



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:12 PM UTC

PDB ID : 1H29 / pdb\_00001h29  
Title : Sulfate respiration in *Desulfovibrio vulgaris* Hildenborough: Structure of the 16-heme Cytochrome c HmcA at 2.5 Å resolution and a view of its role in transmembrane electron transfer  
Authors : Matias, P.M.; Coelho, A.V.; Valente, F.M.A.; Placido, D.; Legall, J.; Xavier, A.V.; Pereira, I.A.C.; Carrondo, M.A.  
Deposited on : 2002-08-01  
Resolution : 2.51 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

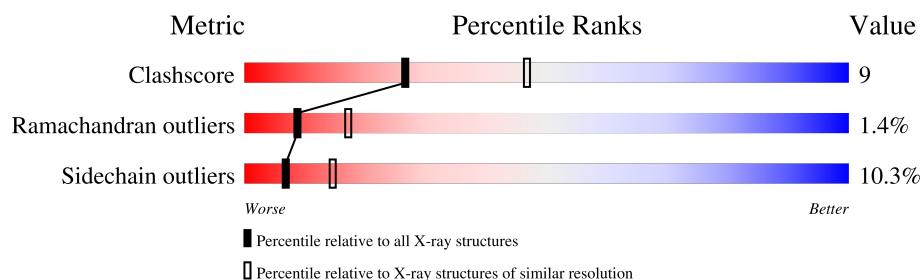
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 6492 (2.50-2.50)                                      |
| Ramachandran outliers | 187476                      | 6378 (2.50-2.50)                                      |
| Sidechain outliers    | 187428                      | 6380 (2.50-2.50)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 514    |                  |
| 1   | B     | 514    |                  |
| 1   | C     | 514    |                  |
| 1   | D     | 514    |                  |

## 2 Entry composition (i)

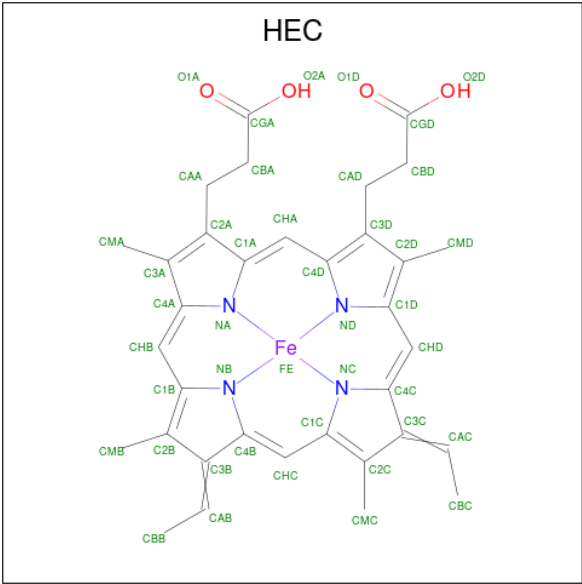
There are 3 unique types of molecules in this entry. The entry contains 18287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIGH-MOLECULAR-WEIGHT CYTOCHROME C.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 501      | Total | C    | N   | O   | S  | 38      | 0       | 0     |
|     |       |          | 3783  | 2323 | 717 | 699 | 44 |         |         |       |
| 1   | B     | 499      | Total | C    | N   | O   | S  | 75      | 0       | 0     |
|     |       |          | 3763  | 2312 | 712 | 695 | 44 |         |         |       |
| 1   | C     | 501      | Total | C    | N   | O   | S  | 90      | 0       | 0     |
|     |       |          | 3777  | 2320 | 714 | 699 | 44 |         |         |       |
| 1   | D     | 492      | Total | C    | N   | O   | S  | 70      | 0       | 0     |
|     |       |          | 3715  | 2284 | 699 | 688 | 44 |         |         |       |

- Molecule 2 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | 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 |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 3 is water.

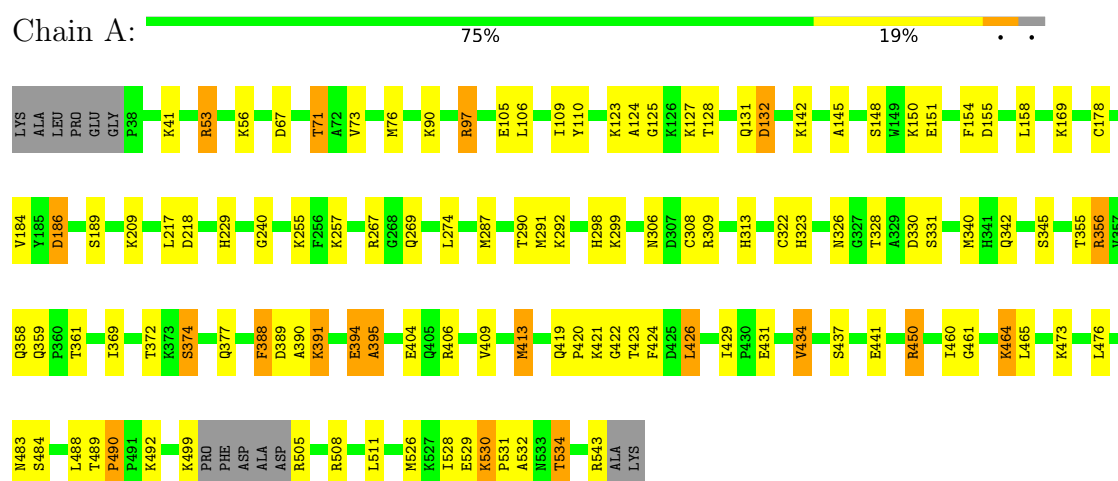
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | A     | 123      | Total<br>123 | O<br>123 | 0       | 0       |
| 3   | B     | 126      | Total<br>126 | O<br>126 | 0       | 0       |
| 3   | C     | 136      | Total<br>136 | O<br>136 | 0       | 0       |
| 3   | D     | 112      | Total<br>112 | O<br>112 | 0       | 0       |

### 3 Residue-property plots

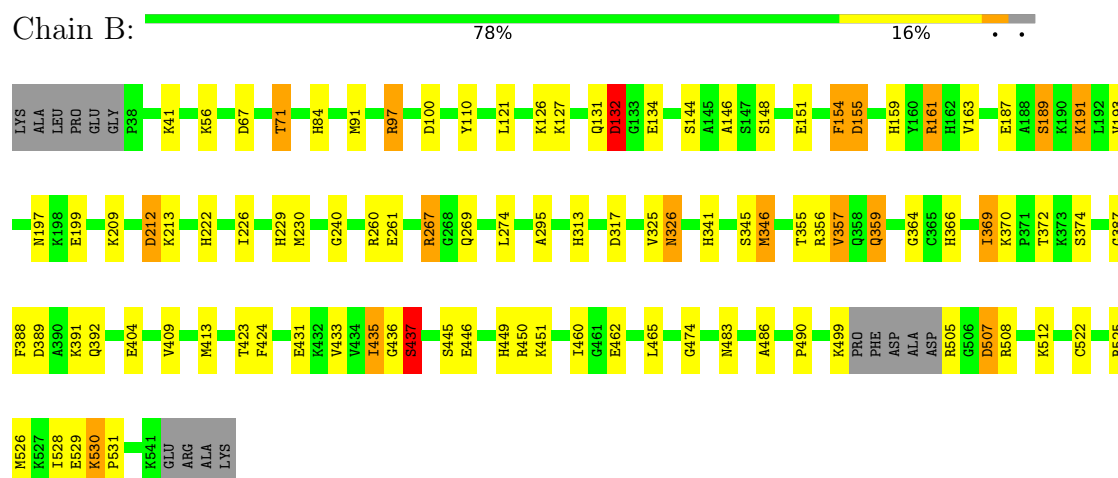
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

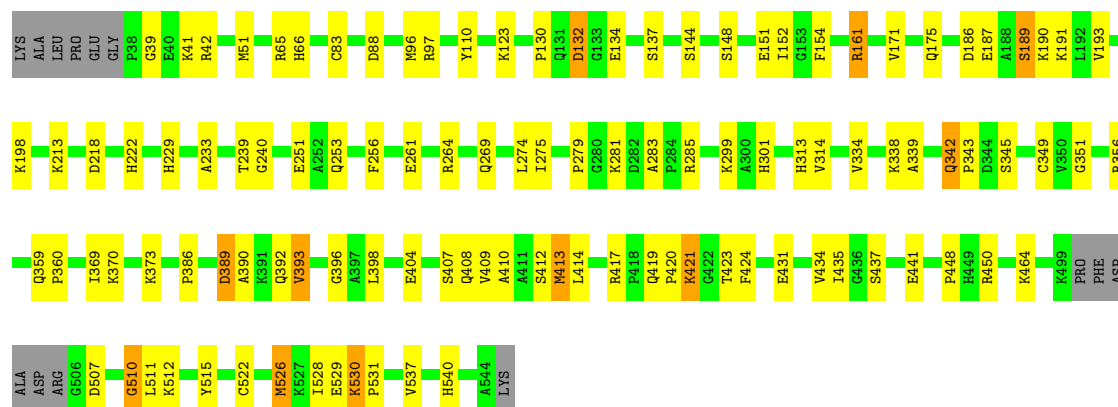


#### • Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C



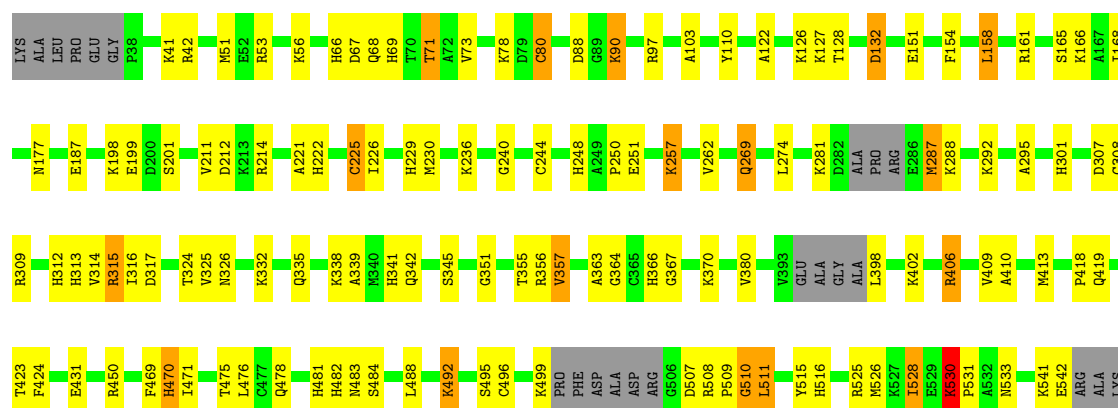
#### • Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C





• Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain D: 70% 22%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                            | Source    |
|----------------------------------------------------------|--------------------------------------------------|-----------|
| Space group                                              | P 62                                             | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 220.39Å 220.39Å 102.64Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å)                                           | 30.00 – 2.51                                     | Depositor |
| % Data completeness<br>(in resolution range)             | 92.1 (30.00-2.51)                                | Depositor |
| $R_{merge}$                                              | 0.06                                             | Depositor |
| $R_{sym}$                                                | (Not available)                                  | Depositor |
| Refinement program                                       | REFMAC 5.1.24                                    | Depositor |
| R, $R_{free}$                                            | 0.192 , 0.258                                    | Depositor |
| Estimated twinning fraction                              | No twinning to report.                           | Xtriage   |
| Total number of atoms                                    | 18287                                            | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 31.0                                             | wwPDB-VP  |

