around HEC E 606:**

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



**Electron density around HEC S 603:**

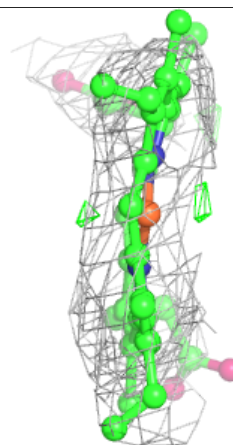
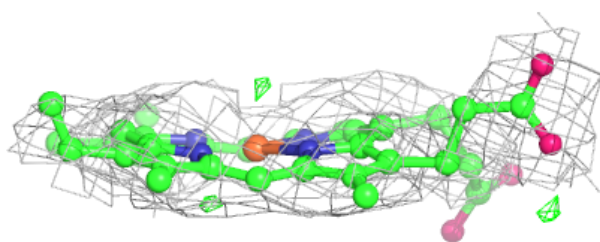
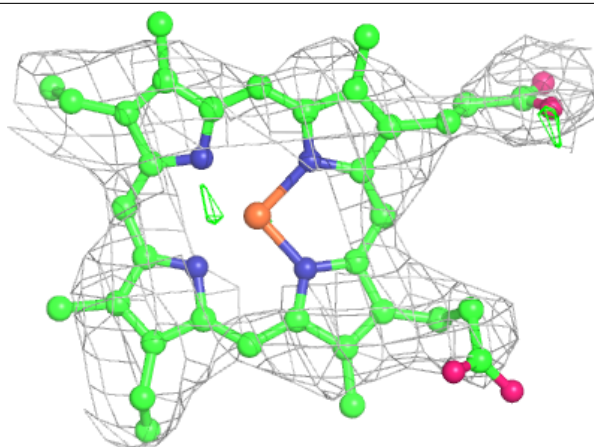
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





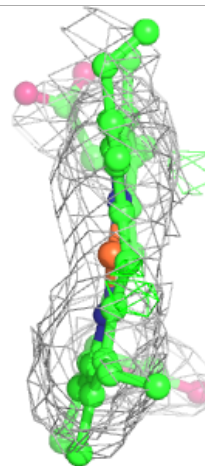
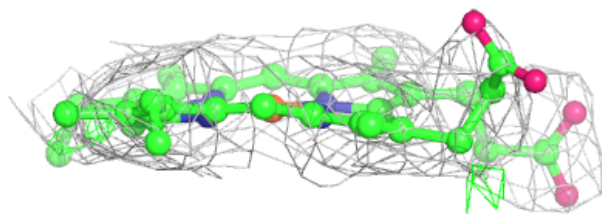
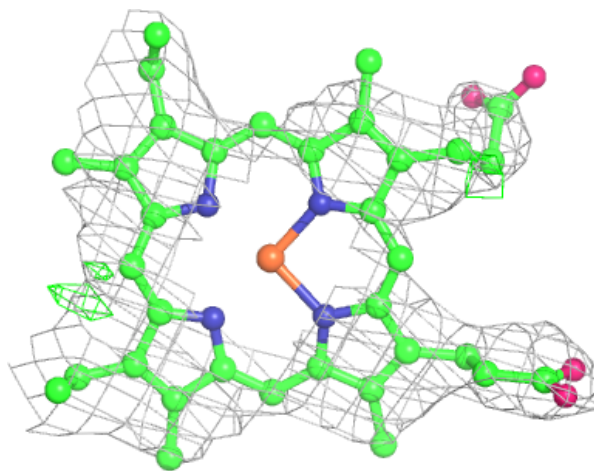
**Electron density around HEC F 602:**

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



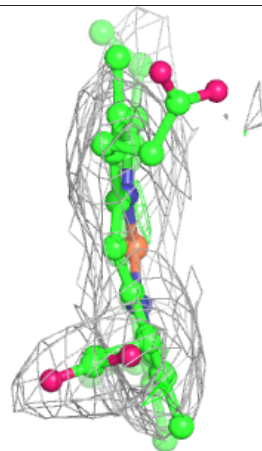
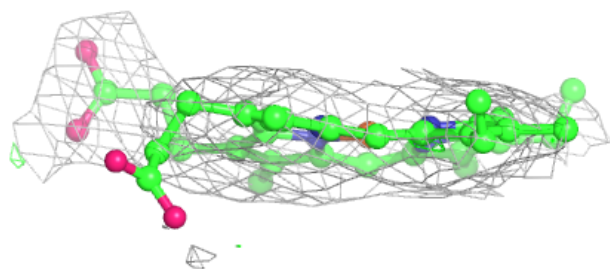
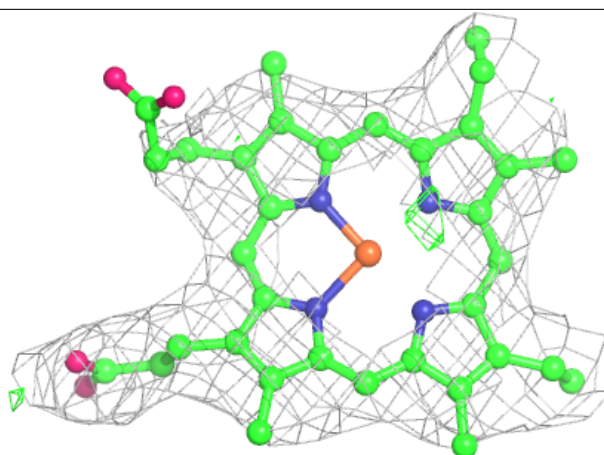
**Electron density around HEC S 602:**

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



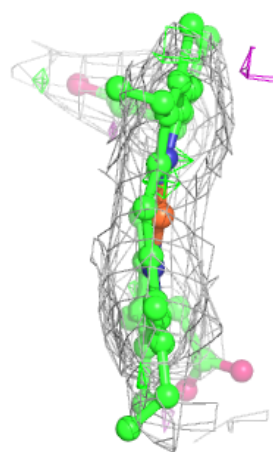
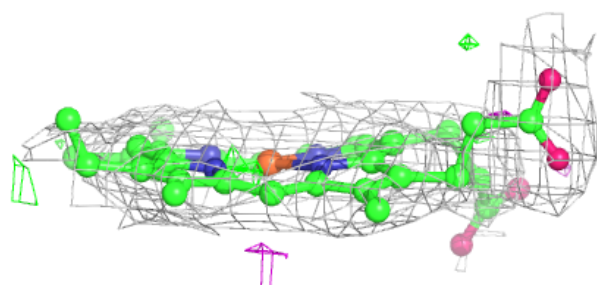
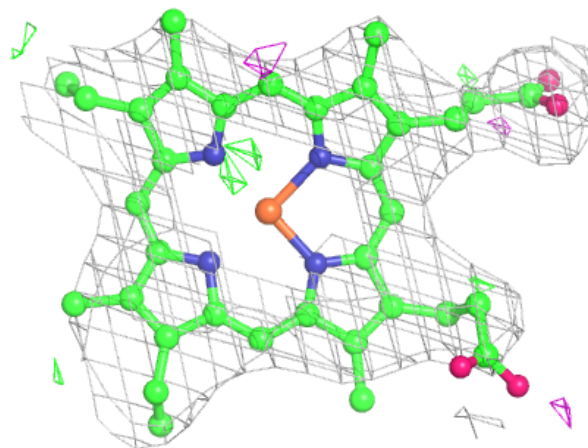
**Electron density around HEC W 602:**

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



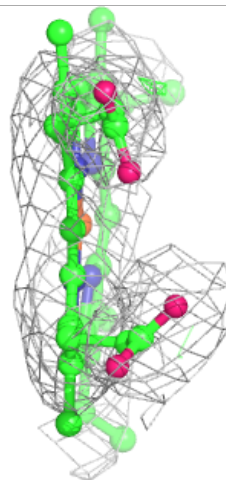
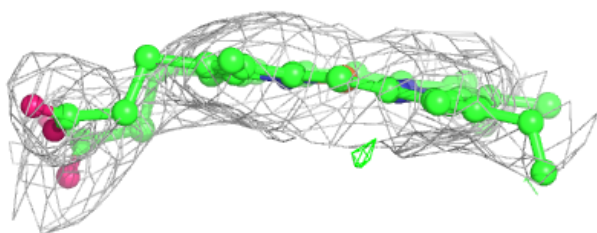
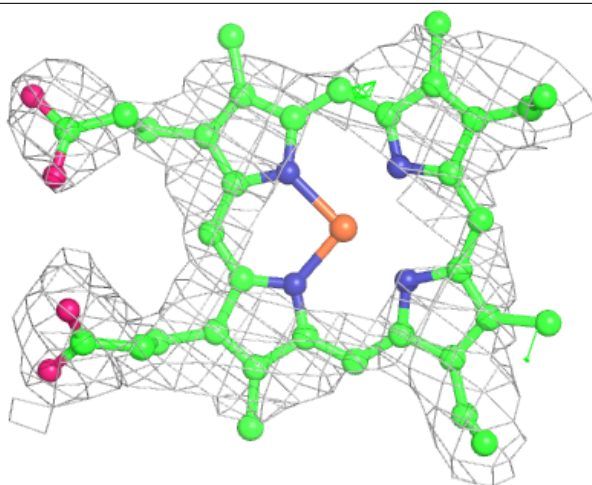
**Electron density around HEC E 602:**

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



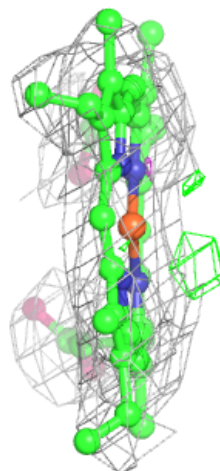
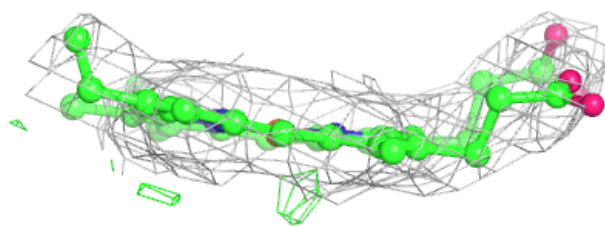
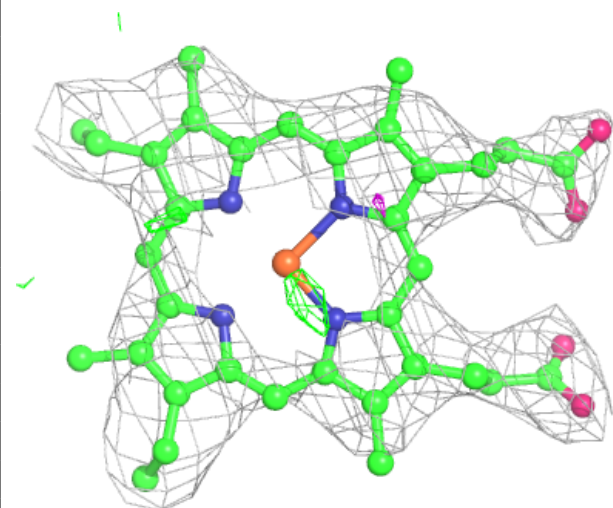
**Electron density around HEC X 604:**

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



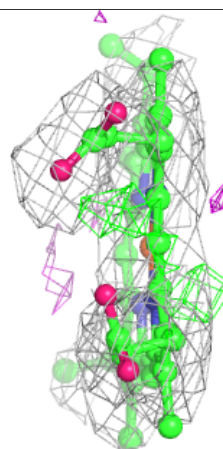
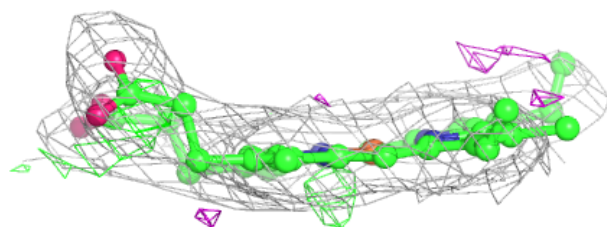
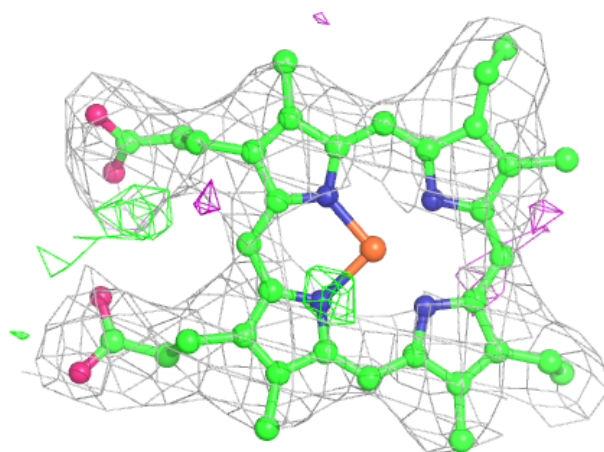
**Electron density around HEC V 604:**

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



**Electron density around HEC A 604:**

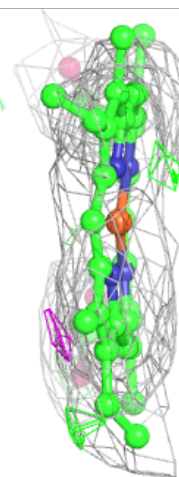
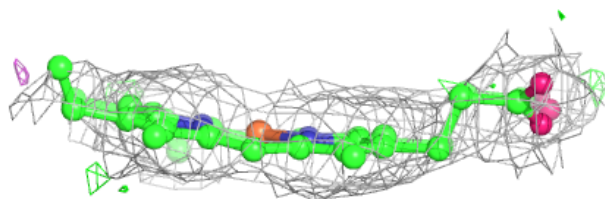
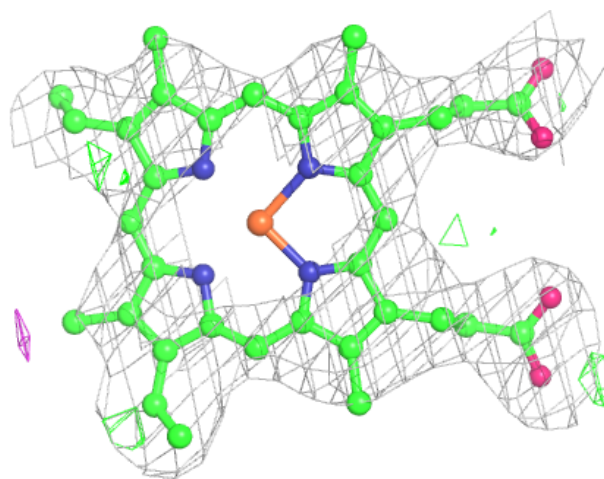
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC C 600:**

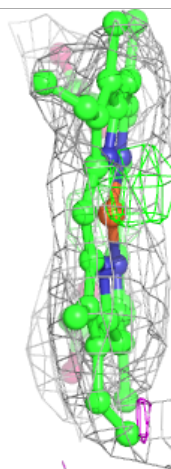
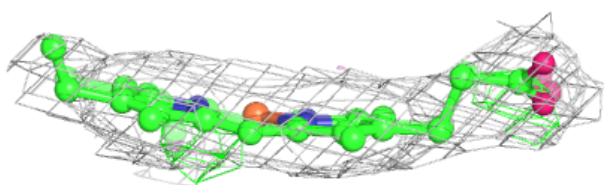
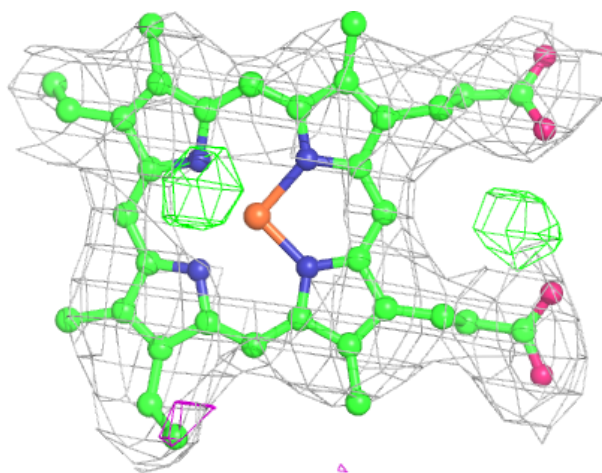
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





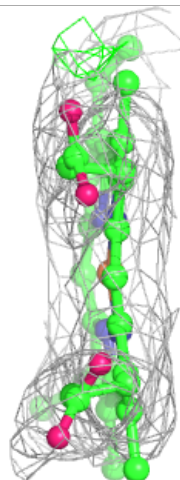
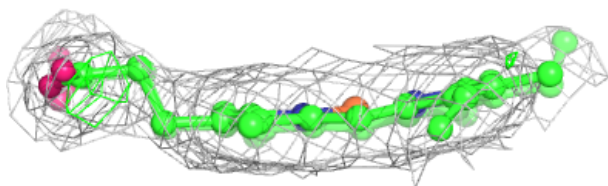
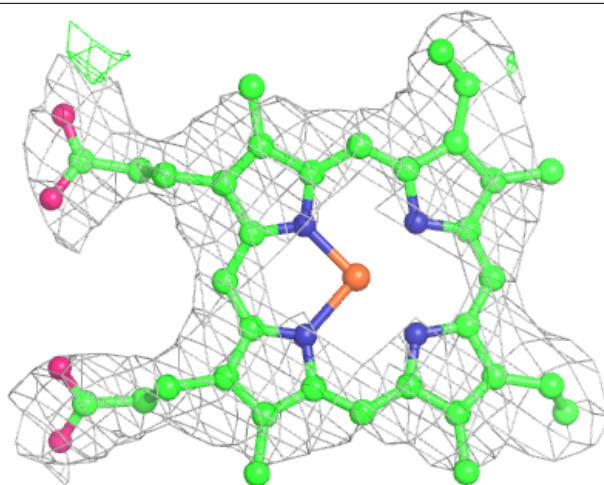
**Electron density around HEC E 600:**

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



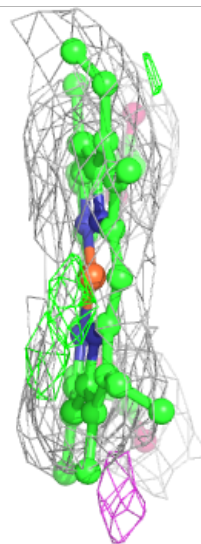
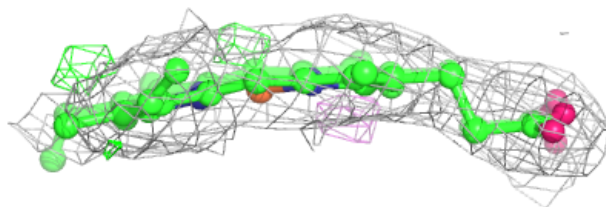
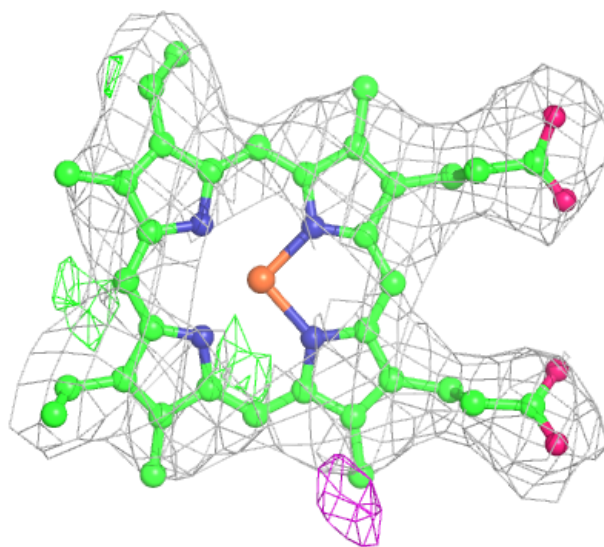
**Electron density around HEC T 600:**

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



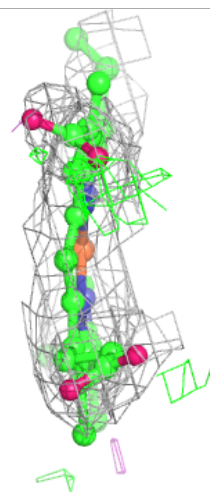
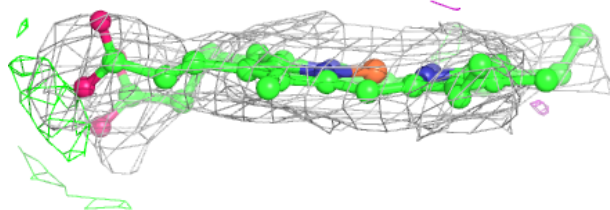
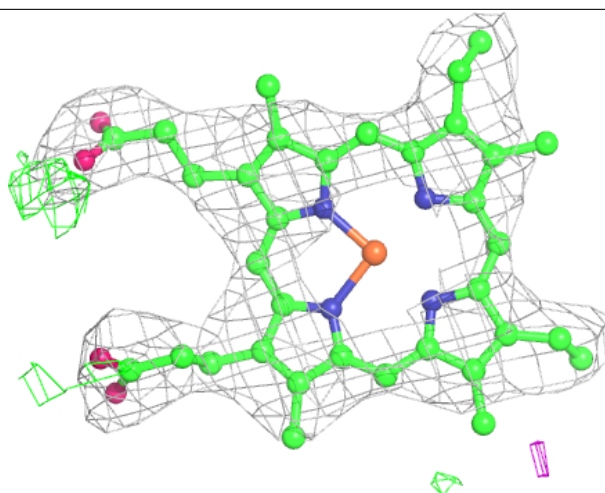
**Electron density around HEC L 600:**

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



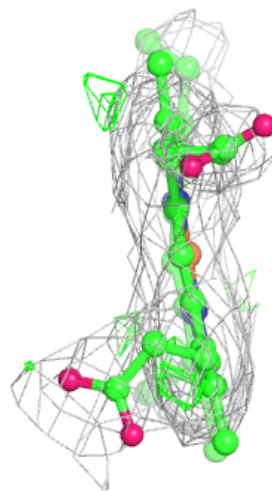
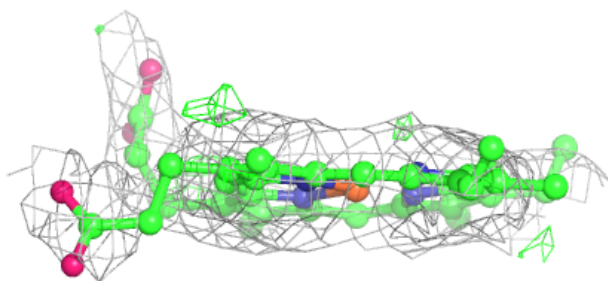
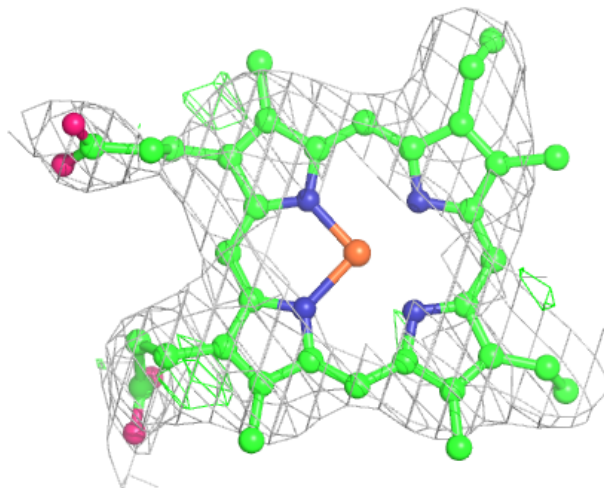
**Electron density around HEC F 605:**

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



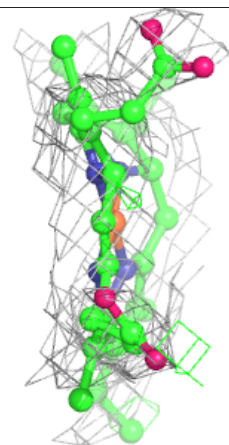
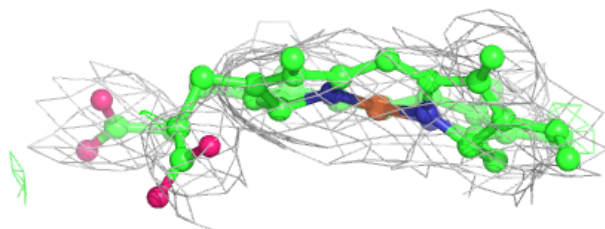
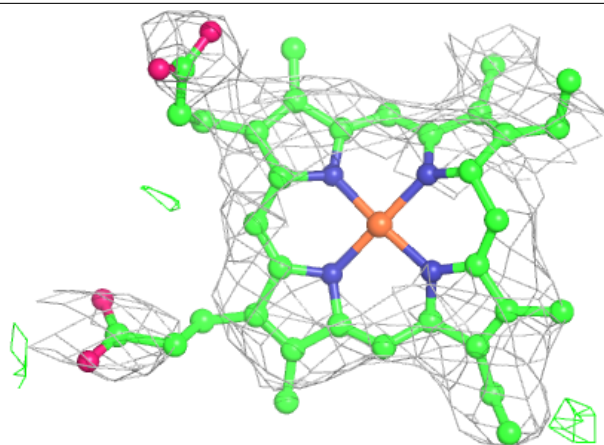
**Electron density around HEC S 601:**

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



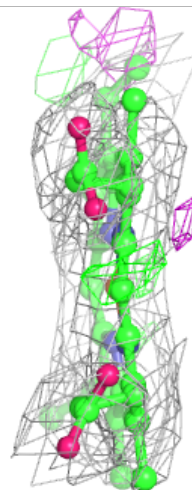
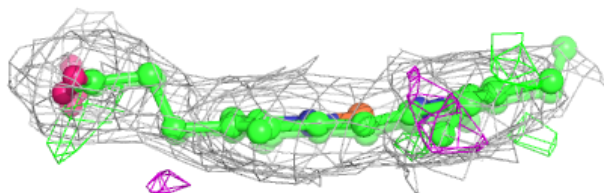
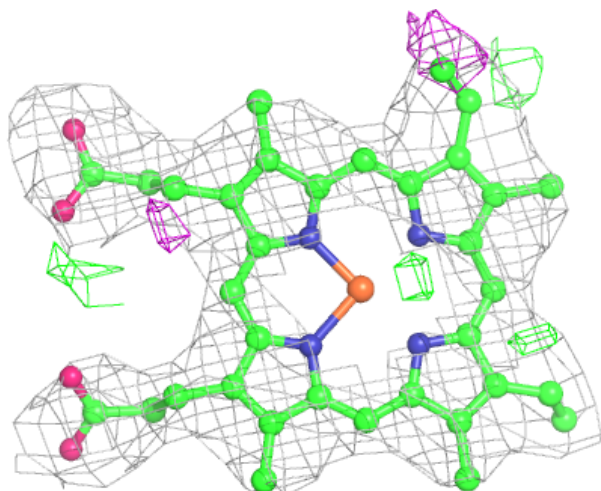
**Electron density around HEC X 603:**

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



**Electron density around HEC K 600:**

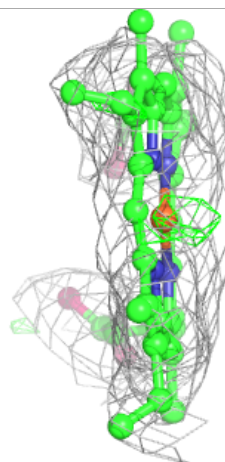
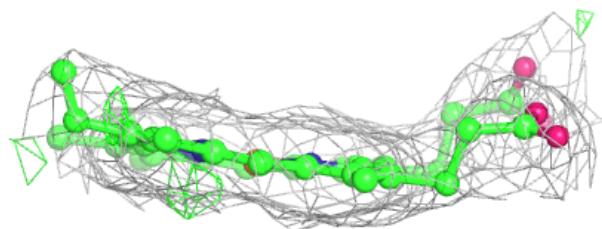
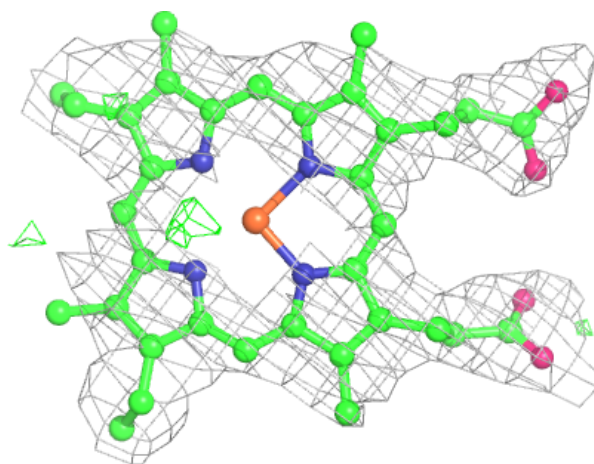
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC C 604:**

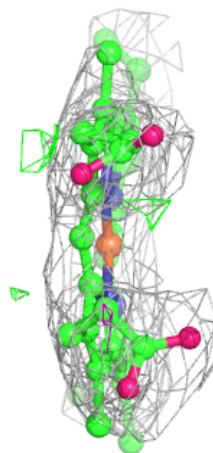
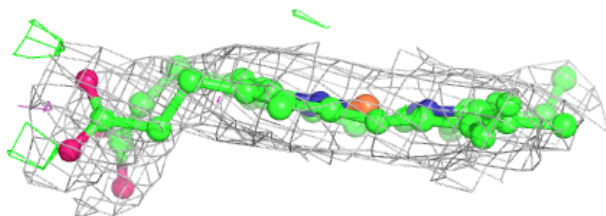
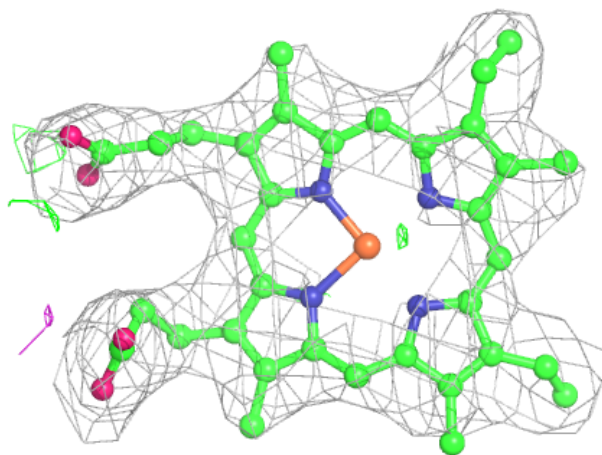
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





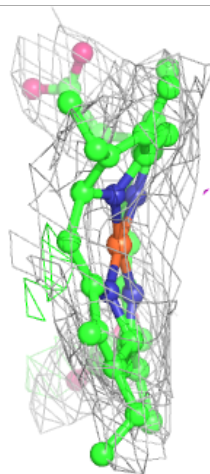
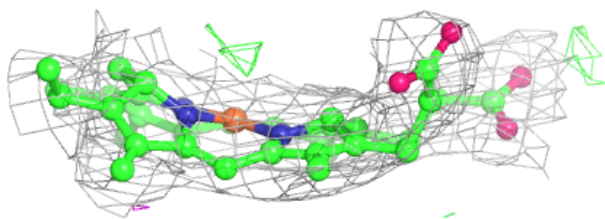
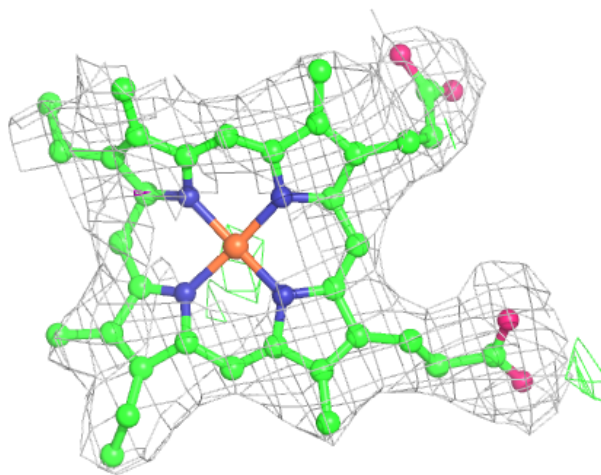
**Electron density around HEC Q 607:**

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



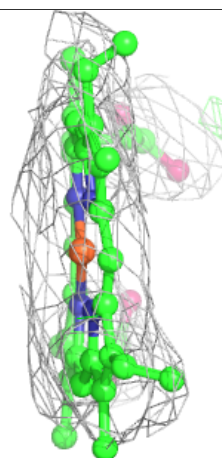
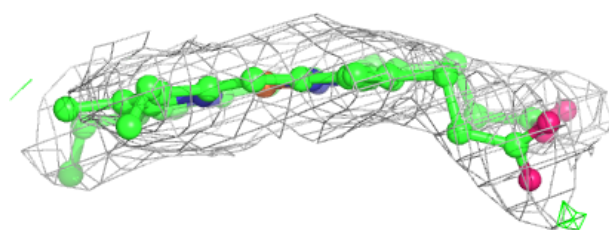
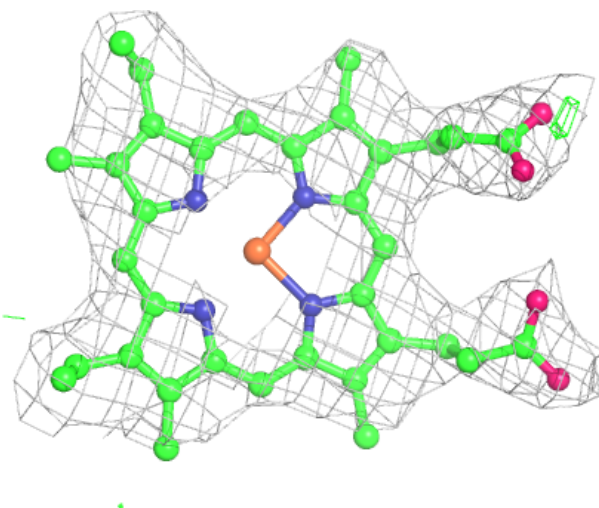
**Electron density around HEC R 603:**

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



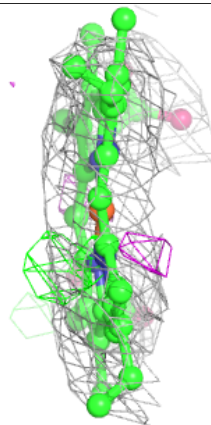
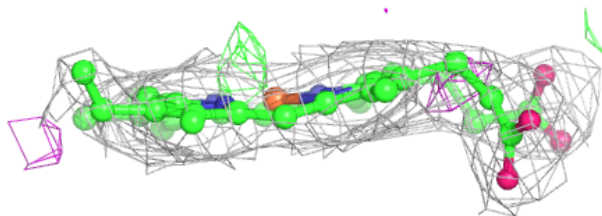
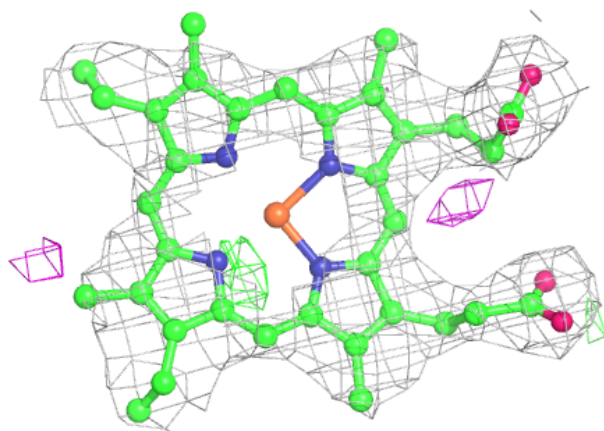
**Electron density around HEC W 604:**

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



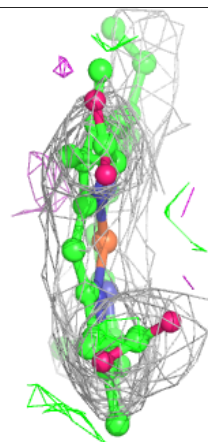
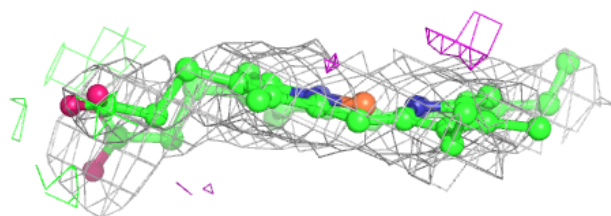
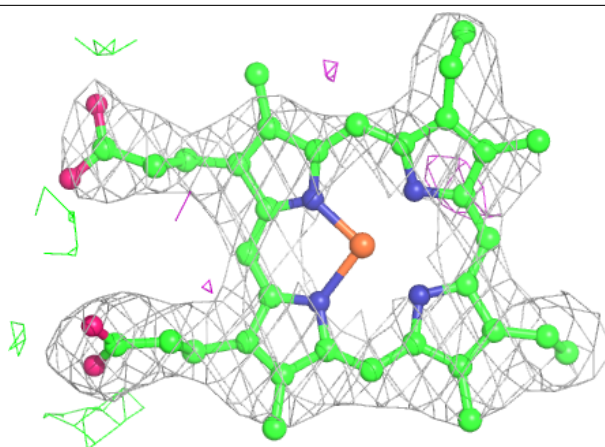
**Electron density around HEC A 607:**