## 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: 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     | 0.76         | 4/3864 (0.1%)   | 1.01        | 4/5201 (0.1%)   |
| 1   | B     | 0.74         | 4/3844 (0.1%)   | 1.00        | 0/5175          |
| 1   | C     | 0.73         | 2/3858 (0.1%)   | 1.04        | 7/5194 (0.1%)   |
| 1   | D     | 0.68         | 0/3793          | 1.01        | 3/5103 (0.1%)   |
| All | All   | 0.73         | 10/15359 (0.1%) | 1.02        | 14/20673 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 2                   |
| 1   | D     | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 413 | MET  | SD-CE | -6.73 | 1.62        | 1.79     |
| 1   | A     | 125 | GLY  | CA-C  | 6.51  | 1.58        | 1.51     |
| 1   | C     | 526 | MET  | SD-CE | -6.28 | 1.63        | 1.79     |
| 1   | B     | 346 | MET  | SD-CE | -6.27 | 1.63        | 1.79     |
| 1   | B     | 189 | SER  | C-O   | 6.18  | 1.32        | 1.24     |
| 1   | A     | 124 | ALA  | C-N   | 6.17  | 1.39        | 1.33     |
| 1   | B     | 260 | ARG  | NE-CZ | 5.82  | 1.39        | 1.33     |
| 1   | A     | 186 | ASP  | C-O   | 5.25  | 1.30        | 1.24     |
| 1   | B     | 189 | SER  | CB-OG | 5.12  | 1.52        | 1.42     |
| 1   | A     | 413 | MET  | SD-CE | -5.10 | 1.66        | 1.79     |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 396 | GLY  | N-CA-C | 12.20 | 126.63      | 113.58   |
| 1   | C     | 421 | LYS  | N-CA-C | -8.04 | 97.50       | 110.20   |
| 1   | D     | 510 | GLY  | N-CA-C | -6.41 | 103.67      | 112.25   |
| 1   | A     | 389 | ASP  | N-CA-C | 6.24  | 118.57      | 108.34   |
| 1   | C     | 96  | MET  | N-CA-C | 6.06  | 119.78      | 111.54   |
| 1   | A     | 490 | PRO  | O-C-N  | 5.92  | 123.93      | 121.15   |
| 1   | A     | 128 | THR  | N-CA-C | 5.89  | 116.06      | 108.34   |
| 1   | C     | 392 | GLN  | N-CA-C | -5.71 | 104.47      | 112.12   |
| 1   | D     | 364 | GLY  | N-CA-C | -5.63 | 99.84       | 113.18   |
| 1   | D     | 363 | ALA  | N-CA-C | -5.40 | 103.35      | 110.43   |
| 1   | C     | 510 | GLY  | N-CA-C | -5.35 | 105.08      | 112.25   |
| 1   | A     | 369 | ILE  | N-CA-C | 5.22  | 116.31      | 109.58   |
| 1   | C     | 448 | PRO  | CA-C-N | 5.01  | 127.75      | 120.79   |
| 1   | C     | 448 | PRO  | C-N-CA | 5.01  | 127.75      | 120.79   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 131 | GLN  | Peptide |
| 1   | A     | 217 | LEU  | Peptide |
| 1   | B     | 131 | GLN  | Peptide |
| 1   | B     | 154 | PHE  | Peptide |
| 1   | D     | 470 | HIS  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3783  | 0        | 3716     | 63      | 0            |
| 1   | B     | 3763  | 0        | 3697     | 68      | 0            |
| 1   | C     | 3777  | 0        | 3708     | 75      | 0            |
| 1   | D     | 3715  | 0        | 3644     | 82      | 0            |
| 2   | A     | 688   | 0        | 480      | 18      | 0            |
| 2   | B     | 688   | 0        | 480      | 23      | 0            |
| 2   | C     | 688   | 0        | 480      | 24      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | D     | 688   | 0        | 480      | 34      | 0            |
| 3   | A     | 123   | 0        | 0        | 1       | 0            |
| 3   | B     | 126   | 0        | 0        | 2       | 0            |
| 3   | C     | 136   | 0        | 0        | 2       | 0            |
| 3   | D     | 112   | 0        | 0        | 1       | 0            |
| All | All   | 18287 | 0        | 16685    | 313     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (313) 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:C:522:CYS:SG   | 1:C:526:MET:HE2  | 1.67                     | 1.35              |
| 1:C:409:VAL:HG12 | 1:C:413:MET:HE2  | 1.21                     | 1.10              |
| 1:D:530:LYS:HB3  | 1:D:531:PRO:CD   | 1.85                     | 1.07              |
| 1:B:530:LYS:HB2  | 1:B:531:PRO:HD3  | 1.34                     | 1.06              |
| 1:D:530:LYS:HB3  | 1:D:531:PRO:HD3  | 1.29                     | 1.06              |
| 1:B:530:LYS:CB   | 1:B:531:PRO:HD3  | 1.89                     | 1.03              |
| 1:D:274:LEU:HD13 | 1:D:413:MET:HE1  | 1.42                     | 1.02              |
| 1:C:522:CYS:SG   | 1:C:526:MET:CE   | 2.54                     | 0.96              |
| 1:C:409:VAL:HG12 | 1:C:413:MET:CE   | 1.97                     | 0.95              |
| 1:D:226:ILE:HG22 | 1:D:230:MET:HE2  | 1.50                     | 0.93              |
| 1:C:274:LEU:HD13 | 1:C:413:MET:HE1  | 1.51                     | 0.93              |
| 1:B:530:LYS:HB2  | 1:B:531:PRO:CD   | 1.99                     | 0.92              |
| 1:C:161:ARG:HG2  | 1:C:161:ARG:HH11 | 1.40                     | 0.87              |
| 1:C:409:VAL:CG1  | 1:C:413:MET:HE2  | 2.03                     | 0.87              |
| 1:B:226:ILE:HG22 | 1:B:230:MET:HE2  | 1.58                     | 0.86              |
| 1:D:528:ILE:CG2  | 1:D:530:LYS:HB2  | 2.06                     | 0.85              |
| 1:D:530:LYS:CB   | 1:D:531:PRO:CD   | 2.55                     | 0.83              |
| 1:A:530:LYS:HB3  | 1:A:531:PRO:HD3  | 1.60                     | 0.82              |
| 1:D:410:ALA:HA   | 1:D:413:MET:HE3  | 1.62                     | 0.80              |
| 1:A:186:ASP:HB3  | 1:A:189:SER:HB2  | 1.62                     | 0.80              |
| 1:B:530:LYS:CB   | 1:B:531:PRO:CD   | 2.58                     | 0.80              |
| 1:B:409:VAL:HG12 | 1:B:413:MET:HE3  | 1.64                     | 0.78              |
| 1:B:189:SER:HB2  | 1:B:191:LYS:HD3  | 1.67                     | 0.76              |
| 1:D:67:ASP:O     | 1:D:71:THR:HG23  | 1.84                     | 0.76              |
| 1:B:356:ARG:O    | 1:B:359:GLN:HG2  | 1.86                     | 0.75              |
| 1:A:356:ARG:O    | 1:A:359:GLN:HG2  | 1.87                     | 0.74              |
| 1:A:426:LEU:O    | 1:A:429:ILE:HB   | 1.88                     | 0.74              |
| 1:A:274:LEU:HD23 | 1:A:406:ARG:HG2  | 1.70                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:526:MET:HE1   | 2:C:1115:HEC:HHD  | 1.72                     | 0.72              |
| 1:C:274:LEU:CD1   | 1:C:413:MET:HE1   | 2.20                     | 0.71              |
| 1:D:410:ALA:HA    | 1:D:413:MET:CE    | 2.20                     | 0.70              |
| 1:C:39:GLY:HA3    | 1:C:144:SER:O     | 1.92                     | 0.70              |
| 1:D:341:HIS:HE1   | 2:D:1112:HEC:NA   | 1.90                     | 0.70              |
| 1:A:419:GLN:HG3   | 1:A:420:PRO:HD2   | 1.74                     | 0.69              |
| 1:C:356:ARG:O     | 1:C:359:GLN:HG2   | 1.92                     | 0.69              |
| 1:A:41:LYS:HB3    | 1:A:148:SER:HB3   | 1.73                     | 0.69              |
| 1:D:528:ILE:HG22  | 1:D:530:LYS:HB2   | 1.75                     | 0.69              |
| 1:A:388:PHE:CD1   | 1:A:388:PHE:N     | 2.60                     | 0.69              |
| 1:C:414:LEU:HA    | 1:C:417:ARG:HE    | 1.58                     | 0.68              |
| 2:C:1106:HEC:HMC3 | 2:C:1106:HEC:HBC3 | 1.76                     | 0.67              |
| 1:A:274:LEU:HD13  | 1:A:413:MET:HE1   | 1.77                     | 0.67              |
| 1:A:409:VAL:HG12  | 1:A:413:MET:CE    | 2.25                     | 0.67              |
| 1:B:526:MET:HE1   | 2:B:1115:HEC:CMD  | 2.24                     | 0.67              |
| 1:C:393:VAL:HG22  | 1:C:398:LEU:HD12  | 1.77                     | 0.66              |
| 1:A:530:LYS:HB3   | 1:A:531:PRO:CD    | 2.25                     | 0.66              |
| 2:D:1104:HEC:CMD  | 2:D:1106:HEC:HBB2 | 2.25                     | 0.66              |
| 1:A:67:ASP:O      | 1:A:71:THR:HG23   | 1.96                     | 0.66              |
| 1:C:154:PHE:HB2   | 2:C:1104:HEC:HBD2 | 1.77                     | 0.65              |
| 1:B:530:LYS:HB3   | 1:B:531:PRO:HD3   | 1.78                     | 0.65              |
| 1:C:510:GLY:HA3   | 3:C:2118:HOH:O    | 1.95                     | 0.65              |
| 1:D:165:SER:HB3   | 1:D:168:ILE:HD12  | 1.78                     | 0.65              |
| 1:B:423:THR:HG22  | 1:B:424:PHE:H     | 1.62                     | 0.65              |
| 1:C:423:THR:HG22  | 1:C:424:PHE:H     | 1.62                     | 0.64              |
| 1:D:211:VAL:HG23  | 1:D:212:ASP:H     | 1.61                     | 0.64              |
| 1:B:41:LYS:HB3    | 1:B:148:SER:HB3   | 1.81                     | 0.63              |
| 1:D:511:LEU:HD13  | 1:D:515:TYR:CE1   | 2.34                     | 0.62              |
| 1:B:326:ASN:H     | 1:B:326:ASN:HD22  | 1.46                     | 0.62              |
| 1:D:423:THR:HG22  | 1:D:424:PHE:N     | 2.14                     | 0.62              |
| 1:C:423:THR:HG22  | 1:C:424:PHE:N     | 2.15                     | 0.61              |
| 1:D:211:VAL:HG21  | 1:D:214:ARG:CZ    | 2.29                     | 0.61              |
| 1:B:526:MET:CE    | 2:B:1115:HEC:HHD  | 2.30                     | 0.61              |
| 1:A:530:LYS:CB    | 1:A:531:PRO:CD    | 2.78                     | 0.61              |
| 1:B:372:THR:CG2   | 1:B:374:SER:HB3   | 2.31                     | 0.61              |
| 1:C:251:GLU:CD    | 1:C:251:GLU:H     | 2.09                     | 0.61              |
| 1:C:389:ASP:CG    | 1:C:390:ALA:H     | 2.08                     | 0.61              |
| 1:D:511:LEU:HD13  | 1:D:515:TYR:HE1   | 1.65                     | 0.61              |
| 1:A:328:THR:HG22  | 1:A:330:ASP:H     | 1.66                     | 0.60              |
| 1:A:356:ARG:HG2   | 1:A:465:LEU:HD12  | 1.82                     | 0.60              |
| 1:B:356:ARG:O     | 1:B:359:GLN:CG    | 2.49                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1106:HEC:HMC3 | 2:B:1106:HEC:HBC3 | 1.84                     | 0.60              |
| 1:B:372:THR:HG22  | 1:B:374:SER:HB3   | 1.84                     | 0.60              |
| 1:B:526:MET:HE1   | 2:B:1115:HEC:HMD1 | 1.84                     | 0.59              |
| 1:B:474:GLY:HA3   | 1:B:486:ALA:HB1   | 1.84                     | 0.59              |
| 1:A:355:THR:HA    | 1:A:358:GLN:HG3   | 1.85                     | 0.58              |
| 1:B:526:MET:HE2   | 2:B:1115:HEC:HHD  | 1.86                     | 0.58              |
| 1:A:73:VAL:HA     | 1:A:76:MET:HE3    | 1.86                     | 0.58              |
| 1:C:41:LYS:HB3    | 1:C:148:SER:HB3   | 1.85                     | 0.57              |
| 2:C:1109:HEC:HBC3 | 2:C:1109:HEC:HMC3 | 1.87                     | 0.57              |
| 2:A:1102:HEC:HMC3 | 2:A:1102:HEC:HBC3 | 1.86                     | 0.57              |
| 1:D:229:HIS:CE1   | 1:D:240:GLY:HA3   | 2.39                     | 0.57              |
| 1:D:269:GLN:HG2   | 2:D:1108:HEC:HMB1 | 1.87                     | 0.56              |
| 1:A:374:SER:HB3   | 1:A:377:GLN:H     | 1.70                     | 0.56              |
| 1:B:97:ARG:NH2    | 1:B:110:TYR:OH    | 2.39                     | 0.56              |
| 1:C:414:LEU:HB3   | 1:C:417:ARG:HH21  | 1.71                     | 0.56              |
| 1:D:496:CYS:O     | 1:D:508:ARG:HD3   | 2.04                     | 0.56              |
| 1:A:431:GLU:HA    | 1:A:450:ARG:HB3   | 1.88                     | 0.56              |
| 1:D:225:CYS:HB3   | 2:D:1106:HEC:C4B  | 2.36                     | 0.56              |
| 2:B:1107:HEC:HMA1 | 2:B:1107:HEC:HBA2 | 1.89                     | 0.55              |
| 1:D:313:HIS:CE1   | 1:D:314:VAL:HG23  | 2.41                     | 0.55              |
| 1:C:339:ALA:HA    | 2:C:1109:HEC:HMA2 | 1.88                     | 0.55              |
| 1:B:161:ARG:NH1   | 1:B:161:ARG:HG2   | 2.21                     | 0.55              |
| 1:B:409:VAL:HG12  | 1:B:413:MET:CE    | 2.36                     | 0.55              |
| 1:D:68:GLN:HE22   | 2:D:1102:HEC:HBA2 | 1.71                     | 0.55              |
| 1:D:80:CYS:HB3    | 2:D:1101:HEC:CHC  | 2.37                     | 0.55              |
| 1:D:154:PHE:CD1   | 1:D:158:LEU:HD13  | 2.42                     | 0.55              |
| 1:A:394:GLU:O     | 1:A:395:ALA:CB    | 2.54                     | 0.55              |
| 1:B:161:ARG:HG2   | 1:B:161:ARG:HH11  | 1.72                     | 0.55              |
| 1:B:189:SER:CB    | 1:B:191:LYS:HD3   | 2.35                     | 0.54              |
| 1:D:301:HIS:CD2   | 2:D:1110:HEC:NC   | 2.75                     | 0.54              |
| 1:A:298:HIS:HE1   | 2:A:1108:HEC:NB   | 2.06                     | 0.54              |
| 1:D:470:HIS:HA    | 1:D:475:THR:HG21  | 1.89                     | 0.54              |
| 1:A:374:SER:HB2   | 1:A:377:GLN:HB2   | 1.89                     | 0.54              |
| 1:C:264:ARG:NH1   | 1:C:299:LYS:HD2   | 2.23                     | 0.54              |
| 1:C:393:VAL:HG22  | 1:C:398:LEU:CD1   | 2.37                     | 0.54              |
| 1:C:526:MET:CE    | 2:C:1115:HEC:HHD  | 2.36                     | 0.54              |
| 1:B:132:ASP:CG    | 1:D:516:HIS:HD1   | 2.17                     | 0.53              |
| 1:B:483:ASN:HD22  | 2:B:1114:HEC:C1D  | 2.22                     | 0.53              |
| 1:C:537:VAL:HA    | 1:C:540:HIS:O     | 2.08                     | 0.53              |
| 1:A:322:CYS:HB3   | 1:A:331:SER:HB3   | 1.91                     | 0.53              |
| 1:C:360:PRO:O     | 1:C:526:MET:HG2   | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:66:HIS:HE1    | 2:D:1101:HEC:NB   | 2.04                     | 0.53              |
| 2:D:1110:HEC:HBC3 | 2:D:1110:HEC:HMC3 | 1.91                     | 0.53              |
| 1:C:419:GLN:NE2   | 1:C:420:PRO:HD2   | 2.24                     | 0.52              |
| 1:D:222:HIS:HA    | 1:D:226:ILE:HD12  | 1.90                     | 0.52              |
| 1:D:69:HIS:CD2    | 2:D:1102:HEC:NC   | 2.78                     | 0.52              |
| 1:A:464:LYS:HB2   | 2:A:1110:HEC:CGD  | 2.39                     | 0.52              |
| 1:C:97:ARG:NH2    | 1:C:110:TYR:CZ    | 2.78                     | 0.52              |
| 1:D:80:CYS:HB3    | 2:D:1101:HEC:C4B  | 2.38                     | 0.52              |
| 1:D:423:THR:HG22  | 1:D:424:PHE:H     | 1.73                     | 0.52              |
| 1:A:423:THR:HG23  | 1:A:473:LYS:O     | 2.10                     | 0.52              |
| 1:B:341:HIS:HE1   | 2:B:1112:HEC:C1A  | 2.23                     | 0.52              |
| 1:C:186:ASP:OD2   | 1:C:189:SER:HB2   | 2.09                     | 0.52              |
| 1:A:388:PHE:H     | 1:A:388:PHE:HD1   | 1.52                     | 0.52              |
| 1:D:431:GLU:HA    | 1:D:450:ARG:HB2   | 1.92                     | 0.52              |
| 1:C:410:ALA:HA    | 1:C:413:MET:HE3   | 1.91                     | 0.51              |
| 1:B:274:LEU:CD1   | 1:B:413:MET:HE1   | 2.40                     | 0.51              |
| 1:D:530:LYS:CB    | 1:D:531:PRO:HD2   | 2.38                     | 0.51              |
| 2:D:1102:HEC:HBC3 | 2:D:1102:HEC:HMC3 | 1.92                     | 0.51              |
| 1:B:121:LEU:HD13  | 2:B:1102:HEC:HMD2 | 1.93                     | 0.51              |
| 1:A:528:ILE:CG2   | 1:A:530:LYS:HB2   | 2.39                     | 0.51              |
| 1:A:340:MET:HG3   | 2:A:1112:HEC:C3D  | 2.41                     | 0.51              |
| 1:B:154:PHE:HB2   | 2:B:1104:HEC:HBD2 | 1.92                     | 0.51              |
| 1:D:51:MET:HE3    | 1:D:103:ALA:O     | 2.11                     | 0.51              |
| 1:D:168:ILE:HG22  | 1:D:177:ASN:HB2   | 1.93                     | 0.51              |
| 1:B:274:LEU:HD13  | 1:B:413:MET:HE1   | 1.93                     | 0.51              |
| 1:A:409:VAL:HG12  | 1:A:413:MET:HE2   | 1.93                     | 0.50              |
| 1:D:367:GLY:HA3   | 1:D:525:ARG:HD3   | 1.93                     | 0.50              |
| 1:D:510:GLY:HA3   | 3:D:2100:HOH:O    | 2.11                     | 0.50              |
| 1:D:541:LYS:O     | 1:D:542:GLU:HB2   | 2.11                     | 0.50              |
| 1:C:66:HIS:CE1    | 2:C:1101:HEC:NB   | 2.80                     | 0.50              |
| 1:A:464:LYS:HD3   | 2:A:1110:HEC:O1D  | 2.11                     | 0.50              |
| 1:A:154:PHE:HB2   | 2:A:1104:HEC:HBD2 | 1.94                     | 0.50              |
| 1:A:186:ASP:OD2   | 1:A:189:SER:N     | 2.45                     | 0.50              |
| 1:A:429:ILE:HD11  | 2:A:1113:HEC:CMB  | 2.41                     | 0.50              |
| 1:B:507:ASP:N     | 1:B:507:ASP:OD2   | 2.45                     | 0.50              |
| 1:B:199:GLU:OE1   | 1:B:267:ARG:HG3   | 2.12                     | 0.50              |
| 2:A:1108:HEC:HBB3 | 2:A:1108:HEC:HMB3 | 1.93                     | 0.49              |
| 1:A:394:GLU:O     | 1:A:395:ALA:HB2   | 2.13                     | 0.49              |
| 1:C:526:MET:HE2   | 2:C:1115:HEC:CAC  | 2.40                     | 0.49              |
| 1:B:295:ALA:HB2   | 1:B:413:MET:SD    | 2.52                     | 0.49              |
| 1:B:134:GLU:OE2   | 1:D:533:ASN:ND2   | 2.25                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:295:ALA:HB2   | 1:D:413:MET:HE3   | 1.95                     | 0.49              |
| 1:C:233:ALA:HB2   | 1:C:239:THR:HG21  | 1.94                     | 0.49              |
| 1:C:97:ARG:NH2    | 1:C:110:TYR:OH    | 2.39                     | 0.49              |
| 1:C:161:ARG:HG2   | 1:C:161:ARG:NH1   | 2.16                     | 0.49              |
| 1:C:386:PRO:HG3   | 1:C:412:SER:OG    | 2.13                     | 0.49              |
| 1:C:530:LYS:HB2   | 1:C:531:PRO:CD    | 2.43                     | 0.49              |
| 1:D:287:MET:SD    | 1:D:325:VAL:HG12  | 2.52                     | 0.49              |
| 1:A:423:THR:HG22  | 1:A:424:PHE:H     | 1.77                     | 0.49              |
| 1:C:431:GLU:HA    | 1:C:450:ARG:HB2   | 1.95                     | 0.48              |
| 1:D:73:VAL:HG13   | 1:D:78:LYS:HB2    | 1.93                     | 0.48              |
| 1:A:229:HIS:CE1   | 1:A:240:GLY:HA3   | 2.48                     | 0.48              |
| 1:D:250:PRO:HD2   | 1:D:251:GLU:OE2   | 2.14                     | 0.48              |
| 1:B:41:LYS:HA     | 1:B:146:ALA:O     | 2.13                     | 0.48              |
| 1:B:526:MET:HE1   | 2:B:1115:HEC:HMD2 | 1.94                     | 0.48              |
| 1:A:530:LYS:HB3   | 2:A:1115:HEC:HBA1 | 1.96                     | 0.48              |
| 1:C:338:LYS:HE2   | 1:C:342:GLN:OE1   | 2.14                     | 0.48              |
| 1:D:221:ALA:O     | 1:D:225:CYS:SG    | 2.71                     | 0.48              |
| 2:A:1109:HEC:HBA2 | 2:A:1109:HEC:CMA  | 2.43                     | 0.48              |
| 1:B:67:ASP:O      | 1:B:71:THR:HG23   | 2.13                     | 0.48              |
| 1:B:346:MET:HE1   | 1:B:355:THR:HB    | 1.96                     | 0.48              |
| 1:C:370:LYS:HG3   | 2:C:1114:HEC:O2D  | 2.14                     | 0.47              |
| 1:A:526:MET:HB2   | 1:A:528:ILE:HG12  | 1.95                     | 0.47              |
| 2:B:1102:HEC:HMC1 | 2:B:1102:HEC:HBC3 | 1.95                     | 0.47              |
| 1:C:530:LYS:CB    | 1:C:531:PRO:CD    | 2.92                     | 0.47              |
| 1:D:211:VAL:CG2   | 1:D:214:ARG:HB2   | 2.45                     | 0.47              |
| 1:D:248:HIS:CD2   | 2:D:1107:HEC:NB   | 2.83                     | 0.47              |
| 2:D:1104:HEC:HMD2 | 2:D:1106:HEC:HBB2 | 1.95                     | 0.47              |
| 2:D:1112:HEC:HBA2 | 2:D:1112:HEC:O2D  | 2.14                     | 0.47              |
| 1:B:226:ILE:CG2   | 1:B:230:MET:HE2   | 2.37                     | 0.47              |
| 1:B:387:GLY:O     | 1:B:388:PHE:C     | 2.57                     | 0.47              |
| 1:D:274:LEU:HB3   | 1:D:406:ARG:HG2   | 1.97                     | 0.47              |
| 1:D:380:VAL:HG11  | 1:D:469:PHE:CE2   | 2.50                     | 0.47              |
| 1:D:345:SER:O     | 1:D:351:GLY:HA3   | 2.15                     | 0.47              |
| 1:D:88:ASP:C      | 1:D:90:LYS:H      | 2.22                     | 0.47              |
| 1:A:342:GLN:HG2   | 1:A:345:SER:HB2   | 1.96                     | 0.46              |
| 1:A:530:LYS:CB    | 1:A:531:PRO:HD3   | 2.36                     | 0.46              |
| 2:C:1115:HEC:HMC3 | 2:C:1115:HEC:HBC3 | 1.96                     | 0.46              |
| 1:B:229:HIS:CE1   | 1:B:240:GLY:HA3   | 2.51                     | 0.46              |
| 1:B:431:GLU:HA    | 1:B:450:ARG:HB2   | 1.97                     | 0.46              |
| 1:C:51:MET:HG3    | 2:C:1103:HEC:O1D  | 2.15                     | 0.46              |
| 1:C:404:GLU:CD    | 1:C:404:GLU:H     | 2.23                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:483:ASN:HD22  | 2:D:1114:HEC:C1D  | 2.28                     | 0.46              |
| 1:A:423:THR:OG1   | 1:A:476:LEU:HD12  | 2.14                     | 0.46              |
| 1:D:339:ALA:HA    | 2:D:1109:HEC:HMA1 | 1.96                     | 0.46              |
| 1:C:389:ASP:OD1   | 1:C:390:ALA:N     | 2.46                     | 0.46              |
| 1:D:211:VAL:HG23  | 1:D:212:ASP:N     | 2.30                     | 0.46              |
| 1:C:313:HIS:HE1   | 2:C:1109:HEC:ND   | 2.11                     | 0.46              |
| 1:C:389:ASP:CG    | 1:C:390:ALA:N     | 2.74                     | 0.46              |
| 1:A:422:GLY:O     | 1:A:473:LYS:HA    | 2.15                     | 0.46              |
| 1:C:186:ASP:HB3   | 1:C:191:LYS:O     | 2.16                     | 0.46              |
| 1:D:357:VAL:HG13  | 1:D:366:HIS:HB3   | 1.98                     | 0.46              |
| 1:C:130:PRO:HA    | 1:C:134:GLU:OE1   | 2.16                     | 0.45              |
| 1:C:313:HIS:HE1   | 2:C:1109:HEC:C1D  | 2.29                     | 0.45              |
| 1:D:307:ASP:HB2   | 2:D:1104:HEC:O1A  | 2.16                     | 0.45              |
| 1:D:66:HIS:HB3    | 1:D:244:CYS:SG    | 2.56                     | 0.45              |
| 1:A:308:CYS:SG    | 2:A:1104:HEC:HBA1 | 2.56                     | 0.45              |
| 1:B:222:HIS:CD2   | 2:B:1107:HEC:NC   | 2.83                     | 0.45              |
| 1:C:152:ILE:O     | 2:C:1107:HEC:O1D  | 2.34                     | 0.45              |
| 1:C:161:ARG:HH11  | 1:C:161:ARG:CG    | 2.18                     | 0.45              |
| 1:C:526:MET:CE    | 2:C:1115:HEC:CAC  | 2.95                     | 0.45              |
| 1:D:476:LEU:HB3   | 2:D:1111:HEC:HBC2 | 1.98                     | 0.45              |
| 1:D:423:THR:CG2   | 1:D:424:PHE:N     | 2.80                     | 0.45              |
| 1:D:508:ARG:HA    | 1:D:509:PRO:HD2   | 1.85                     | 0.45              |
| 2:B:1115:HEC:HMC3 | 2:B:1115:HEC:HBC3 | 1.99                     | 0.45              |
| 1:D:201:SER:HA    | 2:D:1104:HEC:HAD2 | 1.99                     | 0.45              |
| 2:A:1102:HEC:HMC3 | 2:A:1102:HEC:CBC  | 2.46                     | 0.45              |
| 1:B:346:MET:HE1   | 1:B:355:THR:CB    | 2.47                     | 0.45              |
| 1:D:51:MET:HE1    | 2:D:1103:HEC:HAA2 | 1.99                     | 0.45              |
| 1:C:313:HIS:CE1   | 1:C:314:VAL:HG23  | 2.51                     | 0.45              |
| 1:A:532:ALA:C     | 1:A:534:THR:H     | 2.25                     | 0.45              |
| 1:B:529:GLU:O     | 1:B:530:LYS:C     | 2.60                     | 0.45              |
| 2:B:1107:HEC:HBA2 | 2:B:1107:HEC:CMA  | 2.46                     | 0.45              |
| 1:C:274:LEU:HD13  | 1:C:413:MET:CE    | 2.34                     | 0.45              |
| 1:A:97:ARG:NH2    | 1:A:110:TYR:OH    | 2.50                     | 0.44              |
| 1:B:212:ASP:O     | 1:B:213:LYS:HB2   | 2.17                     | 0.44              |
| 1:A:372:THR:HG21  | 3:A:2088:HOH:O    | 2.17                     | 0.44              |
| 1:B:528:ILE:HG23  | 1:B:530:LYS:HG2   | 1.98                     | 0.44              |
| 1:C:301:HIS:CE1   | 2:C:1110:HEC:NA   | 2.85                     | 0.44              |
| 2:C:1108:HEC:HBC1 | 2:C:1110:HEC:CMC  | 2.48                     | 0.44              |
| 1:D:409:VAL:HG12  | 1:D:413:MET:HE2   | 1.99                     | 0.44              |
| 1:A:460:ILE:HG12  | 2:A:1111:HEC:HBB2 | 2.00                     | 0.44              |
| 1:B:435:ILE:O     | 2:B:1116:HEC:HBD1 | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1106:HEC:HMC3 | 2:B:1106:HEC:CBC  | 2.47                     | 0.44              |
| 1:D:492:LYS:HD3   | 2:D:1113:HEC:O1A  | 2.17                     | 0.44              |
| 1:C:342:GLN:NE2   | 2:C:1109:HEC:O2A  | 2.49                     | 0.44              |
| 1:B:346:MET:CE    | 1:B:355:THR:OG1   | 2.66                     | 0.44              |
| 1:C:511:LEU:HG    | 1:C:515:TYR:CE1   | 2.52                     | 0.44              |
| 1:D:161:ARG:NH1   | 1:D:257:LYS:O     | 2.46                     | 0.44              |
| 1:B:460:ILE:HD11  | 2:B:1111:HEC:HMC2 | 1.99                     | 0.44              |
| 1:B:465:LEU:HD13  | 2:B:1110:HEC:CHA  | 2.48                     | 0.44              |
| 1:C:349:CYS:HA    | 2:C:1110:HEC:CHC  | 2.48                     | 0.43              |
| 2:C:1111:HEC:HBA2 | 2:C:1111:HEC:CHA  | 2.48                     | 0.43              |
| 2:D:1108:HEC:HBC1 | 2:D:1110:HEC:C2C  | 2.48                     | 0.43              |
| 1:C:342:GLN:HG2   | 1:C:345:SER:HB2   | 2.00                     | 0.43              |
| 1:D:313:HIS:HE1   | 2:D:1109:HEC:C1D  | 2.32                     | 0.43              |
| 1:D:316:ILE:HD11  | 2:D:1104:HEC:HAA2 | 1.99                     | 0.43              |
| 1:A:323:HIS:CE1   | 2:A:1109:HEC:ND   | 2.86                     | 0.43              |
| 1:B:526:MET:HE1   | 2:B:1115:HEC:HHD  | 1.99                     | 0.43              |
| 1:C:83:CYS:HB2    | 2:C:1101:HEC:C2C  | 2.48                     | 0.43              |
| 1:C:161:ARG:NH1   | 1:C:161:ARG:CG    | 2.79                     | 0.43              |
| 1:C:423:THR:CG2   | 1:C:424:PHE:H     | 2.29                     | 0.43              |
| 1:C:528:ILE:CG2   | 1:C:530:LYS:HB2   | 2.48                     | 0.43              |
| 1:D:308:CYS:SG    | 2:D:1104:HEC:HBA1 | 2.58                     | 0.43              |
| 1:D:211:VAL:HG22  | 1:D:214:ARG:HB2   | 1.99                     | 0.43              |
| 2:C:1102:HEC:CBC  | 2:C:1102:HEC:HMC3 | 2.49                     | 0.43              |
| 1:A:106:LEU:HA    | 1:A:106:LEU:HD23  | 1.74                     | 0.42              |
| 1:C:253:GLN:HA    | 1:C:256:PHE:CE2   | 2.54                     | 0.42              |
| 1:C:274:LEU:HD21  | 1:C:398:LEU:HD22  | 2.00                     | 0.42              |
| 1:C:423:THR:CG2   | 1:C:424:PHE:N     | 2.81                     | 0.42              |
| 2:C:1114:HEC:HMB3 | 2:C:1114:HEC:HBB3 | 2.01                     | 0.42              |
| 1:A:105:GLU:HG2   | 1:A:109:ILE:HD12  | 2.01                     | 0.42              |
| 1:A:328:THR:HG22  | 1:A:330:ASP:N     | 2.34                     | 0.42              |
| 1:C:334:VAL:HG13  | 1:C:338:LYS:HD3   | 2.01                     | 0.42              |
| 1:D:122:ALA:HB2   | 1:D:128:THR:HG21  | 2.02                     | 0.42              |
| 2:D:1115:HEC:HBC3 | 2:D:1115:HEC:HMC3 | 2.01                     | 0.42              |
| 1:B:357:VAL:HG13  | 1:B:366:HIS:HB3   | 2.01                     | 0.42              |
| 1:D:211:VAL:HG21  | 1:D:214:ARG:NH2   | 2.35                     | 0.42              |
| 1:D:482:HIS:HE1   | 2:D:1114:HEC:CHA  | 2.33                     | 0.42              |
| 2:D:1103:HEC:HMC3 | 2:D:1103:HEC:HBC3 | 2.00                     | 0.42              |
| 1:A:483:ASN:HD22  | 2:A:1114:HEC:C1D  | 2.33                     | 0.42              |
| 1:B:161:ARG:HG3   | 3:B:2113:HOH:O    | 2.19                     | 0.42              |
| 1:B:436:GLY:O     | 1:B:437:SER:C     | 2.62                     | 0.42              |
| 1:C:42:ARG:HE     | 1:C:65:ARG:HG2    | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:478:GLN:HA    | 1:D:481:HIS:O     | 2.20                     | 0.42              |
| 1:A:429:ILE:CD1   | 2:A:1113:HEC:HMB1 | 2.50                     | 0.42              |
| 1:D:199:GLU:H     | 1:D:199:GLU:CD    | 2.28                     | 0.42              |
| 1:A:53:ARG:H      | 1:A:53:ARG:HG2    | 1.66                     | 0.42              |
| 1:C:222:HIS:CD2   | 2:C:1107:HEC:NC   | 2.87                     | 0.42              |
| 1:B:522:CYS:SG    | 1:B:526:MET:HE2   | 2.60                     | 0.41              |
| 1:D:66:HIS:ND1    | 2:D:1107:HEC:HBB1 | 2.35                     | 0.41              |
| 1:C:229:HIS:CE1   | 1:C:240:GLY:HA3   | 2.56                     | 0.41              |
| 2:D:1108:HEC:HBC1 | 2:D:1110:HEC:CMC  | 2.50                     | 0.41              |
| 2:D:1104:HEC:HBC1 | 2:D:1106:HEC:C2C  | 2.50                     | 0.41              |
| 1:B:84:HIS:CG     | 1:B:91:MET:HE3    | 2.55                     | 0.41              |
| 1:D:339:ALA:HA    | 2:D:1109:HEC:CMA  | 2.51                     | 0.41              |
| 1:A:291:MET:HG3   | 2:A:1112:HEC:CHB  | 2.51                     | 0.41              |
| 1:B:313:HIS:HE1   | 2:B:1109:HEC:ND   | 2.17                     | 0.41              |
| 1:C:345:SER:O     | 1:C:351:GLY:HA3   | 2.21                     | 0.41              |
| 1:A:529:GLU:O     | 1:A:530:LYS:C     | 2.63                     | 0.41              |
| 1:C:342:GLN:HA    | 1:C:343:PRO:HD3   | 1.93                     | 0.41              |
| 1:A:309:ARG:NH1   | 2:A:1104:HEC:CGD  | 2.84                     | 0.41              |
| 1:A:488:LEU:C     | 1:A:490:PRO:HD3   | 2.45                     | 0.41              |
| 1:C:420:PRO:HG3   | 3:C:2100:HOH:O    | 2.21                     | 0.41              |
| 1:D:526:MET:HE2   | 1:D:526:MET:HB3   | 1.98                     | 0.41              |
| 1:A:423:THR:HA    | 1:A:473:LYS:O     | 2.20                     | 0.41              |
| 1:B:372:THR:HG21  | 1:B:374:SER:HB3   | 2.01                     | 0.41              |
| 1:B:490:PRO:HD2   | 2:B:1113:HEC:HMA1 | 2.02                     | 0.41              |
| 1:C:279:PRO:HB2   | 1:C:283:ALA:CB    | 2.50                     | 0.41              |
| 1:A:313:HIS:H     | 1:A:313:HIS:CD2   | 2.39                     | 0.40              |
| 1:B:159:HIS:O     | 1:B:163:VAL:HG23  | 2.21                     | 0.40              |
| 1:D:97:ARG:NH2    | 1:D:110:TYR:OH    | 2.52                     | 0.40              |
| 1:D:313:HIS:CE1   | 2:D:1109:HEC:C1D  | 3.04                     | 0.40              |
| 1:D:326:ASN:HA    | 1:D:335:GLN:HE21  | 1.85                     | 0.40              |
| 1:B:364:GLY:O     | 1:B:525:ARG:NH1   | 2.54                     | 0.40              |
| 1:A:434:VAL:O     | 1:A:434:VAL:HG22  | 2.21                     | 0.40              |
| 1:B:346:MET:CE    | 1:B:355:THR:CB    | 2.99                     | 0.40              |
| 1:B:369:ILE:HD12  | 2:B:1111:HEC:HMD2 | 2.03                     | 0.40              |
| 1:B:197:ASN:HA    | 1:B:267:ARG:HG2   | 2.02                     | 0.40              |
| 1:D:312:HIS:HB3   | 1:D:315:ARG:O     | 2.21                     | 0.40              |
| 1:A:287:MET:SD    | 1:A:326:ASN:HA    | 2.62                     | 0.40              |
| 1:A:528:ILE:HG22  | 1:A:530:LYS:HB2   | 2.04                     | 0.40              |
| 1:B:71:THR:HG22   | 3:B:2059:HOH:O    | 2.20                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 497/514 (97%)   | 463 (93%)  | 25 (5%)  | 9 (2%)   | 6           | 12 |
| 1   | B     | 495/514 (96%)   | 460 (93%)  | 28 (6%)  | 7 (1%)   | 9           | 17 |
| 1   | C     | 497/514 (97%)   | 468 (94%)  | 24 (5%)  | 5 (1%)   | 12          | 24 |
| 1   | D     | 484/514 (94%)   | 451 (93%)  | 26 (5%)  | 7 (1%)   | 9           | 17 |
| All | All   | 1973/2056 (96%) | 1842 (93%) | 103 (5%) | 28 (1%)  | 9           | 17 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 132 | ASP  |
| 1   | A     | 218 | ASP  |
| 1   | A     | 390 | ALA  |
| 1   | A     | 395 | ALA  |
| 1   | B     | 132 | ASP  |
| 1   | B     | 530 | LYS  |
| 1   | C     | 132 | ASP  |
| 1   | C     | 218 | ASP  |
| 1   | D     | 530 | LYS  |
| 1   | A     | 530 | LYS  |
| 1   | B     | 212 | ASP  |
| 1   | B     | 317 | ASP  |
| 1   | C     | 507 | ASP  |
| 1   | D     | 132 | ASP  |
| 1   | D     | 495 | SER  |
| 1   | A     | 391 | LYS  |
| 1   | B     | 155 | ASP  |
| 1   | B     | 437 | SER  |
| 1   | C     | 530 | LYS  |
| 1   | D     | 317 | ASP  |
| 1   | D     | 507 | ASP  |
| 1   | A     | 145 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 437 | SER  |
| 1   | A     | 461 | GLY  |
| 1   | B     | 449 | HIS  |
| 1   | C     | 393 | VAL  |
| 1   | D     | 418 | PRO  |
| 1   | D     | 309 | ARG  |