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



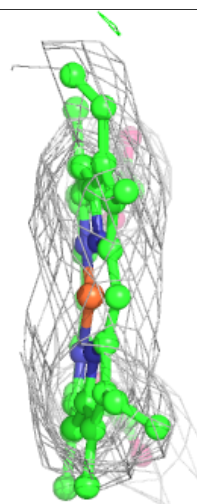
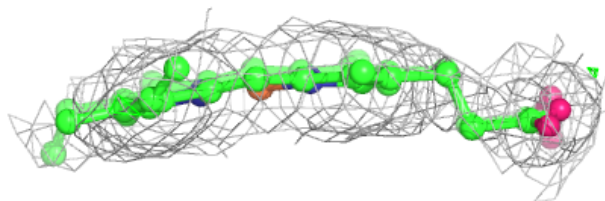
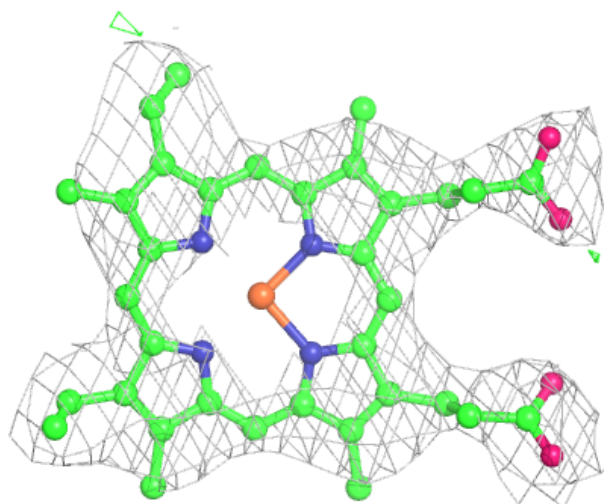
**Electron density around HEC T 606:**

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



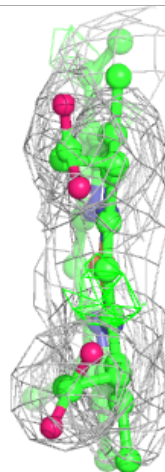
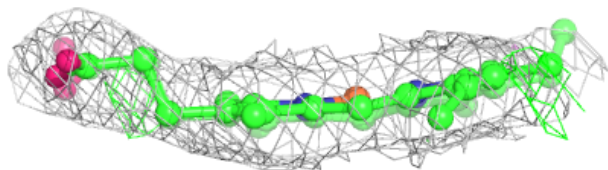
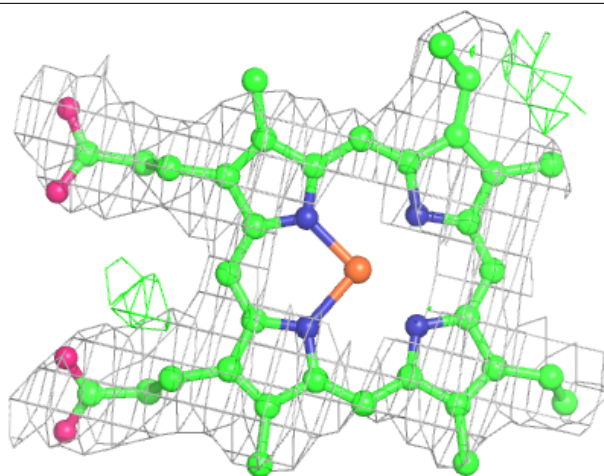
**Electron density around HEC S 600:**

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



**Electron density around HEC N 600:**

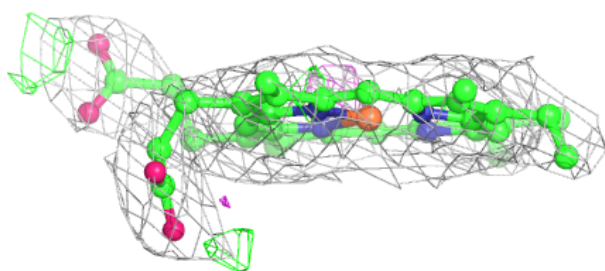
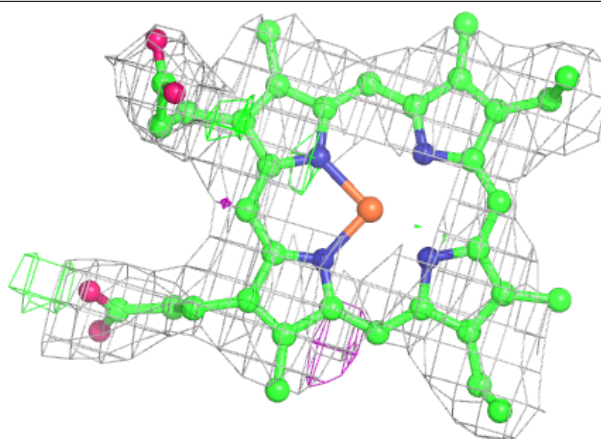
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC N 601:**

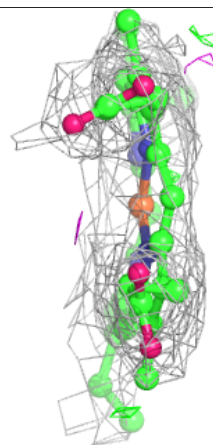
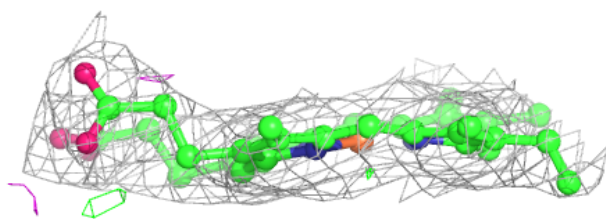
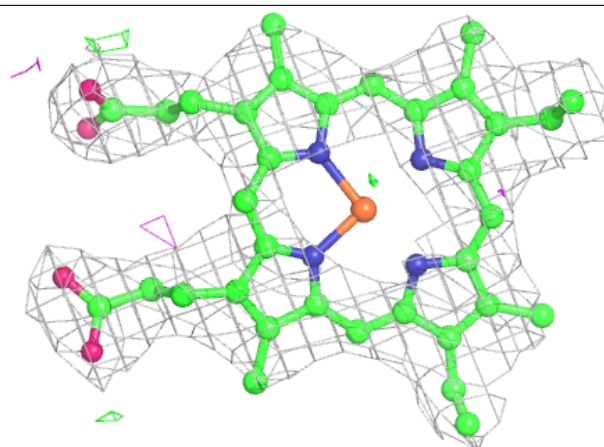
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





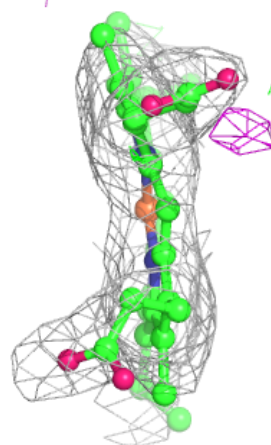
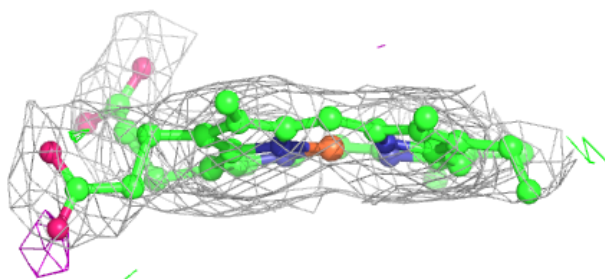
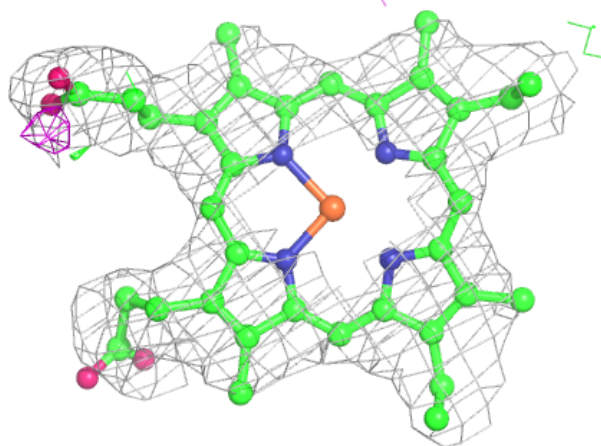
**Electron density around HEC P 606:**

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



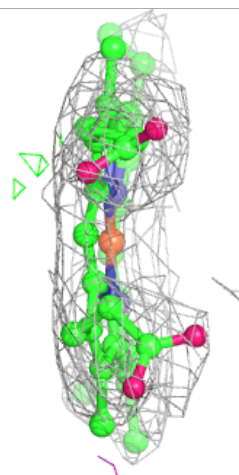
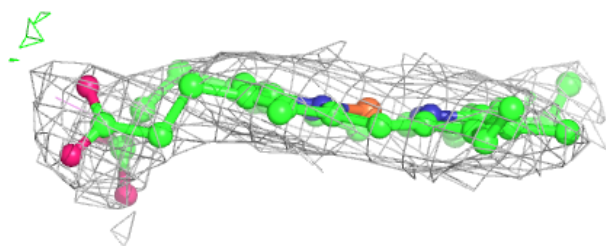
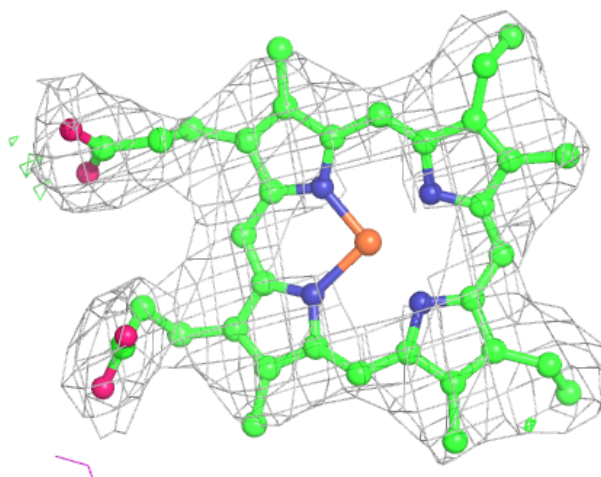
**Electron density around HEC L 602:**

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



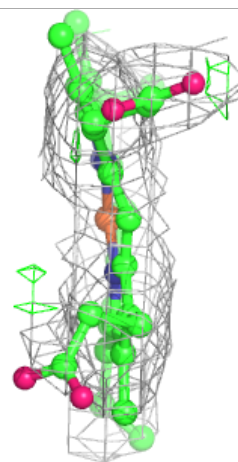
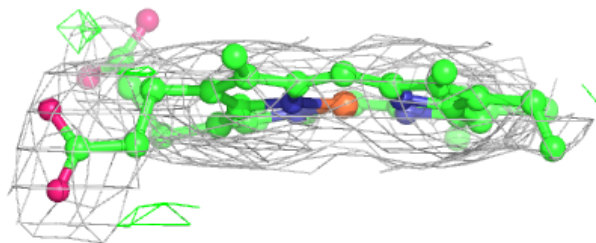
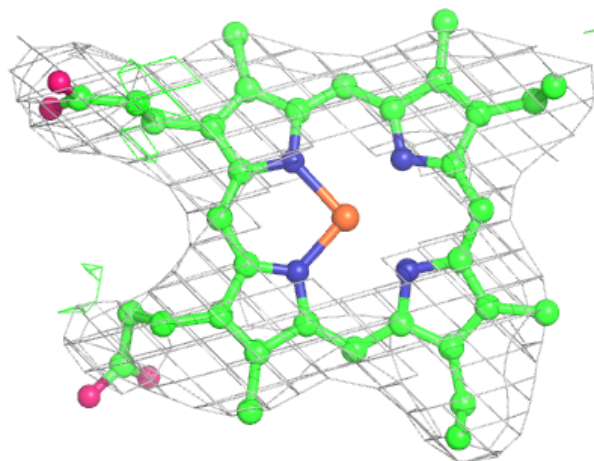
**Electron density around HEC M 607:**

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



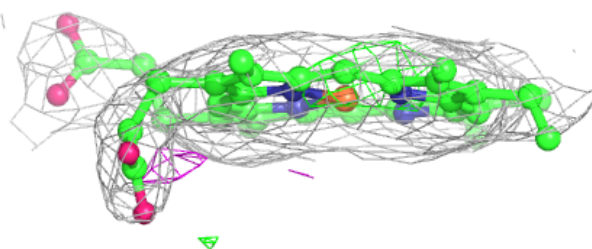
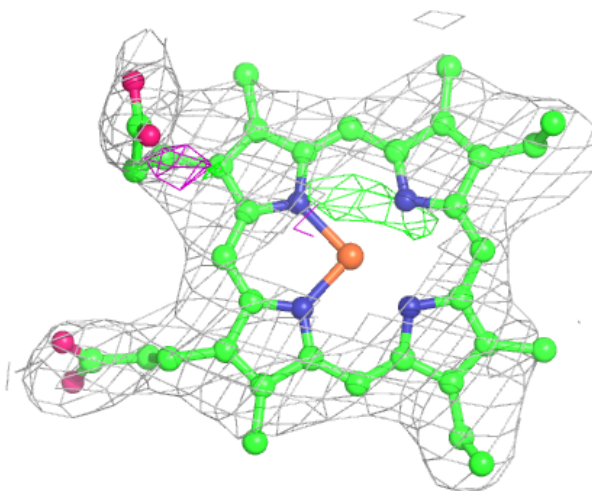
**Electron density around HEC N 602:**

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



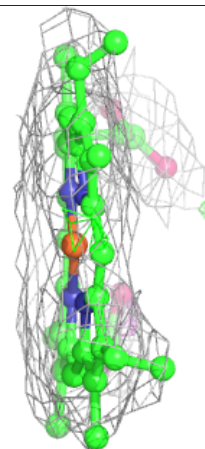
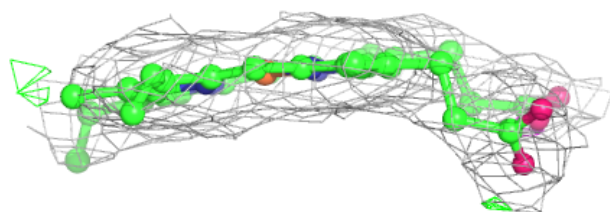
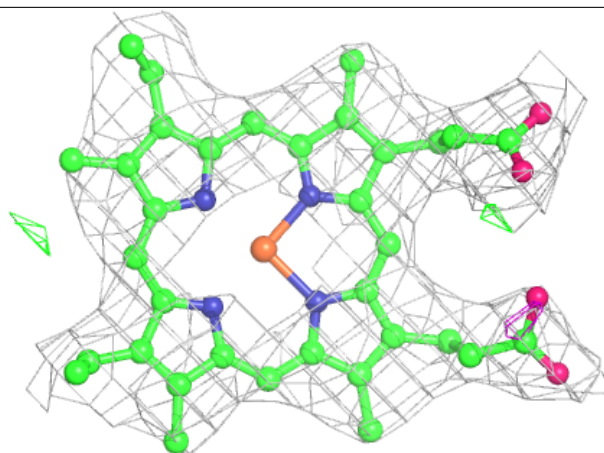
**Electron density around HEC F 601:**

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



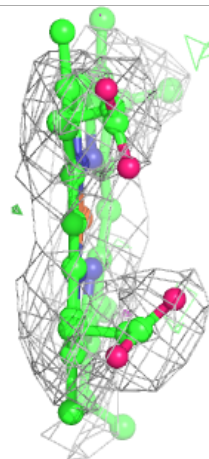
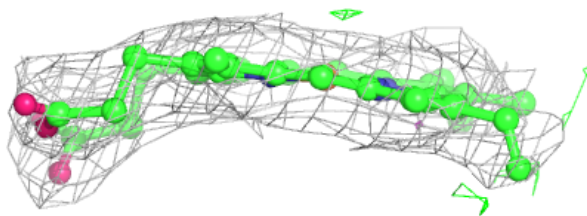
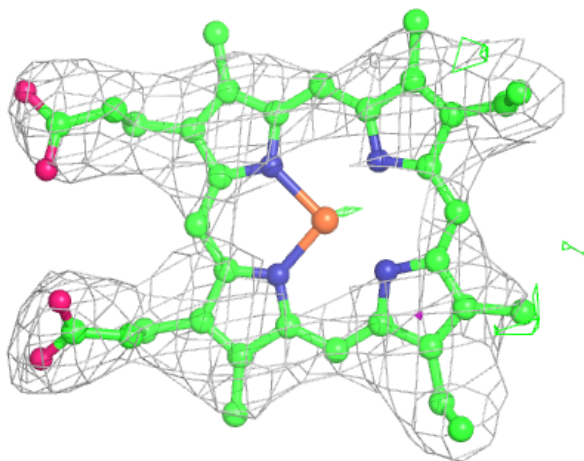
**Electron density around HEC P 604:**

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



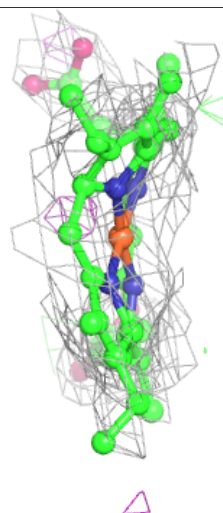
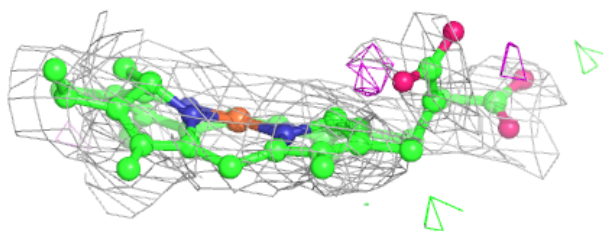
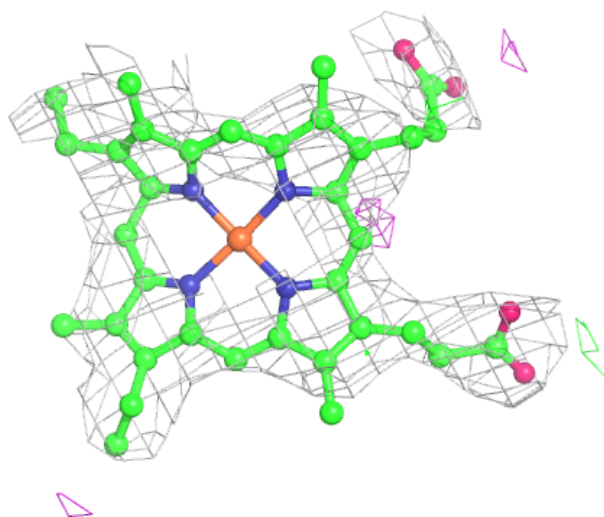
**Electron density around HEC T 604:**

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



**Electron density around HEC E 603:**

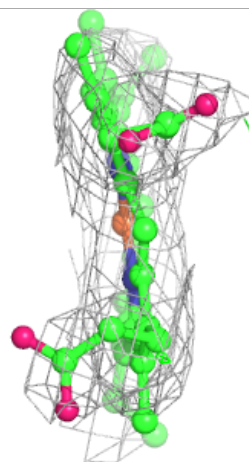
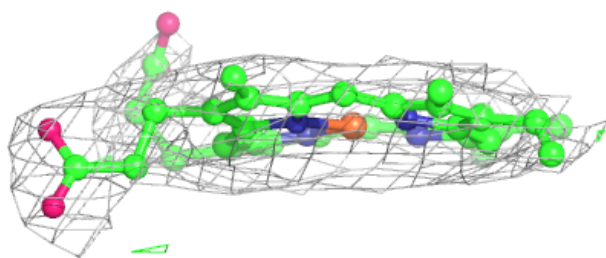
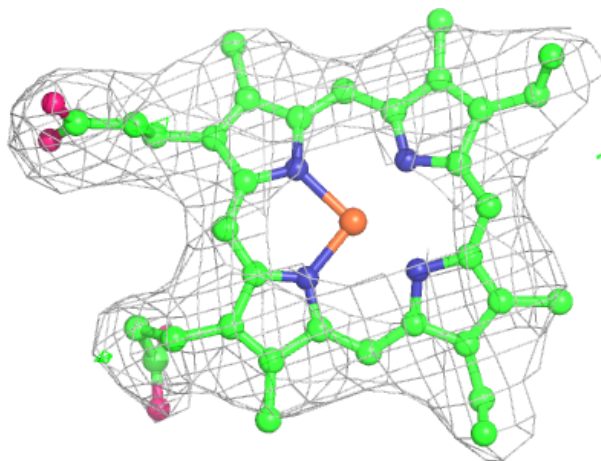
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





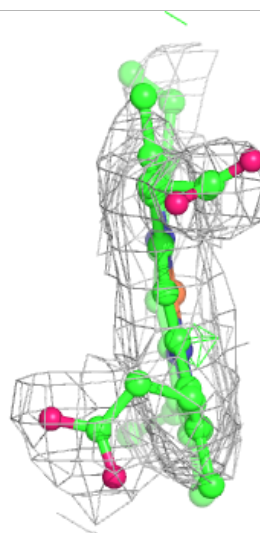
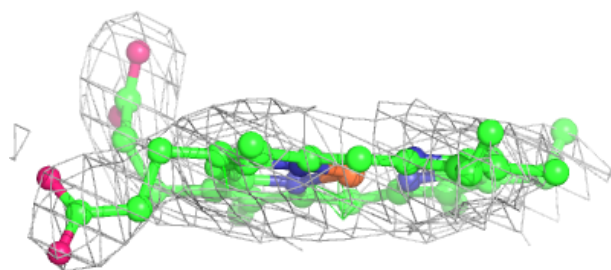
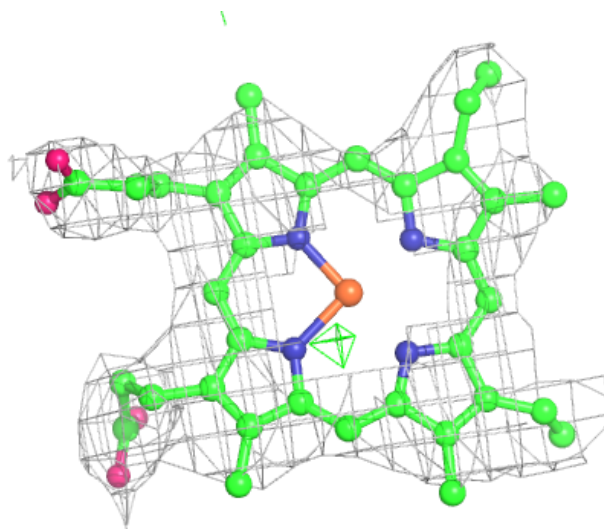
**Electron density around HEC D 602:**

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



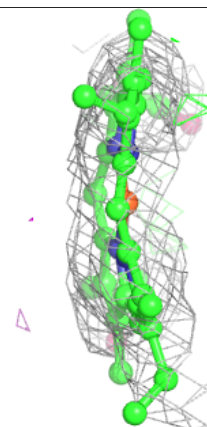
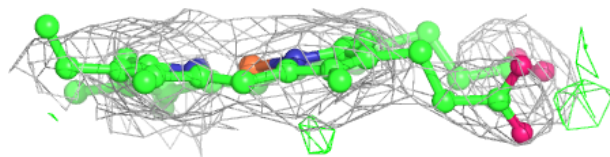
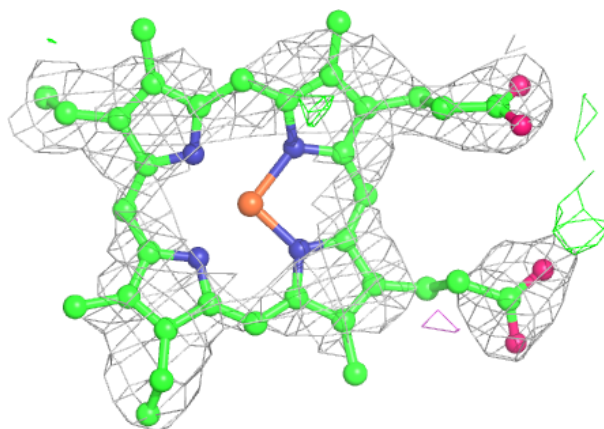
**Electron density around HEC U 601:**

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



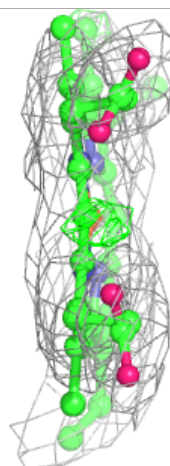
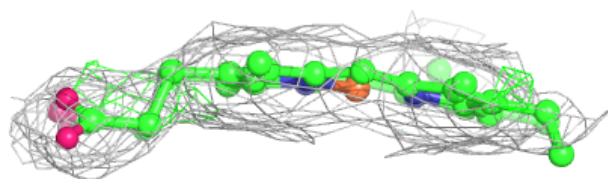
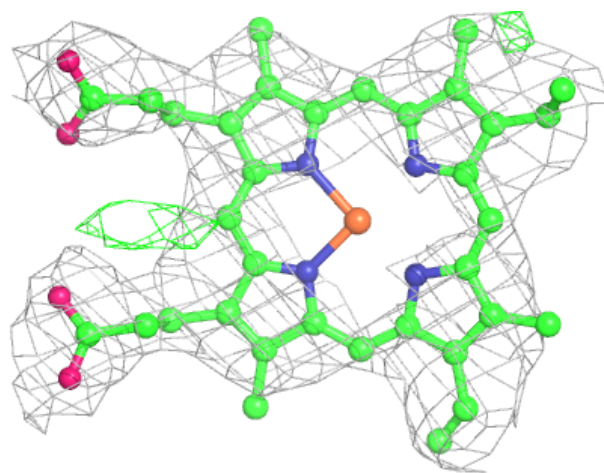
**Electron density around HEC W 606:**

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



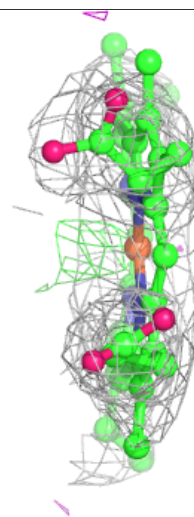
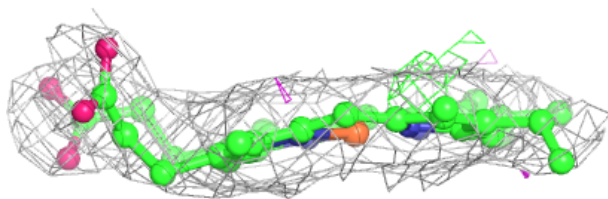
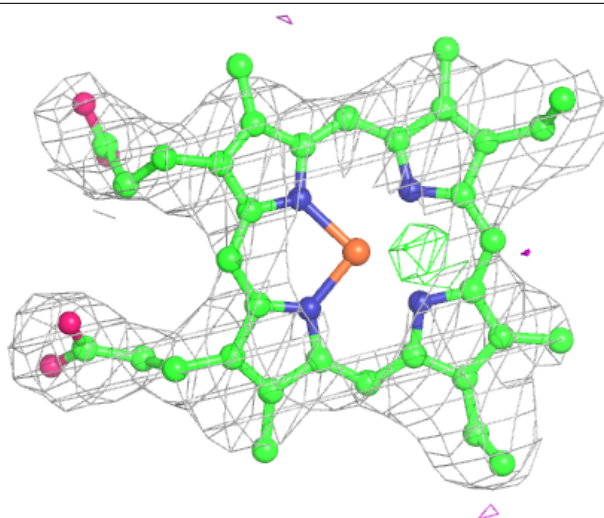
**Electron density around HEC Q 600:**

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



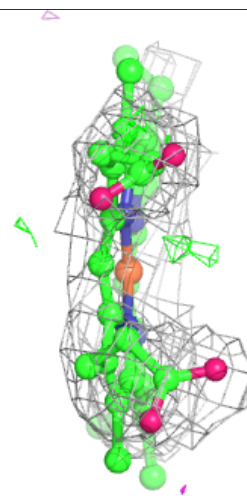
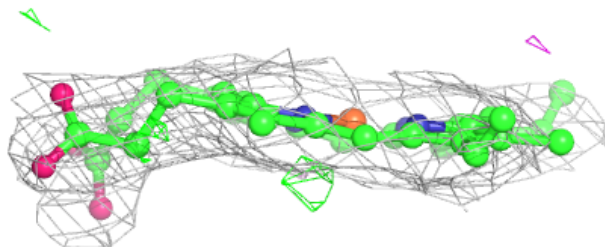
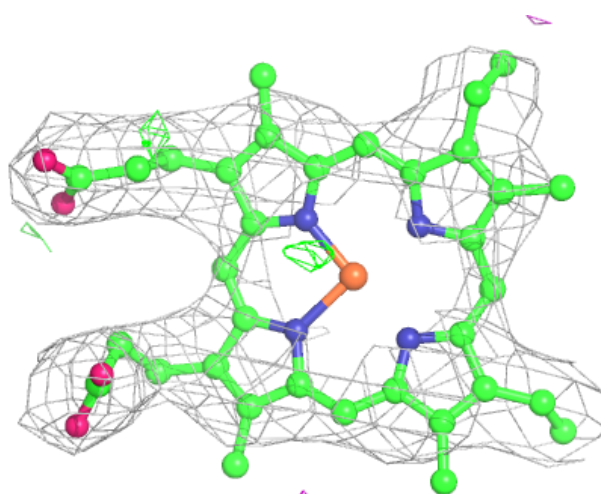
**Electron density around HEC S 607:**

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



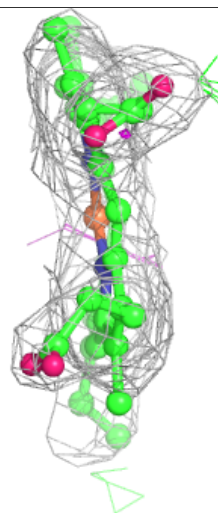
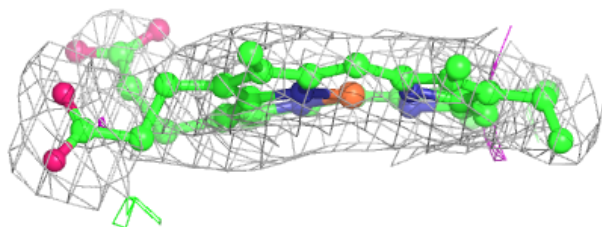
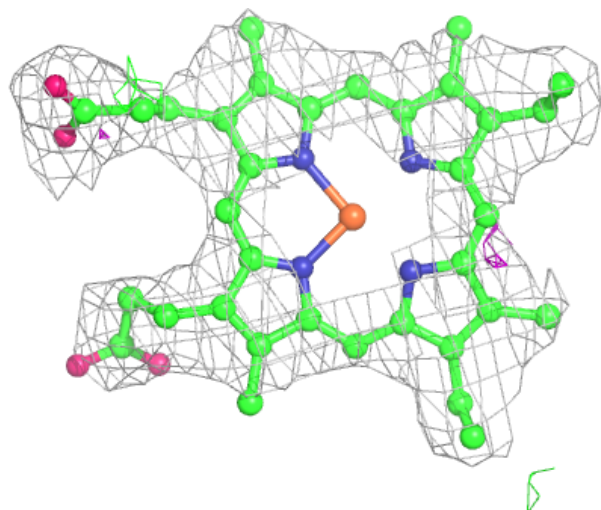
**Electron density around HEC W 607:**

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



**Electron density around HEC I 602:**

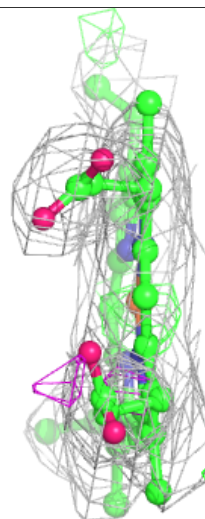
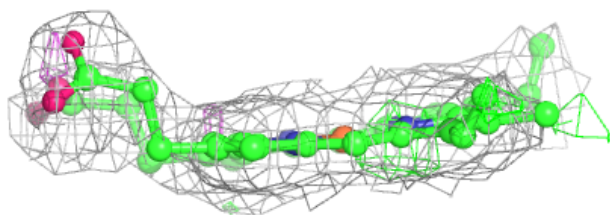
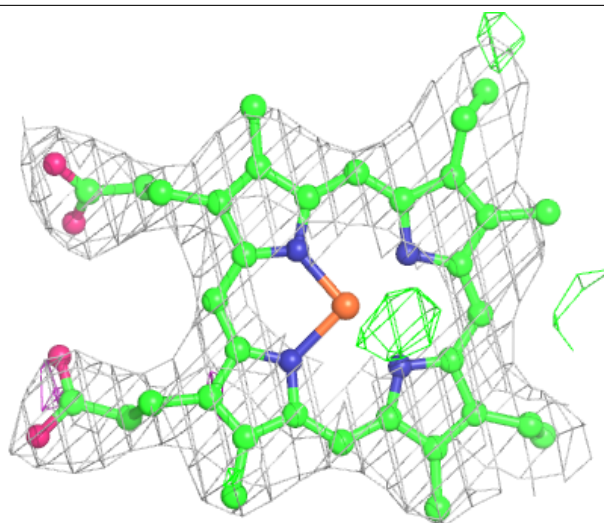
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC B 604:**

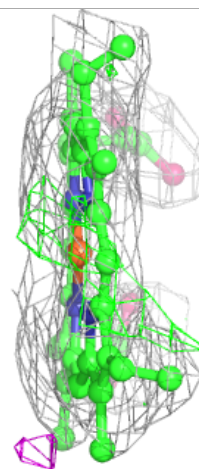
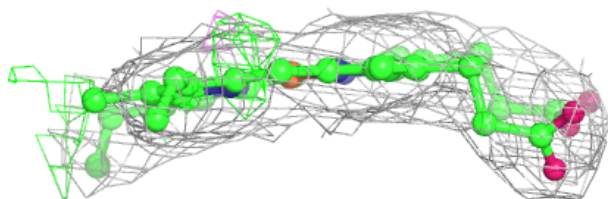
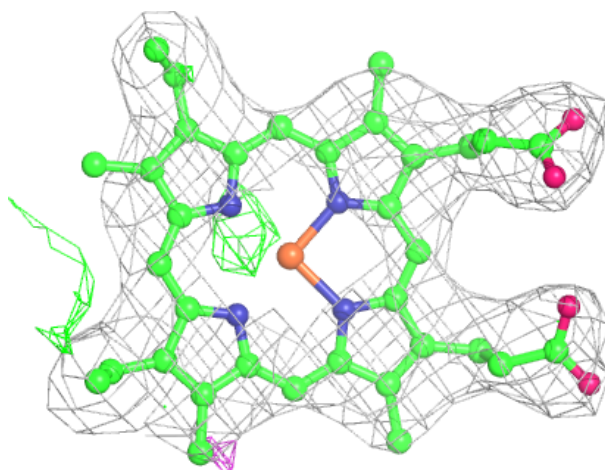
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





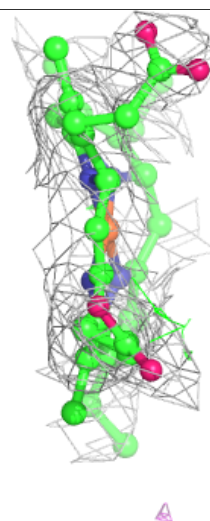
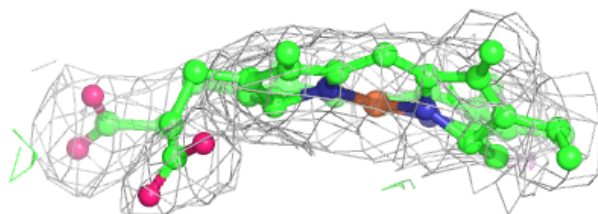
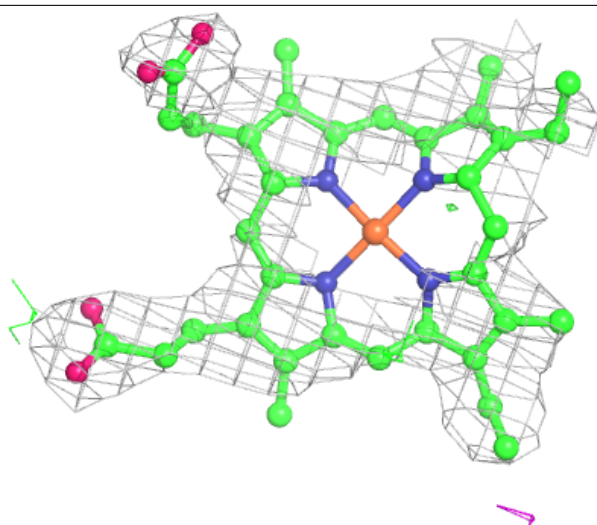
**Electron density around HEC O 604:**