### 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     | 405/414 (98%)   | 358 (88%)  | 47 (12%)  | 5           | 11 |
| 1   | B     | 403/414 (97%)   | 362 (90%)  | 41 (10%)  | 7           | 15 |
| 1   | C     | 404/414 (98%)   | 371 (92%)  | 33 (8%)   | 10          | 23 |
| 1   | D     | 400/414 (97%)   | 355 (89%)  | 45 (11%)  | 5           | 12 |
| All | All   | 1612/1656 (97%) | 1446 (90%) | 166 (10%) | 7           | 14 |

All (166) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 53  | ARG  |
| 1   | A     | 56  | LYS  |
| 1   | A     | 71  | THR  |
| 1   | A     | 90  | LYS  |
| 1   | A     | 97  | ARG  |
| 1   | A     | 123 | LYS  |
| 1   | A     | 127 | LYS  |
| 1   | A     | 132 | ASP  |
| 1   | A     | 142 | LYS  |
| 1   | A     | 150 | LYS  |
| 1   | A     | 151 | GLU  |
| 1   | A     | 155 | ASP  |
| 1   | A     | 158 | LEU  |
| 1   | A     | 169 | LYS  |
| 1   | A     | 178 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 184 | VAL  |
| 1   | A     | 209 | LYS  |
| 1   | A     | 255 | LYS  |
| 1   | A     | 257 | LYS  |
| 1   | A     | 267 | ARG  |
| 1   | A     | 269 | GLN  |
| 1   | A     | 290 | THR  |
| 1   | A     | 292 | LYS  |
| 1   | A     | 299 | LYS  |
| 1   | A     | 306 | ASN  |
| 1   | A     | 356 | ARG  |
| 1   | A     | 361 | THR  |
| 1   | A     | 374 | SER  |
| 1   | A     | 388 | PHE  |
| 1   | A     | 391 | LYS  |
| 1   | A     | 394 | GLU  |
| 1   | A     | 404 | GLU  |
| 1   | A     | 421 | LYS  |
| 1   | A     | 426 | LEU  |
| 1   | A     | 434 | VAL  |
| 1   | A     | 441 | GLU  |
| 1   | A     | 450 | ARG  |
| 1   | A     | 464 | LYS  |
| 1   | A     | 484 | SER  |
| 1   | A     | 489 | THR  |
| 1   | A     | 492 | LYS  |
| 1   | A     | 499 | LYS  |
| 1   | A     | 505 | ARG  |
| 1   | A     | 508 | ARG  |
| 1   | A     | 511 | LEU  |
| 1   | A     | 534 | THR  |
| 1   | A     | 543 | ARG  |
| 1   | B     | 56  | LYS  |
| 1   | B     | 71  | THR  |
| 1   | B     | 97  | ARG  |
| 1   | B     | 100 | ASP  |
| 1   | B     | 126 | LYS  |
| 1   | B     | 127 | LYS  |
| 1   | B     | 132 | ASP  |
| 1   | B     | 144 | SER  |
| 1   | B     | 151 | GLU  |
| 1   | B     | 155 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 161 | ARG  |
| 1   | B     | 187 | GLU  |
| 1   | B     | 191 | LYS  |
| 1   | B     | 193 | VAL  |
| 1   | B     | 209 | LYS  |
| 1   | B     | 261 | GLU  |
| 1   | B     | 267 | ARG  |
| 1   | B     | 269 | GLN  |
| 1   | B     | 325 | VAL  |
| 1   | B     | 326 | ASN  |
| 1   | B     | 345 | SER  |
| 1   | B     | 357 | VAL  |
| 1   | B     | 359 | GLN  |
| 1   | B     | 369 | ILE  |
| 1   | B     | 370 | LYS  |
| 1   | B     | 389 | ASP  |
| 1   | B     | 391 | LYS  |
| 1   | B     | 392 | GLN  |
| 1   | B     | 404 | GLU  |
| 1   | B     | 433 | VAL  |
| 1   | B     | 435 | ILE  |
| 1   | B     | 437 | SER  |
| 1   | B     | 445 | SER  |
| 1   | B     | 446 | GLU  |
| 1   | B     | 451 | LYS  |
| 1   | B     | 462 | GLU  |
| 1   | B     | 499 | LYS  |
| 1   | B     | 505 | ARG  |
| 1   | B     | 507 | ASP  |
| 1   | B     | 508 | ARG  |
| 1   | B     | 512 | LYS  |
| 1   | C     | 88  | ASP  |
| 1   | C     | 123 | LYS  |
| 1   | C     | 132 | ASP  |
| 1   | C     | 137 | SER  |
| 1   | C     | 151 | GLU  |
| 1   | C     | 161 | ARG  |
| 1   | C     | 171 | VAL  |
| 1   | C     | 175 | GLN  |
| 1   | C     | 187 | GLU  |
| 1   | C     | 189 | SER  |
| 1   | C     | 190 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 193 | VAL  |
| 1   | C     | 198 | LYS  |
| 1   | C     | 213 | LYS  |
| 1   | C     | 261 | GLU  |
| 1   | C     | 269 | GLN  |
| 1   | C     | 275 | ILE  |
| 1   | C     | 281 | LYS  |
| 1   | C     | 285 | ARG  |
| 1   | C     | 342 | GLN  |
| 1   | C     | 369 | ILE  |
| 1   | C     | 373 | LYS  |
| 1   | C     | 389 | ASP  |
| 1   | C     | 407 | SER  |
| 1   | C     | 408 | GLN  |
| 1   | C     | 421 | LYS  |
| 1   | C     | 434 | VAL  |
| 1   | C     | 435 | ILE  |
| 1   | C     | 437 | SER  |
| 1   | C     | 441 | GLU  |
| 1   | C     | 464 | LYS  |
| 1   | C     | 512 | LYS  |
| 1   | C     | 529 | GLU  |
| 1   | D     | 41  | LYS  |
| 1   | D     | 42  | ARG  |
| 1   | D     | 53  | ARG  |
| 1   | D     | 56  | LYS  |
| 1   | D     | 71  | THR  |
| 1   | D     | 80  | CYS  |
| 1   | D     | 90  | LYS  |
| 1   | D     | 126 | LYS  |
| 1   | D     | 127 | LYS  |
| 1   | D     | 132 | ASP  |
| 1   | D     | 151 | GLU  |
| 1   | D     | 158 | LEU  |
| 1   | D     | 166 | LYS  |
| 1   | D     | 187 | GLU  |
| 1   | D     | 198 | LYS  |
| 1   | D     | 225 | CYS  |
| 1   | D     | 236 | LYS  |
| 1   | D     | 257 | LYS  |
| 1   | D     | 262 | VAL  |
| 1   | D     | 269 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 281 | LYS  |
| 1   | D     | 287 | MET  |
| 1   | D     | 288 | LYS  |
| 1   | D     | 292 | LYS  |
| 1   | D     | 315 | ARG  |
| 1   | D     | 324 | THR  |
| 1   | D     | 332 | LYS  |
| 1   | D     | 338 | LYS  |
| 1   | D     | 342 | GLN  |
| 1   | D     | 355 | THR  |
| 1   | D     | 356 | ARG  |
| 1   | D     | 357 | VAL  |
| 1   | D     | 370 | LYS  |
| 1   | D     | 398 | LEU  |
| 1   | D     | 402 | LYS  |
| 1   | D     | 406 | ARG  |
| 1   | D     | 419 | GLN  |
| 1   | D     | 471 | ILE  |
| 1   | D     | 484 | SER  |
| 1   | D     | 488 | LEU  |
| 1   | D     | 492 | LYS  |
| 1   | D     | 499 | LYS  |
| 1   | D     | 511 | LEU  |
| 1   | D     | 528 | ILE  |
| 1   | D     | 530 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 68  | GLN  |
| 1   | A     | 359 | GLN  |
| 1   | A     | 408 | GLN  |
| 1   | A     | 483 | ASN  |
| 1   | B     | 101 | ASN  |
| 1   | B     | 197 | ASN  |
| 1   | B     | 326 | ASN  |
| 1   | B     | 335 | GLN  |
| 1   | B     | 342 | GLN  |
| 1   | B     | 358 | GLN  |
| 1   | B     | 377 | GLN  |
| 1   | B     | 392 | GLN  |
| 1   | B     | 419 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 427 | ASN  |
| 1   | B     | 483 | ASN  |
| 1   | C     | 68  | GLN  |
| 1   | C     | 358 | GLN  |
| 1   | C     | 377 | GLN  |
| 1   | C     | 419 | GLN  |
| 1   | D     | 68  | GLN  |
| 1   | D     | 335 | GLN  |
| 1   | D     | 342 | GLN  |
| 1   | D     | 354 | ASN  |
| 1   | D     | 358 | GLN  |
| 1   | D     | 377 | GLN  |
| 1   | D     | 405 | GLN  |
| 1   | D     | 443 | GLN  |
| 1   | D     | 483 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

64 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | HEC  | A     | 1111 | 1    | 46,50,50     | 2.06 | 11 (23%) | 58,82,82    | 1.26 | 5 (8%)   |
| 2   | HEC  | C     | 1113 | 1    | 46,50,50     | 2.01 | 11 (23%) | 58,82,82    | 1.48 | 9 (15%)  |
| 2   | HEC  | D     | 1102 | 1    | 46,50,50     | 2.06 | 9 (19%)  | 58,82,82    | 1.32 | 6 (10%)  |
| 2   | HEC  | A     | 1114 | 1    | 46,50,50     | 2.08 | 7 (15%)  | 58,82,82    | 1.28 | 5 (8%)   |
| 2   | HEC  | B     | 1103 | 1    | 46,50,50     | 2.09 | 9 (19%)  | 58,82,82    | 1.33 | 4 (6%)   |
| 2   | HEC  | C     | 1108 | 1    | 46,50,50     | 2.03 | 9 (19%)  | 58,82,82    | 1.13 | 5 (8%)   |
| 2   | HEC  | B     | 1107 | 1    | 46,50,50     | 1.99 | 8 (17%)  | 58,82,82    | 1.44 | 7 (12%)  |
| 2   | HEC  | A     | 1102 | 1    | 46,50,50     | 2.05 | 8 (17%)  | 58,82,82    | 1.33 | 4 (6%)   |
| 2   | HEC  | B     | 1109 | 1    | 46,50,50     | 2.09 | 10 (21%) | 58,82,82    | 1.08 | 3 (5%)   |
| 2   | HEC  | B     | 1113 | 1    | 46,50,50     | 2.04 | 8 (17%)  | 58,82,82    | 1.50 | 9 (15%)  |
| 2   | HEC  | B     | 1116 | 1    | 46,50,50     | 2.05 | 10 (21%) | 58,82,82    | 1.28 | 8 (13%)  |
| 2   | HEC  | C     | 1103 | 1    | 46,50,50     | 2.04 | 9 (19%)  | 58,82,82    | 1.34 | 4 (6%)   |
| 2   | HEC  | C     | 1104 | 1    | 46,50,50     | 2.03 | 8 (17%)  | 58,82,82    | 1.23 | 6 (10%)  |
| 2   | HEC  | B     | 1108 | 1    | 46,50,50     | 2.03 | 9 (19%)  | 58,82,82    | 1.22 | 5 (8%)   |
| 2   | HEC  | A     | 1113 | 1    | 46,50,50     | 2.02 | 9 (19%)  | 58,82,82    | 1.25 | 5 (8%)   |
| 2   | HEC  | A     | 1116 | 1    | 46,50,50     | 1.99 | 7 (15%)  | 58,82,82    | 1.31 | 7 (12%)  |
| 2   | HEC  | D     | 1109 | 1    | 46,50,50     | 2.08 | 10 (21%) | 58,82,82    | 1.11 | 5 (8%)   |
| 2   | HEC  | D     | 1107 | 1    | 46,50,50     | 2.04 | 8 (17%)  | 58,82,82    | 1.30 | 4 (6%)   |
| 2   | HEC  | D     | 1114 | 1    | 46,50,50     | 2.04 | 9 (19%)  | 58,82,82    | 1.41 | 5 (8%)   |
| 2   | HEC  | C     | 1107 | 1    | 46,50,50     | 2.03 | 6 (13%)  | 58,82,82    | 1.40 | 7 (12%)  |
| 2   | HEC  | A     | 1106 | 1    | 46,50,50     | 2.05 | 10 (21%) | 58,82,82    | 1.18 | 5 (8%)   |
| 2   | HEC  | A     | 1101 | 1    | 46,50,50     | 2.08 | 8 (17%)  | 58,82,82    | 1.14 | 4 (6%)   |
| 2   | HEC  | B     | 1102 | 1    | 46,50,50     | 2.07 | 9 (19%)  | 58,82,82    | 1.19 | 5 (8%)   |
| 2   | HEC  | A     | 1115 | 1    | 46,50,50     | 1.97 | 7 (15%)  | 58,82,82    | 1.34 | 6 (10%)  |
| 2   | HEC  | D     | 1108 | 1    | 46,50,50     | 2.01 | 8 (17%)  | 58,82,82    | 1.41 | 10 (17%) |
| 2   | HEC  | A     | 1105 | 1    | 46,50,50     | 2.02 | 9 (19%)  | 58,82,82    | 1.21 | 5 (8%)   |
| 2   | HEC  | C     | 1109 | 1    | 46,50,50     | 2.03 | 8 (17%)  | 58,82,82    | 1.22 | 4 (6%)   |
| 2   | HEC  | D     | 1104 | 1    | 46,50,50     | 2.04 | 7 (15%)  | 58,82,82    | 1.21 | 6 (10%)  |
| 2   | HEC  | B     | 1112 | 1    | 46,50,50     | 2.05 | 9 (19%)  | 58,82,82    | 1.49 | 6 (10%)  |
| 2   | HEC  | D     | 1106 | 1    | 46,50,50     | 2.05 | 8 (17%)  | 58,82,82    | 1.05 | 2 (3%)   |
| 2   | HEC  | A     | 1112 | 1    | 46,50,50     | 2.08 | 9 (19%)  | 58,82,82    | 1.20 | 4 (6%)   |
| 2   | HEC  | D     | 1115 | 1    | 46,50,50     | 2.05 | 9 (19%)  | 58,82,82    | 1.32 | 6 (10%)  |
| 2   | HEC  | A     | 1103 | 1    | 46,50,50     | 2.01 | 9 (19%)  | 58,82,82    | 1.37 | 6 (10%)  |
| 2   | HEC  | B     | 1111 | 1    | 46,50,50     | 2.09 | 10 (21%) | 58,82,82    | 1.23 | 6 (10%)  |
| 2   | HEC  | A     | 1107 | 1    | 46,50,50     | 2.09 | 7 (15%)  | 58,82,82    | 1.52 | 9 (15%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | HEC  | B     | 1114 | 1    | 46,50,50     | 2.14 | 8 (17%)  | 58,82,82    | 1.17 | 3 (5%)   |
| 2   | HEC  | C     | 1116 | 1    | 46,50,50     | 2.12 | 8 (17%)  | 58,82,82    | 1.24 | 5 (8%)   |
| 2   | HEC  | D     | 1103 | 1    | 46,50,50     | 2.06 | 8 (17%)  | 58,82,82    | 1.36 | 7 (12%)  |
| 2   | HEC  | A     | 1110 | 1    | 46,50,50     | 2.02 | 8 (17%)  | 58,82,82    | 1.30 | 3 (5%)   |
| 2   | HEC  | C     | 1110 | 1    | 46,50,50     | 1.98 | 8 (17%)  | 58,82,82    | 1.38 | 8 (13%)  |
| 2   | HEC  | D     | 1116 | 1    | 46,50,50     | 2.08 | 10 (21%) | 58,82,82    | 1.39 | 8 (13%)  |
| 2   | HEC  | B     | 1110 | 1    | 46,50,50     | 2.05 | 8 (17%)  | 58,82,82    | 1.37 | 9 (15%)  |
| 2   | HEC  | A     | 1109 | 1    | 46,50,50     | 2.03 | 9 (19%)  | 58,82,82    | 1.39 | 6 (10%)  |
| 2   | HEC  | B     | 1104 | 1    | 46,50,50     | 2.00 | 7 (15%)  | 58,82,82    | 1.24 | 6 (10%)  |
| 2   | HEC  | A     | 1108 | 1    | 46,50,50     | 2.13 | 8 (17%)  | 58,82,82    | 1.27 | 6 (10%)  |
| 2   | HEC  | C     | 1102 | 1    | 46,50,50     | 2.07 | 10 (21%) | 58,82,82    | 1.19 | 5 (8%)   |
| 2   | HEC  | C     | 1106 | 1    | 46,50,50     | 2.02 | 10 (21%) | 58,82,82    | 1.25 | 6 (10%)  |
| 2   | HEC  | C     | 1114 | 1    | 46,50,50     | 2.10 | 11 (23%) | 58,82,82    | 1.36 | 4 (6%)   |
| 2   | HEC  | C     | 1115 | 1    | 46,50,50     | 2.07 | 10 (21%) | 58,82,82    | 1.49 | 7 (12%)  |
| 2   | HEC  | B     | 1106 | 1    | 46,50,50     | 2.04 | 7 (15%)  | 58,82,82    | 1.20 | 6 (10%)  |
| 2   | HEC  | D     | 1111 | 1    | 46,50,50     | 2.06 | 9 (19%)  | 58,82,82    | 1.32 | 5 (8%)   |
| 2   | HEC  | D     | 1112 | 1    | 46,50,50     | 2.05 | 9 (19%)  | 58,82,82    | 1.30 | 4 (6%)   |
| 2   | HEC  | C     | 1111 | 1    | 46,50,50     | 2.08 | 10 (21%) | 58,82,82    | 1.20 | 4 (6%)   |
| 2   | HEC  | A     | 1104 | 1    | 46,50,50     | 2.02 | 7 (15%)  | 58,82,82    | 1.36 | 7 (12%)  |
| 2   | HEC  | C     | 1112 | 1    | 46,50,50     | 2.02 | 8 (17%)  | 58,82,82    | 1.23 | 5 (8%)   |
| 2   | HEC  | D     | 1105 | 1    | 46,50,50     | 2.10 | 8 (17%)  | 58,82,82    | 1.21 | 5 (8%)   |
| 2   | HEC  | B     | 1115 | 1    | 46,50,50     | 2.07 | 9 (19%)  | 58,82,82    | 1.23 | 7 (12%)  |
| 2   | HEC  | D     | 1110 | 1    | 46,50,50     | 2.12 | 10 (21%) | 58,82,82    | 1.27 | 4 (6%)   |
| 2   | HEC  | B     | 1101 | 1    | 46,50,50     | 2.05 | 8 (17%)  | 58,82,82    | 1.31 | 3 (5%)   |
| 2   | HEC  | D     | 1101 | 1    | 46,50,50     | 2.11 | 9 (19%)  | 58,82,82    | 1.31 | 3 (5%)   |
| 2   | HEC  | C     | 1105 | 1    | 46,50,50     | 2.02 | 9 (19%)  | 58,82,82    | 1.25 | 6 (10%)  |
| 2   | HEC  | D     | 1113 | 1    | 46,50,50     | 1.97 | 9 (19%)  | 58,82,82    | 1.50 | 4 (6%)   |
| 2   | HEC  | B     | 1105 | 1    | 46,50,50     | 2.07 | 9 (19%)  | 58,82,82    | 1.23 | 3 (5%)   |
| 2   | HEC  | C     | 1101 | 1    | 46,50,50     | 2.01 | 7 (15%)  | 58,82,82    | 1.32 | 6 (10%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings |
|-----|------|-------|------|------|---------|-------------|-------|
| 2   | HEC  | A     | 1111 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | C     | 1113 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | D     | 1102 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1114 | 1    | -       | 5/14/54/54  | -     |
| 2   | HEC  | B     | 1103 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | C     | 1108 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | B     | 1107 | 1    | -       | 10/14/54/54 | -     |
| 2   | HEC  | A     | 1102 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | B     | 1109 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | B     | 1113 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | B     | 1116 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | C     | 1103 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | C     | 1104 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | B     | 1108 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1113 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | A     | 1116 | 1    | -       | 4/14/54/54  | -     |
| 2   | HEC  | D     | 1109 | 1    | -       | 11/14/54/54 | -     |
| 2   | HEC  | D     | 1107 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | D     | 1114 | 1    | -       | 5/14/54/54  | -     |
| 2   | HEC  | C     | 1107 | 1    | -       | 9/14/54/54  | -     |
| 2   | HEC  | A     | 1106 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1101 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | B     | 1102 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1115 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | D     | 1108 | 1    | -       | 9/14/54/54  | -     |
| 2   | HEC  | A     | 1105 | 1    | -       | 10/14/54/54 | -     |
| 2   | HEC  | C     | 1109 | 1    | -       | 9/14/54/54  | -     |
| 2   | HEC  | D     | 1104 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | B     | 1112 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | D     | 1106 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1112 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | D     | 1115 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1103 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | B     | 1111 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1107 | 1    | -       | 8/14/54/54  | -     |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings |
|-----|------|-------|------|------|---------|-------------|-------|
| 2   | HEC  | B     | 1114 | 1    | -       | 4/14/54/54  | -     |
| 2   | HEC  | C     | 1116 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | D     | 1103 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | A     | 1110 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | C     | 1110 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | D     | 1116 | 1    | -       | 5/14/54/54  | -     |
| 2   | HEC  | B     | 1110 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | A     | 1109 | 1    | -       | 11/14/54/54 | -     |
| 2   | HEC  | B     | 1104 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | A     | 1108 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | C     | 1102 | 1    | -       | 4/14/54/54  | -     |
| 2   | HEC  | C     | 1106 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | C     | 1114 | 1    | -       | 4/14/54/54  | -     |
| 2   | HEC  | C     | 1115 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | B     | 1106 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | D     | 1111 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | D     | 1112 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | C     | 1111 | 1    | -       | 10/14/54/54 | -     |
| 2   | HEC  | A     | 1104 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | C     | 1112 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | D     | 1105 | 1    | -       | 10/14/54/54 | -     |
| 2   | HEC  | B     | 1115 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | D     | 1110 | 1    | -       | 9/14/54/54  | -     |
| 2   | HEC  | B     | 1101 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | D     | 1101 | 1    | -       | 7/14/54/54  | -     |
| 2   | HEC  | C     | 1105 | 1    | -       | 11/14/54/54 | -     |
| 2   | HEC  | D     | 1113 | 1    | -       | 6/14/54/54  | -     |
| 2   | HEC  | B     | 1105 | 1    | -       | 8/14/54/54  | -     |
| 2   | HEC  | C     | 1101 | 1    | -       | 7/14/54/54  | -     |

All (553) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | B     | 1103 | HEC  | CAC-C3C | 6.92 | 1.57        | 1.35     |
| 2   | D     | 1105 | HEC  | CAC-C3C | 6.91 | 1.57        | 1.35     |
| 2   | A     | 1101 | HEC  | CAC-C3C | 6.85 | 1.57        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | B     | 1110 | HEC  | CAC-C3C | 6.83 | 1.57        | 1.35     |
| 2   | A     | 1107 | HEC  | CAC-C3C | 6.82 | 1.57        | 1.35     |
| 2   | C     | 1103 | HEC  | CAC-C3C | 6.81 | 1.57        | 1.35     |
| 2   | A     | 1114 | HEC  | CAC-C3C | 6.75 | 1.56        | 1.35     |
| 2   | B     | 1104 | HEC  | CAC-C3C | 6.69 | 1.56        | 1.35     |
| 2   | B     | 1114 | HEC  | CAC-C3C | 6.67 | 1.56        | 1.35     |
| 2   | D     | 1115 | HEC  | CAC-C3C | 6.66 | 1.56        | 1.35     |
| 2   | D     | 1103 | HEC  | CAC-C3C | 6.66 | 1.56        | 1.35     |
| 2   | B     | 1115 | HEC  | CAC-C3C | 6.63 | 1.56        | 1.35     |
| 2   | C     | 1114 | HEC  | CAC-C3C | 6.63 | 1.56        | 1.35     |
| 2   | A     | 1103 | HEC  | CAC-C3C | 6.62 | 1.56        | 1.35     |
| 2   | C     | 1110 | HEC  | CAC-C3C | 6.62 | 1.56        | 1.35     |
| 2   | B     | 1105 | HEC  | CAC-C3C | 6.62 | 1.56        | 1.35     |
| 2   | C     | 1106 | HEC  | CAB-C3B | 6.59 | 1.56        | 1.35     |
| 2   | A     | 1108 | HEC  | CAB-C3B | 6.57 | 1.56        | 1.35     |
| 2   | D     | 1110 | HEC  | CAC-C3C | 6.57 | 1.56        | 1.35     |
| 2   | D     | 1104 | HEC  | CAC-C3C | 6.56 | 1.56        | 1.35     |
| 2   | D     | 1107 | HEC  | CAC-C3C | 6.55 | 1.56        | 1.35     |
| 2   | A     | 1112 | HEC  | CAC-C3C | 6.54 | 1.56        | 1.35     |
| 2   | A     | 1113 | HEC  | CAC-C3C | 6.54 | 1.56        | 1.35     |
| 2   | B     | 1106 | HEC  | CAC-C3C | 6.54 | 1.56        | 1.35     |
| 2   | C     | 1105 | HEC  | CAC-C3C | 6.53 | 1.56        | 1.35     |
| 2   | C     | 1104 | HEC  | CAB-C3B | 6.52 | 1.56        | 1.35     |
| 2   | B     | 1101 | HEC  | CAC-C3C | 6.51 | 1.56        | 1.35     |
| 2   | C     | 1107 | HEC  | CAC-C3C | 6.51 | 1.56        | 1.35     |
| 2   | D     | 1109 | HEC  | CAB-C3B | 6.49 | 1.56        | 1.35     |
| 2   | C     | 1107 | HEC  | CAB-C3B | 6.47 | 1.56        | 1.35     |
| 2   | D     | 1108 | HEC  | CAB-C3B | 6.47 | 1.56        | 1.35     |
| 2   | B     | 1104 | HEC  | CAB-C3B | 6.46 | 1.56        | 1.35     |
| 2   | A     | 1108 | HEC  | CAC-C3C | 6.46 | 1.56        | 1.35     |
| 2   | D     | 1106 | HEC  | CAC-C3C | 6.44 | 1.55        | 1.35     |
| 2   | C     | 1104 | HEC  | CAC-C3C | 6.44 | 1.55        | 1.35     |
| 2   | C     | 1116 | HEC  | CAB-C3B | 6.44 | 1.55        | 1.35     |
| 2   | B     | 1109 | HEC  | CAC-C3C | 6.41 | 1.55        | 1.35     |
| 2   | B     | 1113 | HEC  | CAC-C3C | 6.41 | 1.55        | 1.35     |
| 2   | D     | 1111 | HEC  | CAC-C3C | 6.39 | 1.55        | 1.35     |
| 2   | C     | 1112 | HEC  | CAC-C3C | 6.39 | 1.55        | 1.35     |
| 2   | D     | 1101 | HEC  | CAC-C3C | 6.38 | 1.55        | 1.35     |
| 2   | C     | 1102 | HEC  | CAC-C3C | 6.37 | 1.55        | 1.35     |
| 2   | D     | 1105 | HEC  | CAB-C3B | 6.36 | 1.55        | 1.35     |
| 2   | C     | 1115 | HEC  | CAC-C3C | 6.36 | 1.55        | 1.35     |
| 2   | A     | 1107 | HEC  | CAB-C3B | 6.35 | 1.55        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | B     | 1102 | HEC  | CAC-C3C | 6.35 | 1.55        | 1.35     |
| 2   | D     | 1106 | HEC  | CAB-C3B | 6.34 | 1.55        | 1.35     |
| 2   | B     | 1116 | HEC  | CAC-C3C | 6.34 | 1.55        | 1.35     |
| 2   | C     | 1108 | HEC  | CAB-C3B | 6.34 | 1.55        | 1.35     |
| 2   | D     | 1116 | HEC  | CAB-C3B | 6.33 | 1.55        | 1.35     |
| 2   | B     | 1107 | HEC  | CAC-C3C | 6.30 | 1.55        | 1.35     |
| 2   | D     | 1101 | HEC  | CAB-C3B | 6.30 | 1.55        | 1.35     |
| 2   | C     | 1101 | HEC  | CAC-C3C | 6.30 | 1.55        | 1.35     |
| 2   | A     | 1115 | HEC  | CAC-C3C | 6.30 | 1.55        | 1.35     |
| 2   | B     | 1108 | HEC  | CAC-C3C | 6.29 | 1.55        | 1.35     |
| 2   | D     | 1110 | HEC  | C3D-C2D | 6.28 | 1.55        | 1.38     |
| 2   | D     | 1107 | HEC  | CAB-C3B | 6.28 | 1.55        | 1.35     |
| 2   | B     | 1108 | HEC  | CAB-C3B | 6.28 | 1.55        | 1.35     |
| 2   | C     | 1102 | HEC  | CAB-C3B | 6.27 | 1.55        | 1.35     |
| 2   | D     | 1102 | HEC  | CAB-C3B | 6.27 | 1.55        | 1.35     |
| 2   | A     | 1102 | HEC  | CAC-C3C | 6.26 | 1.55        | 1.35     |
| 2   | D     | 1108 | HEC  | CAC-C3C | 6.26 | 1.55        | 1.35     |
| 2   | A     | 1102 | HEC  | CAB-C3B | 6.26 | 1.55        | 1.35     |
| 2   | B     | 1111 | HEC  | CAC-C3C | 6.25 | 1.55        | 1.35     |
| 2   | B     | 1101 | HEC  | CAB-C3B | 6.25 | 1.55        | 1.35     |
| 2   | B     | 1109 | HEC  | CAB-C3B | 6.25 | 1.55        | 1.35     |
| 2   | A     | 1111 | HEC  | CAC-C3C | 6.23 | 1.55        | 1.35     |
| 2   | D     | 1112 | HEC  | CAB-C3B | 6.22 | 1.55        | 1.35     |
| 2   | D     | 1102 | HEC  | CAC-C3C | 6.21 | 1.55        | 1.35     |
| 2   | A     | 1103 | HEC  | CAB-C3B | 6.21 | 1.55        | 1.35     |
| 2   | A     | 1108 | HEC  | C3D-C2D | 6.21 | 1.55        | 1.38     |
| 2   | A     | 1113 | HEC  | CAB-C3B | 6.21 | 1.55        | 1.35     |
| 2   | B     | 1115 | HEC  | CAB-C3B | 6.20 | 1.55        | 1.35     |
| 2   | B     | 1102 | HEC  | CAB-C3B | 6.20 | 1.55        | 1.35     |
| 2   | A     | 1101 | HEC  | CAB-C3B | 6.20 | 1.55        | 1.35     |
| 2   | B     | 1103 | HEC  | CAB-C3B | 6.19 | 1.55        | 1.35     |
| 2   | A     | 1116 | HEC  | CAC-C3C | 6.19 | 1.55        | 1.35     |
| 2   | B     | 1106 | HEC  | CAB-C3B | 6.19 | 1.55        | 1.35     |
| 2   | A     | 1105 | HEC  | CAB-C3B | 6.19 | 1.55        | 1.35     |
| 2   | A     | 1104 | HEC  | CAB-C3B | 6.18 | 1.55        | 1.35     |
| 2   | C     | 1115 | HEC  | CAB-C3B | 6.18 | 1.55        | 1.35     |
| 2   | D     | 1109 | HEC  | CAC-C3C | 6.18 | 1.55        | 1.35     |
| 2   | C     | 1111 | HEC  | CAC-C3C | 6.17 | 1.55        | 1.35     |
| 2   | D     | 1114 | HEC  | CAC-C3C | 6.16 | 1.55        | 1.35     |
| 2   | D     | 1115 | HEC  | CAB-C3B | 6.13 | 1.54        | 1.35     |
| 2   | A     | 1110 | HEC  | CAC-C3C | 6.13 | 1.54        | 1.35     |
| 2   | B     | 1107 | HEC  | CAB-C3B | 6.12 | 1.54        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | A     | 1105 | HEC  | CAC-C3C | 6.12 | 1.54        | 1.35     |
| 2   | A     | 1116 | HEC  | CAB-C3B | 6.12 | 1.54        | 1.35     |
| 2   | C     | 1109 | HEC  | CAC-C3C | 6.11 | 1.54        | 1.35     |
| 2   | B     | 1114 | HEC  | C3D-C2D | 6.11 | 1.54        | 1.38     |
| 2   | D     | 1105 | HEC  | C3D-C2D | 6.10 | 1.54        | 1.38     |
| 2   | A     | 1114 | HEC  | CAB-C3B | 6.10 | 1.54        | 1.35     |
| 2   | B     | 1114 | HEC  | CAB-C3B | 6.10 | 1.54        | 1.35     |
| 2   | C     | 1113 | HEC  | CAB-C3B | 6.10 | 1.54        | 1.35     |
| 2   | D     | 1111 | HEC  | CAB-C3B | 6.09 | 1.54        | 1.35     |
| 2   | C     | 1109 | HEC  | CAB-C3B | 6.09 | 1.54        | 1.35     |
| 2   | C     | 1116 | HEC  | CAC-C3C | 6.09 | 1.54        | 1.35     |
| 2   | C     | 1111 | HEC  | CAB-C3B | 6.08 | 1.54        | 1.35     |
| 2   | A     | 1115 | HEC  | CAB-C3B | 6.08 | 1.54        | 1.35     |
| 2   | D     | 1116 | HEC  | CAC-C3C | 6.07 | 1.54        | 1.35     |
| 2   | D     | 1110 | HEC  | CAB-C3B | 6.06 | 1.54        | 1.35     |
| 2   | C     | 1101 | HEC  | CAB-C3B | 6.06 | 1.54        | 1.35     |
| 2   | B     | 1116 | HEC  | CAB-C3B | 6.05 | 1.54        | 1.35     |
| 2   | D     | 1112 | HEC  | CAC-C3C | 6.05 | 1.54        | 1.35     |
| 2   | D     | 1104 | HEC  | CAB-C3B | 6.05 | 1.54        | 1.35     |
| 2   | A     | 1111 | HEC  | CAB-C3B | 6.04 | 1.54        | 1.35     |
| 2   | A     | 1106 | HEC  | CAC-C3C | 6.03 | 1.54        | 1.35     |
| 2   | A     | 1104 | HEC  | CAC-C3C | 6.02 | 1.54        | 1.35     |
| 2   | C     | 1108 | HEC  | CAC-C3C | 6.00 | 1.54        | 1.35     |
| 2   | D     | 1114 | HEC  | C3D-C2D | 5.99 | 1.54        | 1.38     |
| 2   | A     | 1114 | HEC  | C3D-C2D | 5.99 | 1.54        | 1.38     |
| 2   | A     | 1112 | HEC  | CAB-C3B | 5.98 | 1.54        | 1.35     |
| 2   | B     | 1111 | HEC  | CAB-C3B | 5.97 | 1.54        | 1.35     |
| 2   | A     | 1110 | HEC  | CAB-C3B | 5.96 | 1.54        | 1.35     |
| 2   | A     | 1109 | HEC  | CAB-C3B | 5.95 | 1.54        | 1.35     |
| 2   | A     | 1109 | HEC  | CAC-C3C | 5.93 | 1.54        | 1.35     |
| 2   | D     | 1109 | HEC  | C3D-C2D | 5.92 | 1.54        | 1.38     |
| 2   | B     | 1110 | HEC  | CAB-C3B | 5.91 | 1.54        | 1.35     |
| 2   | C     | 1112 | HEC  | CAB-C3B | 5.91 | 1.54        | 1.35     |
| 2   | C     | 1114 | HEC  | CAB-C3B | 5.89 | 1.54        | 1.35     |
| 2   | B     | 1111 | HEC  | C3D-C2D | 5.89 | 1.54        | 1.38     |
| 2   | C     | 1103 | HEC  | CAB-C3B | 5.89 | 1.54        | 1.35     |
| 2   | B     | 1102 | HEC  | C3D-C2D | 5.89 | 1.54        | 1.38     |
| 2   | A     | 1106 | HEC  | CAB-C3B | 5.88 | 1.54        | 1.35     |
| 2   | D     | 1103 | HEC  | CAB-C3B | 5.87 | 1.54        | 1.35     |
| 2   | D     | 1113 | HEC  | CAB-C3B | 5.87 | 1.54        | 1.35     |
| 2   | C     | 1114 | HEC  | C3D-C2D | 5.86 | 1.54        | 1.38     |
| 2   | C     | 1102 | HEC  | C3D-C2D | 5.86 | 1.54        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 2   | B     | 1112 | HEC  | CAC-C3C | 5.86 | 1.54        | 1.35     |
| 2   | C     | 1113 | HEC  | CAC-C3C | 5.85 | 1.54        | 1.35     |
| 2   | B     | 1105 | HEC  | CAB-C3B | 5.84 | 1.54        | 1.35     |
| 2   | D     | 1114 | HEC  | CAB-C3B | 5.83 | 1.53        | 1.35     |
| 2   | C     | 1106 | HEC  | CAC-C3C | 5.83 | 1.53        | 1.35     |
| 2   | A     | 1102 | HEC  | C3D-C2D | 5.82 | 1.54        | 1.38     |
| 2   | C     | 1110 | HEC  | CAB-C3B | 5.78 | 1.53        | 1.35     |
| 2   | B     | 1112 | HEC  | CAB-C3B | 5.77 | 1.53        | 1.35     |
| 2   | D     | 1111 | HEC  | C3D-C2D | 5.77 | 1.53        | 1.38     |
| 2   | D     | 1102 | HEC  | C3D-C2D | 5.75 | 1.53        | 1.38     |
| 2   | C     | 1116 | HEC  | C3D-C2D | 5.75 | 1.53        | 1.38     |
| 2   | C     | 1111 | HEC  | C3D-C2D | 5.73 | 1.53        | 1.38     |
| 2   | A     | 1111 | HEC  | C3D-C2D | 5.72 | 1.53        | 1.38     |
| 2   | C     | 1105 | HEC  | CAB-C3B | 5.72 | 1.53        | 1.35     |
| 2   | D     | 1106 | HEC  | C3D-C2D | 5.70 | 1.53        | 1.38     |
| 2   | B     | 1113 | HEC  | CAB-C3B | 5.69 | 1.53        | 1.35     |
| 2   | B     | 1113 | HEC  | C3D-C2D | 5.69 | 1.53        | 1.38     |
| 2   | D     | 1101 | HEC  | C3D-C2D | 5.69 | 1.53        | 1.38     |
| 2   | A     | 1110 | HEC  | C3D-C2D | 5.67 | 1.53        | 1.38     |
| 2   | C     | 1115 | HEC  | C3D-C2D | 5.67 | 1.53        | 1.38     |
| 2   | D     | 1113 | HEC  | CAC-C3C | 5.66 | 1.53        | 1.35     |
| 2   | A     | 1109 | HEC  | C3D-C2D | 5.62 | 1.53        | 1.38     |
| 2   | D     | 1103 | HEC  | C3D-C2D | 5.62 | 1.53        | 1.38     |
| 2   | B     | 1115 | HEC  | C3D-C2D | 5.55 | 1.53        | 1.38     |
| 2   | D     | 1104 | HEC  | C3D-C2D | 5.55 | 1.53        | 1.38     |
| 2   | C     | 1105 | HEC  | C3D-C2D | 5.54 | 1.53        | 1.38     |
| 2   | A     | 1113 | HEC  | C3D-C2D | 5.53 | 1.53        | 1.38     |
| 2   | A     | 1106 | HEC  | C3D-C2D | 5.53 | 1.53        | 1.38     |
| 2   | B     | 1108 | HEC  | C3D-C2D | 5.53 | 1.53        | 1.38     |
| 2   | A     | 1101 | HEC  | C3D-C2D | 5.51 | 1.53        | 1.38     |
| 2   | B     | 1101 | HEC  | C3D-C2D | 5.50 | 1.53        | 1.38     |
| 2   | D     | 1107 | HEC  | C3D-C2D | 5.50 | 1.53        | 1.38     |
| 2   | B     | 1105 | HEC  | C3D-C2D | 5.49 | 1.53        | 1.38     |
| 2   | A     | 1112 | HEC  | C3D-C2D | 5.49 | 1.53        | 1.38     |
| 2   | B     | 1116 | HEC  | C3D-C2D | 5.47 | 1.53        | 1.38     |
| 2   | B     | 1110 | HEC  | C3D-C2D | 5.42 | 1.53        | 1.38     |
| 2   | C     | 1101 | HEC  | C3D-C2D | 5.41 | 1.53        | 1.38     |
| 2   | C     | 1108 | HEC  | C3D-C2D | 5.40 | 1.53        | 1.38     |
| 2   | A     | 1107 | HEC  | C3D-C2D | 5.39 | 1.53        | 1.38     |
| 2   | A     | 1104 | HEC  | C3D-C2D | 5.39 | 1.52        | 1.38     |
| 2   | A     | 1105 | HEC  | C3D-C2D | 5.38 | 1.52        | 1.38     |
| 2   | C     | 1106 | HEC  | C3D-C2D | 5.32 | 1.52        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | C     | 1113 | HEC  | C3D-C2D | 5.29  | 1.52        | 1.38     |
| 2   | D     | 1112 | HEC  | C3D-C2D | 5.29  | 1.52        | 1.38     |
| 2   | C     | 1109 | HEC  | C3D-C2D | 5.28  | 1.52        | 1.38     |
| 2   | B     | 1109 | HEC  | C3D-C2D | 5.25  | 1.52        | 1.38     |
| 2   | D     | 1116 | HEC  | C3D-C2D | 5.24  | 1.52        | 1.38     |
| 2   | C     | 1103 | HEC  | C3D-C2D | 5.24  | 1.52        | 1.38     |
| 2   | C     | 1110 | HEC  | C3D-C2D | 5.22  | 1.52        | 1.38     |
| 2   | B     | 1112 | HEC  | C3D-C2D | 5.19  | 1.52        | 1.38     |
| 2   | A     | 1116 | HEC  | C3D-C2D | 5.19  | 1.52        | 1.38     |
| 2   | C     | 1107 | HEC  | C3D-C2D | 5.15  | 1.52        | 1.38     |
| 2   | B     | 1106 | HEC  | C3D-C2D | 5.15  | 1.52        | 1.38     |
| 2   | B     | 1107 | HEC  | C3D-C2D | 5.14  | 1.52        | 1.38     |
| 2   | C     | 1112 | HEC  | C3D-C2D | 5.10  | 1.52        | 1.38     |
| 2   | D     | 1115 | HEC  | C3D-C2D | 5.08  | 1.52        | 1.38     |