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



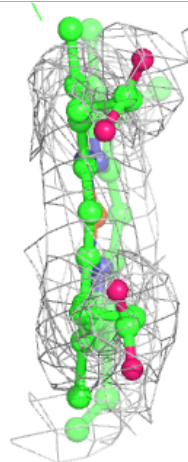
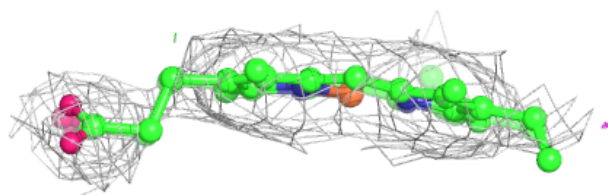
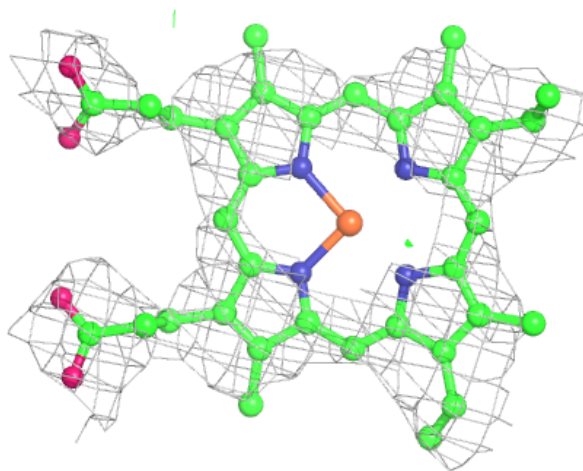
**Electron density around HEC U 603:**

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



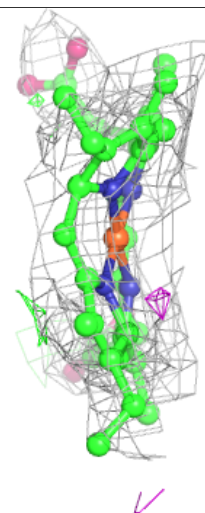
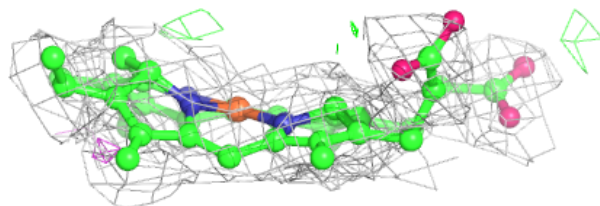
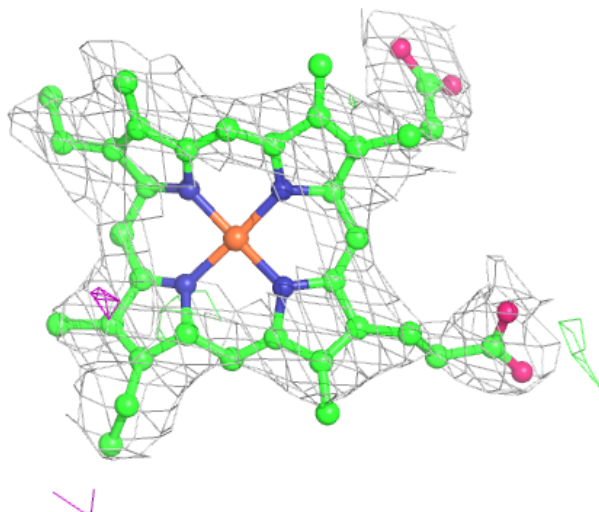
**Electron density around HEC V 600:**

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



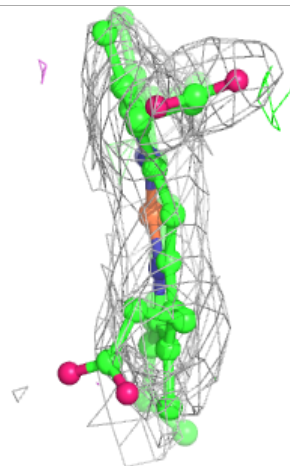
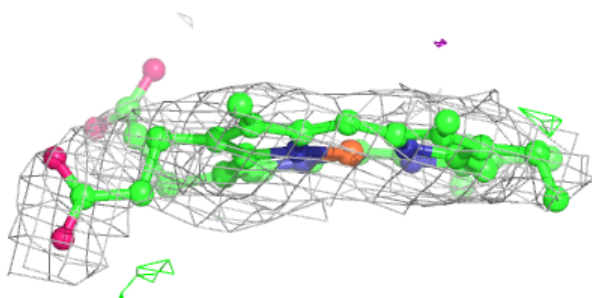
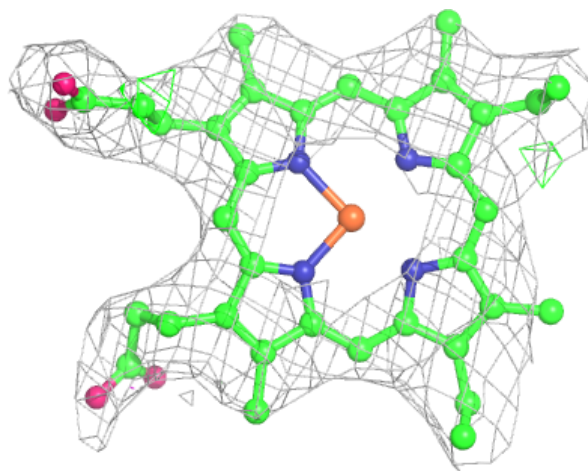
**Electron density around HEC A 603:**

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



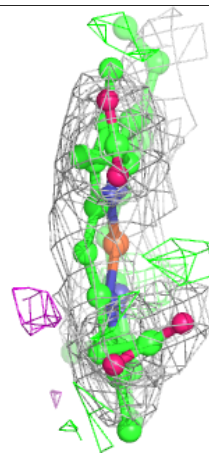
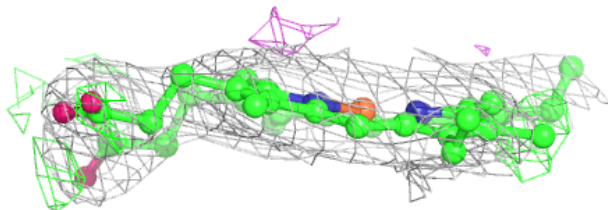
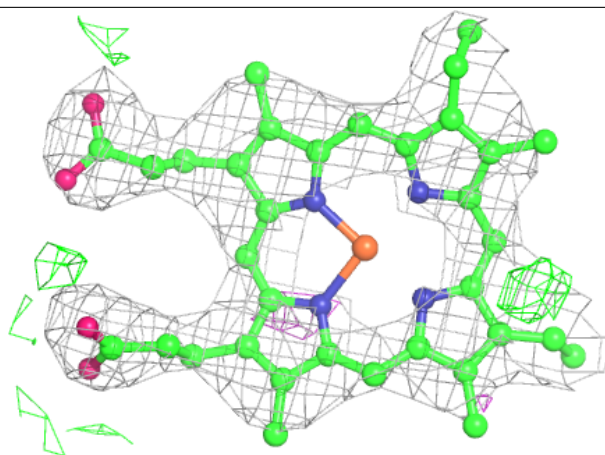
**Electron density around HEC O 602:**

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



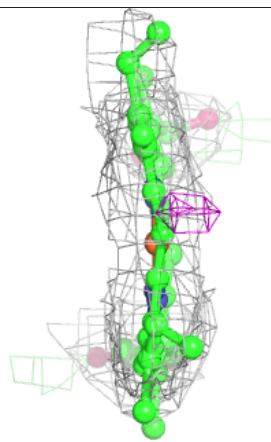
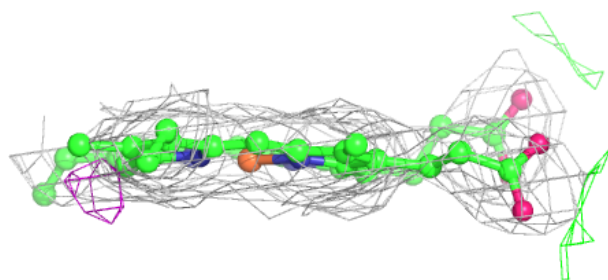
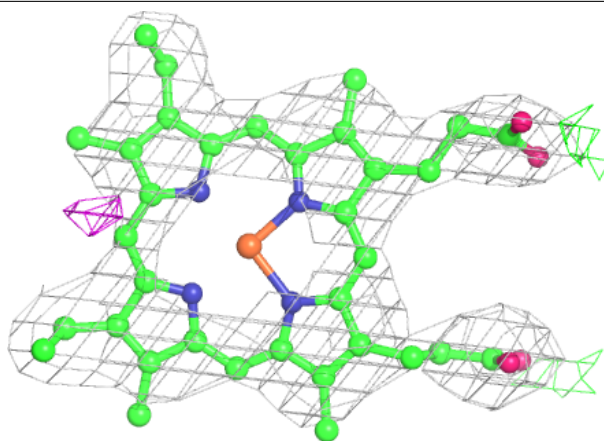
**Electron density around HEC F 606:**

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



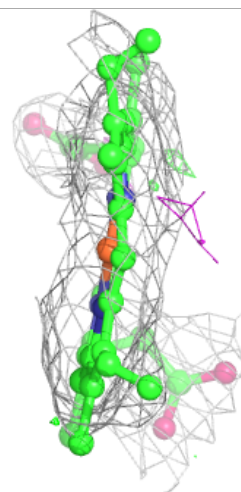
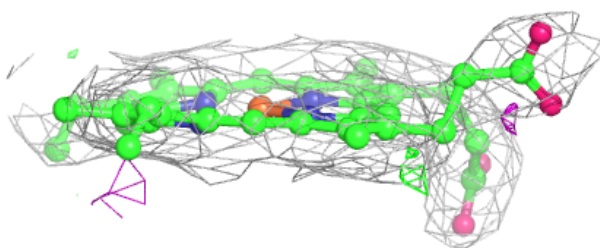
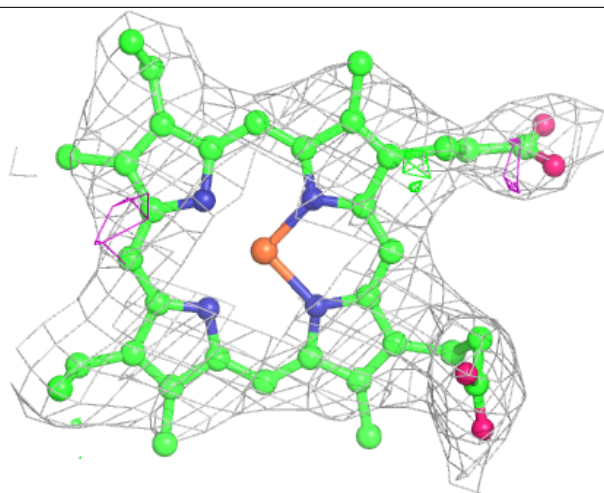
**Electron density around HEC D 605:**

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



**Electron density around HEC Q 601:**

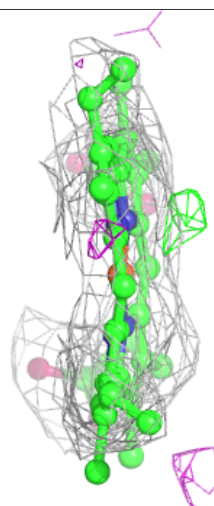
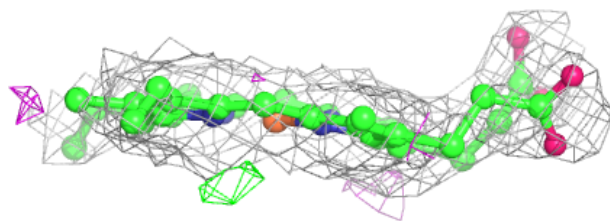
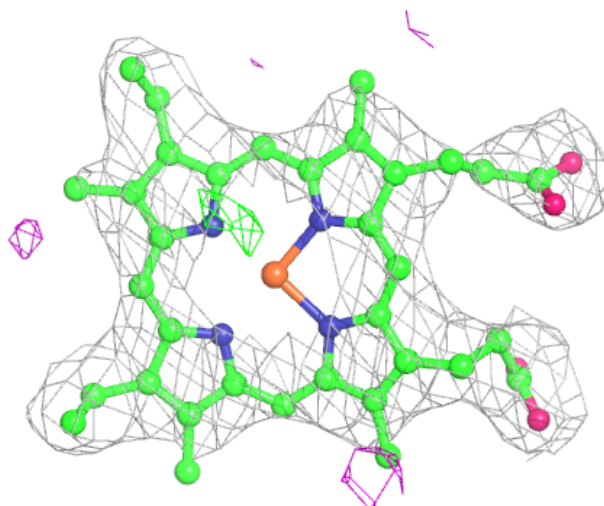
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





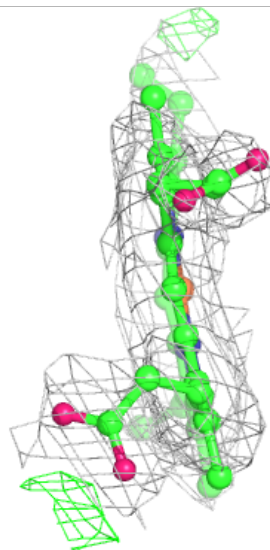
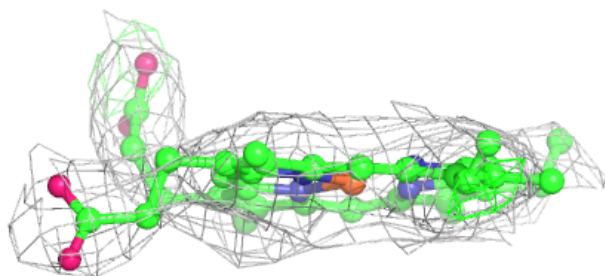
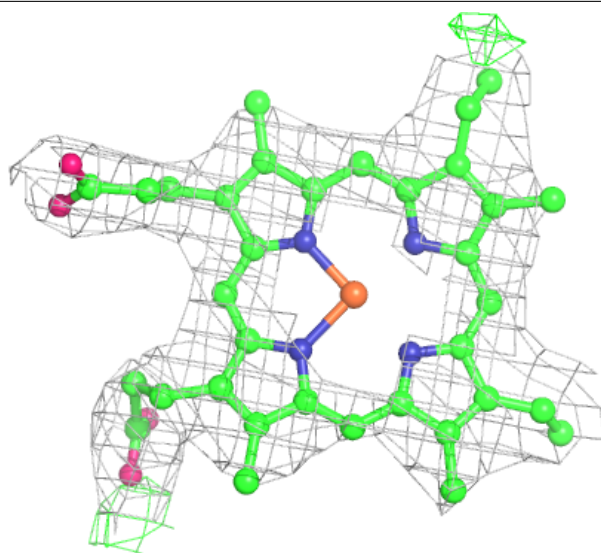
**Electron density around HEC F 607:**

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



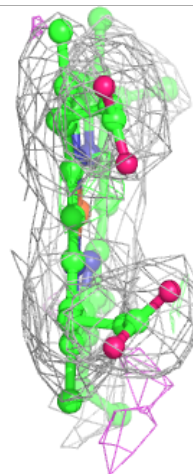
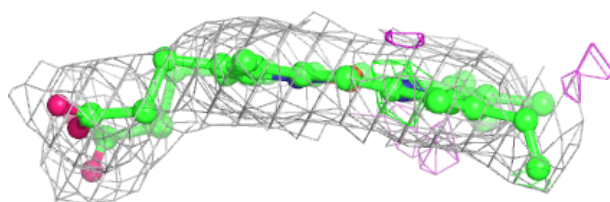
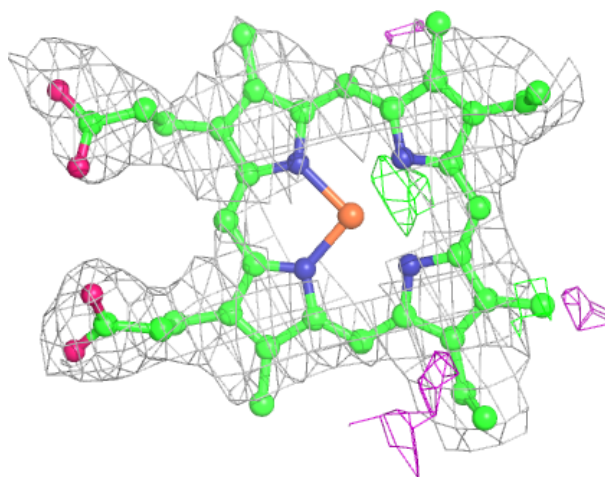
**Electron density around HEC V 601:**

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



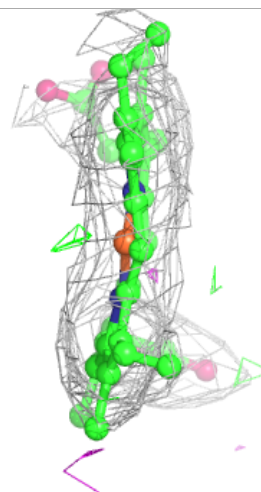
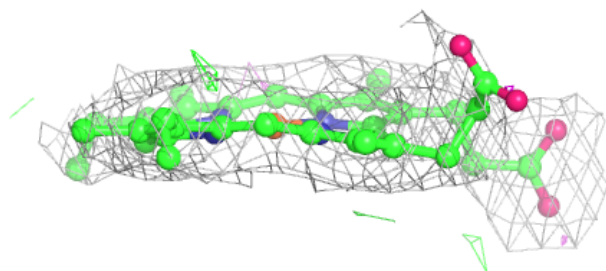
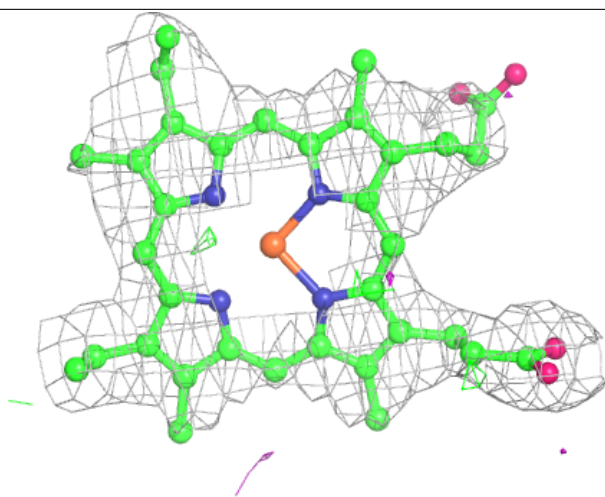
**Electron density around HEC M 604:**

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



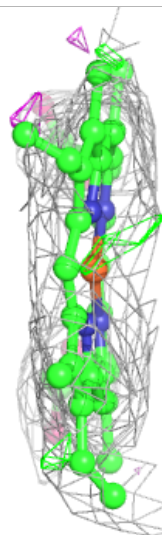
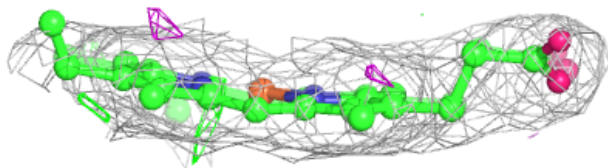
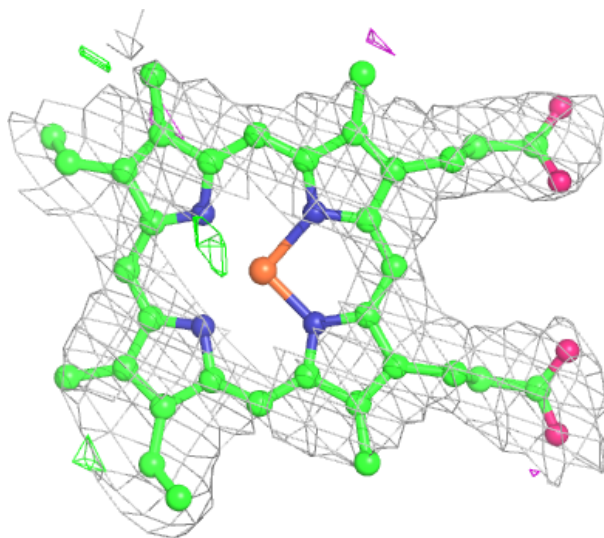
**Electron density around HEC M 602:**

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



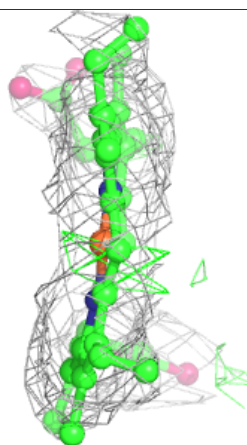
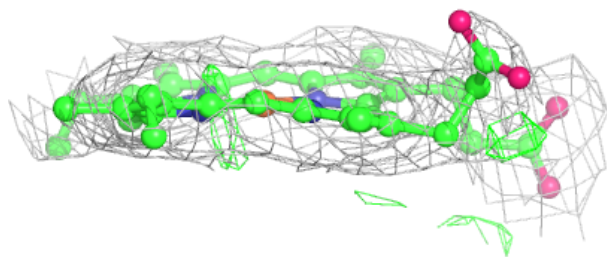
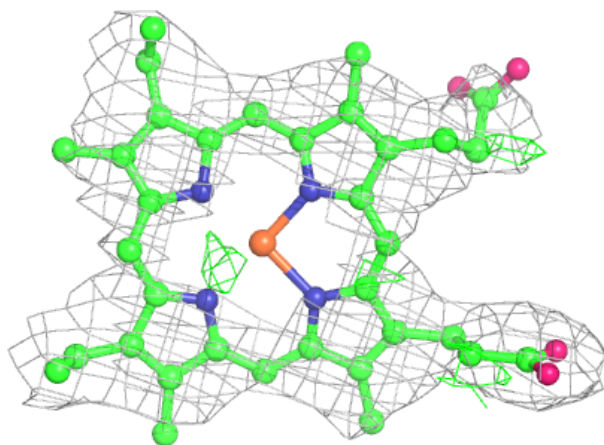
**Electron density around HEC A 600:**

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



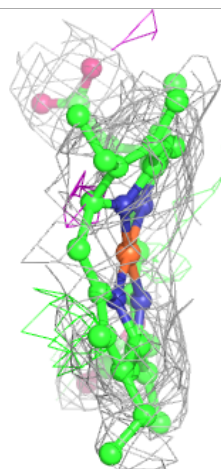
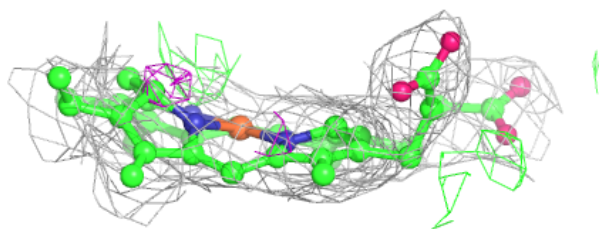
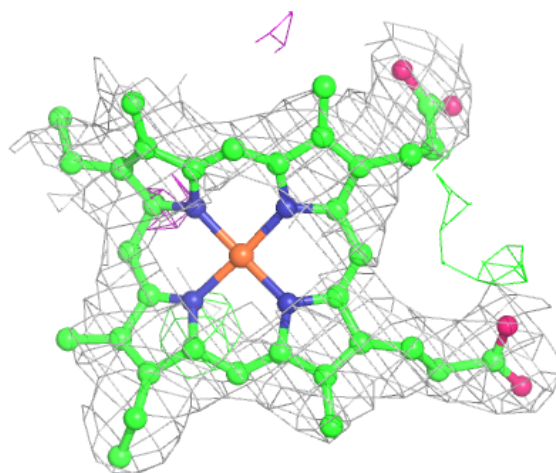
**Electron density around HEC C 602:**

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



**Electron density around HEC O 603:**

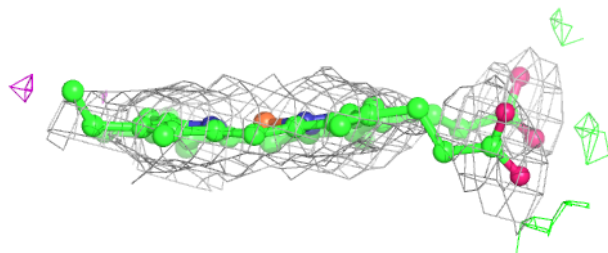
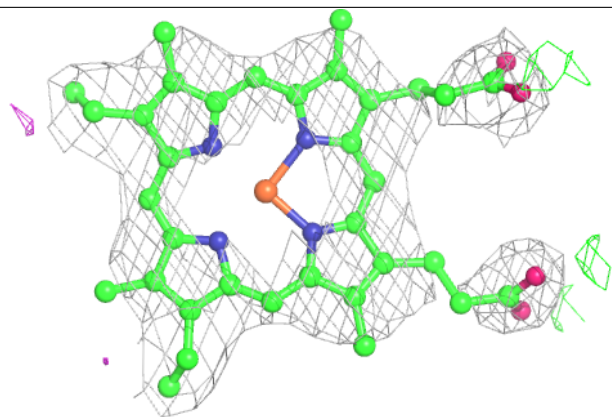
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



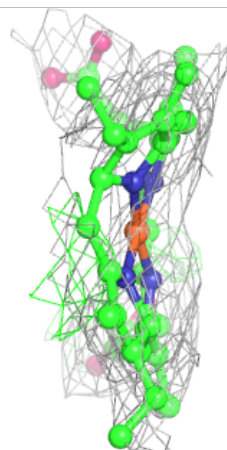
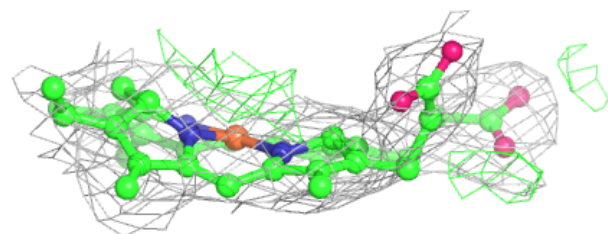
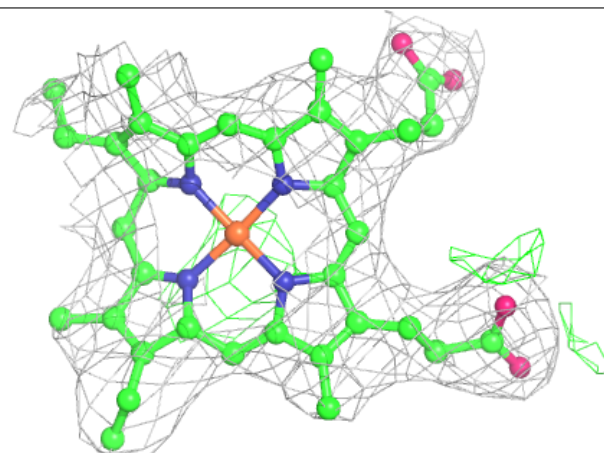


**Electron density around HEC T 605:**

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

**Electron density around HEC C 603:**

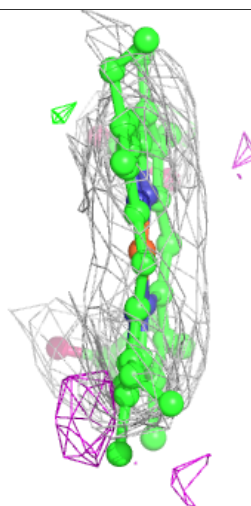
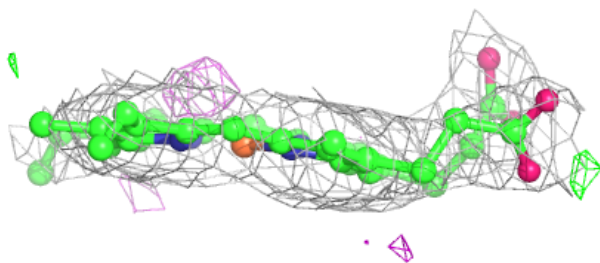
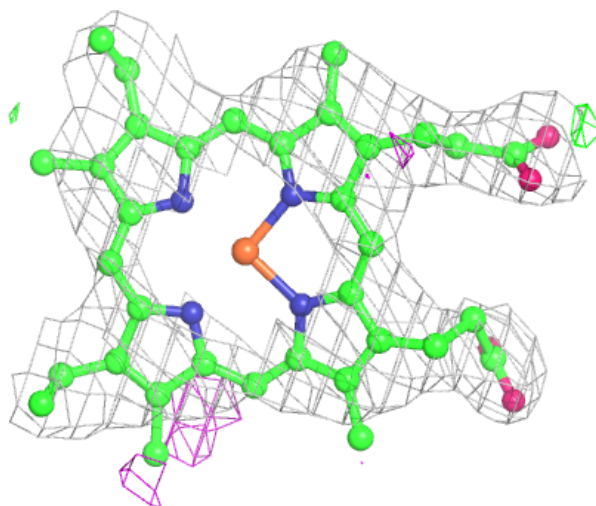
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





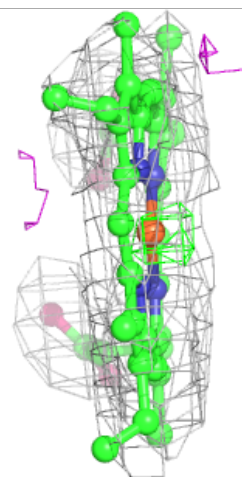
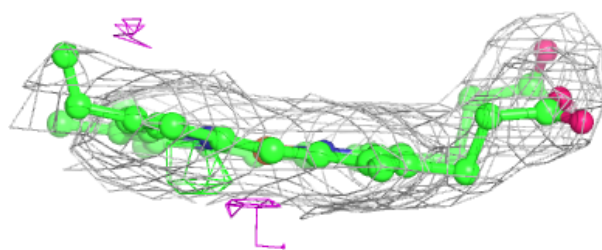
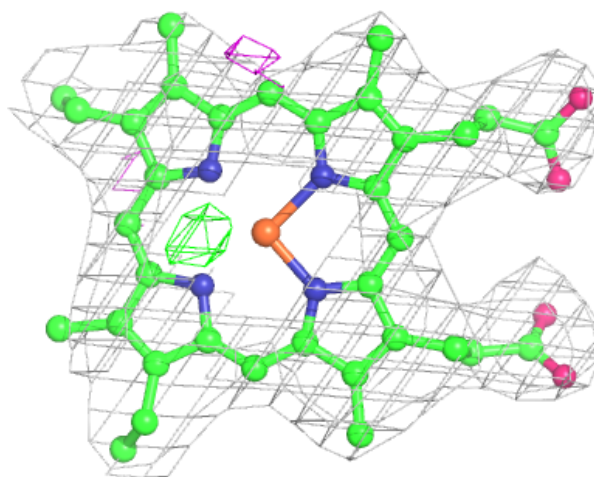
**Electron density around HEC E 607:**

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



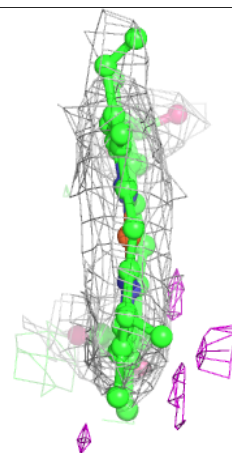
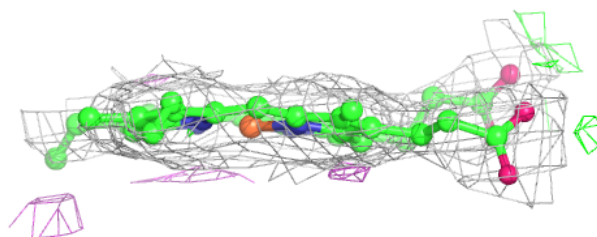
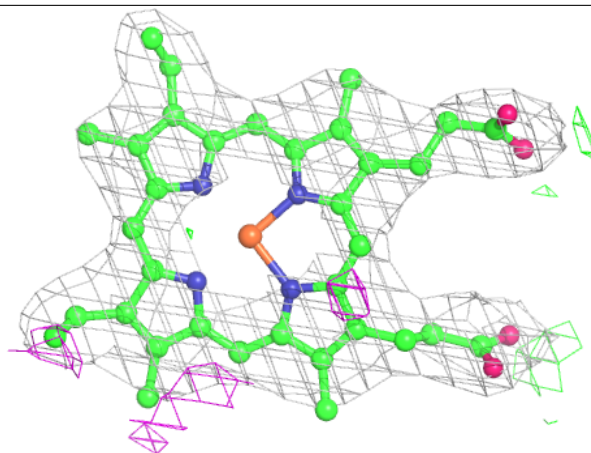
**Electron density around HEC E 604:**

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



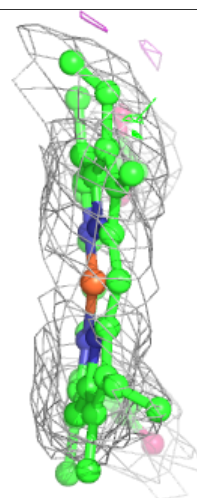
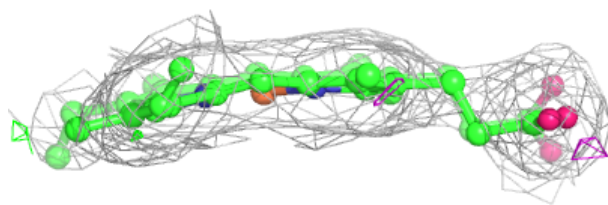
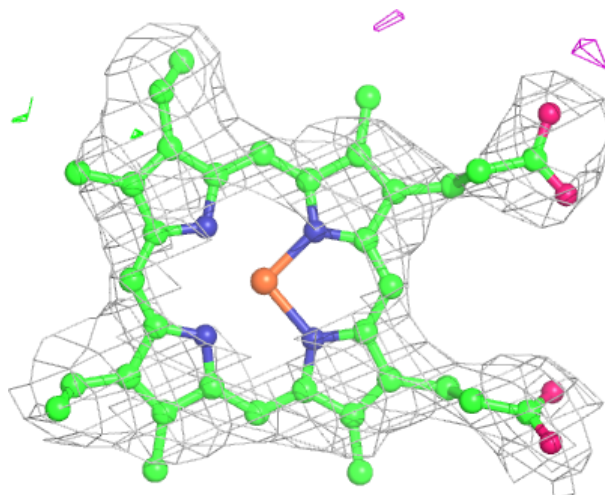
**Electron density around HEC M 605:**

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



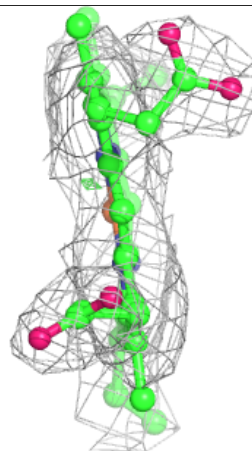
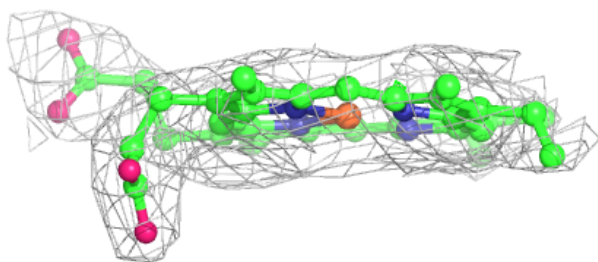
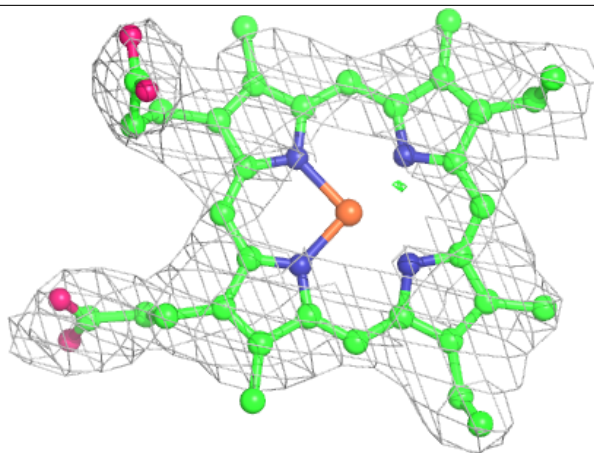
**Electron density around HEC D 600:**

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



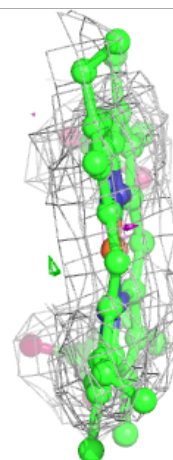
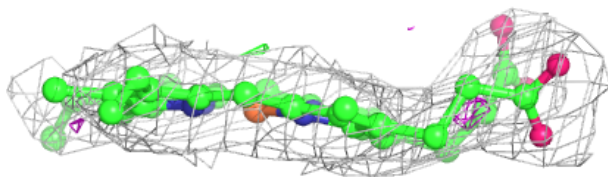
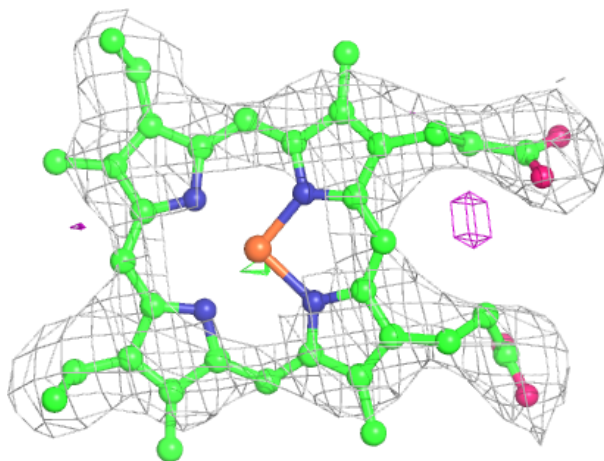
**Electron density around HEC O 601:**