| 2   | B     | 1103 | HEC  | C3D-C2D | 5.04  | 1.52        | 1.38     |
| 2   | C     | 1104 | HEC  | C3D-C2D | 5.02  | 1.52        | 1.38     |
| 2   | D     | 1108 | HEC  | C3D-C2D | 4.99  | 1.51        | 1.38     |
| 2   | B     | 1104 | HEC  | C3D-C2D | 4.93  | 1.51        | 1.38     |
| 2   | A     | 1115 | HEC  | C3D-C2D | 4.90  | 1.51        | 1.38     |
| 2   | A     | 1103 | HEC  | C3D-C2D | 4.89  | 1.51        | 1.38     |
| 2   | D     | 1113 | HEC  | C3D-C2D | 4.87  | 1.51        | 1.38     |
| 2   | A     | 1106 | HEC  | CBC-CAC | -4.42 | 1.33        | 1.49     |
| 2   | A     | 1105 | HEC  | CBC-CAC | -4.40 | 1.33        | 1.49     |
| 2   | B     | 1112 | HEC  | CBC-CAC | -4.38 | 1.33        | 1.49     |
| 2   | B     | 1116 | HEC  | CBC-CAC | -4.38 | 1.33        | 1.49     |
| 2   | D     | 1107 | HEC  | CBB-CAB | -4.35 | 1.33        | 1.49     |
| 2   | C     | 1116 | HEC  | CBC-CAC | -4.35 | 1.33        | 1.49     |
| 2   | C     | 1110 | HEC  | CBB-CAB | -4.34 | 1.33        | 1.49     |
| 2   | C     | 1113 | HEC  | CBC-CAC | -4.32 | 1.33        | 1.49     |
| 2   | B     | 1111 | HEC  | CBB-CAB | -4.32 | 1.33        | 1.49     |
| 2   | B     | 1108 | HEC  | CBC-CAC | -4.29 | 1.33        | 1.49     |
| 2   | D     | 1114 | HEC  | CBB-CAB | -4.29 | 1.33        | 1.49     |
| 2   | B     | 1116 | HEC  | CBB-CAB | -4.27 | 1.33        | 1.49     |
| 2   | A     | 1114 | HEC  | CBB-CAB | -4.27 | 1.33        | 1.49     |
| 2   | B     | 1106 | HEC  | CBB-CAB | -4.26 | 1.33        | 1.49     |
| 2   | C     | 1109 | HEC  | CBC-CAC | -4.26 | 1.33        | 1.49     |
| 2   | A     | 1115 | HEC  | CBC-CAC | -4.25 | 1.33        | 1.49     |
| 2   | C     | 1116 | HEC  | CBB-CAB | -4.23 | 1.33        | 1.49     |
| 2   | A     | 1111 | HEC  | CBC-CAC | -4.22 | 1.33        | 1.49     |
| 2   | A     | 1112 | HEC  | CBB-CAB | -4.22 | 1.33        | 1.49     |
| 2   | B     | 1110 | HEC  | CBB-CAB | -4.21 | 1.33        | 1.49     |
| 2   | A     | 1108 | HEC  | CBC-CAC | -4.21 | 1.33        | 1.49     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | D     | 1115 | HEC  | CBB-CAB | -4.20 | 1.33        | 1.49     |
| 2   | A     | 1116 | HEC  | CBC-CAC | -4.20 | 1.33        | 1.49     |
| 2   | C     | 1108 | HEC  | CBB-CAB | -4.20 | 1.34        | 1.49     |
| 2   | B     | 1115 | HEC  | CBB-CAB | -4.18 | 1.34        | 1.49     |
| 2   | D     | 1116 | HEC  | CBC-CAC | -4.18 | 1.34        | 1.49     |
| 2   | A     | 1109 | HEC  | CBC-CAC | -4.18 | 1.34        | 1.49     |
| 2   | C     | 1114 | HEC  | CBB-CAB | -4.17 | 1.34        | 1.49     |
| 2   | D     | 1108 | HEC  | CBC-CAC | -4.17 | 1.34        | 1.49     |
| 2   | C     | 1104 | HEC  | CBC-CAC | -4.16 | 1.34        | 1.49     |
| 2   | D     | 1111 | HEC  | CBB-CAB | -4.16 | 1.34        | 1.49     |
| 2   | B     | 1113 | HEC  | CBB-CAB | -4.16 | 1.34        | 1.49     |
| 2   | B     | 1111 | HEC  | CBC-CAC | -4.15 | 1.34        | 1.49     |
| 2   | D     | 1104 | HEC  | CBB-CAB | -4.15 | 1.34        | 1.49     |
| 2   | C     | 1111 | HEC  | CBB-CAB | -4.15 | 1.34        | 1.49     |
| 2   | B     | 1105 | HEC  | CBB-CAB | -4.15 | 1.34        | 1.49     |
| 2   | C     | 1112 | HEC  | CBC-CAC | -4.14 | 1.34        | 1.49     |
| 2   | A     | 1114 | HEC  | CBC-CAC | -4.13 | 1.34        | 1.49     |
| 2   | B     | 1103 | HEC  | CBC-CAC | -4.12 | 1.34        | 1.49     |
| 2   | B     | 1109 | HEC  | CBC-CAC | -4.11 | 1.34        | 1.49     |
| 2   | D     | 1101 | HEC  | CBC-CAC | -4.11 | 1.34        | 1.49     |
| 2   | D     | 1105 | HEC  | CBB-CAB | -4.11 | 1.34        | 1.49     |
| 2   | B     | 1115 | HEC  | CBC-CAC | -4.10 | 1.34        | 1.49     |
| 2   | B     | 1114 | HEC  | CBB-CAB | -4.10 | 1.34        | 1.49     |
| 2   | D     | 1103 | HEC  | CBB-CAB | -4.10 | 1.34        | 1.49     |
| 2   | A     | 1113 | HEC  | CBC-CAC | -4.10 | 1.34        | 1.49     |
| 2   | D     | 1115 | HEC  | CBC-CAC | -4.09 | 1.34        | 1.49     |
| 2   | D     | 1114 | HEC  | CBC-CAC | -4.09 | 1.34        | 1.49     |
| 2   | D     | 1108 | HEC  | CBB-CAB | -4.07 | 1.34        | 1.49     |
| 2   | B     | 1112 | HEC  | CBB-CAB | -4.07 | 1.34        | 1.49     |
| 2   | C     | 1103 | HEC  | CBC-CAC | -4.06 | 1.34        | 1.49     |
| 2   | B     | 1105 | HEC  | CBC-CAC | -4.06 | 1.34        | 1.49     |
| 2   | C     | 1115 | HEC  | CBC-CAC | -4.05 | 1.34        | 1.49     |
| 2   | C     | 1112 | HEC  | CBB-CAB | -4.04 | 1.34        | 1.49     |
| 2   | D     | 1110 | HEC  | CBB-CAB | -4.04 | 1.34        | 1.49     |
| 2   | D     | 1113 | HEC  | CBC-CAC | -4.04 | 1.34        | 1.49     |
| 2   | A     | 1109 | HEC  | CBB-CAB | -4.03 | 1.34        | 1.49     |
| 2   | D     | 1112 | HEC  | CBB-CAB | -4.03 | 1.34        | 1.49     |
| 2   | D     | 1103 | HEC  | CBC-CAC | -4.02 | 1.34        | 1.49     |
| 2   | D     | 1113 | HEC  | CBB-CAB | -4.02 | 1.34        | 1.49     |
| 2   | D     | 1104 | HEC  | CBC-CAC | -4.02 | 1.34        | 1.49     |
| 2   | D     | 1109 | HEC  | CBC-CAC | -4.00 | 1.34        | 1.49     |
| 2   | A     | 1116 | HEC  | CBB-CAB | -4.00 | 1.34        | 1.49     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1102 | HEC  | CBC-CAC | -4.00 | 1.34        | 1.49     |
| 2   | B     | 1101 | HEC  | CBC-CAC | -3.99 | 1.34        | 1.49     |
| 2   | B     | 1109 | HEC  | CBB-CAB | -3.99 | 1.34        | 1.49     |
| 2   | C     | 1105 | HEC  | CBC-CAC | -3.99 | 1.34        | 1.49     |
| 2   | D     | 1106 | HEC  | CBC-CAC | -3.99 | 1.34        | 1.49     |
| 2   | C     | 1115 | HEC  | CBB-CAB | -3.99 | 1.34        | 1.49     |
| 2   | B     | 1106 | HEC  | CBC-CAC | -3.98 | 1.34        | 1.49     |
| 2   | A     | 1115 | HEC  | CBB-CAB | -3.98 | 1.34        | 1.49     |
| 2   | D     | 1107 | HEC  | CBC-CAC | -3.98 | 1.34        | 1.49     |
| 2   | C     | 1107 | HEC  | CBC-CAC | -3.97 | 1.34        | 1.49     |
| 2   | A     | 1108 | HEC  | CBB-CAB | -3.97 | 1.34        | 1.49     |
| 2   | C     | 1105 | HEC  | CBB-CAB | -3.97 | 1.34        | 1.49     |
| 2   | A     | 1106 | HEC  | CBB-CAB | -3.96 | 1.34        | 1.49     |
| 2   | B     | 1108 | HEC  | CBB-CAB | -3.95 | 1.34        | 1.49     |
| 2   | B     | 1103 | HEC  | CBB-CAB | -3.94 | 1.34        | 1.49     |
| 2   | A     | 1104 | HEC  | CBC-CAC | -3.93 | 1.34        | 1.49     |
| 2   | B     | 1107 | HEC  | CBC-CAC | -3.93 | 1.35        | 1.49     |
| 2   | A     | 1107 | HEC  | CBC-CAC | -3.92 | 1.35        | 1.49     |
| 2   | A     | 1110 | HEC  | CBC-CAC | -3.92 | 1.35        | 1.49     |
| 2   | D     | 1116 | HEC  | CBB-CAB | -3.92 | 1.35        | 1.49     |
| 2   | C     | 1108 | HEC  | CBC-CAC | -3.92 | 1.35        | 1.49     |
| 2   | A     | 1112 | HEC  | CBC-CAC | -3.92 | 1.35        | 1.49     |
| 2   | A     | 1110 | HEC  | CBB-CAB | -3.92 | 1.35        | 1.49     |
| 2   | C     | 1104 | HEC  | CBB-CAB | -3.92 | 1.35        | 1.49     |
| 2   | D     | 1102 | HEC  | CBC-CAC | -3.91 | 1.35        | 1.49     |
| 2   | A     | 1104 | HEC  | CBB-CAB | -3.91 | 1.35        | 1.49     |
| 2   | A     | 1111 | HEC  | CBB-CAB | -3.90 | 1.35        | 1.49     |
| 2   | B     | 1114 | HEC  | CBC-CAC | -3.90 | 1.35        | 1.49     |
| 2   | C     | 1102 | HEC  | CBB-CAB | -3.90 | 1.35        | 1.49     |
| 2   | B     | 1104 | HEC  | CBC-CAC | -3.90 | 1.35        | 1.49     |
| 2   | C     | 1106 | HEC  | CBC-CAC | -3.89 | 1.35        | 1.49     |
| 2   | A     | 1105 | HEC  | CBB-CAB | -3.88 | 1.35        | 1.49     |
| 2   | C     | 1106 | HEC  | CBB-CAB | -3.88 | 1.35        | 1.49     |
| 2   | B     | 1107 | HEC  | CBB-CAB | -3.88 | 1.35        | 1.49     |
| 2   | D     | 1109 | HEC  | CBB-CAB | -3.88 | 1.35        | 1.49     |
| 2   | C     | 1113 | HEC  | CBB-CAB | -3.86 | 1.35        | 1.49     |
| 2   | D     | 1112 | HEC  | CBC-CAC | -3.84 | 1.35        | 1.49     |
| 2   | A     | 1101 | HEC  | CBB-CAB | -3.84 | 1.35        | 1.49     |
| 2   | D     | 1110 | HEC  | CBC-CAC | -3.84 | 1.35        | 1.49     |
| 2   | B     | 1113 | HEC  | CBC-CAC | -3.83 | 1.35        | 1.49     |
| 2   | C     | 1110 | HEC  | CBC-CAC | -3.83 | 1.35        | 1.49     |
| 2   | A     | 1103 | HEC  | CBC-CAC | -3.83 | 1.35        | 1.49     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 1102 | HEC  | CBC-CAC | -3.82 | 1.35        | 1.49     |
| 2   | B     | 1101 | HEC  | CBB-CAB | -3.81 | 1.35        | 1.49     |
| 2   | D     | 1106 | HEC  | CBB-CAB | -3.79 | 1.35        | 1.49     |
| 2   | A     | 1107 | HEC  | CBB-CAB | -3.79 | 1.35        | 1.49     |
| 2   | C     | 1114 | HEC  | CBC-CAC | -3.78 | 1.35        | 1.49     |
| 2   | D     | 1101 | HEC  | CBB-CAB | -3.78 | 1.35        | 1.49     |
| 2   | D     | 1105 | HEC  | CBC-CAC | -3.77 | 1.35        | 1.49     |
| 2   | C     | 1102 | HEC  | CBC-CAC | -3.76 | 1.35        | 1.49     |
| 2   | A     | 1113 | HEC  | CBB-CAB | -3.75 | 1.35        | 1.49     |
| 2   | C     | 1103 | HEC  | CBB-CAB | -3.74 | 1.35        | 1.49     |
| 2   | D     | 1102 | HEC  | CBB-CAB | -3.73 | 1.35        | 1.49     |
| 2   | C     | 1109 | HEC  | CBB-CAB | -3.73 | 1.35        | 1.49     |
| 2   | C     | 1101 | HEC  | CBB-CAB | -3.73 | 1.35        | 1.49     |
| 2   | A     | 1101 | HEC  | CBC-CAC | -3.71 | 1.35        | 1.49     |
| 2   | B     | 1104 | HEC  | CBB-CAB | -3.71 | 1.35        | 1.49     |
| 2   | B     | 1110 | HEC  | CBC-CAC | -3.71 | 1.35        | 1.49     |
| 2   | C     | 1111 | HEC  | CBC-CAC | -3.70 | 1.35        | 1.49     |
| 2   | A     | 1102 | HEC  | CBB-CAB | -3.67 | 1.35        | 1.49     |
| 2   | A     | 1103 | HEC  | CBB-CAB | -3.67 | 1.35        | 1.49     |
| 2   | B     | 1102 | HEC  | CBB-CAB | -3.67 | 1.35        | 1.49     |
| 2   | C     | 1101 | HEC  | CBC-CAC | -3.65 | 1.36        | 1.49     |
| 2   | D     | 1111 | HEC  | CBC-CAC | -3.63 | 1.36        | 1.49     |
| 2   | C     | 1107 | HEC  | CBB-CAB | -3.54 | 1.36        | 1.49     |
| 2   | C     | 1109 | HEC  | CMA-C3A | 3.09  | 1.57        | 1.50     |
| 2   | B     | 1103 | HEC  | CMB-C2B | 2.97  | 1.56        | 1.50     |
| 2   | D     | 1101 | HEC  | CMC-C2C | 2.91  | 1.56        | 1.50     |
| 2   | D     | 1116 | HEC  | CMA-C3A | 2.81  | 1.56        | 1.50     |
| 2   | D     | 1110 | HEC  | CMC-C2C | 2.81  | 1.56        | 1.50     |
| 2   | B     | 1112 | HEC  | CMA-C3A | 2.80  | 1.56        | 1.50     |
| 2   | D     | 1103 | HEC  | CMB-C2B | 2.77  | 1.56        | 1.50     |
| 2   | A     | 1101 | HEC  | CMC-C2C | 2.75  | 1.56        | 1.50     |
| 2   | B     | 1101 | HEC  | CMA-C3A | 2.71  | 1.56        | 1.50     |
| 2   | A     | 1104 | HEC  | CMC-C2C | 2.69  | 1.56        | 1.50     |
| 2   | B     | 1110 | HEC  | CMB-C2B | 2.68  | 1.56        | 1.50     |
| 2   | A     | 1106 | HEC  | CMC-C2C | 2.66  | 1.56        | 1.50     |
| 2   | A     | 1110 | HEC  | CMC-C2C | 2.63  | 1.56        | 1.50     |
| 2   | D     | 1104 | HEC  | CMB-C2B | 2.61  | 1.56        | 1.50     |
| 2   | C     | 1112 | HEC  | C3B-C2B | -2.61 | 1.32        | 1.41     |
| 2   | C     | 1112 | HEC  | CMA-C3A | 2.60  | 1.56        | 1.50     |
| 2   | B     | 1106 | HEC  | CMB-C2B | 2.60  | 1.56        | 1.50     |
| 2   | C     | 1114 | HEC  | CMD-C2D | 2.60  | 1.56        | 1.50     |
| 2   | B     | 1109 | HEC  | CMB-C2B | 2.60  | 1.56        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 1105 | HEC  | CMB-C2B | 2.60  | 1.56        | 1.50     |
| 2   | B     | 1113 | HEC  | CMD-C2D | 2.59  | 1.56        | 1.50     |
| 2   | D     | 1108 | HEC  | C3B-C2B | -2.58 | 1.32        | 1.41     |
| 2   | D     | 1102 | HEC  | CMA-C3A | 2.57  | 1.56        | 1.50     |
| 2   | C     | 1115 | HEC  | CMA-C3A | 2.57  | 1.56        | 1.50     |
| 2   | D     | 1113 | HEC  | C3C-C2C | -2.55 | 1.32        | 1.41     |
| 2   | D     | 1109 | HEC  | CMD-C2D | 2.55  | 1.56        | 1.50     |
| 2   | B     | 1114 | HEC  | CMD-C2D | 2.54  | 1.56        | 1.50     |
| 2   | A     | 1103 | HEC  | CMB-C2B | 2.54  | 1.56        | 1.50     |
| 2   | C     | 1113 | HEC  | C3C-C2C | -2.53 | 1.32        | 1.41     |
| 2   | A     | 1102 | HEC  | CMD-C2D | 2.52  | 1.55        | 1.50     |
| 2   | C     | 1106 | HEC  | CMD-C2D | 2.51  | 1.55        | 1.50     |
| 2   | C     | 1115 | HEC  | CMB-C2B | 2.51  | 1.55        | 1.50     |
| 2   | C     | 1116 | HEC  | CMC-C2C | 2.51  | 1.55        | 1.50     |
| 2   | B     | 1101 | HEC  | CMC-C2C | 2.51  | 1.55        | 1.50     |
| 2   | D     | 1111 | HEC  | CMB-C2B | 2.50  | 1.55        | 1.50     |
| 2   | D     | 1115 | HEC  | CMB-C2B | 2.48  | 1.55        | 1.50     |
| 2   | C     | 1103 | HEC  | CMB-C2B | 2.48  | 1.55        | 1.50     |
| 2   | B     | 1109 | HEC  | C3C-C2C | -2.48 | 1.32        | 1.41     |
| 2   | D     | 1116 | HEC  | C3B-C2B | -2.47 | 1.32        | 1.41     |
| 2   | C     | 1111 | HEC  | CMB-C2B | 2.47  | 1.55        | 1.50     |
| 2   | C     | 1104 | HEC  | CMB-C2B | 2.46  | 1.55        | 1.50     |
| 2   | D     | 1115 | HEC  | CMD-C2D | 2.44  | 1.55        | 1.50     |
| 2   | B     | 1111 | HEC  | C3B-C2B | -2.44 | 1.32        | 1.41     |
| 2   | A     | 1111 | HEC  | CMA-C3A | 2.44  | 1.55        | 1.50     |
| 2   | A     | 1115 | HEC  | CMA-C3A | 2.43  | 1.55        | 1.50     |
| 2   | A     | 1103 | HEC  | C3B-C2B | -2.42 | 1.33        | 1.41     |
| 2   | B     | 1113 | HEC  | C3B-C2B | -2.42 | 1.33        | 1.41     |
| 2   | D     | 1102 | HEC  | CMC-C2C | 2.41  | 1.55        | 1.50     |
| 2   | D     | 1107 | HEC  | CMA-C3A | 2.40  | 1.55        | 1.50     |