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



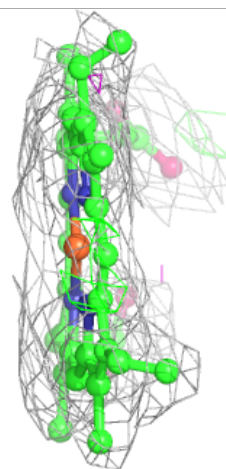
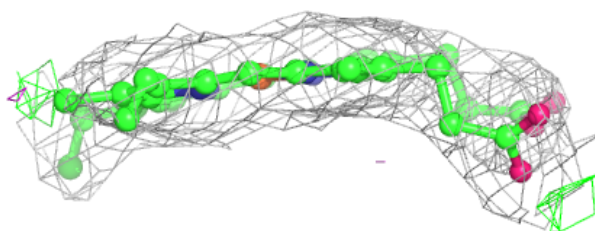
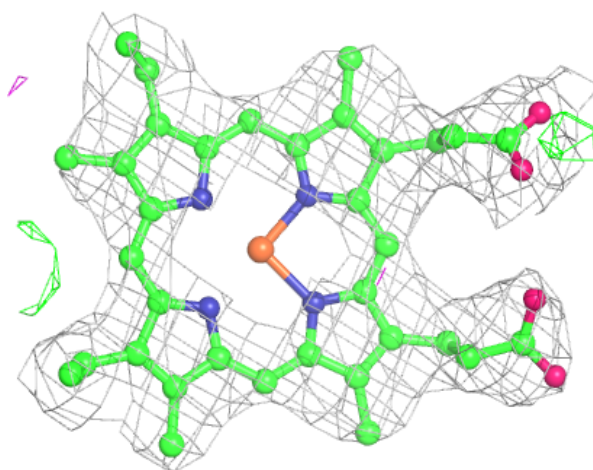
**Electron density around HEC V 607:**

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



**Electron density around HEC K 604:**

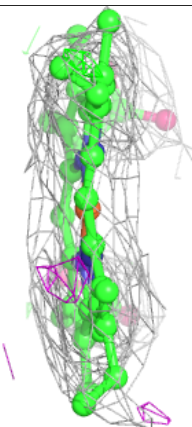
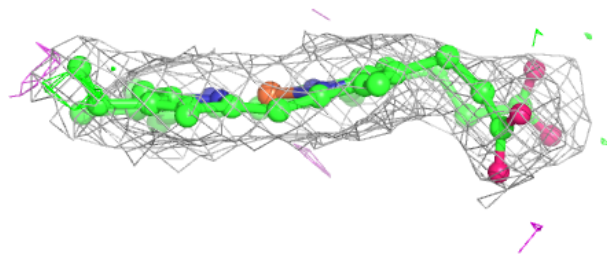
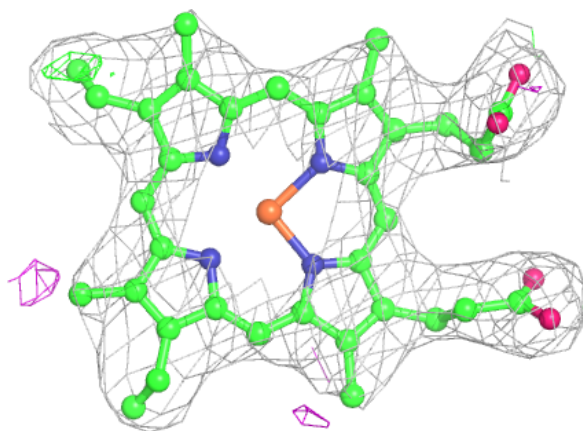
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC P 607:**

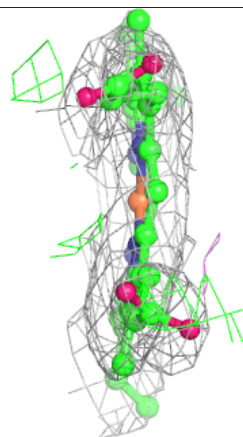
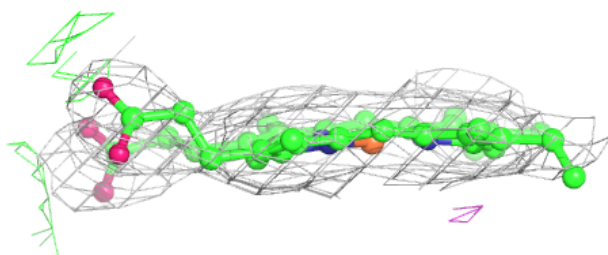
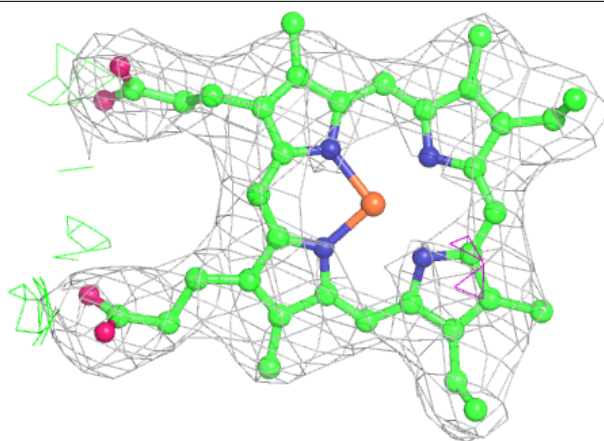
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





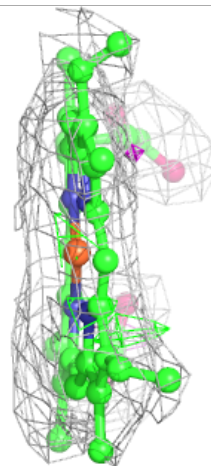
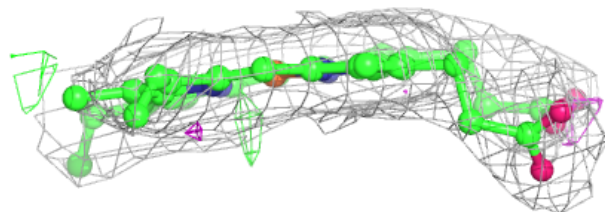
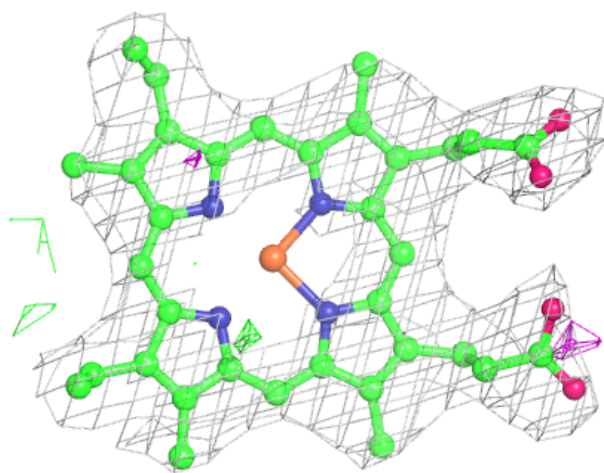
**Electron density around HEC C 605:**

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



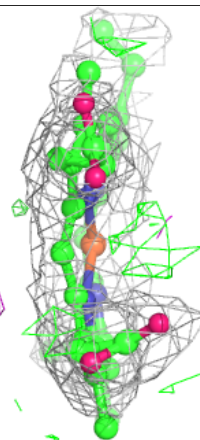
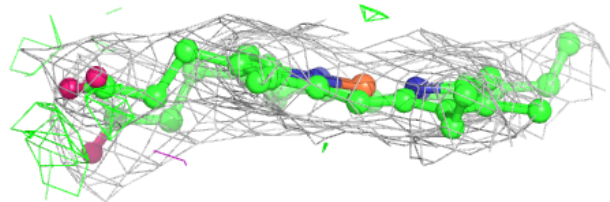
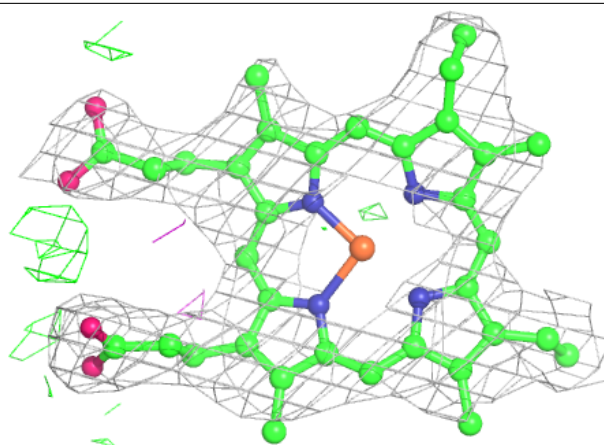
**Electron density around HEC G 604:**

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



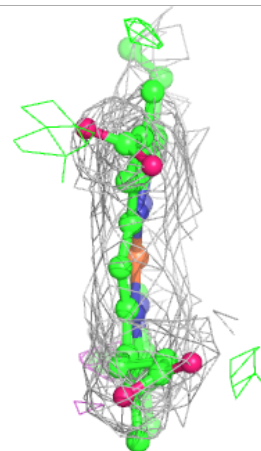
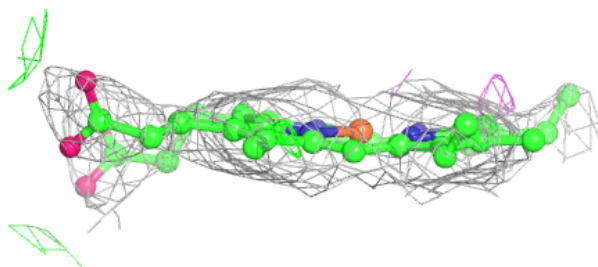
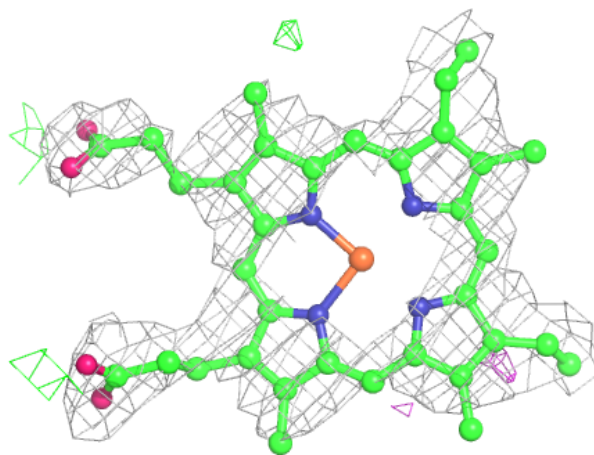
**Electron density around HEC Q 606:**

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



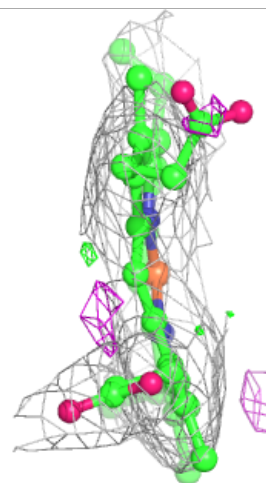
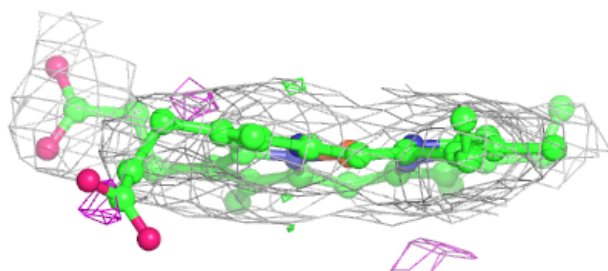
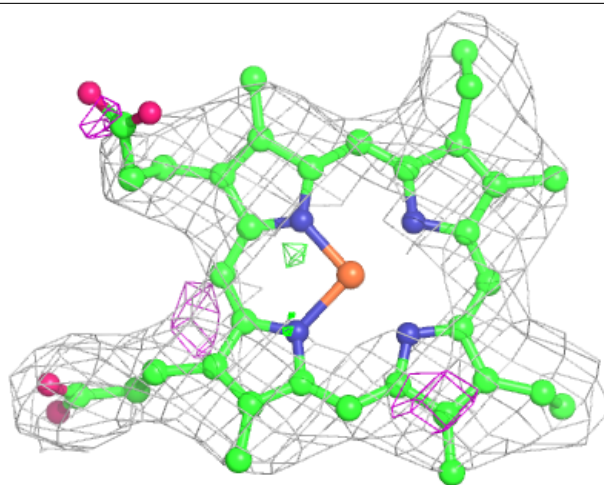
**Electron density around HEC U 605:**

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



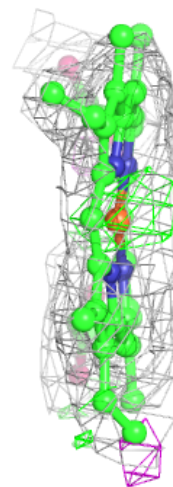
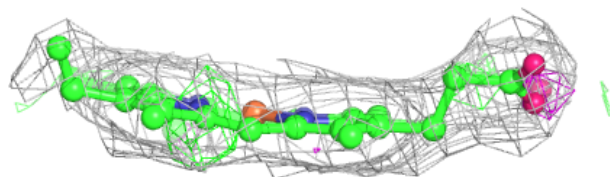
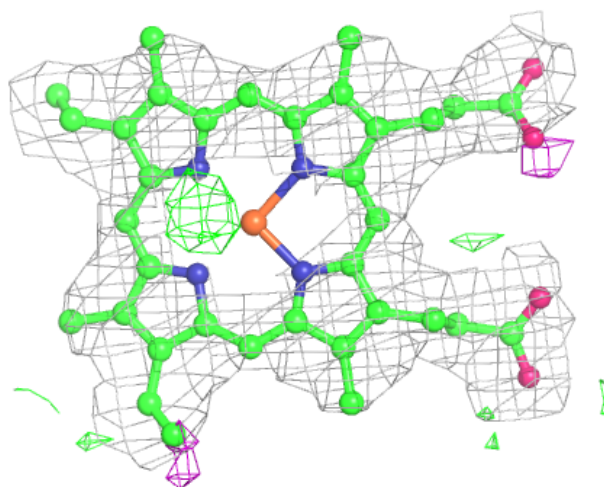
**Electron density around HEC J 602:**

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



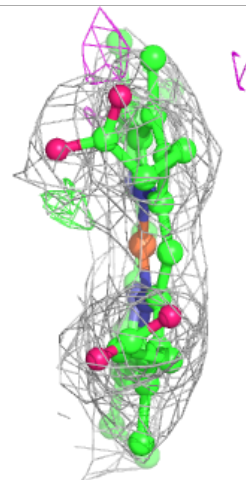
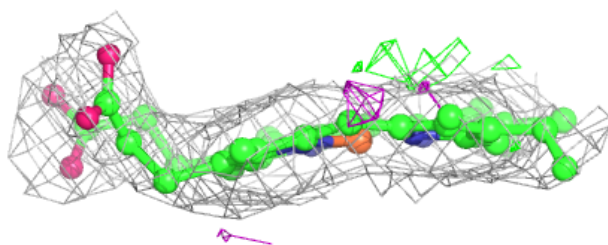
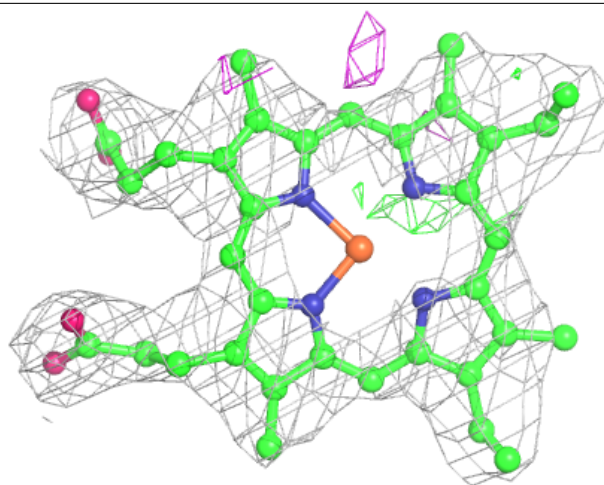
**Electron density around HEC J 600:**

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



**Electron density around HEC C 607:**

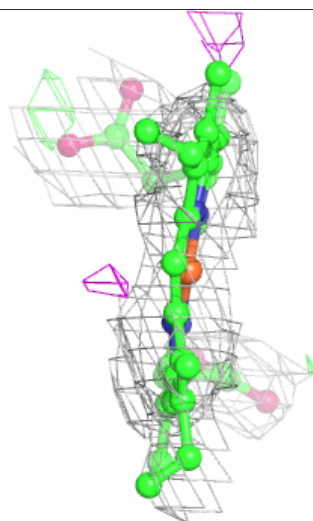
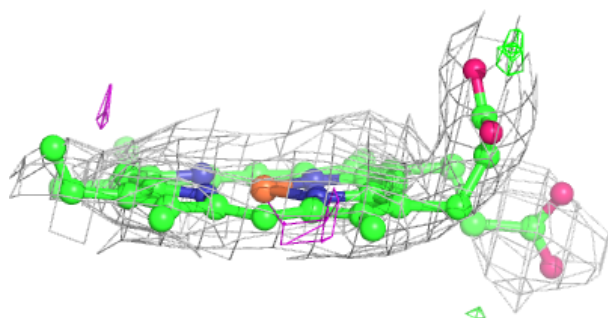
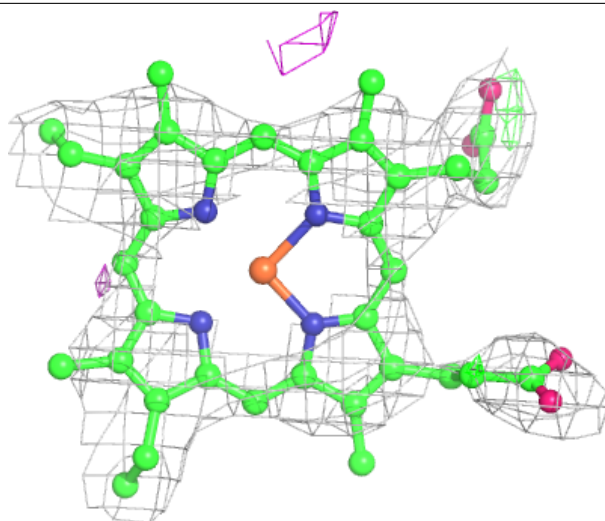
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC W 601:**

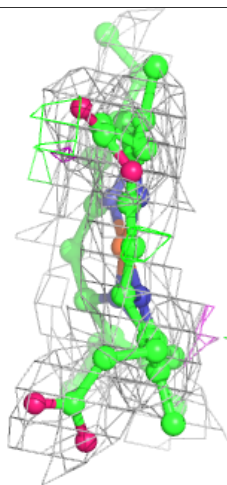
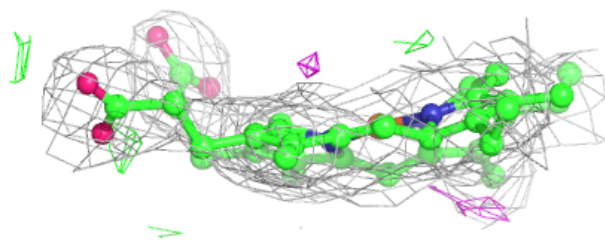
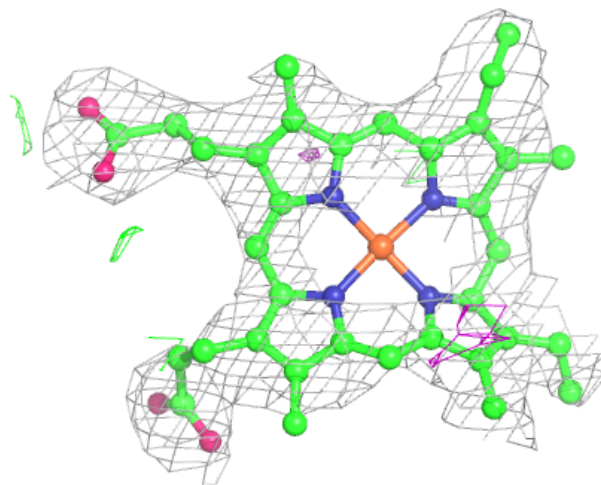
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





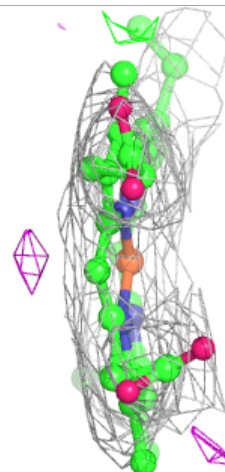
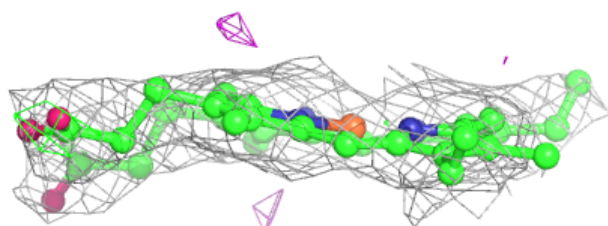
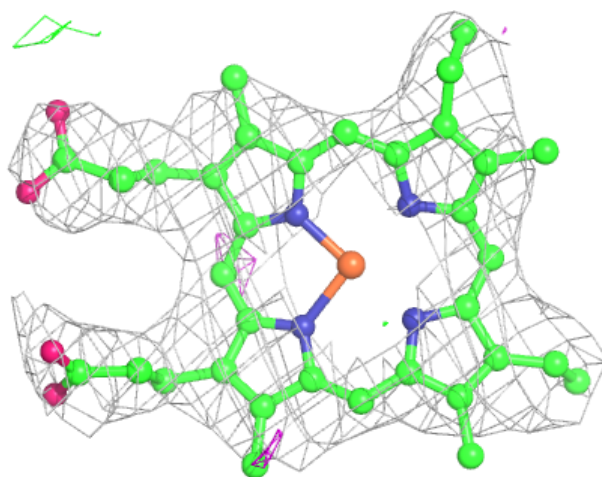
**Electron density around HEC M 603:**

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



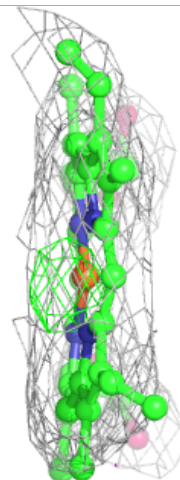
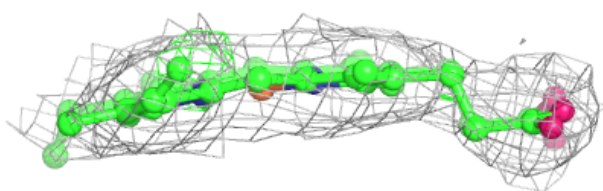
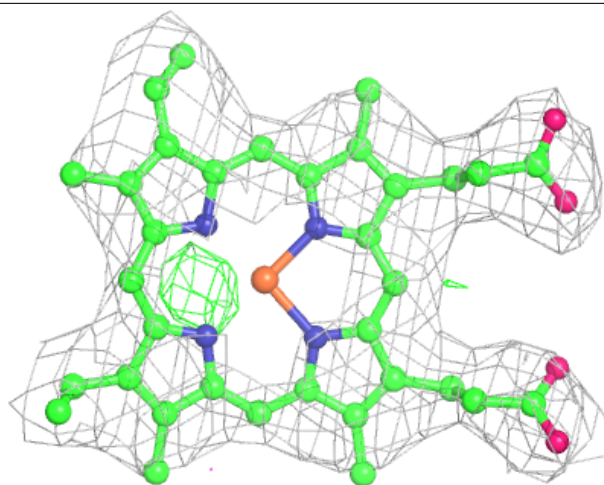
**Electron density around HEC V 606:**

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



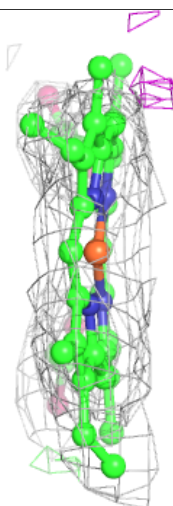
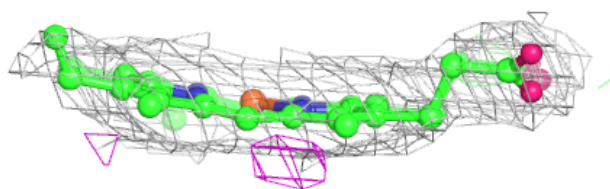
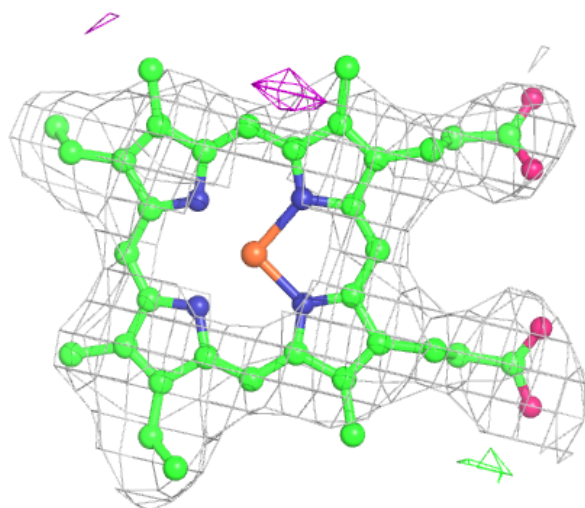
**Electron density around HEC X 600:**

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



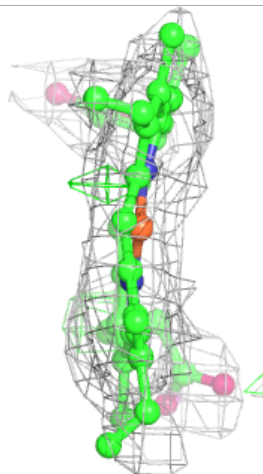
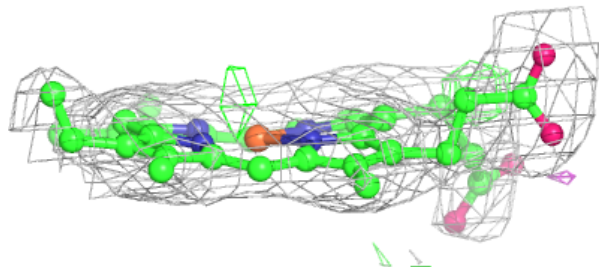
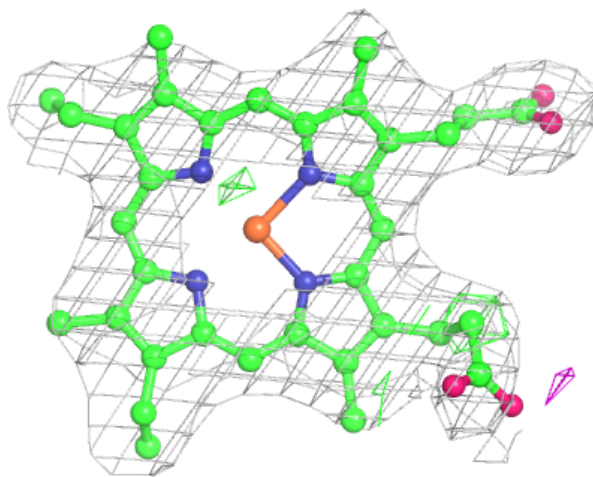
**Electron density around HEC B 600:**

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



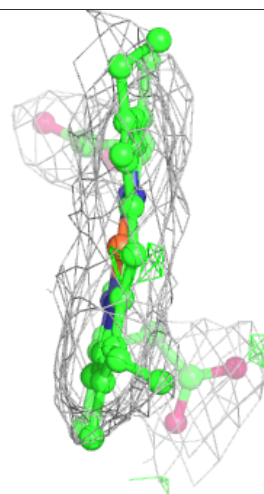
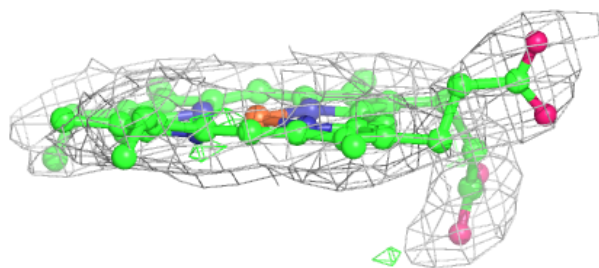
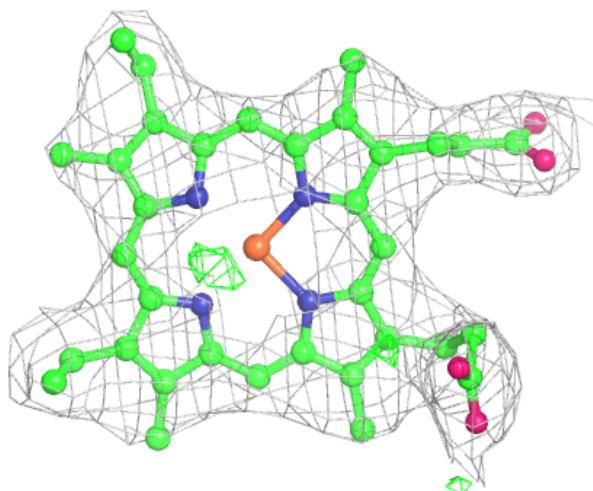
**Electron density around HEC G 602:**

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



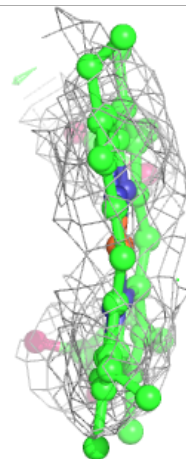
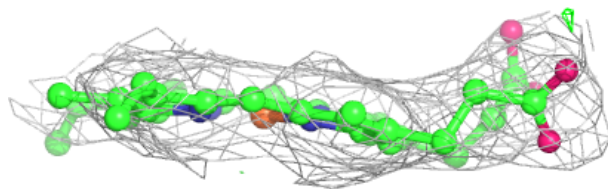
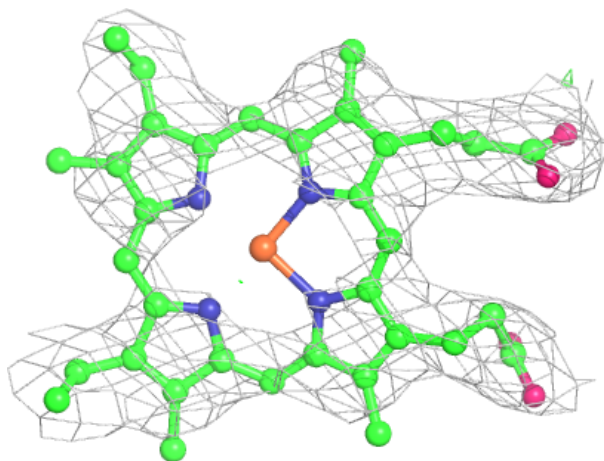
**Electron density around HEC L 601:**

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



**Electron density around HEC U 607:**

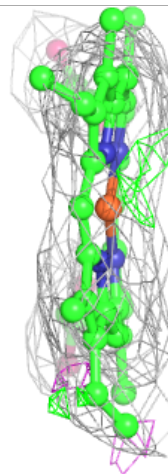
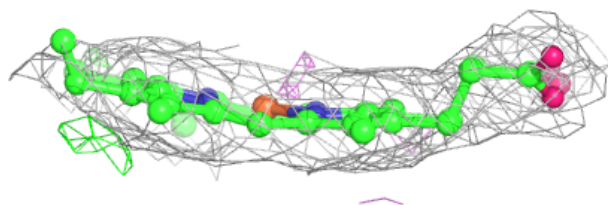
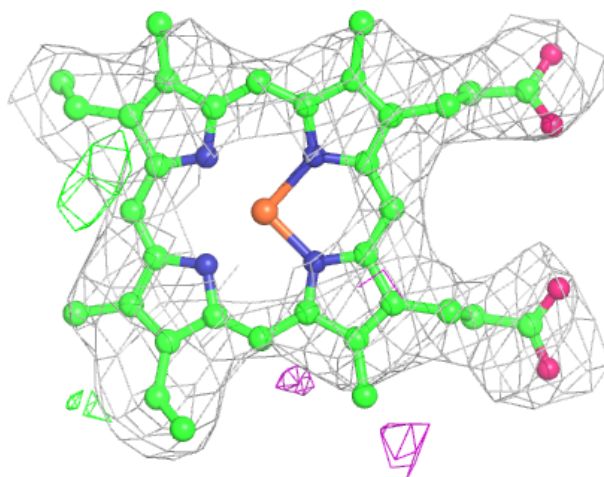
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC M 600:**

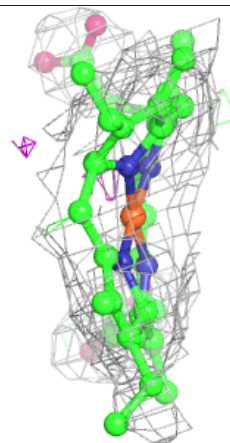
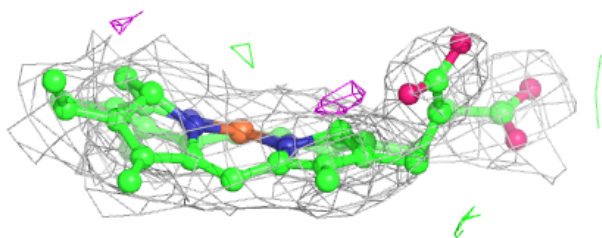
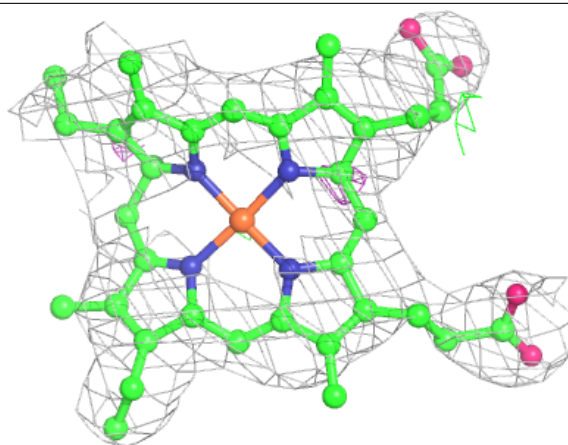
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





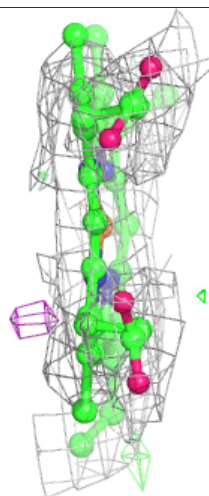
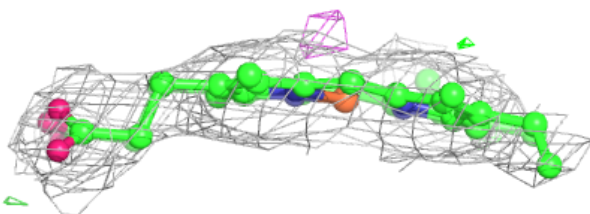
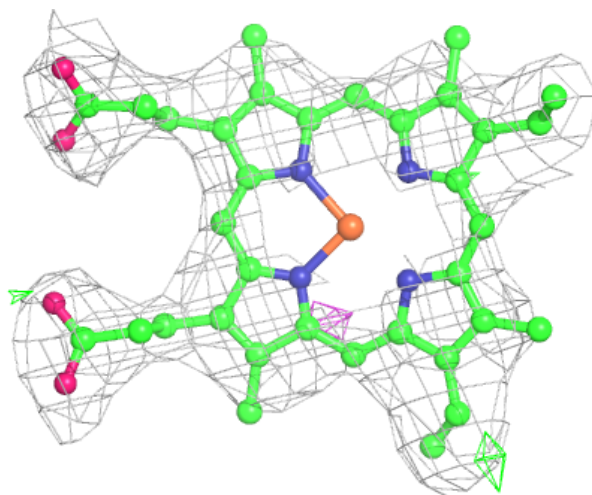
**Electron density around HEC T 603:**