| 2   | B     | 1111 | HEC  | CMA-C3A | 2.40  | 1.55        | 1.50     |
| 2   | A     | 1110 | HEC  | C3B-C2B | -2.39 | 1.33        | 1.41     |
| 2   | D     | 1113 | HEC  | CMA-C3A | 2.39  | 1.55        | 1.50     |
| 2   | A     | 1112 | HEC  | CMA-C3A | 2.39  | 1.55        | 1.50     |
| 2   | B     | 1115 | HEC  | CMB-C2B | 2.39  | 1.55        | 1.50     |
| 2   | D     | 1110 | HEC  | CMD-C2D | 2.38  | 1.55        | 1.50     |
| 2   | D     | 1111 | HEC  | CMC-C2C | 2.37  | 1.55        | 1.50     |
| 2   | D     | 1116 | HEC  | CMC-C2C | 2.37  | 1.55        | 1.50     |
| 2   | D     | 1114 | HEC  | CMB-C2B | 2.37  | 1.55        | 1.50     |
| 2   | A     | 1108 | HEC  | CMB-C2B | 2.37  | 1.55        | 1.50     |
| 2   | B     | 1104 | HEC  | CMB-C2B | 2.36  | 1.55        | 1.50     |
| 2   | A     | 1116 | HEC  | CMC-C2C | 2.36  | 1.55        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | D     | 1116 | HEC  | C3C-C2C | -2.36 | 1.33        | 1.41     |
| 2   | D     | 1110 | HEC  | CMB-C2B | 2.35  | 1.55        | 1.50     |
| 2   | B     | 1116 | HEC  | CMA-C3A | 2.35  | 1.55        | 1.50     |
| 2   | A     | 1106 | HEC  | C3C-C2C | -2.35 | 1.33        | 1.41     |
| 2   | A     | 1104 | HEC  | C3B-C2B | -2.34 | 1.33        | 1.41     |
| 2   | D     | 1109 | HEC  | CMA-C3A | 2.34  | 1.55        | 1.50     |
| 2   | C     | 1110 | HEC  | CMC-C2C | 2.34  | 1.55        | 1.50     |
| 2   | D     | 1113 | HEC  | CMB-C2B | 2.34  | 1.55        | 1.50     |
| 2   | D     | 1116 | HEC  | CMD-C2D | 2.34  | 1.55        | 1.50     |
| 2   | A     | 1106 | HEC  | CMB-C2B | 2.33  | 1.55        | 1.50     |
| 2   | C     | 1111 | HEC  | CMA-C3A | 2.33  | 1.55        | 1.50     |
| 2   | C     | 1116 | HEC  | CMD-C2D | 2.33  | 1.55        | 1.50     |
| 2   | A     | 1105 | HEC  | C3C-C2C | -2.32 | 1.33        | 1.41     |
| 2   | C     | 1108 | HEC  | CMD-C2D | 2.32  | 1.55        | 1.50     |
| 2   | B     | 1110 | HEC  | CMC-C2C | 2.32  | 1.55        | 1.50     |
| 2   | B     | 1106 | HEC  | CMC-C2C | 2.32  | 1.55        | 1.50     |
| 2   | C     | 1103 | HEC  | C3B-C2B | -2.32 | 1.33        | 1.41     |
| 2   | C     | 1115 | HEC  | C3B-C2B | -2.31 | 1.33        | 1.41     |
| 2   | D     | 1112 | HEC  | CMA-C3A | 2.31  | 1.55        | 1.50     |
| 2   | A     | 1112 | HEC  | CMC-C2C | 2.31  | 1.55        | 1.50     |
| 2   | B     | 1103 | HEC  | C3B-C2B | -2.31 | 1.33        | 1.41     |
| 2   | D     | 1102 | HEC  | CMD-C2D | 2.30  | 1.55        | 1.50     |
| 2   | D     | 1106 | HEC  | CMB-C2B | 2.30  | 1.55        | 1.50     |
| 2   | C     | 1114 | HEC  | CMB-C2B | 2.30  | 1.55        | 1.50     |
| 2   | B     | 1109 | HEC  | CMA-C3A | 2.29  | 1.55        | 1.50     |
| 2   | D     | 1108 | HEC  | CMA-C3A | 2.29  | 1.55        | 1.50     |
| 2   | B     | 1114 | HEC  | CMC-C2C | 2.29  | 1.55        | 1.50     |
| 2   | C     | 1105 | HEC  | C3B-C2B | -2.29 | 1.33        | 1.41     |
| 2   | A     | 1103 | HEC  | CMA-C3A | 2.29  | 1.55        | 1.50     |
| 2   | D     | 1114 | HEC  | CMD-C2D | 2.29  | 1.55        | 1.50     |
| 2   | C     | 1114 | HEC  | CMC-C2C | 2.28  | 1.55        | 1.50     |
| 2   | B     | 1110 | HEC  | CMD-C2D | 2.28  | 1.55        | 1.50     |
| 2   | B     | 1112 | HEC  | CMC-C2C | 2.28  | 1.55        | 1.50     |
| 2   | A     | 1111 | HEC  | CMB-C2B | 2.27  | 1.55        | 1.50     |
| 2   | C     | 1102 | HEC  | C3C-C2C | -2.27 | 1.33        | 1.41     |
| 2   | A     | 1102 | HEC  | CMA-C3A | 2.27  | 1.55        | 1.50     |
| 2   | C     | 1112 | HEC  | CMC-C2C | 2.27  | 1.55        | 1.50     |
| 2   | A     | 1109 | HEC  | CMD-C2D | 2.27  | 1.55        | 1.50     |
| 2   | D     | 1101 | HEC  | CMA-C3A | 2.27  | 1.55        | 1.50     |
| 2   | A     | 1105 | HEC  | CMD-C2D | 2.27  | 1.55        | 1.50     |
| 2   | A     | 1101 | HEC  | CMB-C2B | 2.26  | 1.55        | 1.50     |
| 2   | C     | 1114 | HEC  | C3B-C2B | -2.26 | 1.33        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1112 | HEC  | C3B-C2B | -2.25 | 1.33        | 1.41     |
| 2   | D     | 1111 | HEC  | CMA-C3A | 2.25  | 1.55        | 1.50     |
| 2   | B     | 1105 | HEC  | C3B-C2B | -2.25 | 1.33        | 1.41     |
| 2   | B     | 1112 | HEC  | C3B-C2B | -2.25 | 1.33        | 1.41     |
| 2   | A     | 1106 | HEC  | CMA-C3A | 2.25  | 1.55        | 1.50     |
| 2   | A     | 1108 | HEC  | CMA-C3A | 2.25  | 1.55        | 1.50     |
| 2   | B     | 1108 | HEC  | CMA-C3A | 2.24  | 1.55        | 1.50     |
| 2   | B     | 1107 | HEC  | C3C-C2C | -2.24 | 1.33        | 1.41     |
| 2   | A     | 1101 | HEC  | CMA-C3A | 2.23  | 1.55        | 1.50     |
| 2   | B     | 1113 | HEC  | C3C-C2C | -2.23 | 1.33        | 1.41     |
| 2   | C     | 1115 | HEC  | CMD-C2D | 2.23  | 1.55        | 1.50     |
| 2   | B     | 1107 | HEC  | CMA-C3A | 2.23  | 1.55        | 1.50     |
| 2   | C     | 1113 | HEC  | CMD-C2D | 2.23  | 1.55        | 1.50     |
| 2   | C     | 1104 | HEC  | CMC-C2C | 2.22  | 1.55        | 1.50     |
| 2   | C     | 1111 | HEC  | C3C-C2C | -2.22 | 1.33        | 1.41     |
| 2   | B     | 1114 | HEC  | CMB-C2B | 2.21  | 1.55        | 1.50     |
| 2   | C     | 1111 | HEC  | CMC-C2C | 2.21  | 1.55        | 1.50     |
| 2   | C     | 1105 | HEC  | C3C-C2C | -2.21 | 1.33        | 1.41     |
| 2   | A     | 1111 | HEC  | C3C-C2C | -2.21 | 1.33        | 1.41     |
| 2   | C     | 1113 | HEC  | CMB-C2B | 2.21  | 1.55        | 1.50     |
| 2   | B     | 1102 | HEC  | C3B-C2B | -2.21 | 1.33        | 1.41     |
| 2   | B     | 1112 | HEC  | CMB-C2B | 2.21  | 1.55        | 1.50     |
| 2   | C     | 1101 | HEC  | CMC-C2C | 2.20  | 1.55        | 1.50     |
| 2   | A     | 1111 | HEC  | C3B-C2B | -2.20 | 1.33        | 1.41     |
| 2   | D     | 1105 | HEC  | CMC-C2C | 2.20  | 1.55        | 1.50     |
| 2   | C     | 1109 | HEC  | CMB-C2B | 2.20  | 1.55        | 1.50     |
| 2   | A     | 1111 | HEC  | CAA-C2A | 2.20  | 1.57        | 1.51     |
| 2   | D     | 1109 | HEC  | CMC-C2C | 2.19  | 1.55        | 1.50     |
| 2   | D     | 1110 | HEC  | CMA-C3A | 2.19  | 1.55        | 1.50     |
| 2   | C     | 1103 | HEC  | CMA-C3A | 2.19  | 1.55        | 1.50     |
| 2   | B     | 1116 | HEC  | C3B-C2B | -2.18 | 1.33        | 1.41     |
| 2   | C     | 1106 | HEC  | CMA-C3A | 2.17  | 1.55        | 1.50     |
| 2   | D     | 1112 | HEC  | C3B-C2B | -2.17 | 1.33        | 1.41     |
| 2   | D     | 1112 | HEC  | CMD-C2D | 2.16  | 1.55        | 1.50     |
| 2   | B     | 1108 | HEC  | C3B-C2B | -2.16 | 1.33        | 1.41     |
| 2   | C     | 1101 | HEC  | CMA-C3A | 2.15  | 1.55        | 1.50     |
| 2   | D     | 1113 | HEC  | C3B-C2B | -2.15 | 1.33        | 1.41     |
| 2   | A     | 1107 | HEC  | CMC-C2C | 2.15  | 1.55        | 1.50     |
| 2   | D     | 1108 | HEC  | C3C-C2C | -2.15 | 1.33        | 1.41     |
| 2   | A     | 1109 | HEC  | CMA-C3A | 2.15  | 1.55        | 1.50     |
| 2   | B     | 1103 | HEC  | CMC-C2C | 2.15  | 1.55        | 1.50     |
| 2   | D     | 1115 | HEC  | C3B-C2B | -2.15 | 1.33        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | B     | 1105 | HEC  | CMA-C3A | 2.15  | 1.55        | 1.50     |
| 2   | C     | 1115 | HEC  | C3C-C2C | -2.15 | 1.33        | 1.41     |
| 2   | B     | 1103 | HEC  | CMA-C3A | 2.15  | 1.55        | 1.50     |
| 2   | D     | 1115 | HEC  | CMA-C3A | 2.14  | 1.55        | 1.50     |
| 2   | A     | 1114 | HEC  | CMD-C2D | 2.13  | 1.55        | 1.50     |
| 2   | B     | 1111 | HEC  | C3C-C2C | -2.13 | 1.34        | 1.41     |
| 2   | C     | 1108 | HEC  | CMA-C3A | 2.13  | 1.55        | 1.50     |
| 2   | D     | 1101 | HEC  | CMB-C2B | 2.13  | 1.55        | 1.50     |
| 2   | D     | 1103 | HEC  | C3B-C2B | -2.13 | 1.34        | 1.41     |
| 2   | D     | 1103 | HEC  | C3C-C2C | -2.13 | 1.34        | 1.41     |
| 2   | D     | 1111 | HEC  | CMD-C2D | 2.13  | 1.55        | 1.50     |
| 2   | A     | 1113 | HEC  | CMA-C3A | 2.13  | 1.55        | 1.50     |
| 2   | B     | 1116 | HEC  | C3C-C2C | -2.12 | 1.34        | 1.41     |
| 2   | B     | 1111 | HEC  | CMB-C2B | 2.12  | 1.55        | 1.50     |
| 2   | A     | 1114 | HEC  | C3B-C2B | -2.12 | 1.34        | 1.41     |
| 2   | A     | 1103 | HEC  | CMC-C2C | 2.11  | 1.55        | 1.50     |
| 2   | A     | 1116 | HEC  | CMA-C3A | 2.11  | 1.55        | 1.50     |
| 2   | C     | 1113 | HEC  | C3B-C2B | -2.11 | 1.34        | 1.41     |
| 2   | D     | 1112 | HEC  | CMC-C2C | 2.11  | 1.55        | 1.50     |
| 2   | C     | 1106 | HEC  | C3C-C2C | -2.11 | 1.34        | 1.41     |
| 2   | B     | 1104 | HEC  | CMA-C3A | 2.11  | 1.55        | 1.50     |
| 2   | B     | 1116 | HEC  | O1D-CGD | 2.11  | 1.29        | 1.22     |
| 2   | A     | 1108 | HEC  | O1D-CGD | 2.10  | 1.29        | 1.22     |
| 2   | D     | 1109 | HEC  | C3C-C2C | -2.10 | 1.34        | 1.41     |
| 2   | D     | 1101 | HEC  | C3B-C2B | -2.10 | 1.34        | 1.41     |
| 2   | D     | 1114 | HEC  | CMC-C2C | 2.10  | 1.55        | 1.50     |
| 2   | A     | 1113 | HEC  | C3B-C2B | -2.10 | 1.34        | 1.41     |
| 2   | C     | 1106 | HEC  | CMB-C2B | 2.10  | 1.55        | 1.50     |
| 2   | C     | 1103 | HEC  | CAD-C3D | 2.09  | 1.56        | 1.51     |
| 2   | B     | 1102 | HEC  | CMA-C3A | 2.09  | 1.55        | 1.50     |
| 2   | A     | 1112 | HEC  | CMB-C2B | 2.09  | 1.55        | 1.50     |
| 2   | C     | 1113 | HEC  | CMC-C2C | 2.09  | 1.55        | 1.50     |
| 2   | A     | 1105 | HEC  | C3B-C2B | -2.09 | 1.34        | 1.41     |
| 2   | C     | 1107 | HEC  | CMC-C2C | 2.09  | 1.55        | 1.50     |
| 2   | A     | 1113 | HEC  | C3C-C2C | -2.08 | 1.34        | 1.41     |
| 2   | A     | 1106 | HEC  | C3B-C2B | -2.08 | 1.34        | 1.41     |
| 2   | A     | 1105 | HEC  | CMB-C2B | 2.08  | 1.55        | 1.50     |
| 2   | C     | 1109 | HEC  | C3B-C2B | -2.08 | 1.34        | 1.41     |
| 2   | B     | 1115 | HEC  | CMD-C2D | 2.08  | 1.55        | 1.50     |
| 2   | C     | 1110 | HEC  | C3B-C2B | -2.08 | 1.34        | 1.41     |
| 2   | A     | 1113 | HEC  | CMB-C2B | 2.08  | 1.55        | 1.50     |
| 2   | B     | 1108 | HEC  | C3C-C2C | -2.07 | 1.34        | 1.41     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | A     | 1111 | HEC  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 2   | A     | 1107 | HEC  | CAA-C2A | 2.07  | 1.56        | 1.51     |
| 2   | C     | 1102 | HEC  | C3B-C2B | -2.07 | 1.34        | 1.41     |
| 2   | C     | 1106 | HEC  | CAA-C2A | 2.06  | 1.56        | 1.51     |
| 2   | C     | 1110 | HEC  | CMA-C3A | 2.06  | 1.55        | 1.50     |
| 2   | B     | 1102 | HEC  | CMC-C2C | 2.06  | 1.55        | 1.50     |
| 2   | C     | 1116 | HEC  | C3C-C2C | -2.06 | 1.34        | 1.41     |
| 2   | A     | 1102 | HEC  | CMC-C2C | 2.06  | 1.55        | 1.50     |
| 2   | B     | 1105 | HEC  | CMD-C2D | 2.05  | 1.55        | 1.50     |
| 2   | A     | 1109 | HEC  | CMB-C2B | 2.05  | 1.55        | 1.50     |
| 2   | C     | 1104 | HEC  | C3C-C2C | -2.05 | 1.34        | 1.41     |
| 2   | B     | 1115 | HEC  | C3B-C2B | -2.05 | 1.34        | 1.41     |
| 2   | D     | 1106 | HEC  | CMD-C2D | 2.05  | 1.55        | 1.50     |
| 2   | C     | 1105 | HEC  | CMC-C2C | 2.05  | 1.55        | 1.50     |
| 2   | C     | 1102 | HEC  | CMD-C2D | 2.05  | 1.55        | 1.50     |
| 2   | C     | 1114 | HEC  | C3C-C2C | -2.05 | 1.34        | 1.41     |
| 2   | C     | 1108 | HEC  | C3C-C2C | -2.05 | 1.34        | 1.41     |
| 2   | A     | 1115 | HEC  | C3B-C2B | -2.05 | 1.34        | 1.41     |
| 2   | D     | 1107 | HEC  | CMB-C2B | 2.05  | 1.55        | 1.50     |
| 2   | C     | 1114 | HEC  | CMA-C3A | 2.04  | 1.55        | 1.50     |
| 2   | D     | 1105 | HEC  | CMD-C2D | 2.04  | 1.55        | 1.50     |
| 2   | C     | 1102 | HEC  | CMC-C2C | 2.04  | 1.54        | 1.50     |
| 2   | B     | 1109 | HEC  | C3B-C2B | -2.04 | 1.34        | 1.41     |
| 2   | C     | 1105 | HEC  | CMA-C3A | 2.04  | 1.54        | 1.50     |
| 2   | C     | 1108 | HEC  | C3B-C2B | -2.03 | 1.34        | 1.41     |
| 2   | B     | 1101 | HEC  | O1A-CGA | 2.03  | 1.28        | 1.22     |
| 2   | A     | 1109 | HEC  | C3C-C2C | -2.03 | 1.34        | 1.41     |
| 2   | D     | 1105 | HEC  | CAD-C3D | 2.02  | 1.56        | 1.51     |
| 2   | A     | 1110 | HEC  | CMD-C2D | 2.02  | 1.54        | 1.50     |
| 2   | C     | 1113 | HEC  | CMA-C3A | 2.02  | 1.54        | 1.50     |
| 2   | D     | 1114 | HEC  | CMA-C3A | 2.02  | 1.54        | 1.50     |
| 2   | B     | 1111 | HEC  | CMC-C2C | 2.02  | 1.54        | 1.50     |
| 2   | B     | 1107 | HEC  | C3B-C2B | -2.02 | 1.34        | 1.41     |
| 2   | B     | 1115 | HEC  | CMA-C3A | 2.02  | 1.54        | 1.50     |
| 2   | D     | 1106 | HEC  | C3C-C2C | -2.02 | 1.34        | 1.41     |
| 2   | C     | 1111 | HEC  | CMD-C2D | 2.01  | 1.54        | 1.50     |
| 2   | C     | 1102 | HEC  | CMA-C3A | 2.01  | 1.54        | 1.50     |
| 2   | B     | 1109 | HEC  | CAA-C2A | 2.01  | 1.56        | 1.51     |
| 2   | B     | 1108 | HEC  | CAA-C2A | 2.01  | 1.56        | 1.51     |
| 2   | D     | 1102 | HEC  | C3B-C2B | -2.01 | 1.34        | 1.41     |
| 2   | B     | 1116 | HEC  | CMD-C2D | 2.01  | 1.54        | 1.50     |
| 2   | B     | 1102 | HEC  | O2D-CGD | -2.00 | 1.24        | 1.30     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | D     | 1104 | HEC  | CMC-C2C | 2.00  | 1.54        | 1.50     |
| 2   | D     | 1107 | HEC  | CMC-C2C | 2.00  | 1.54        | 1.50     |
| 2   | D     | 1110 | HEC  | CAD-C3D | 2.00  | 1.56        | 1.51     |
| 2   | D     | 1109 | HEC  | C3B-C2B | -2.00 | 1.34        | 1.41     |