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



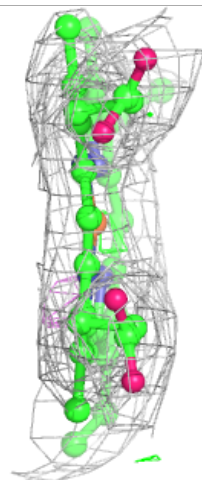
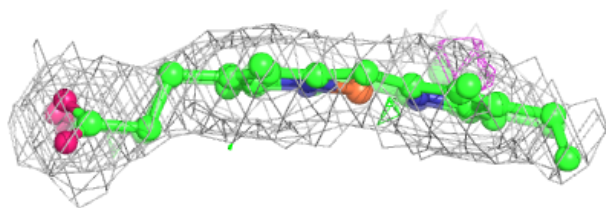
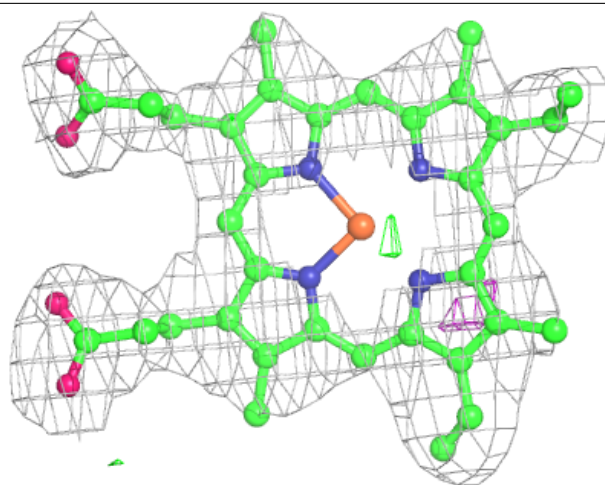
**Electron density around HEC R 600:**

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



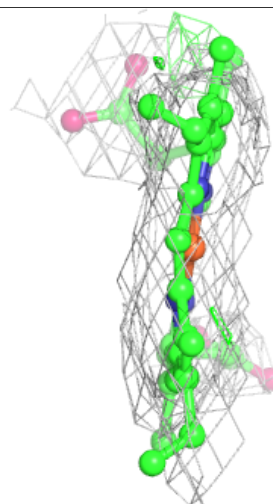
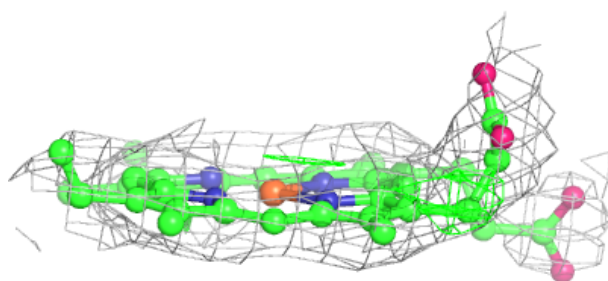
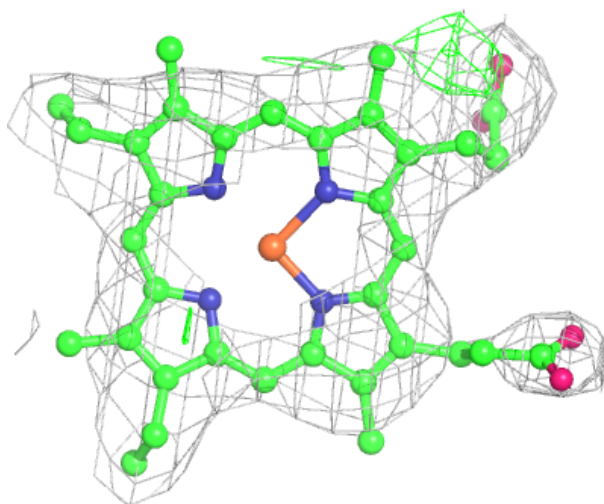
**Electron density around HEC G 600:**

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



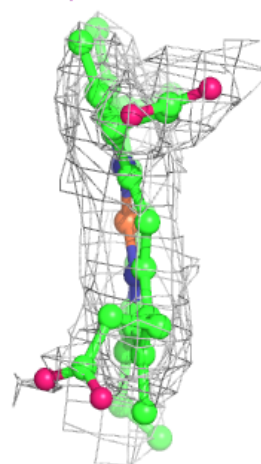
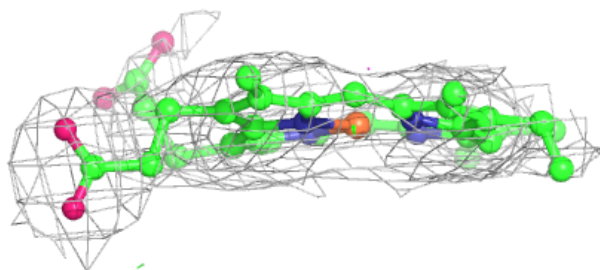
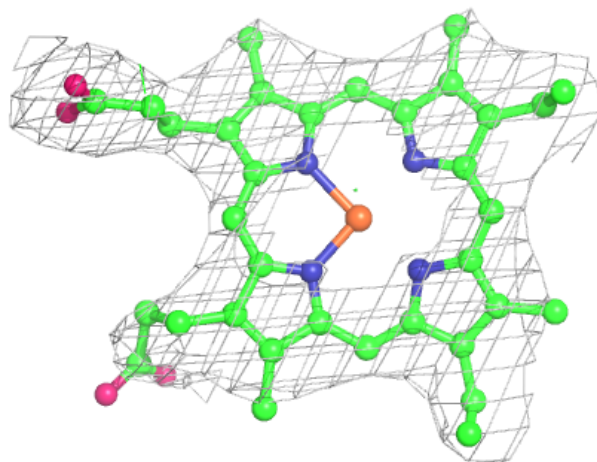
**Electron density around HEC X 601:**

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



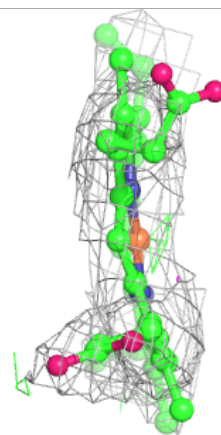
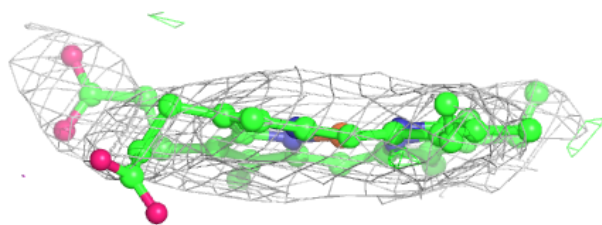
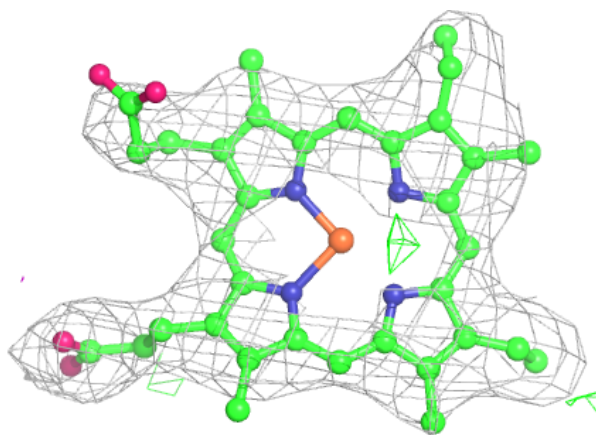
**Electron density around HEC R 602:**

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



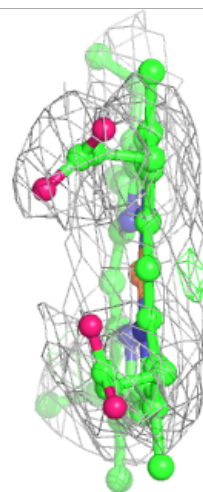
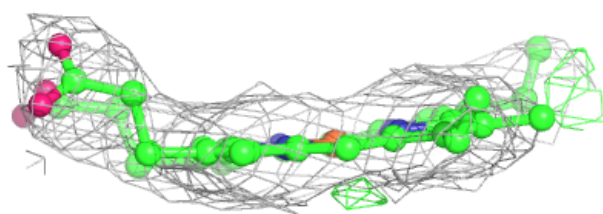
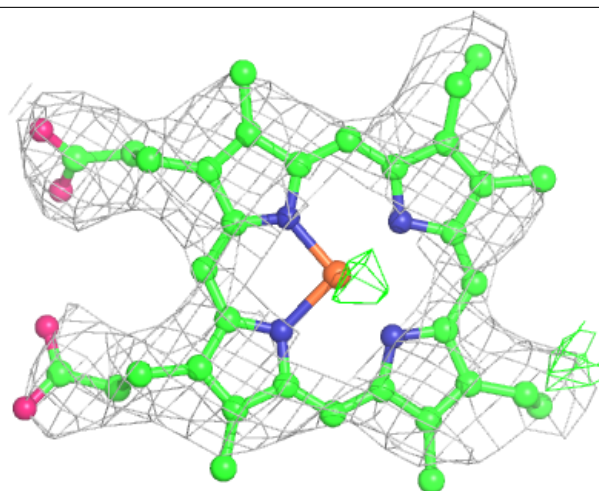
**Electron density around HEC A 602:**

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



**Electron density around HEC F 604:**

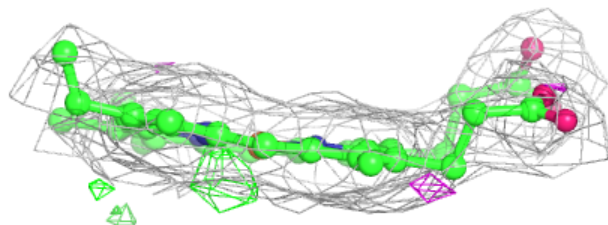
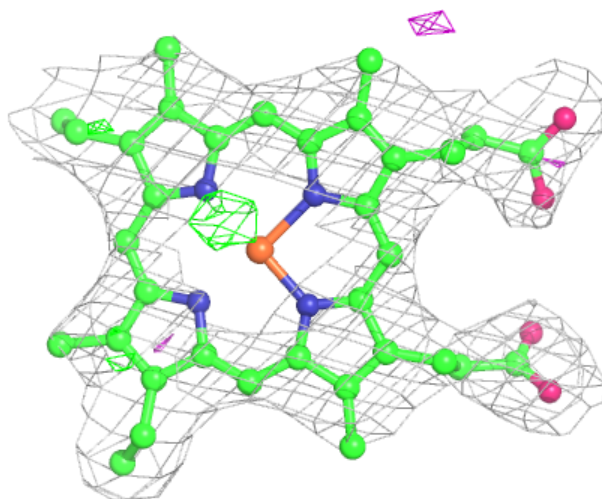
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC R 604:**

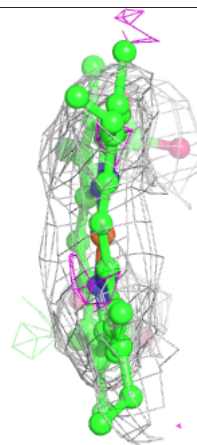
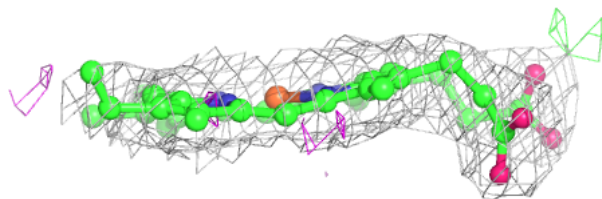
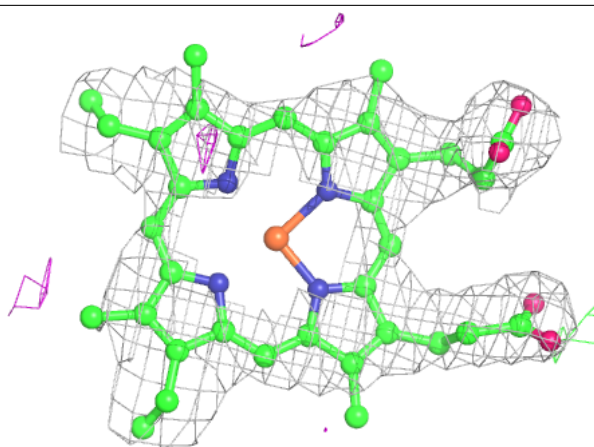
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





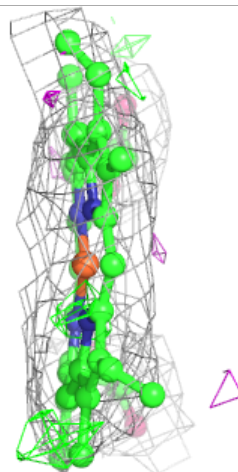
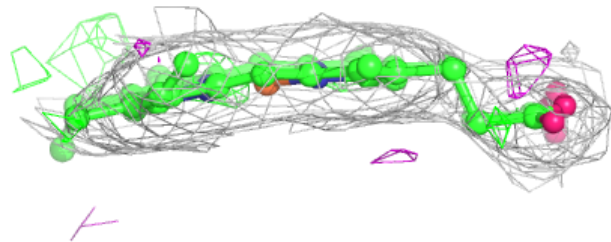
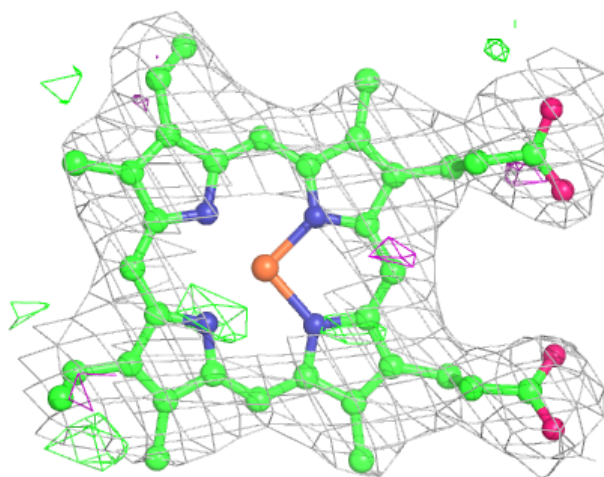
**Electron density around HEC X 607:**

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



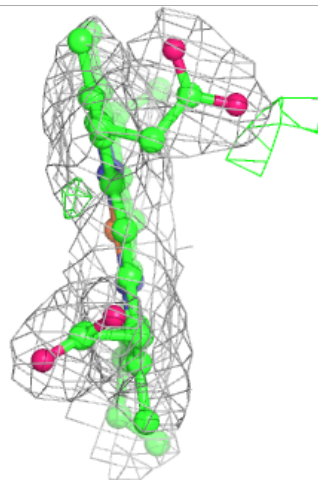
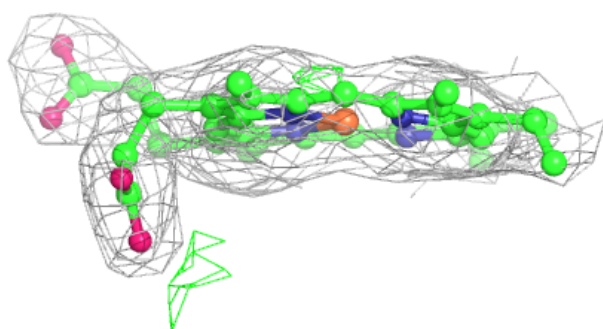
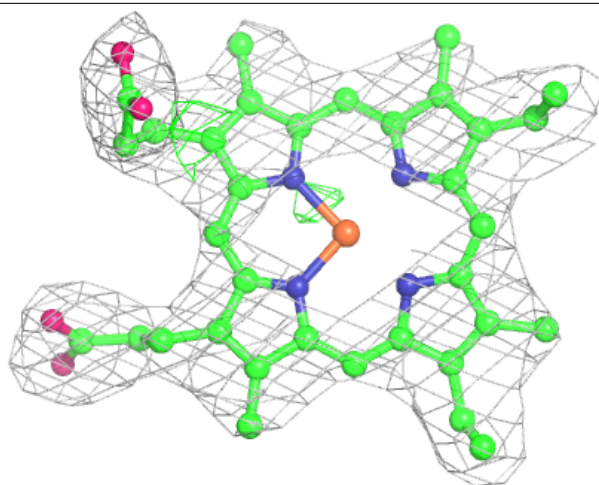
**Electron density around HEC F 600:**

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



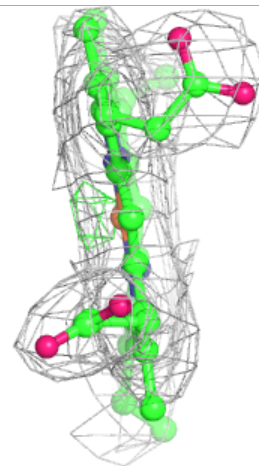
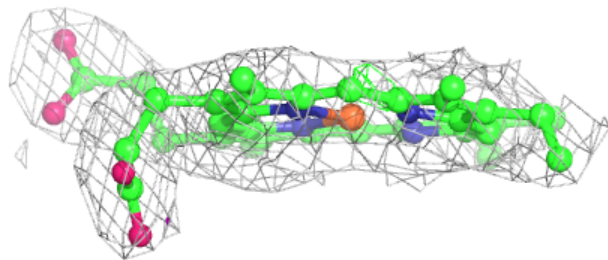
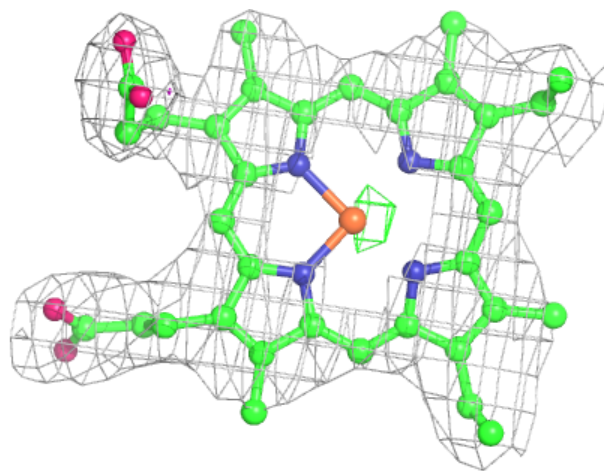
**Electron density around HEC P 601:**

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



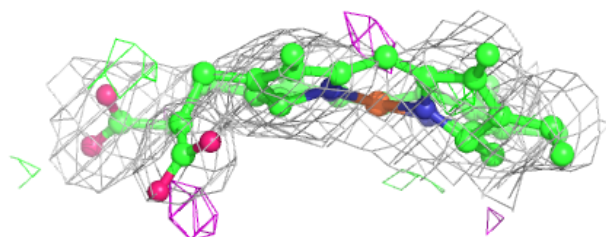
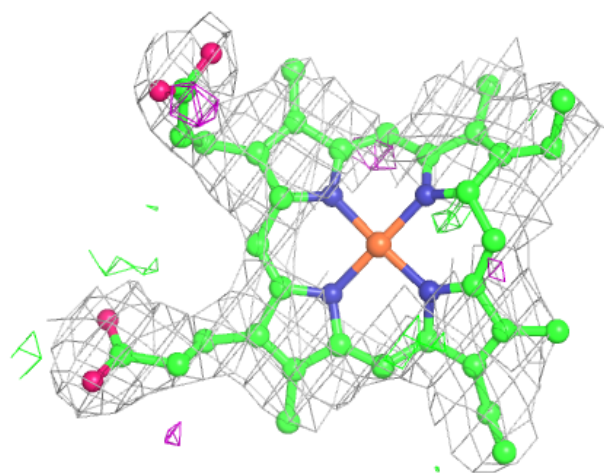
**Electron density around HEC G 601:**

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



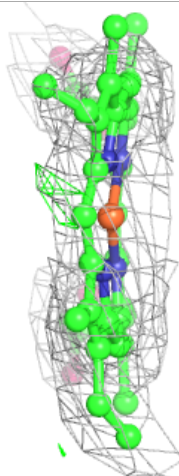
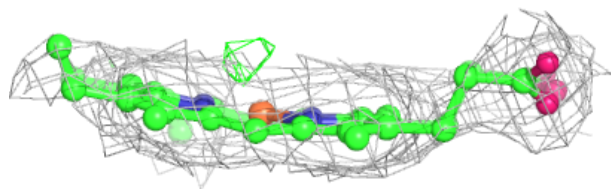
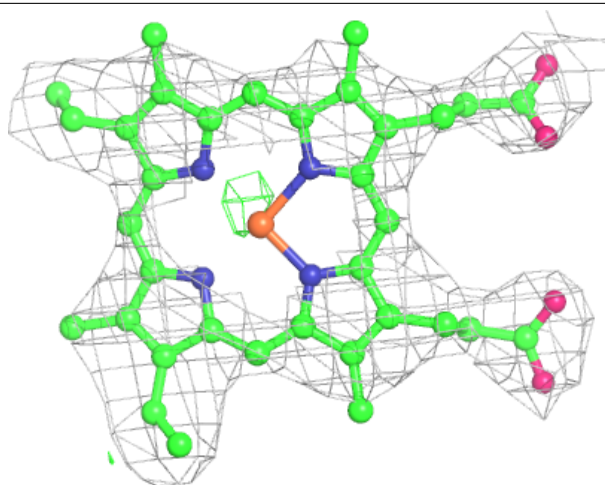
**Electron density around HEC P 603:**

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



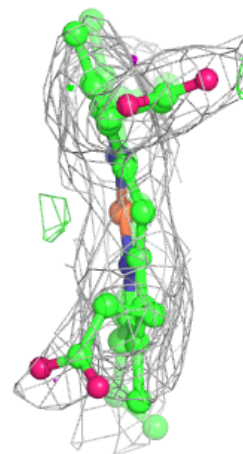
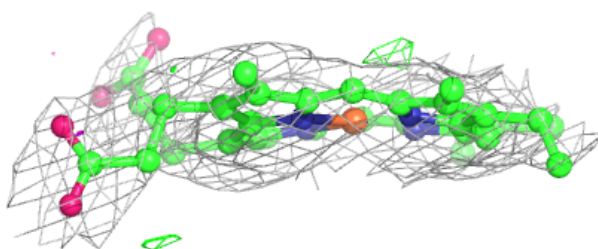
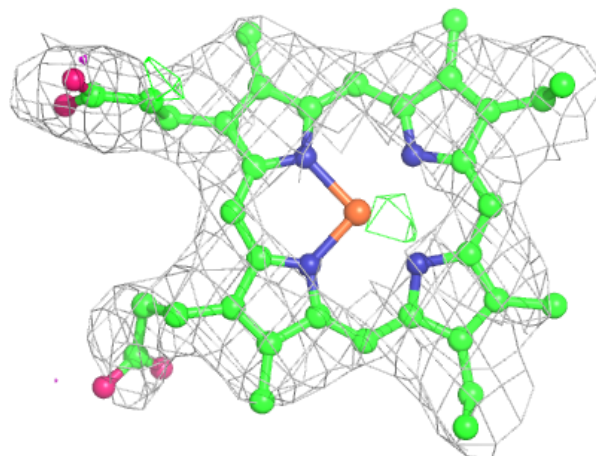
**Electron density around HEC W 600:**

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



**Electron density around HEC K 602:**

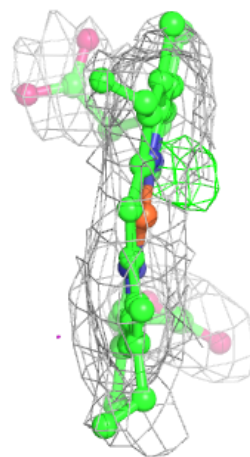
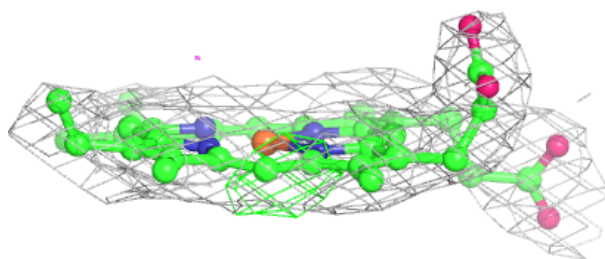
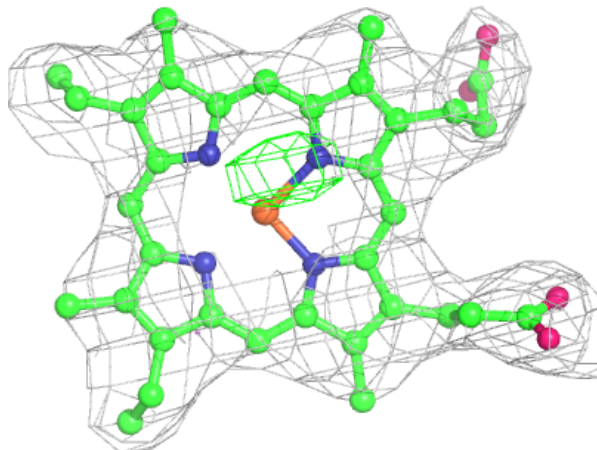
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC E 601:**

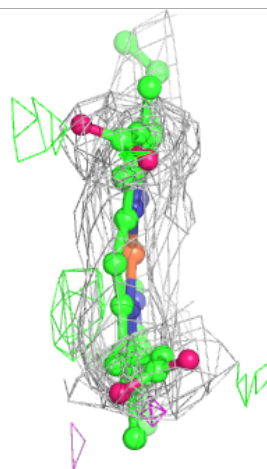
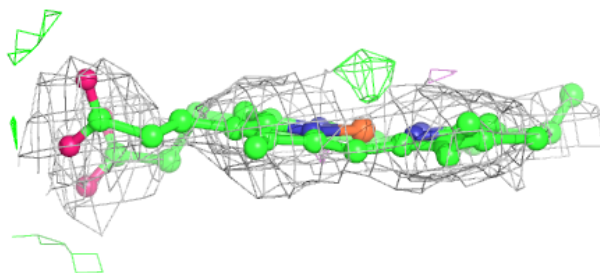
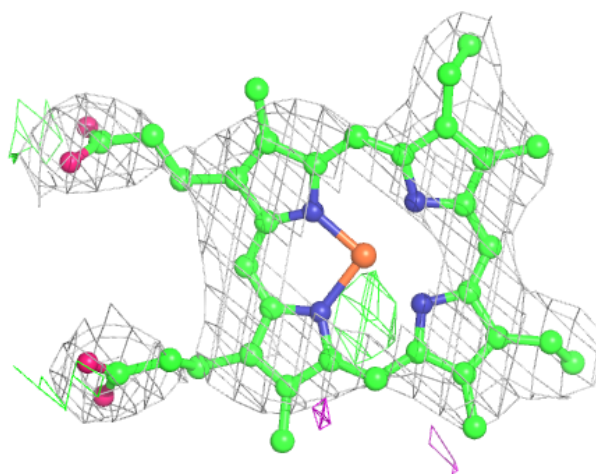
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





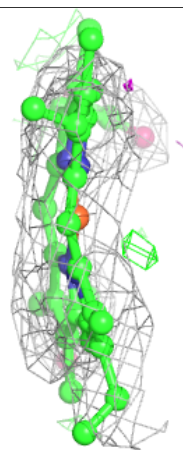
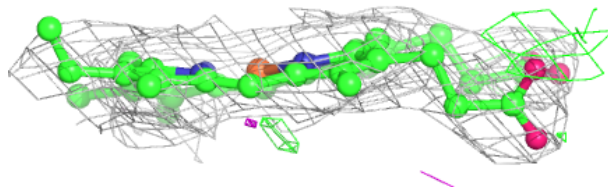
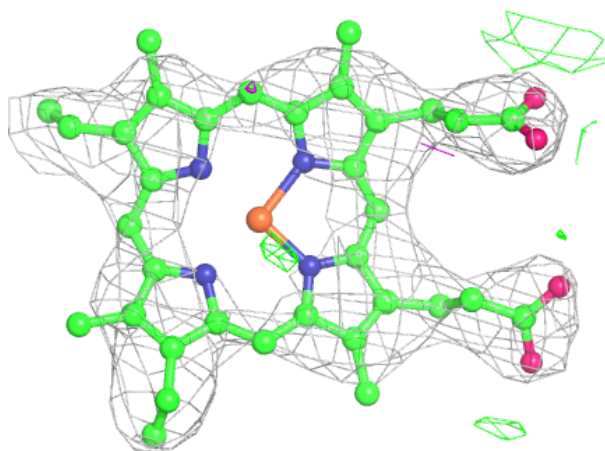
**Electron density around HEC A 605:**

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



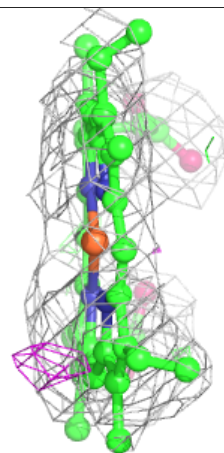
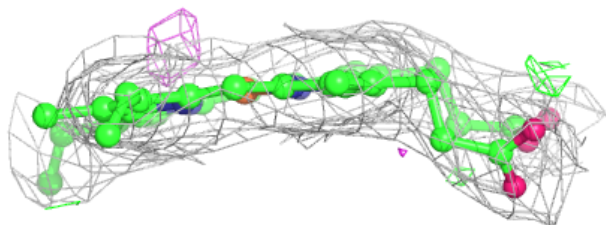
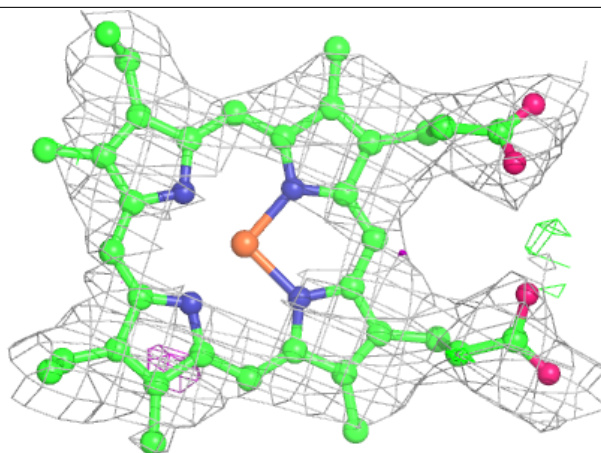
**Electron density around HEC S 606:**

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



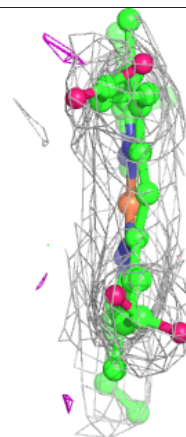
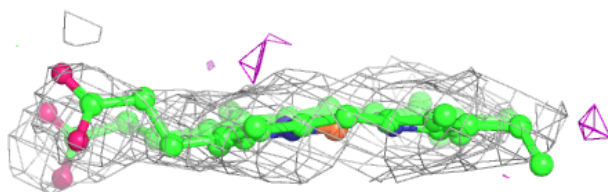
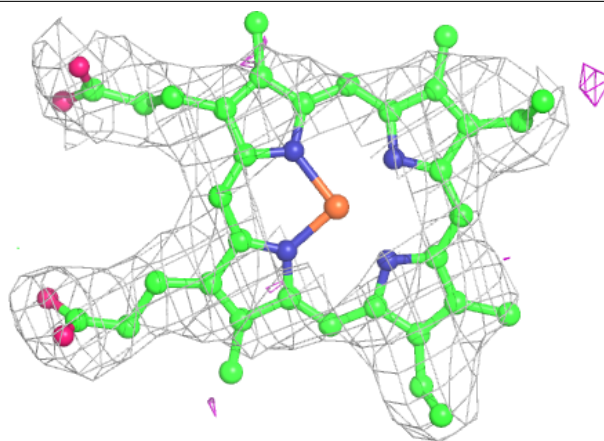
**Electron density around HEC L 604:**

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



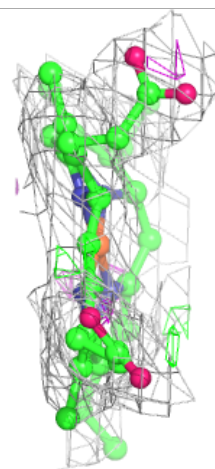
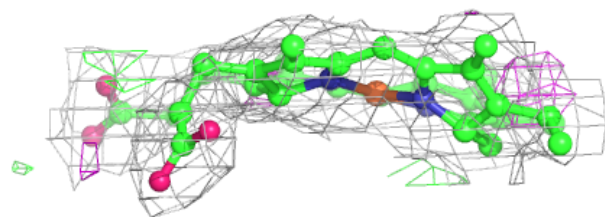
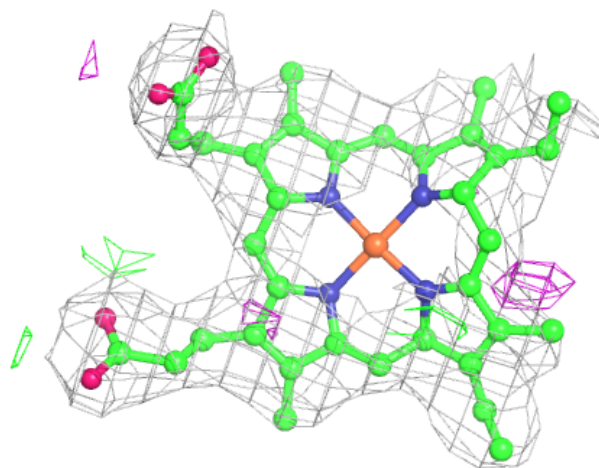
**Electron density around HEC V 605:**

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



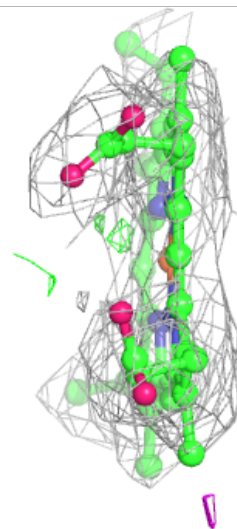
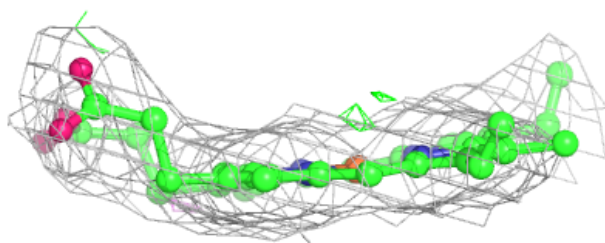
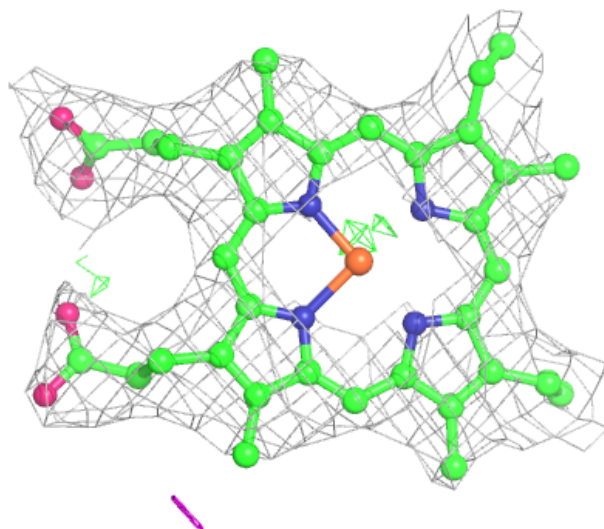
**Electron density around HEC G 603:**

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



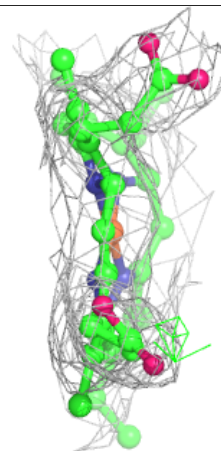
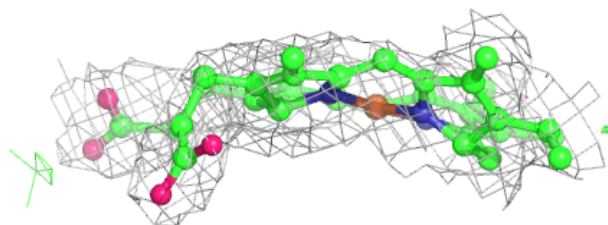
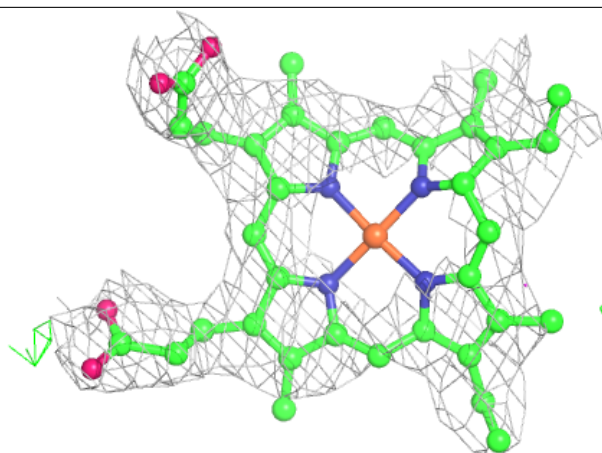
**Electron density around HEC H 604:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



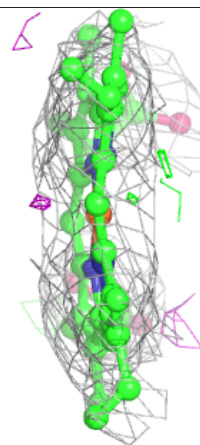
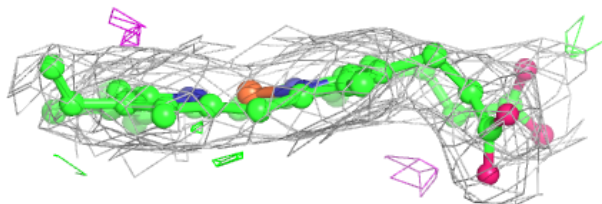
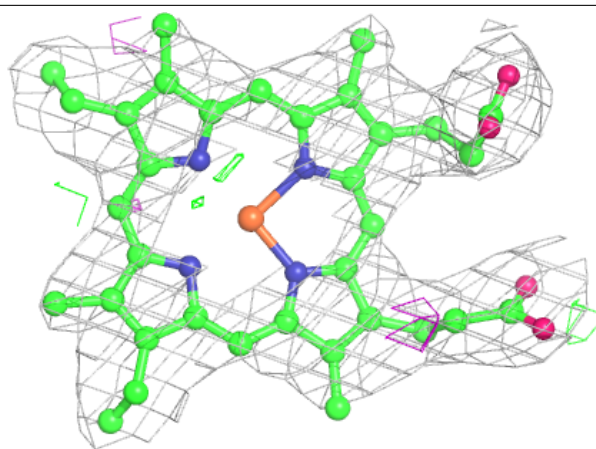
**Electron density around HEC Q 603:**

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



**Electron density around HEC O 607:**

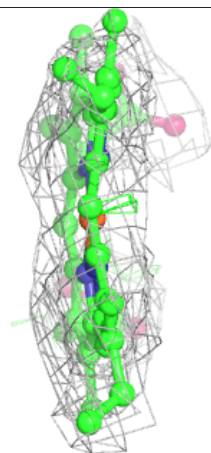
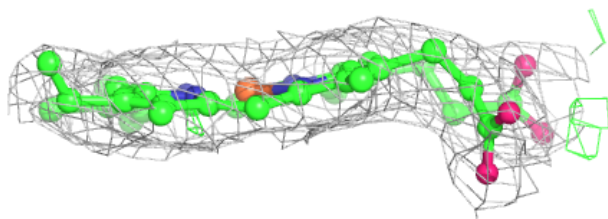
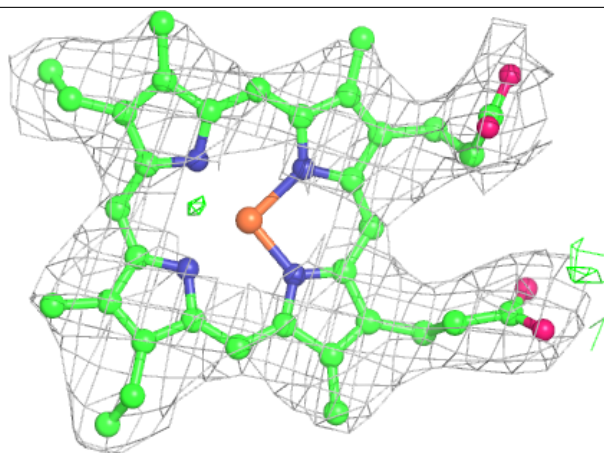
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





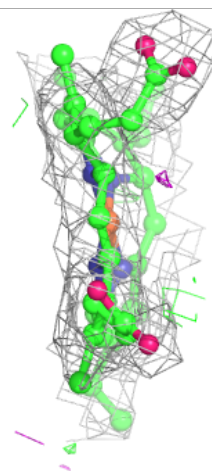
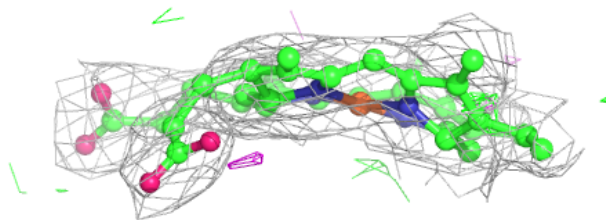
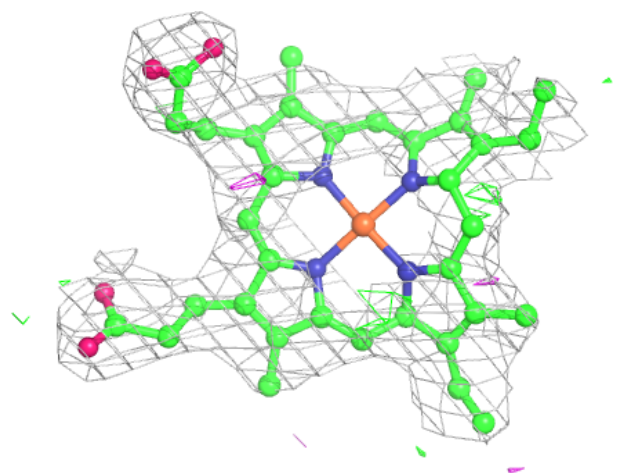
**Electron density around HEC J 607:**

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



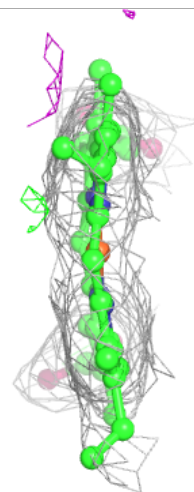
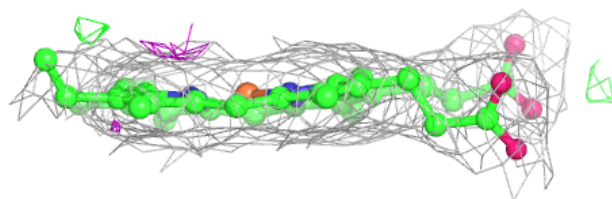
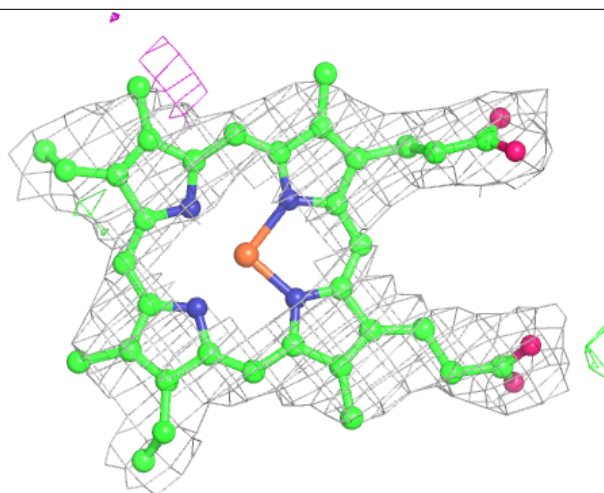
**Electron density around HEC I 603:**

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



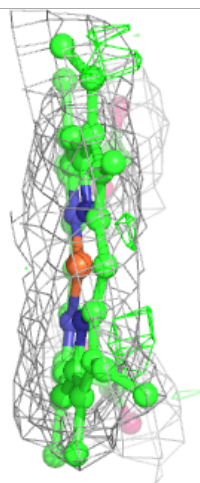
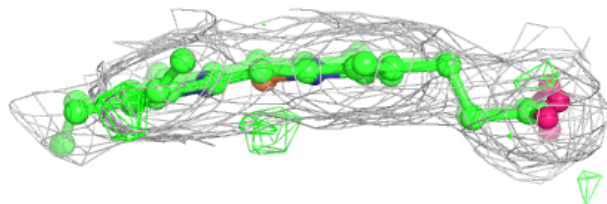
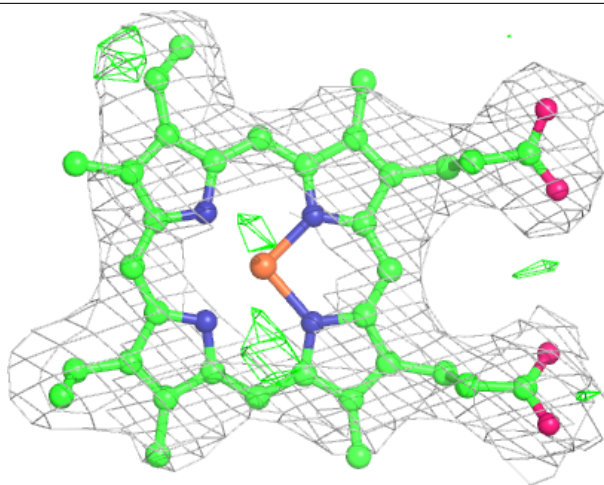
**Electron density around HEC B 605:**

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



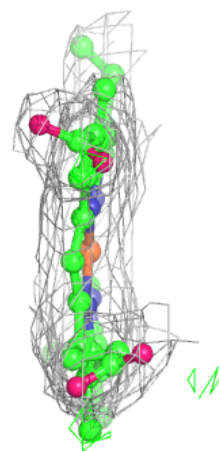
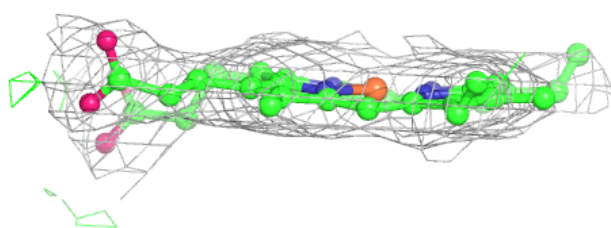
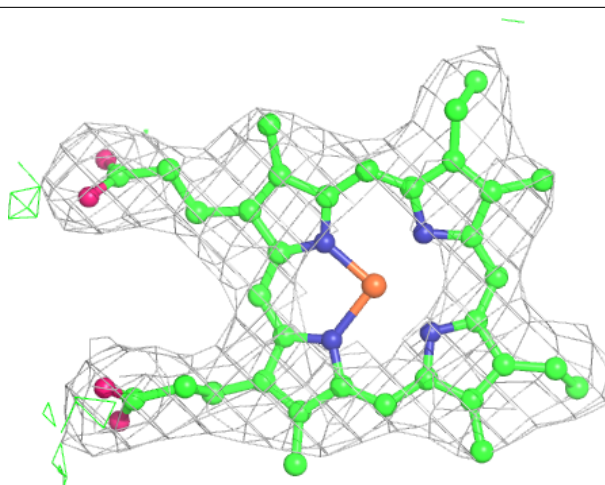
**Electron density around HEC P 600:**

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



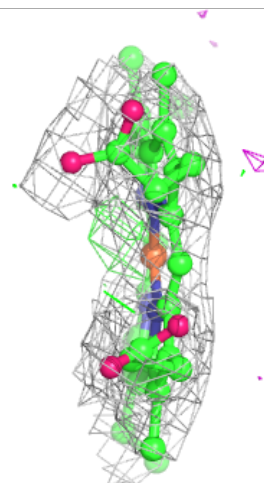
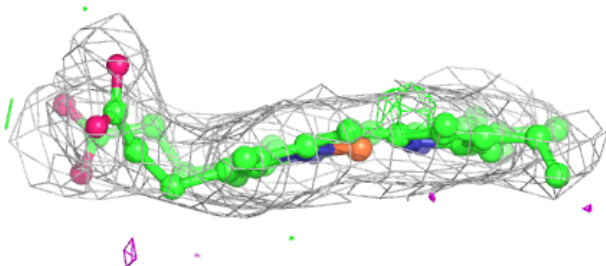
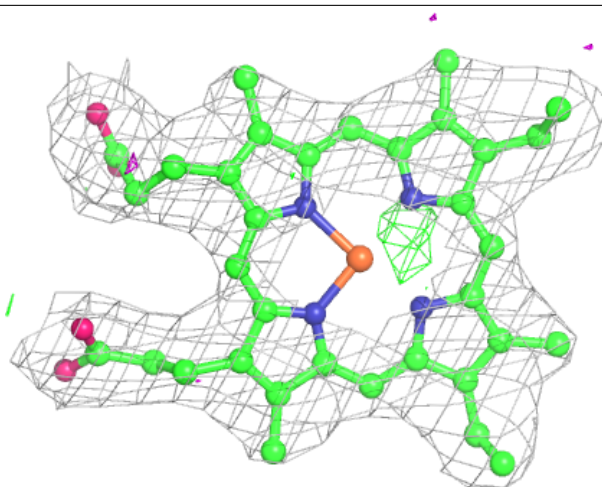
**Electron density around HEC R 605:**

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



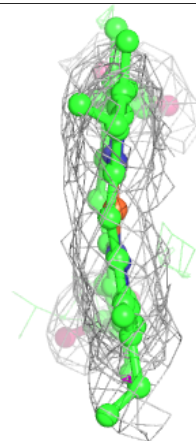
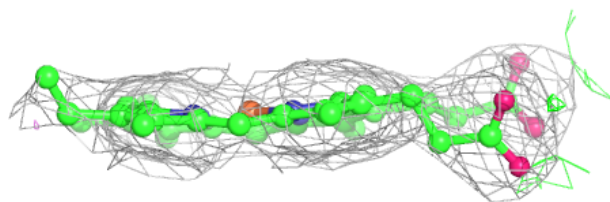
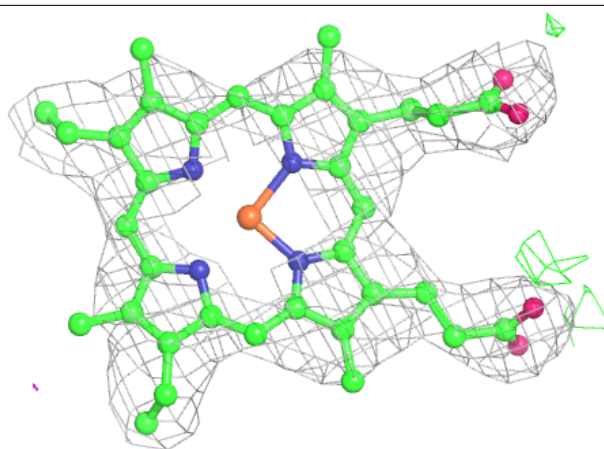
**Electron density around HEC G 607:**

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



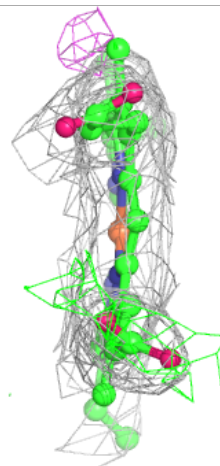
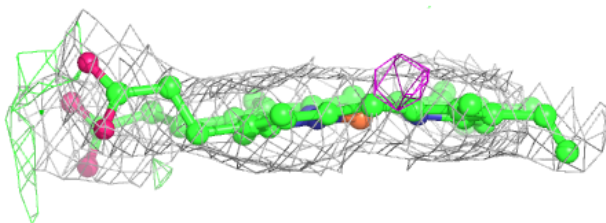
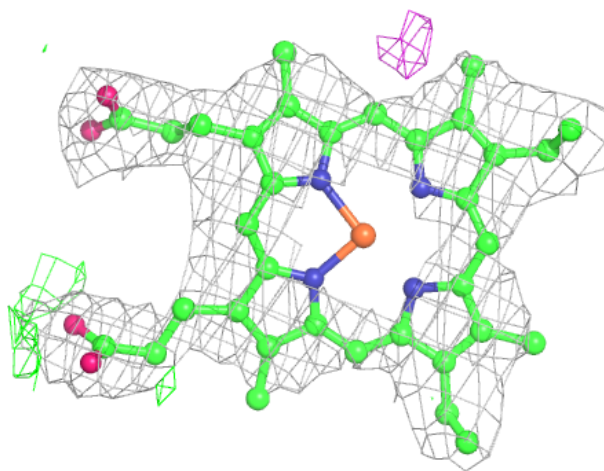
**Electron density around HEC P 605:**

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



**Electron density around HEC O 605:**

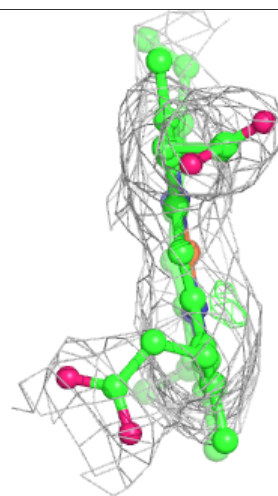
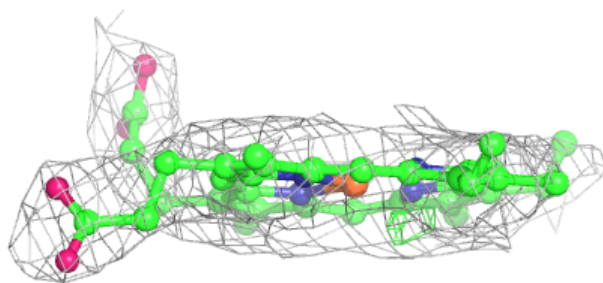
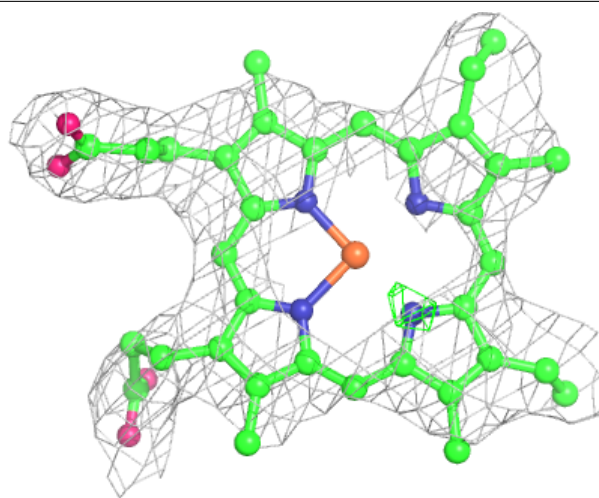
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





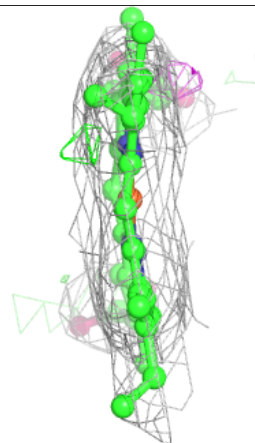
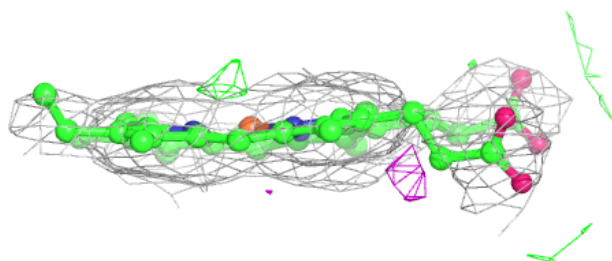
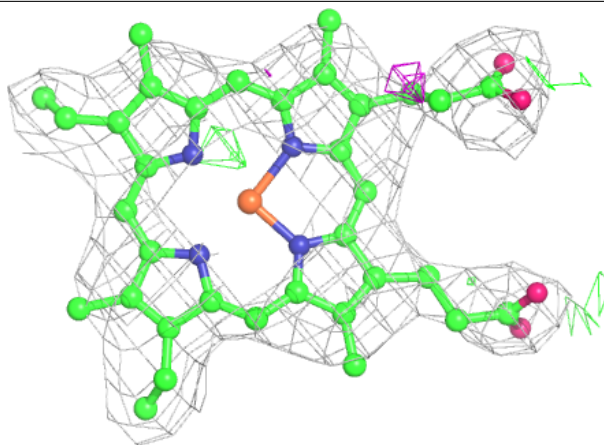
**Electron density around HEC T 601:**

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

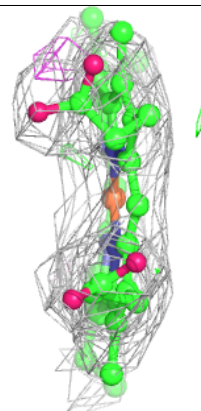
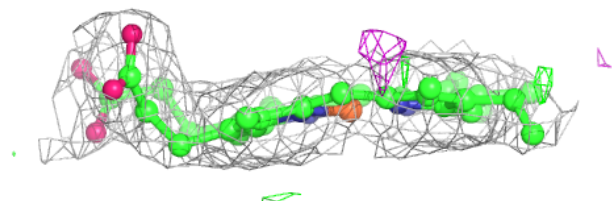
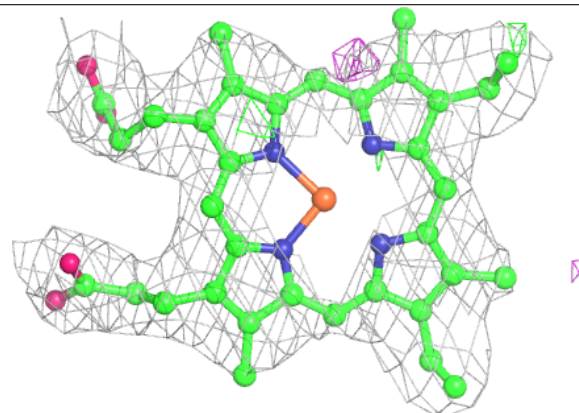


**Electron density around HEC N 605:**

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

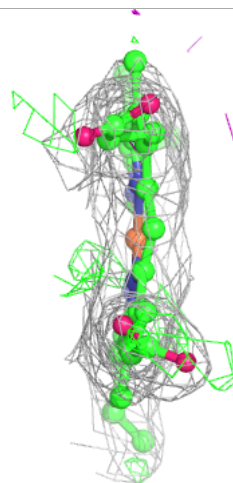
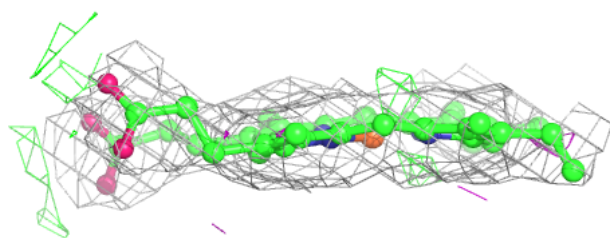
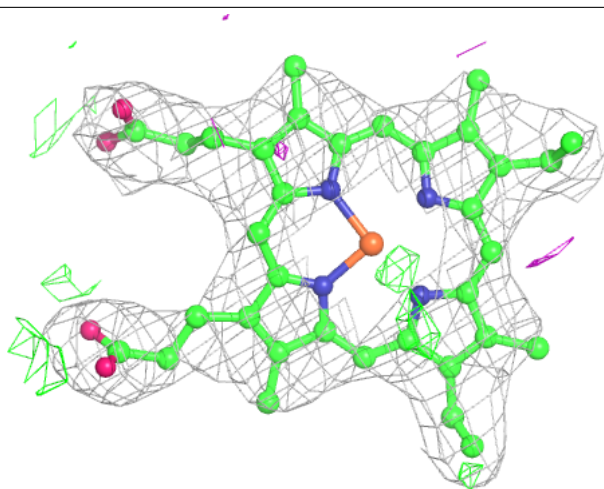
**Electron density around HEC R 607:**

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



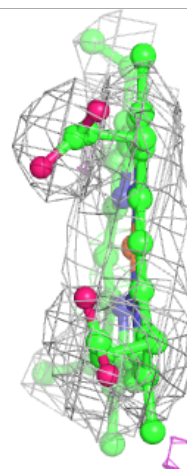
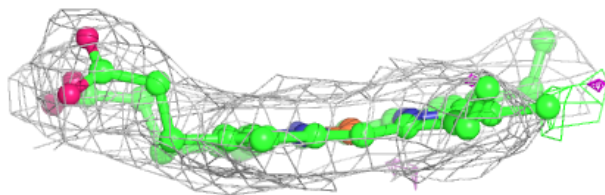
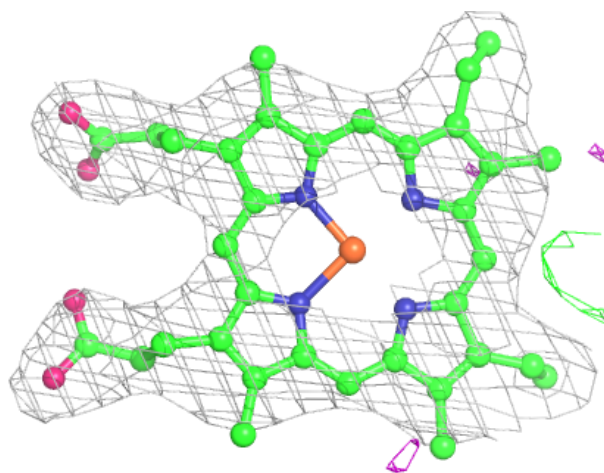
**Electron density around HEC J 605:**

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



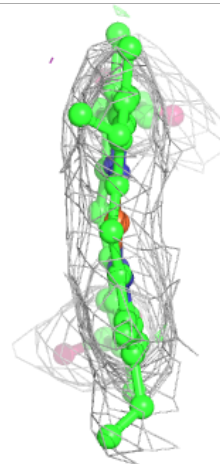
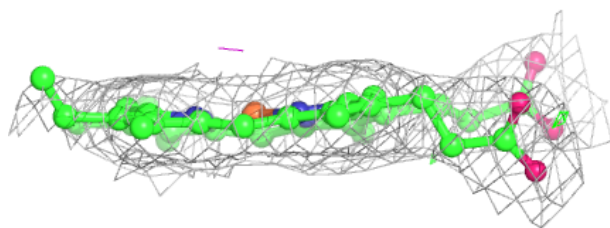
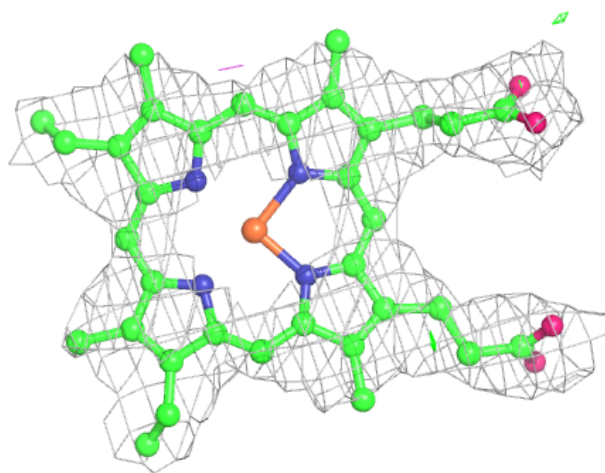
**Electron density around HEC N 604:**

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



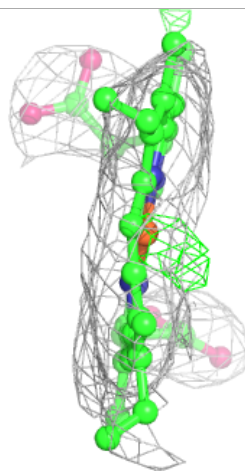
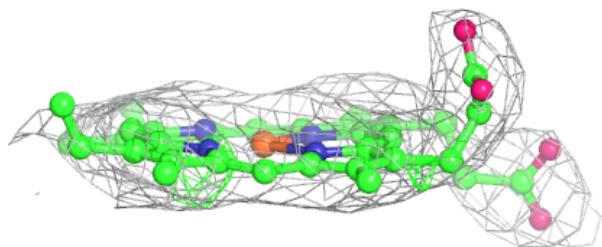
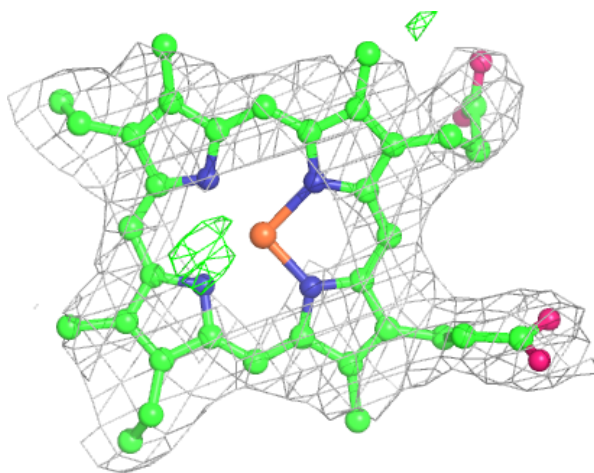
**Electron density around HEC H 605:**

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



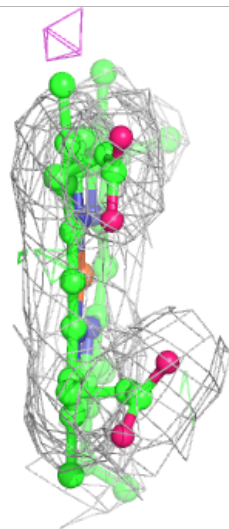
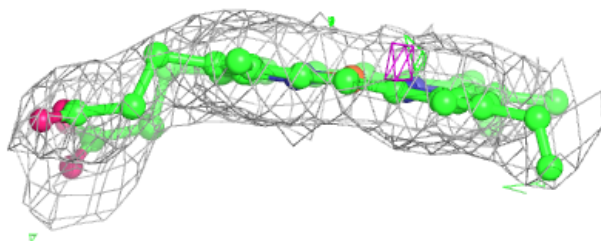
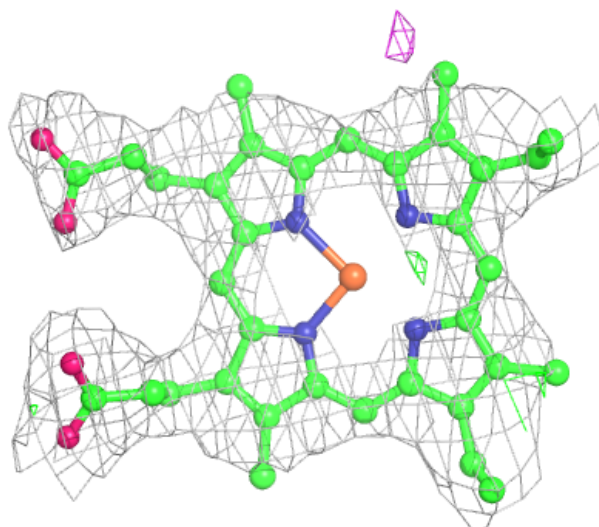
**Electron density around HEC A 601:**

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



**Electron density around HEC I 604:**

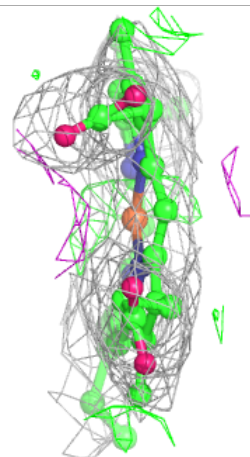
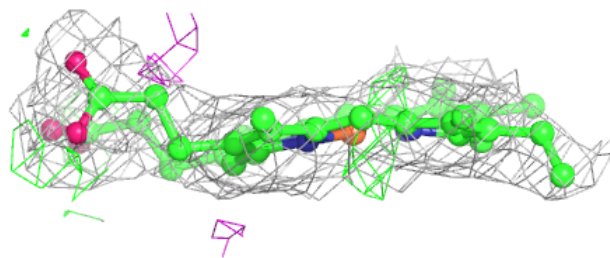
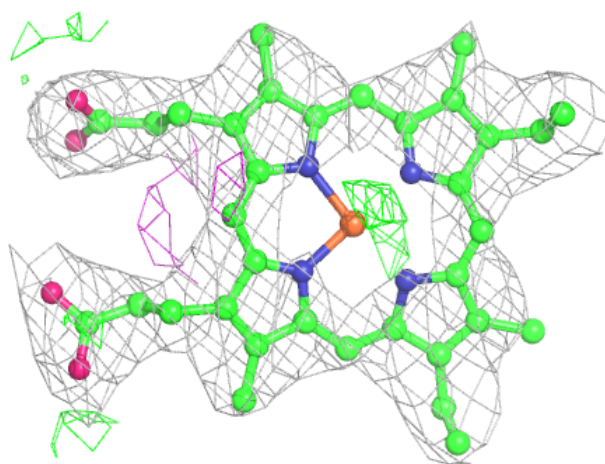
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC J 606:**

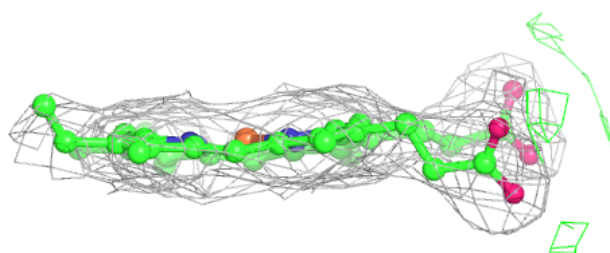
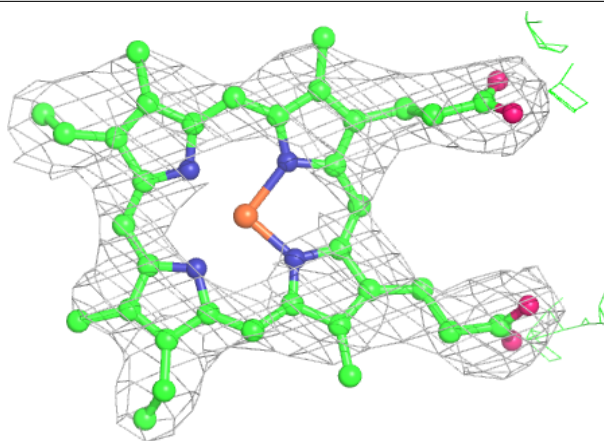
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





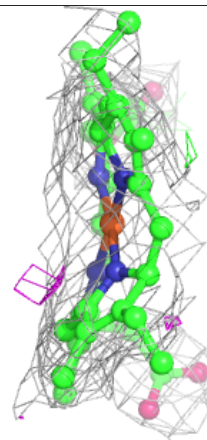
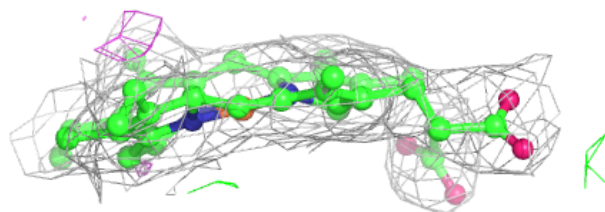
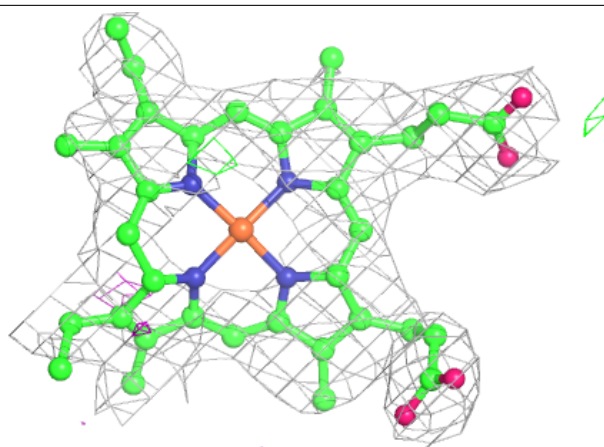
**Electron density around HEC Q 605:**

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



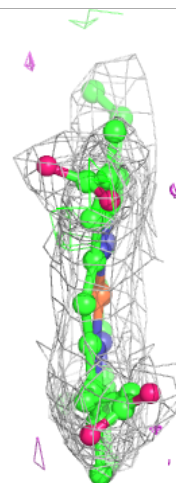
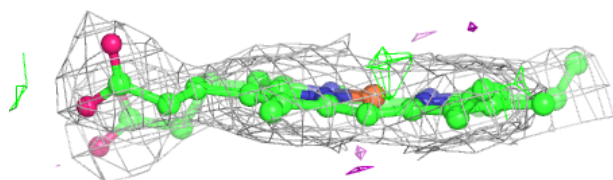
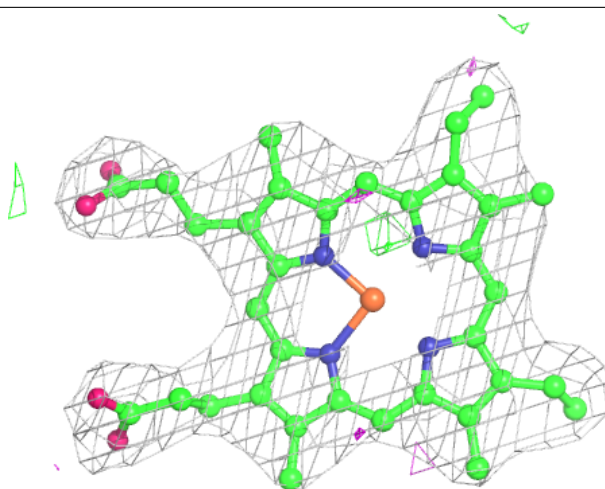
**Electron density around HEC H 603:**

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



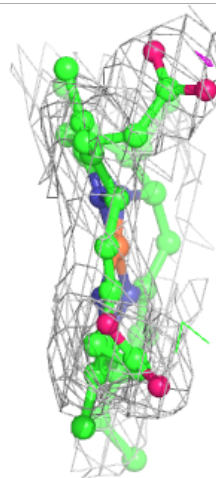
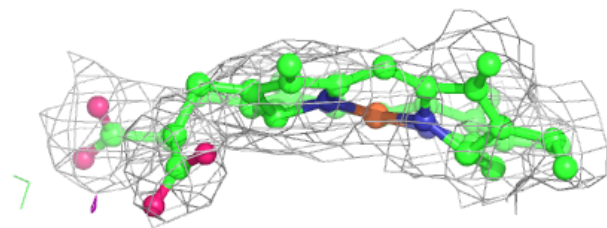
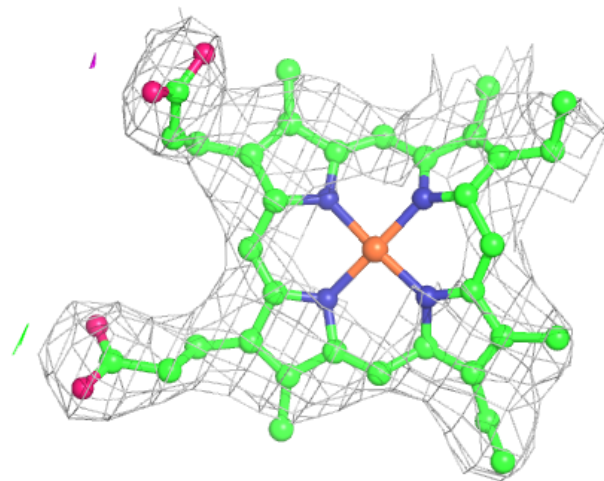
**Electron density around HEC I 605:**

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



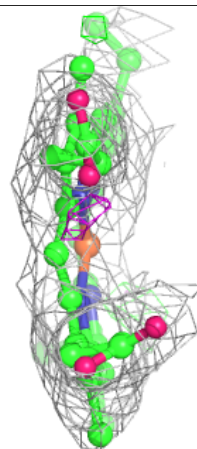
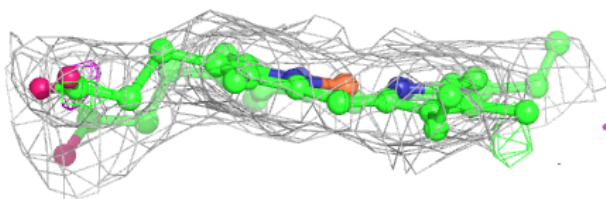
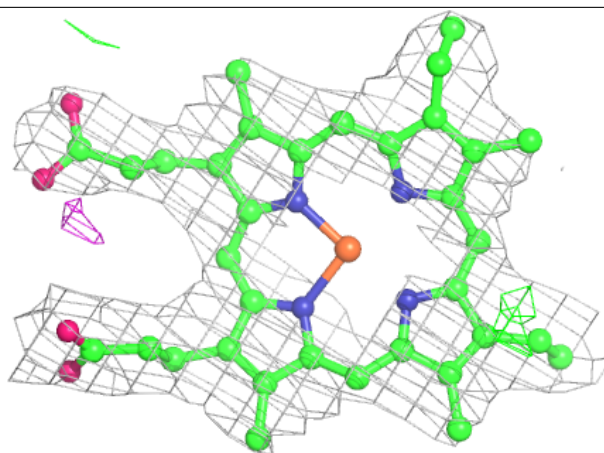
**Electron density around HEC N 603:**

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



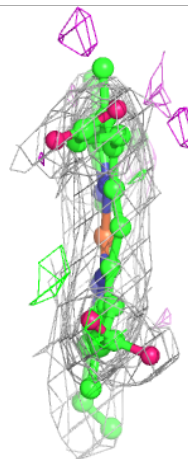
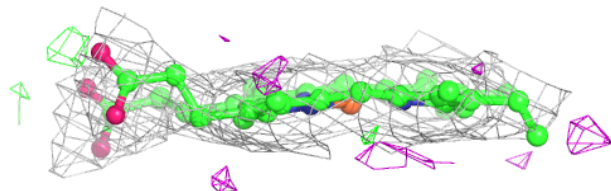
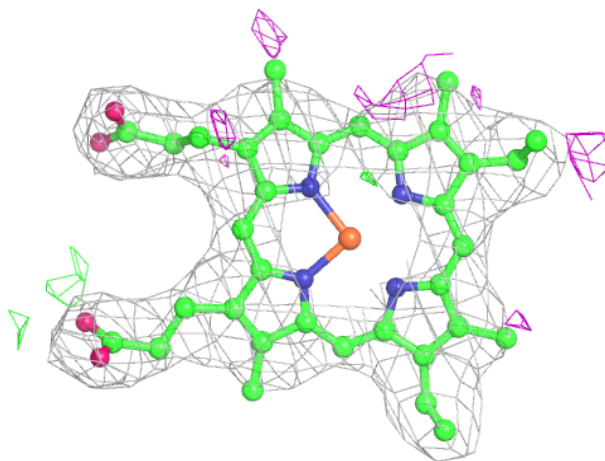
**Electron density around HEC B 606:**

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



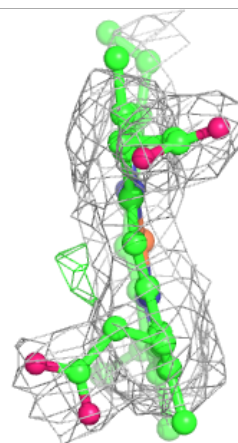
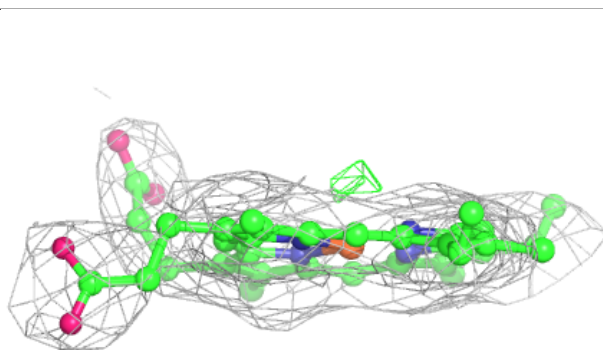
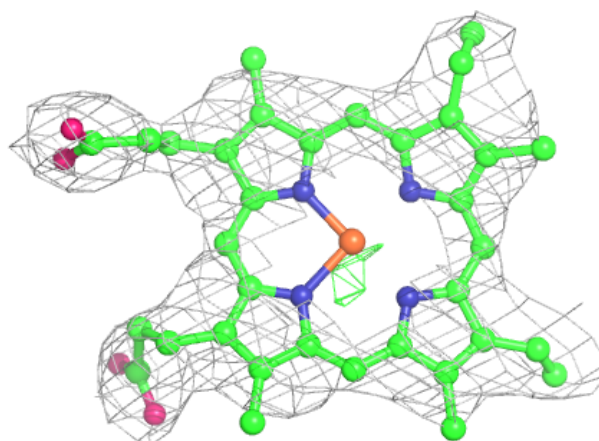
**Electron density around HEC L 605:**

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



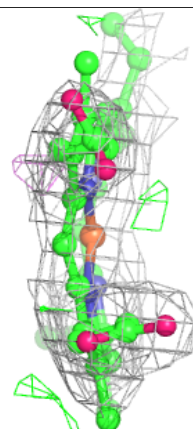
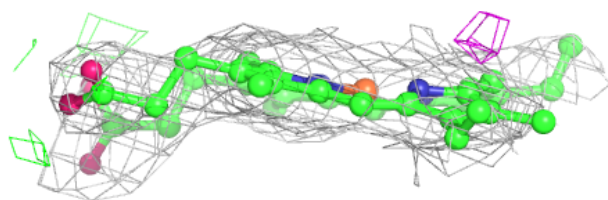
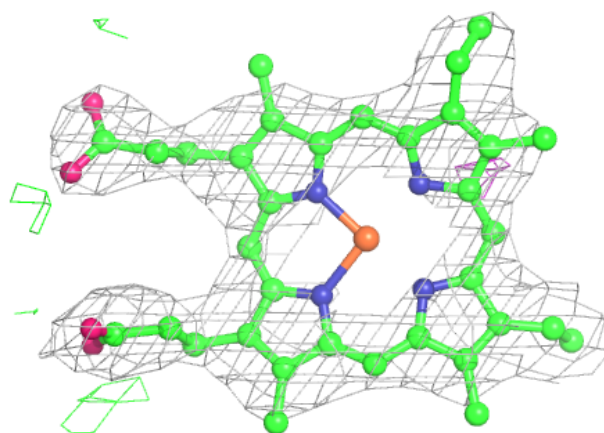
**Electron density around HEC D 601:**

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



**Electron density around HEC D 606:**

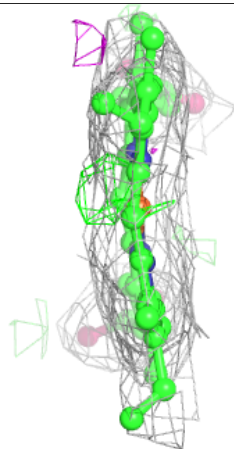
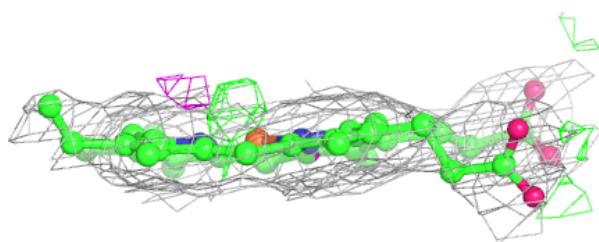
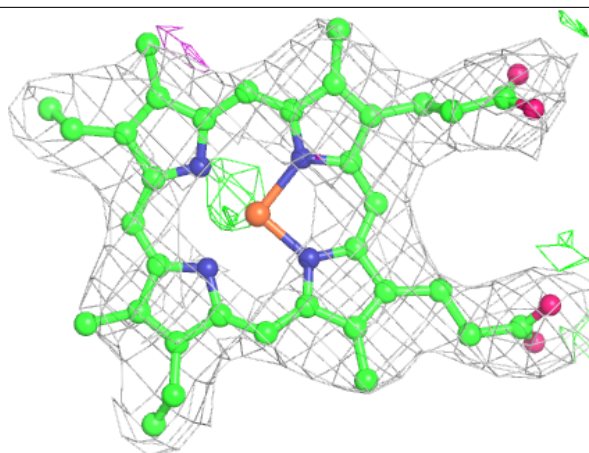
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





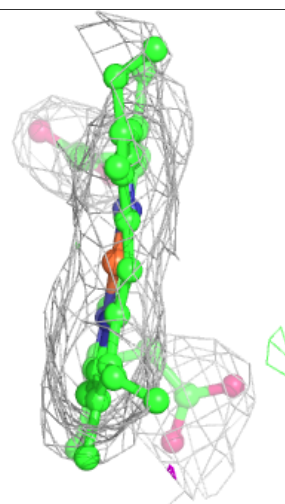
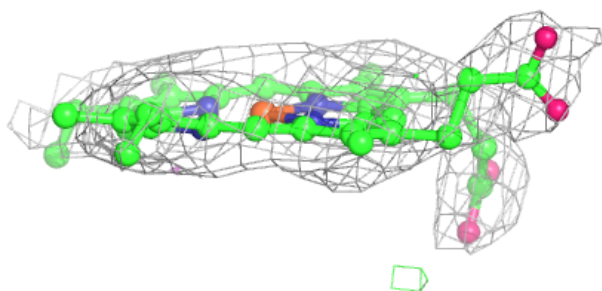
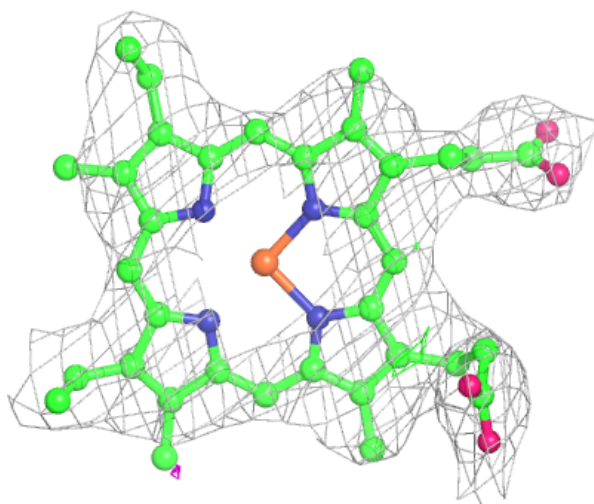
**Electron density around HEC G 605:**

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



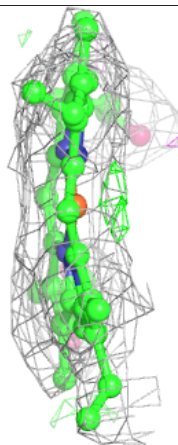
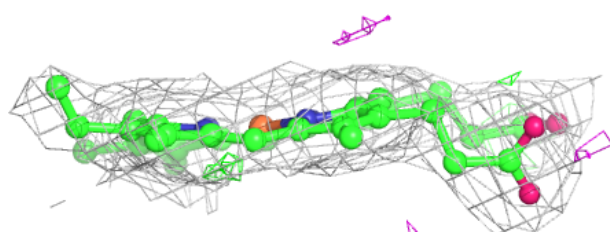
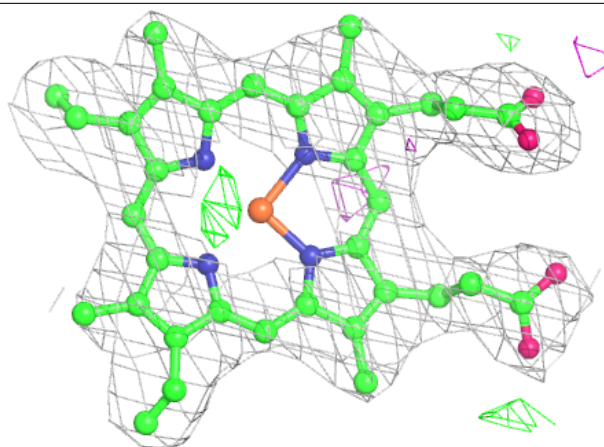
**Electron density around HEC C 601:**

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



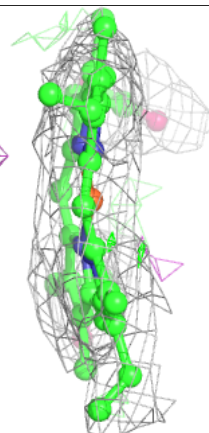
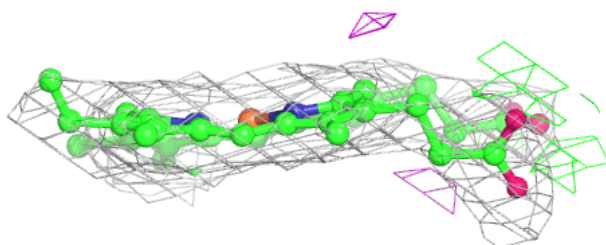
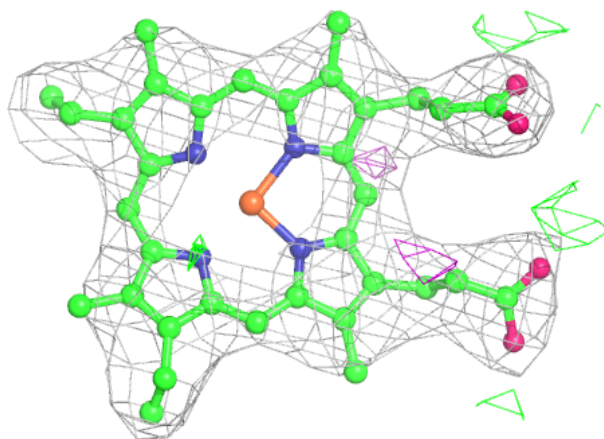
**Electron density around HEC I 606:**

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



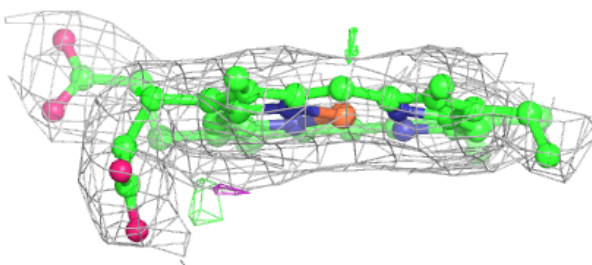
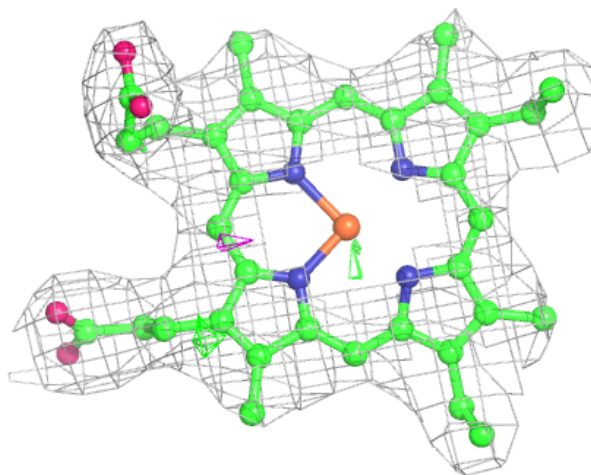
**Electron density around HEC C 606:**

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



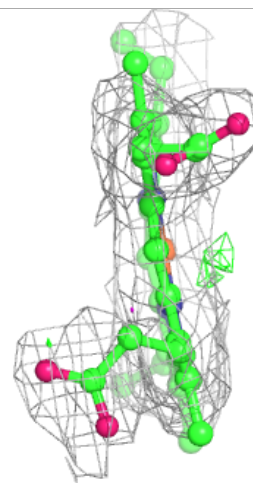
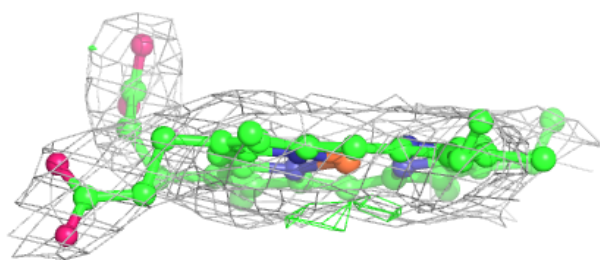
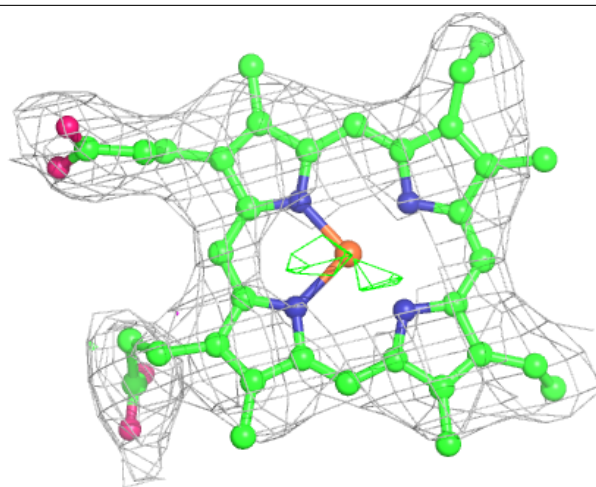
**Electron density around HEC K 601:**

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



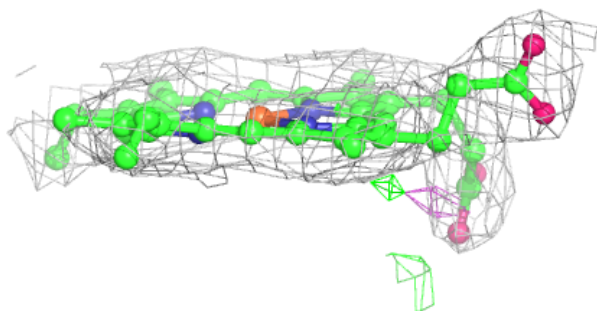
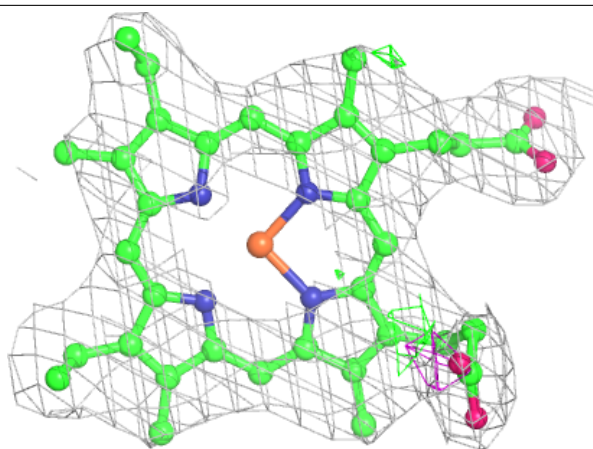
**Electron density around HEC R 601:**

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



**Electron density around HEC H 601:**

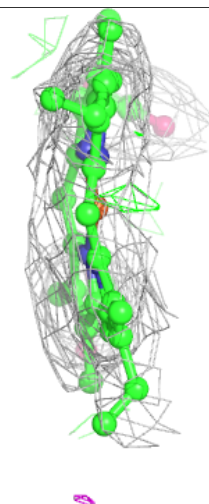
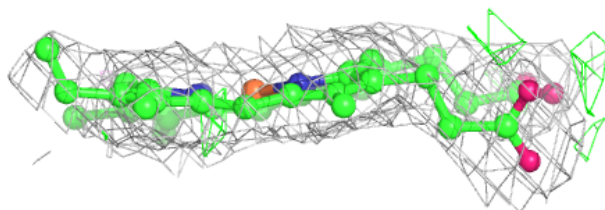
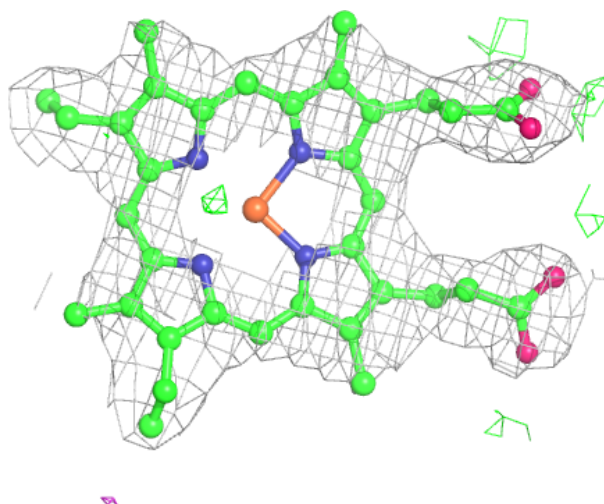
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC O 606:**

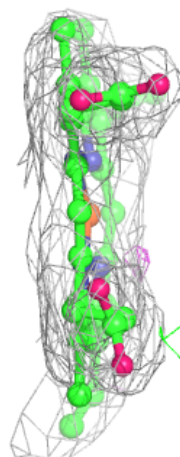
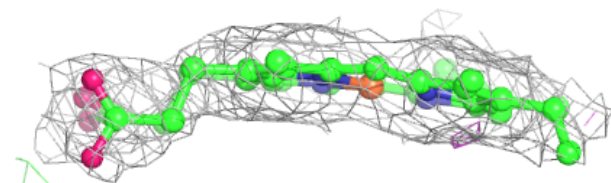
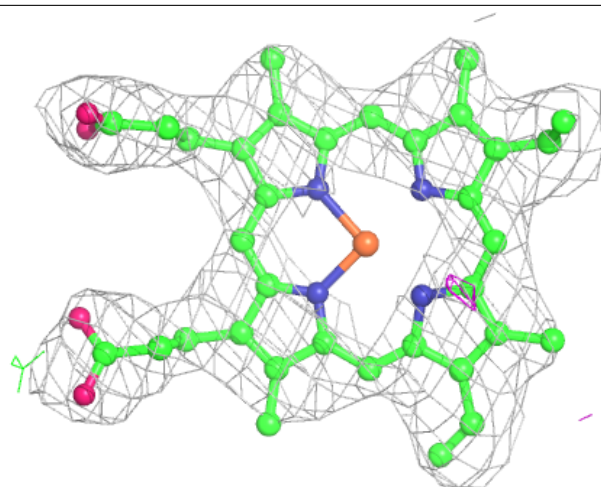
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





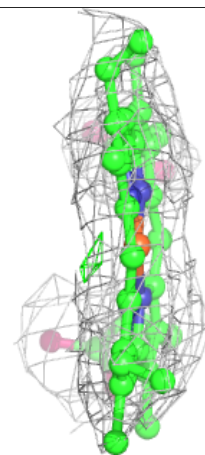
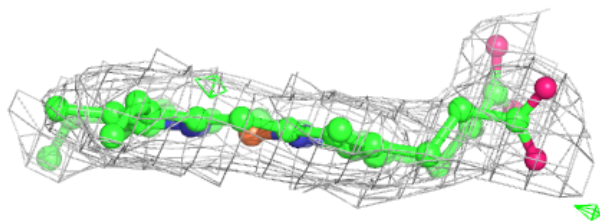
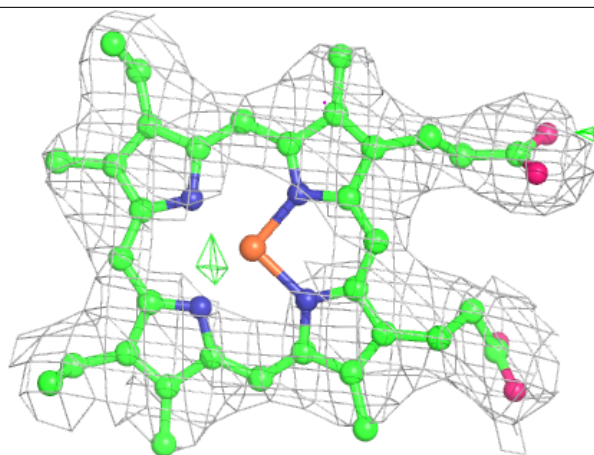
**Electron density around HEC I 600:**

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



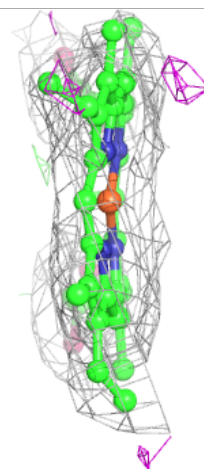
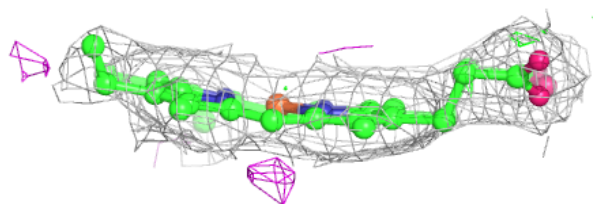
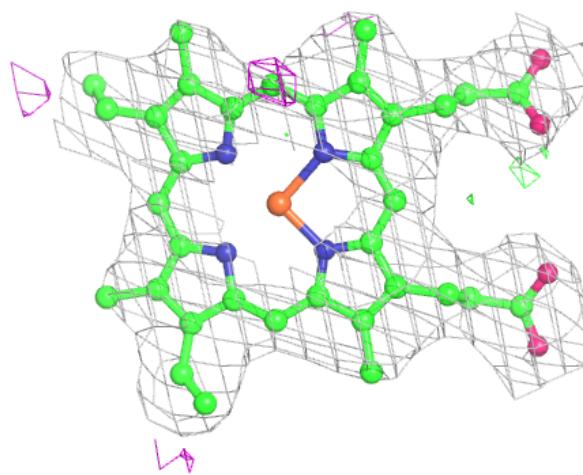
**Electron density around HEC I 607:**

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



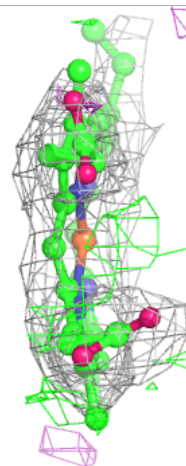
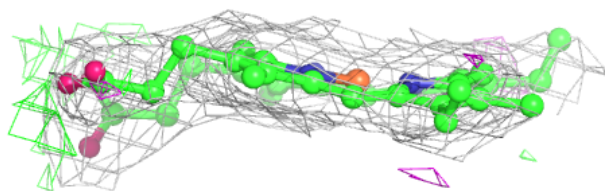
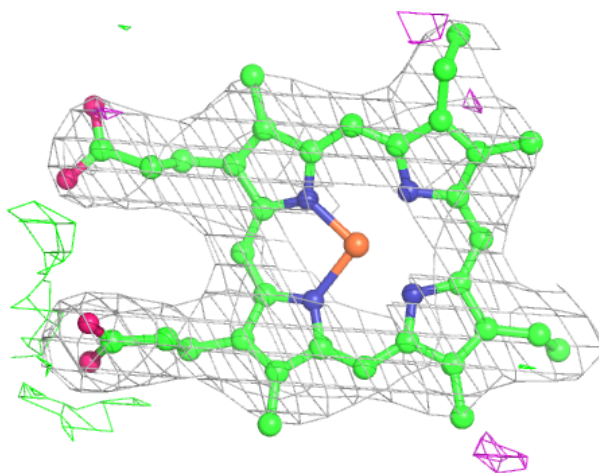
**Electron density around HEC H 600:**

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



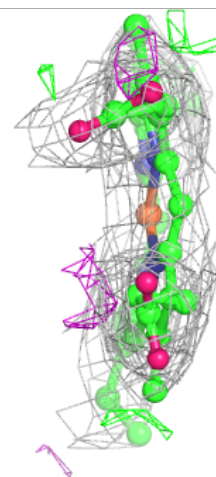
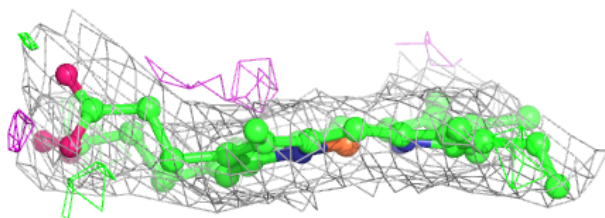
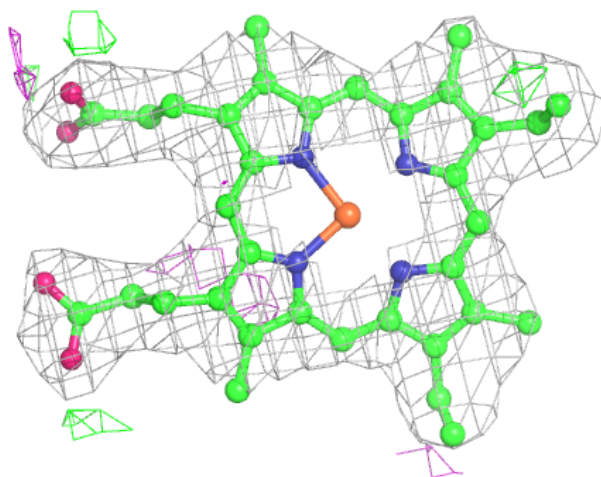
**Electron density around HEC M 606:**

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



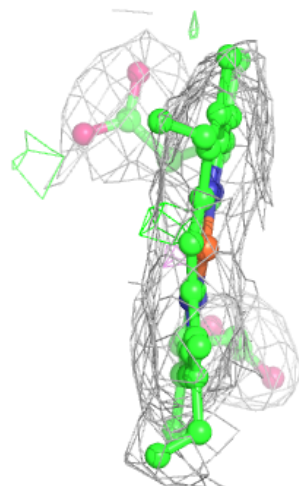
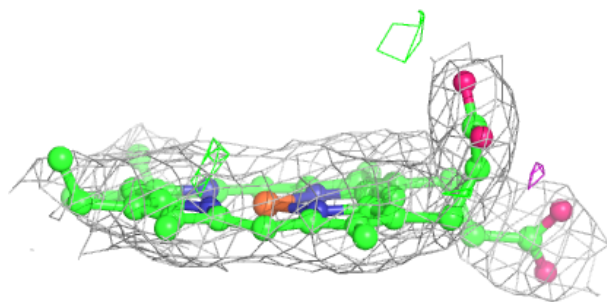
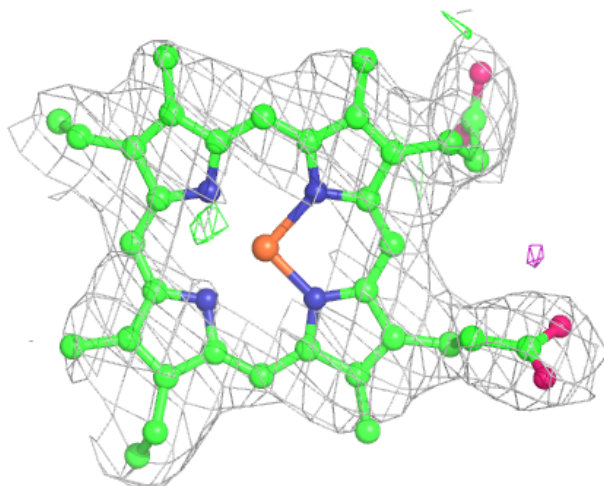
**Electron density around HEC H 606:**

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



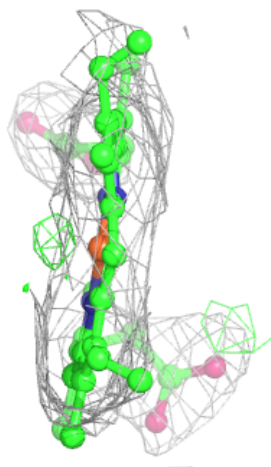
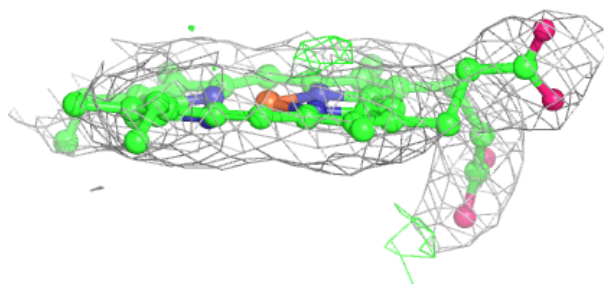
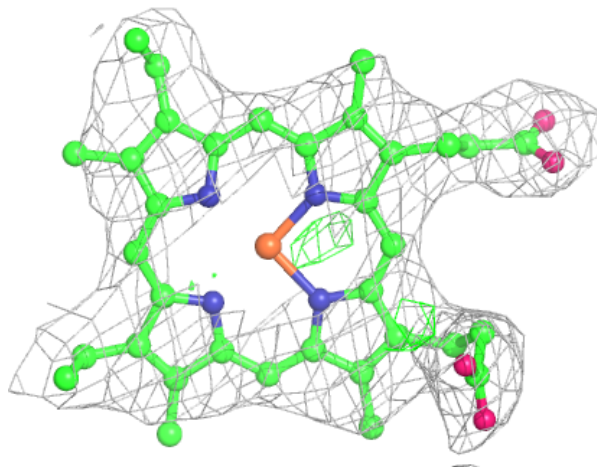
**Electron density around HEC I 601:**

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



**Electron density around HEC M 601:**

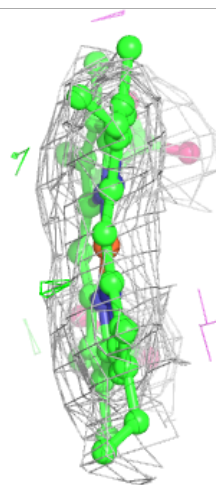
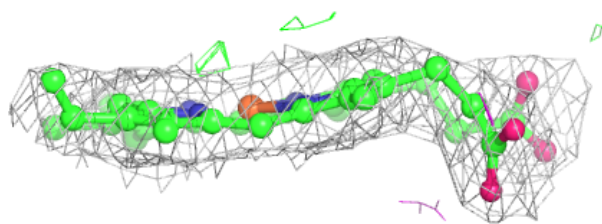
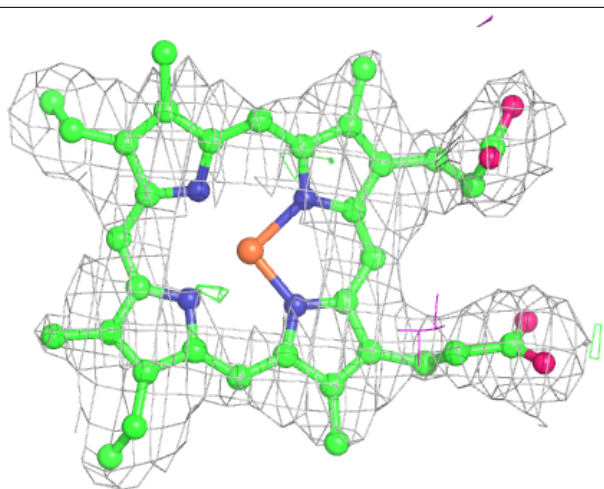
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC L 607:**

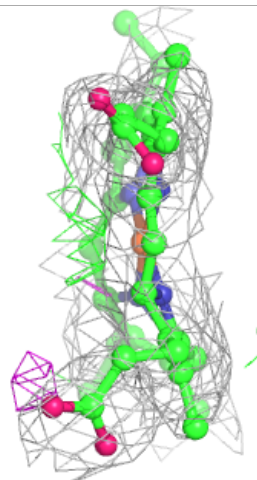
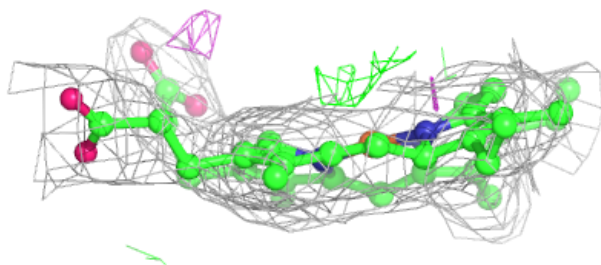
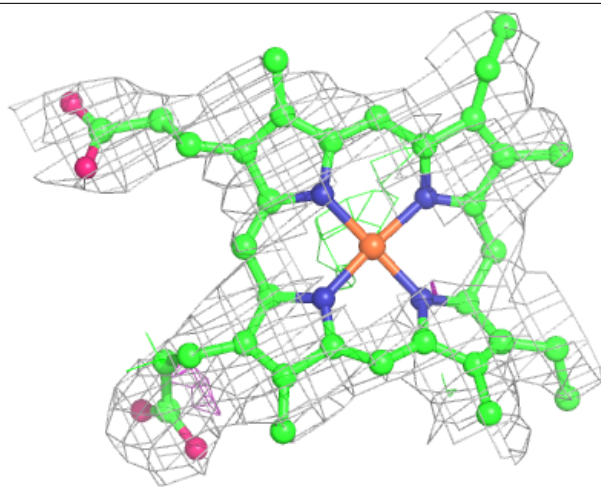
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





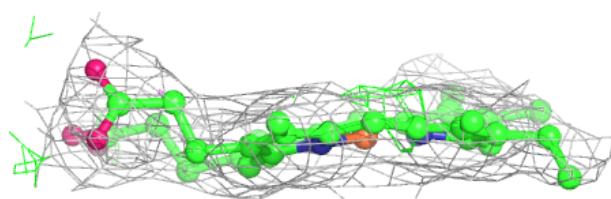
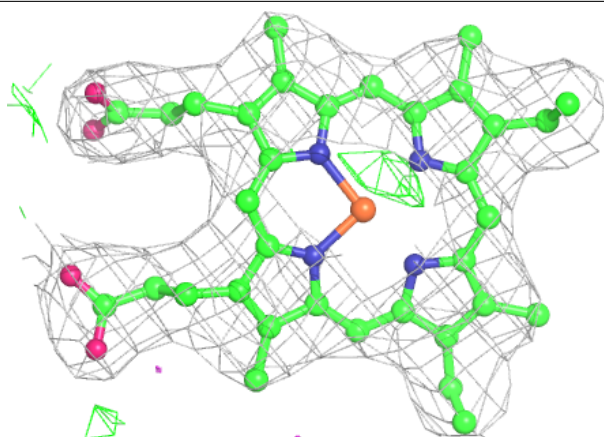
**Electron density around HEC B 603:**

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



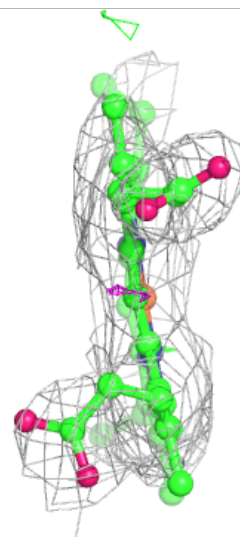
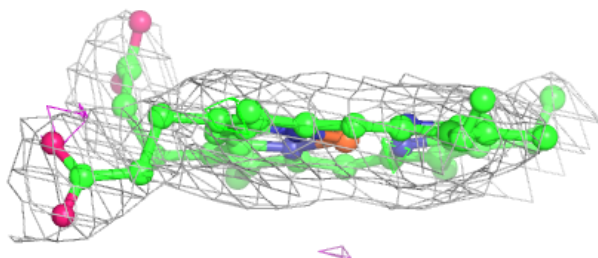
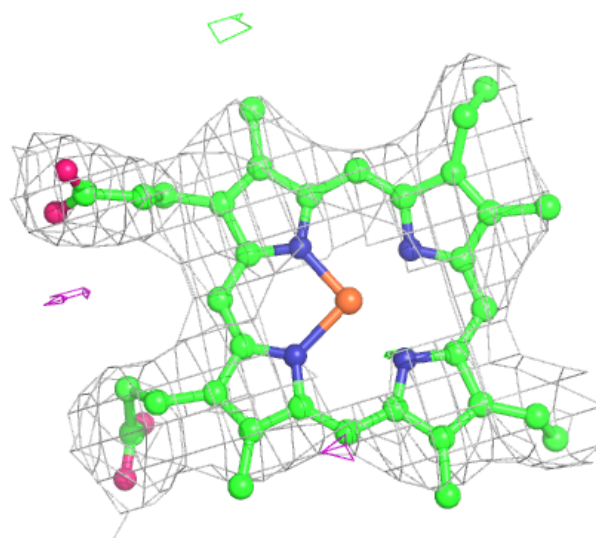
**Electron density around HEC G 606:**

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



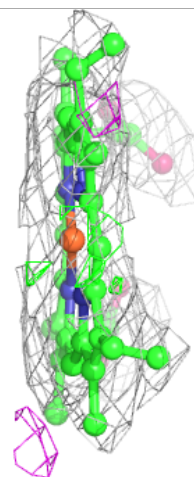
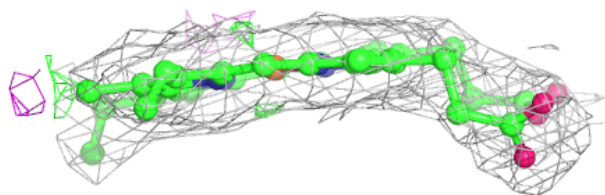
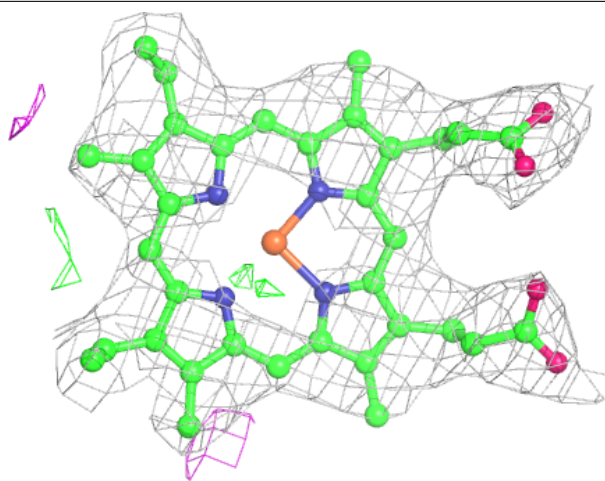
**Electron density around HEC B 601:**

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



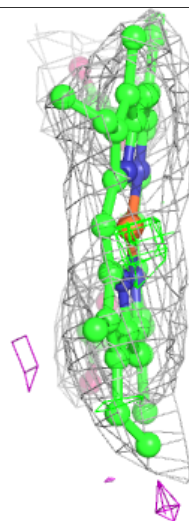
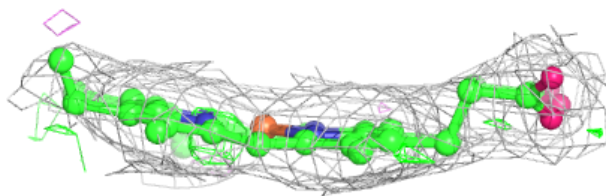
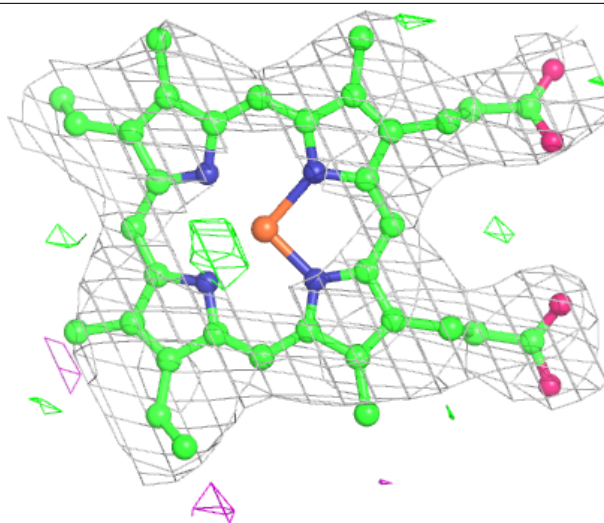
**Electron density around HEC J 604:**

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



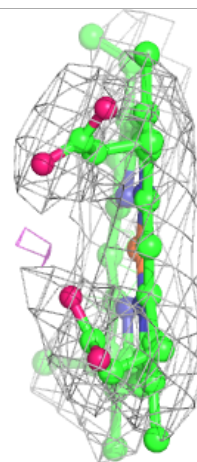
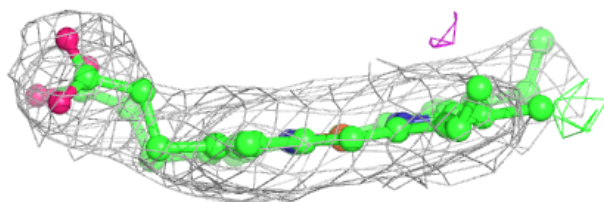
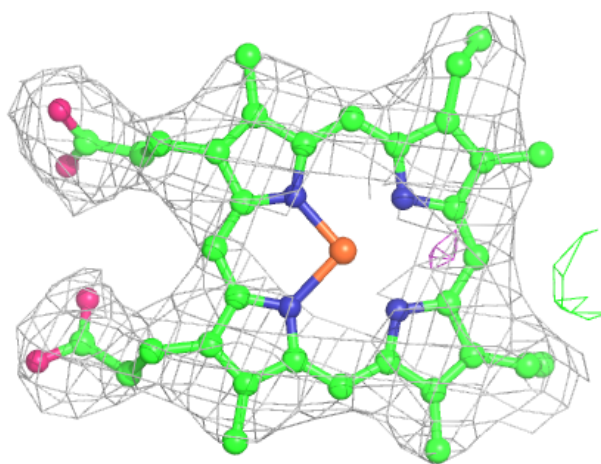
**Electron density around HEC O 600:**

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



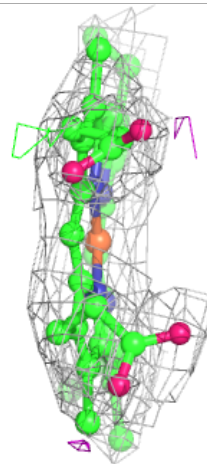
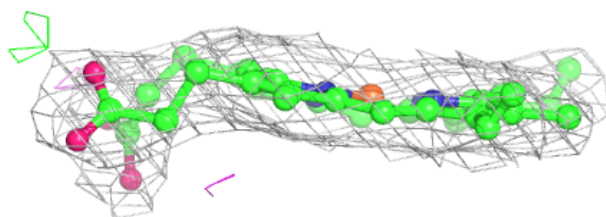
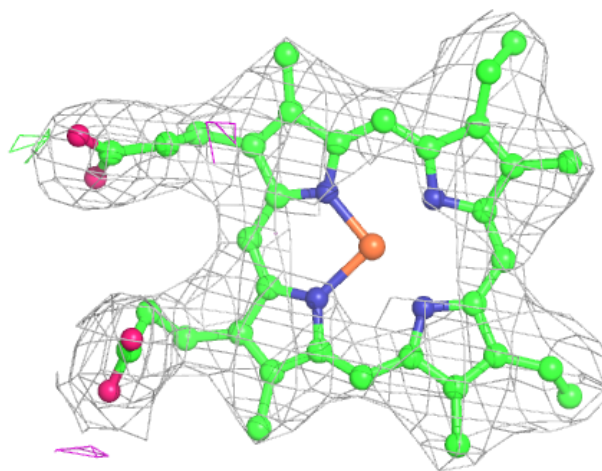
**Electron density around HEC D 604:**

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



**Electron density around HEC K 607:**

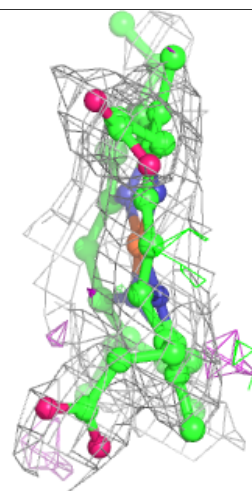
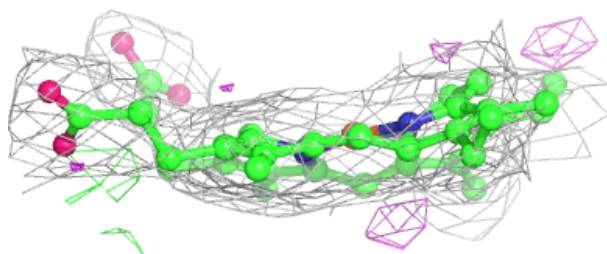
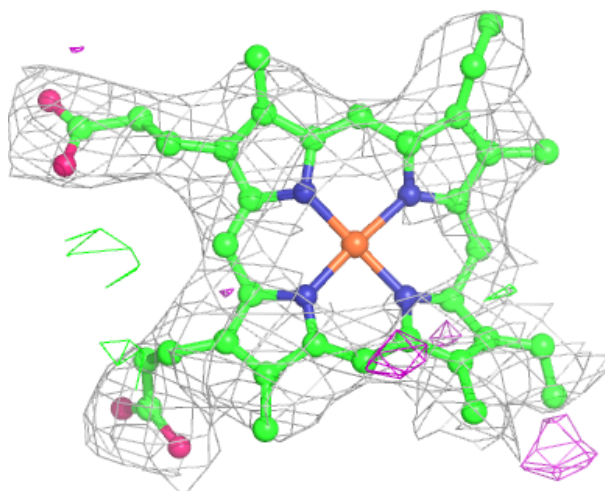
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC L 603:**

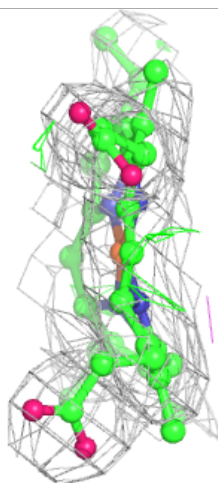
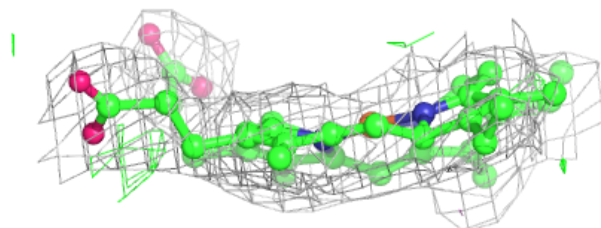
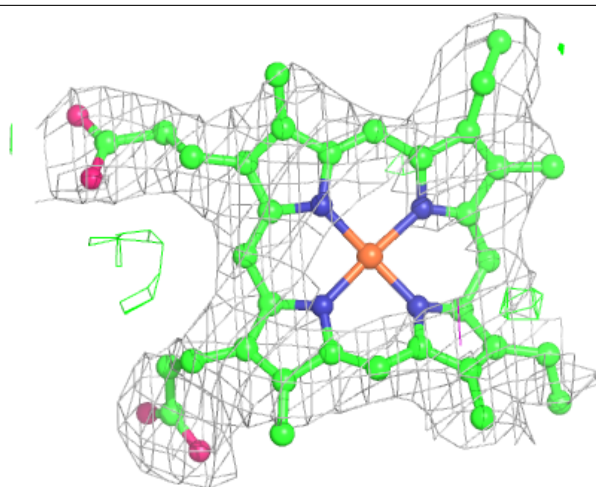
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





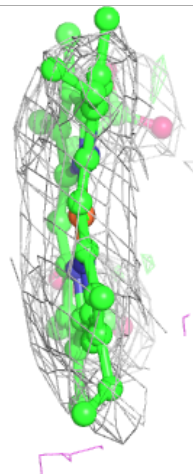
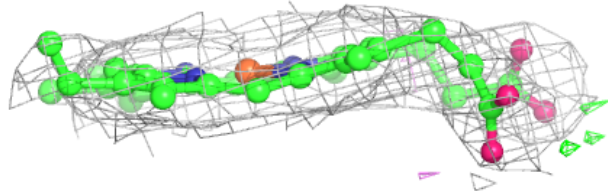
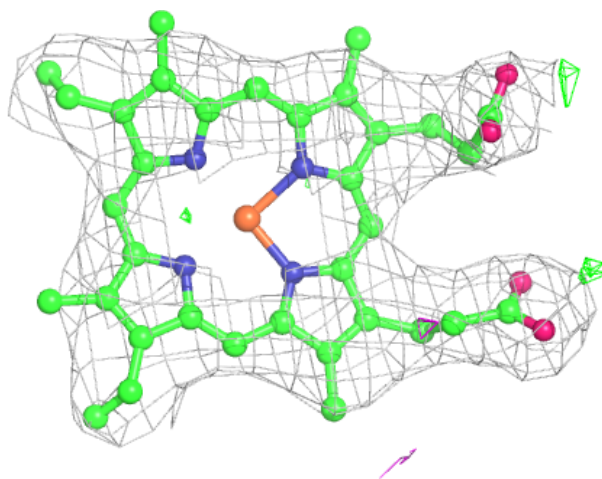
**Electron density around HEC K 603:**

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



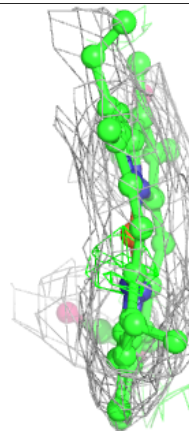
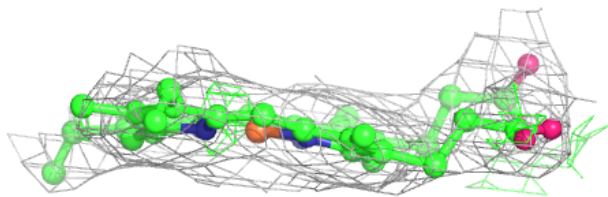
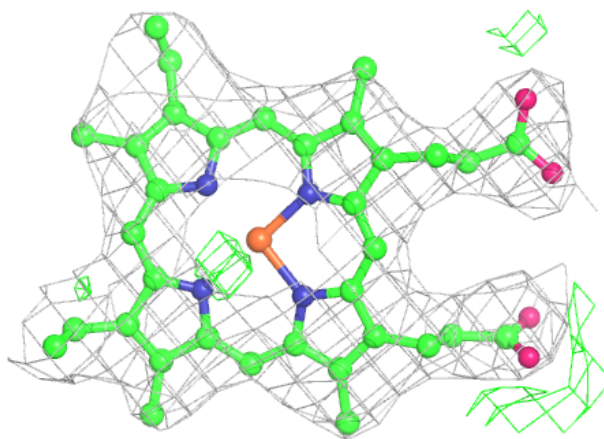
**Electron density around HEC D 607:**

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



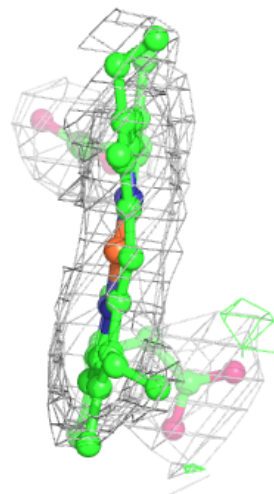
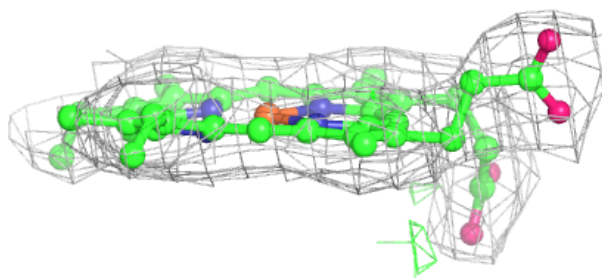
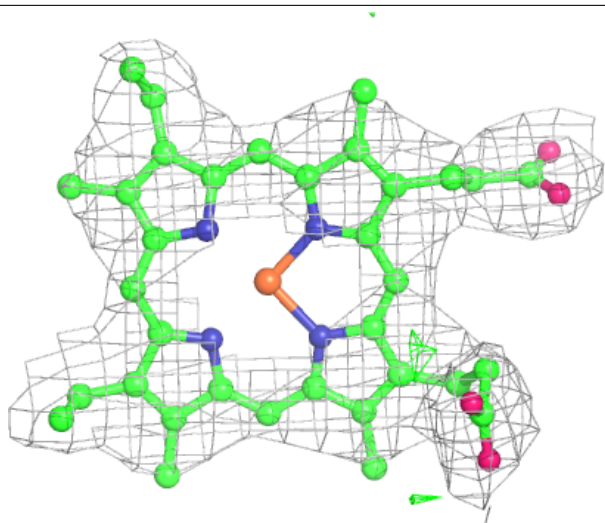
**Electron density around HEC R 606:**

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



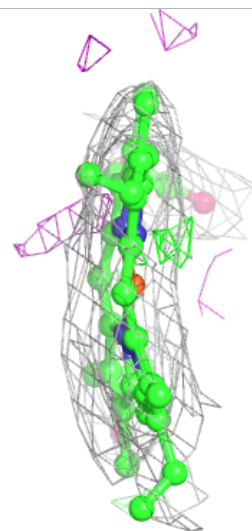
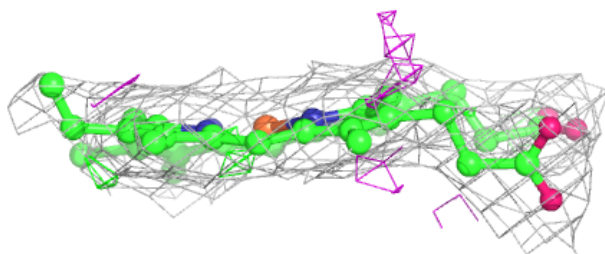
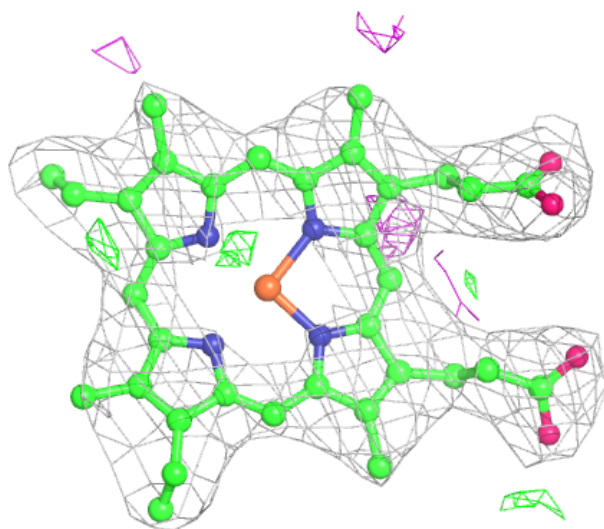
**Electron density around HEC J 601:**

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



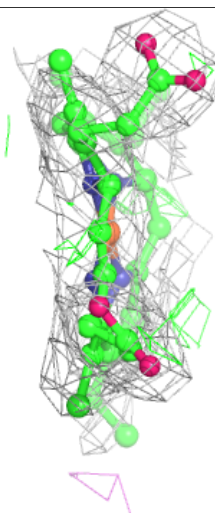
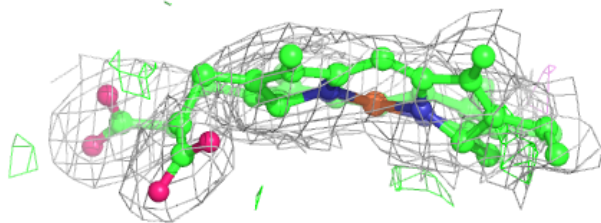
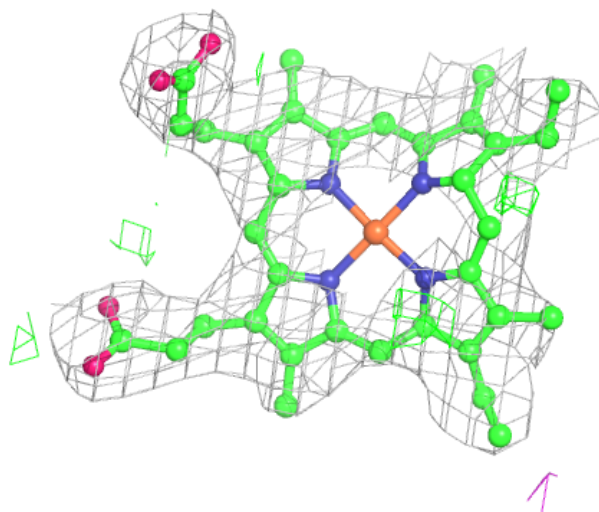
**Electron density around HEC L 606:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



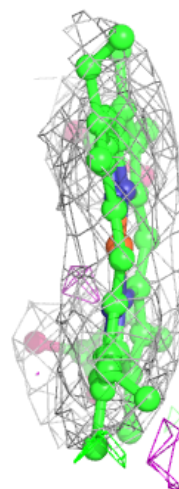
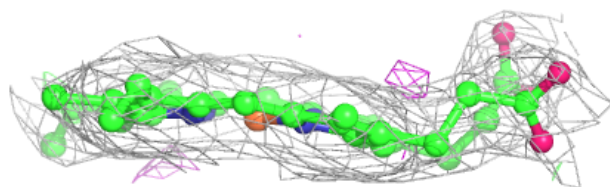
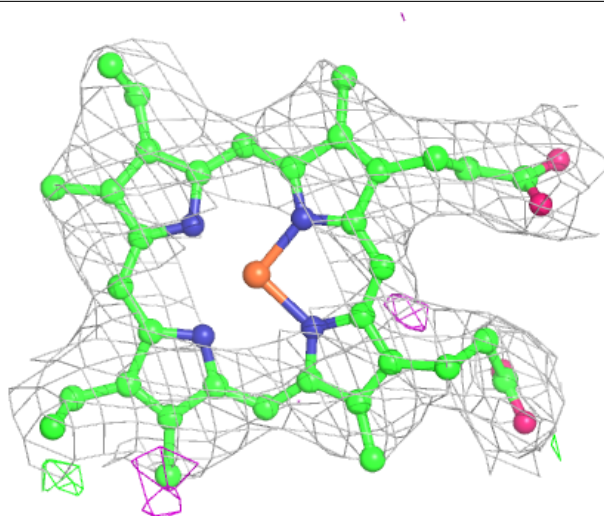
**Electron density around HEC J 603:**

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



**Electron density around HEC B 607:**

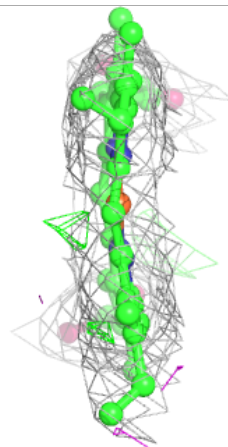
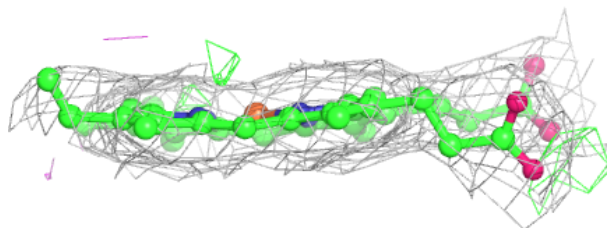
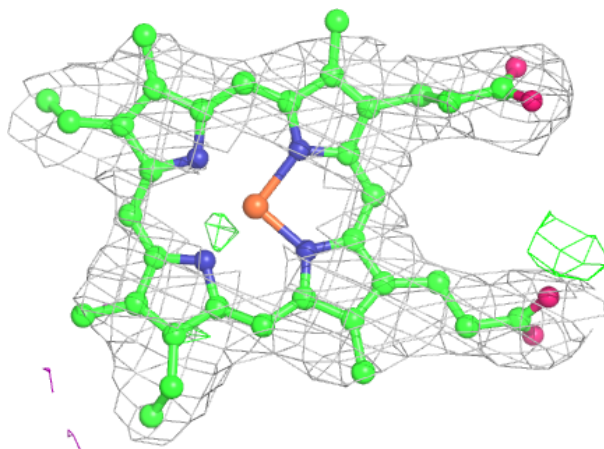
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC K 605:**

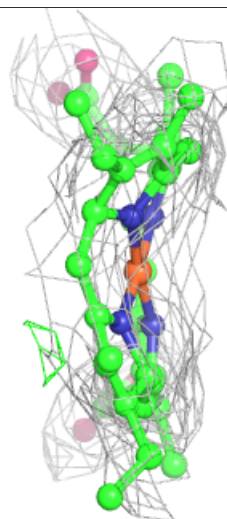
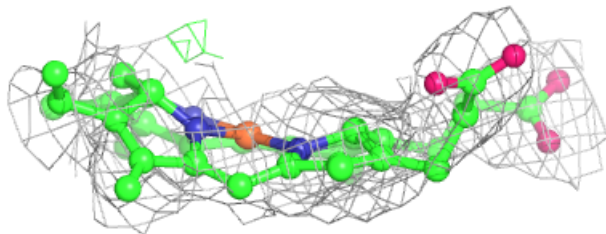
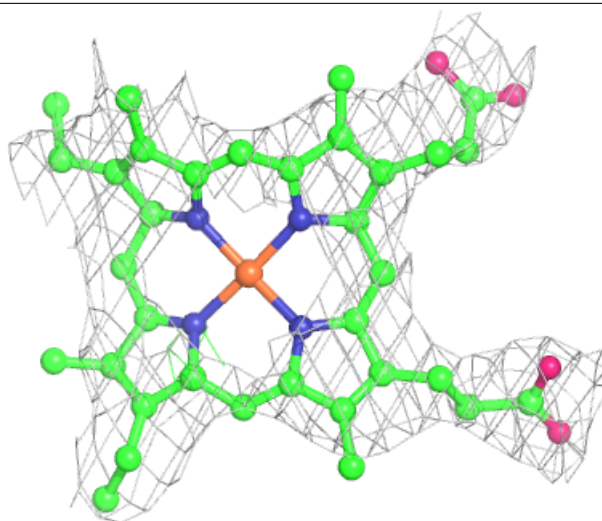
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





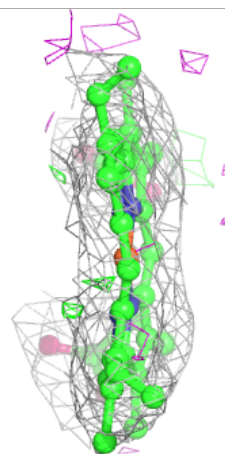
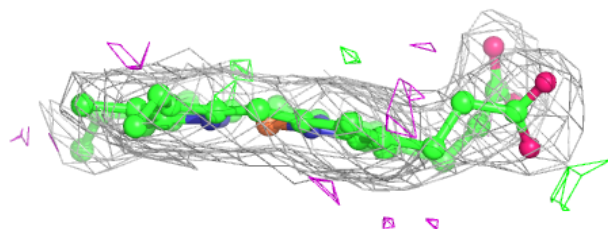
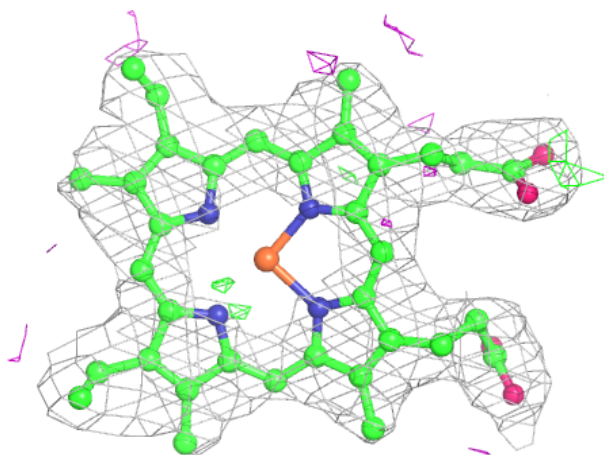
**Electron density around HEC D 603:**

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



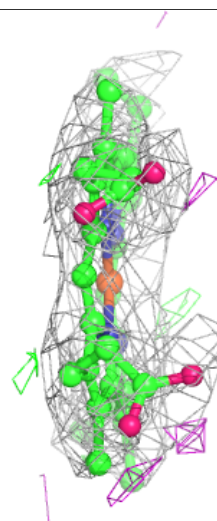
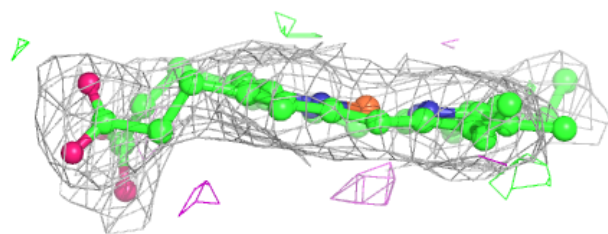
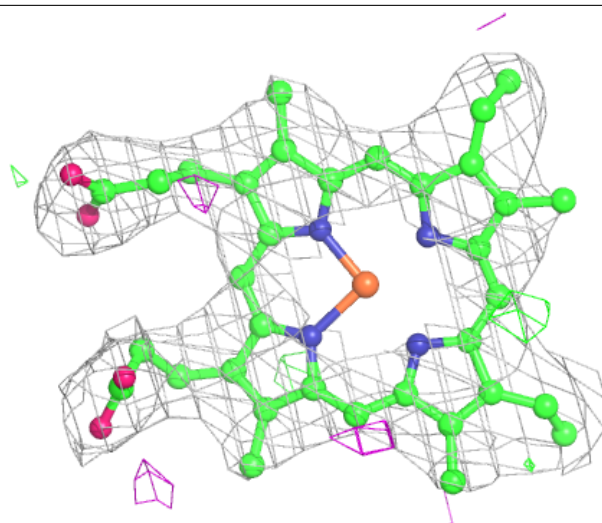
**Electron density around HEC H 607:**

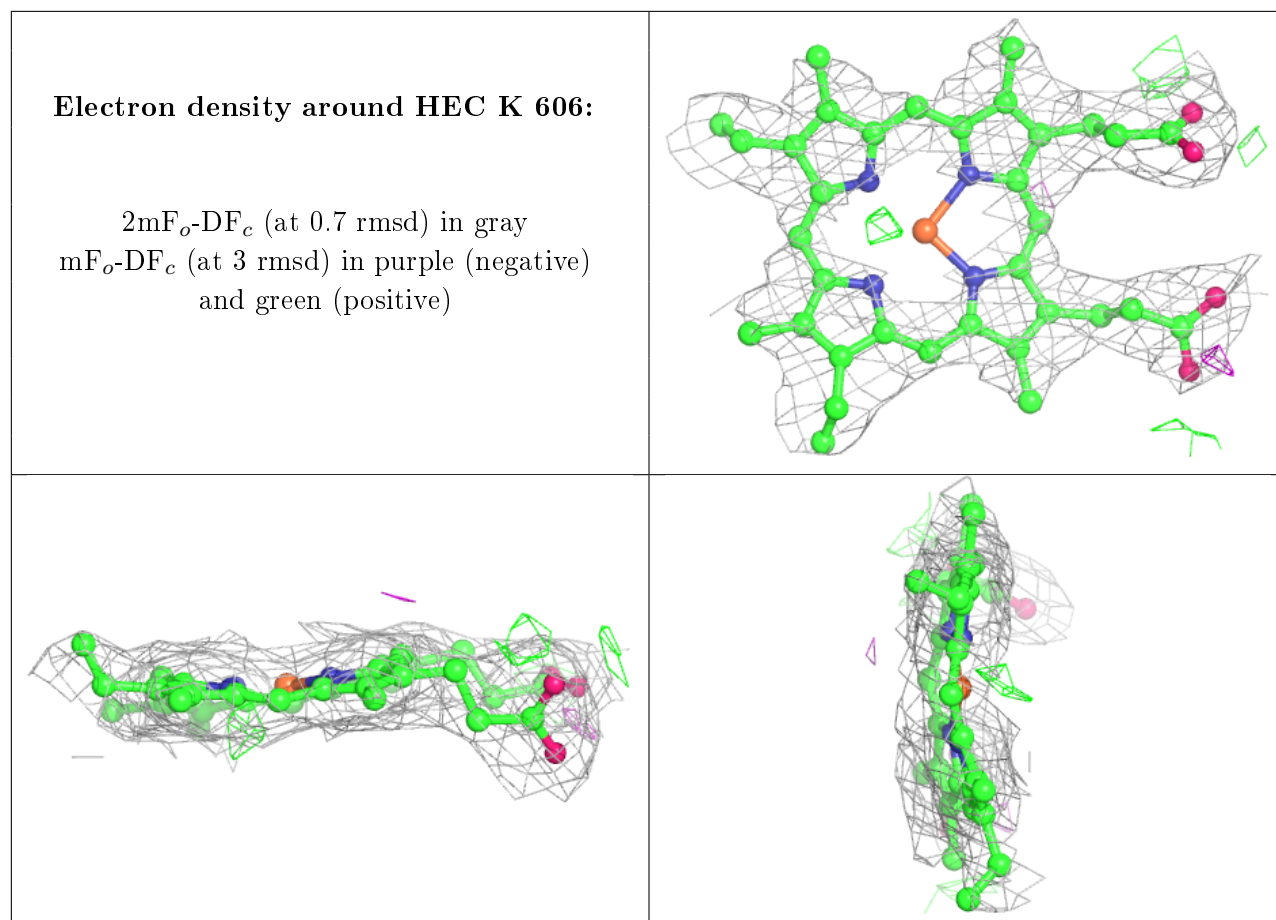
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC N 607:**

$2mF_o-DF_c$  (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.