All (352) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 1112 | HEC  | CBB-CAB-C3B | -6.94 | 113.56      | 127.43   |
| 2   | C     | 1114 | HEC  | CBB-CAB-C3B | -6.21 | 115.03      | 127.43   |
| 2   | B     | 1103 | HEC  | CBB-CAB-C3B | -6.05 | 115.34      | 127.43   |
| 2   | D     | 1114 | HEC  | CBB-CAB-C3B | -5.97 | 115.49      | 127.43   |
| 2   | B     | 1107 | HEC  | CBB-CAB-C3B | -5.76 | 115.93      | 127.43   |
| 2   | D     | 1102 | HEC  | CBB-CAB-C3B | -5.75 | 115.94      | 127.43   |
| 2   | C     | 1103 | HEC  | CBB-CAB-C3B | -5.74 | 115.96      | 127.43   |
| 2   | D     | 1113 | HEC  | CBB-CAB-C3B | -5.66 | 116.11      | 127.43   |
| 2   | A     | 1109 | HEC  | CBB-CAB-C3B | -5.47 | 116.51      | 127.43   |
| 2   | D     | 1116 | HEC  | CBB-CAB-C3B | -5.46 | 116.53      | 127.43   |
| 2   | D     | 1101 | HEC  | CBB-CAB-C3B | -5.44 | 116.56      | 127.43   |
| 2   | C     | 1112 | HEC  | CBB-CAB-C3B | -5.39 | 116.65      | 127.43   |
| 2   | D     | 1115 | HEC  | CBB-CAB-C3B | -5.25 | 116.95      | 127.43   |
| 2   | C     | 1101 | HEC  | CBB-CAB-C3B | -5.10 | 117.25      | 127.43   |
| 2   | B     | 1105 | HEC  | CBB-CAB-C3B | -4.99 | 117.47      | 127.43   |
| 2   | D     | 1113 | HEC  | CBC-CAC-C3C | -4.96 | 117.52      | 127.43   |
| 2   | C     | 1107 | HEC  | CBB-CAB-C3B | -4.92 | 117.60      | 127.43   |
| 2   | C     | 1115 | HEC  | CBB-CAB-C3B | -4.92 | 117.61      | 127.43   |
| 2   | D     | 1107 | HEC  | CBB-CAB-C3B | -4.84 | 117.76      | 127.43   |
| 2   | D     | 1112 | HEC  | CBB-CAB-C3B | -4.81 | 117.81      | 127.43   |
| 2   | C     | 1110 | HEC  | CBB-CAB-C3B | -4.81 | 117.81      | 127.43   |
| 2   | A     | 1110 | HEC  | CBB-CAB-C3B | -4.78 | 117.89      | 127.43   |
| 2   | A     | 1113 | HEC  | CBB-CAB-C3B | -4.69 | 118.06      | 127.43   |
| 2   | C     | 1105 | HEC  | CBB-CAB-C3B | -4.69 | 118.06      | 127.43   |
| 2   | A     | 1103 | HEC  | CBD-CAD-C3D | -4.69 | 99.57       | 112.53   |
| 2   | A     | 1115 | HEC  | CBB-CAB-C3B | -4.69 | 118.07      | 127.43   |
| 2   | B     | 1116 | HEC  | CBB-CAB-C3B | -4.66 | 118.11      | 127.43   |
| 2   | C     | 1109 | HEC  | CBB-CAB-C3B | -4.65 | 118.14      | 127.43   |
| 2   | A     | 1112 | HEC  | CBB-CAB-C3B | -4.63 | 118.18      | 127.43   |
| 2   | B     | 1114 | HEC  | CBB-CAB-C3B | -4.61 | 118.22      | 127.43   |
| 2   | A     | 1104 | HEC  | CBC-CAC-C3C | -4.61 | 118.22      | 127.43   |
| 2   | D     | 1110 | HEC  | CBB-CAB-C3B | -4.59 | 118.25      | 127.43   |
| 2   | A     | 1111 | HEC  | CBB-CAB-C3B | -4.56 | 118.33      | 127.43   |
| 2   | B     | 1102 | HEC  | CBB-CAB-C3B | -4.48 | 118.47      | 127.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1116 | HEC  | CBC-CAC-C3C | -4.47 | 118.50      | 127.43   |
| 2   | A     | 1109 | HEC  | CBC-CAC-C3C | -4.44 | 118.55      | 127.43   |
| 2   | B     | 1112 | HEC  | CBC-CAC-C3C | -4.39 | 118.66      | 127.43   |
| 2   | D     | 1111 | HEC  | CBC-CAC-C3C | -4.39 | 118.66      | 127.43   |
| 2   | B     | 1113 | HEC  | CBB-CAB-C3B | -4.36 | 118.71      | 127.43   |
| 2   | C     | 1106 | HEC  | CBC-CAC-C3C | -4.35 | 118.74      | 127.43   |
| 2   | D     | 1112 | HEC  | CBC-CAC-C3C | -4.33 | 118.78      | 127.43   |
| 2   | A     | 1107 | HEC  | CBB-CAB-C3B | -4.33 | 118.78      | 127.43   |
| 2   | C     | 1111 | HEC  | CBC-CAC-C3C | -4.32 | 118.80      | 127.43   |
| 2   | B     | 1113 | HEC  | CBC-CAC-C3C | -4.31 | 118.82      | 127.43   |
| 2   | D     | 1114 | HEC  | CBC-CAC-C3C | -4.26 | 118.92      | 127.43   |
| 2   | A     | 1102 | HEC  | CBB-CAB-C3B | -4.24 | 118.96      | 127.43   |
| 2   | A     | 1111 | HEC  | CBC-CAC-C3C | -4.23 | 118.97      | 127.43   |
| 2   | A     | 1103 | HEC  | CBB-CAB-C3B | -4.23 | 118.99      | 127.43   |
| 2   | A     | 1116 | HEC  | CBC-CAC-C3C | -4.22 | 119.01      | 127.43   |
| 2   | C     | 1103 | HEC  | CBD-CAD-C3D | -4.21 | 100.89      | 112.53   |
| 2   | B     | 1107 | HEC  | CBC-CAC-C3C | -4.15 | 119.15      | 127.43   |
| 2   | C     | 1113 | HEC  | CBB-CAB-C3B | -4.15 | 119.15      | 127.43   |
| 2   | B     | 1101 | HEC  | CBB-CAB-C3B | -4.14 | 119.15      | 127.43   |
| 2   | A     | 1114 | HEC  | CBB-CAB-C3B | -4.12 | 119.19      | 127.43   |
| 2   | B     | 1101 | HEC  | C4D-ND-C1D  | 4.10  | 112.50      | 105.82   |
| 2   | D     | 1103 | HEC  | CBB-CAB-C3B | -4.08 | 119.27      | 127.43   |
| 2   | C     | 1113 | HEC  | CBC-CAC-C3C | -4.02 | 119.41      | 127.43   |
| 2   | B     | 1115 | HEC  | CBB-CAB-C3B | -4.01 | 119.41      | 127.43   |
| 2   | B     | 1110 | HEC  | CBB-CAB-C3B | -4.00 | 119.44      | 127.43   |
| 2   | A     | 1104 | HEC  | CBB-CAB-C3B | -3.97 | 119.50      | 127.43   |
| 2   | B     | 1108 | HEC  | CBC-CAC-C3C | -3.96 | 119.52      | 127.43   |
| 2   | C     | 1116 | HEC  | CBB-CAB-C3B | -3.94 | 119.56      | 127.43   |
| 2   | D     | 1109 | HEC  | CBB-CAB-C3B | -3.92 | 119.61      | 127.43   |
| 2   | A     | 1114 | HEC  | C4D-ND-C1D  | 3.91  | 112.19      | 105.82   |
| 2   | D     | 1108 | HEC  | C4D-ND-C1D  | 3.88  | 112.14      | 105.82   |
| 2   | B     | 1109 | HEC  | CBB-CAB-C3B | -3.85 | 119.73      | 127.43   |
| 2   | C     | 1111 | HEC  | CBB-CAB-C3B | -3.84 | 119.75      | 127.43   |
| 2   | A     | 1102 | HEC  | C4D-ND-C1D  | 3.81  | 112.03      | 105.82   |
| 2   | B     | 1113 | HEC  | CBD-CAD-C3D | -3.78 | 102.07      | 112.53   |
| 2   | A     | 1116 | HEC  | CBD-CAD-C3D | -3.78 | 102.07      | 112.53   |
| 2   | C     | 1101 | HEC  | CBC-CAC-C3C | -3.74 | 119.95      | 127.43   |
| 2   | A     | 1110 | HEC  | CBC-CAC-C3C | -3.71 | 120.03      | 127.43   |
| 2   | D     | 1114 | HEC  | C4D-ND-C1D  | 3.67  | 111.80      | 105.82   |
| 2   | C     | 1116 | HEC  | CBD-CAD-C3D | -3.66 | 102.40      | 112.53   |
| 2   | A     | 1101 | HEC  | CBB-CAB-C3B | -3.65 | 120.13      | 127.43   |
| 2   | C     | 1102 | HEC  | CBB-CAB-C3B | -3.63 | 120.18      | 127.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1115 | HEC  | C4D-ND-C1D  | 3.62  | 111.73      | 105.82   |
| 2   | A     | 1107 | HEC  | CAA-C2A-C3A | 3.58  | 134.57      | 127.87   |
| 2   | B     | 1111 | HEC  | C4D-ND-C1D  | 3.57  | 111.64      | 105.82   |
| 2   | B     | 1111 | HEC  | CBB-CAB-C3B | -3.53 | 120.38      | 127.43   |
| 2   | C     | 1114 | HEC  | CBC-CAC-C3C | -3.53 | 120.38      | 127.43   |
| 2   | B     | 1113 | HEC  | C4D-ND-C1D  | 3.50  | 111.53      | 105.82   |
| 2   | B     | 1104 | HEC  | CAD-CBD-CGD | -3.50 | 104.37      | 113.67   |
| 2   | A     | 1101 | HEC  | C4D-ND-C1D  | 3.50  | 111.52      | 105.82   |
| 2   | C     | 1110 | HEC  | C4D-ND-C1D  | 3.50  | 111.52      | 105.82   |
| 2   | A     | 1102 | HEC  | CBC-CAC-C3C | -3.48 | 120.47      | 127.43   |
| 2   | A     | 1113 | HEC  | C4D-ND-C1D  | 3.48  | 111.50      | 105.82   |
| 2   | D     | 1103 | HEC  | CBC-CAC-C3C | -3.47 | 120.51      | 127.43   |
| 2   | C     | 1113 | HEC  | C2A-C1A-NA  | -3.45 | 106.99      | 110.32   |
| 2   | A     | 1106 | HEC  | CBB-CAB-C3B | -3.45 | 120.55      | 127.43   |
| 2   | B     | 1108 | HEC  | C4D-ND-C1D  | 3.41  | 111.38      | 105.82   |
| 2   | A     | 1107 | HEC  | CBA-CAA-C2A | 3.40  | 121.94      | 112.53   |
| 2   | B     | 1102 | HEC  | C4D-ND-C1D  | 3.38  | 111.33      | 105.82   |
| 2   | C     | 1102 | HEC  | C4D-ND-C1D  | 3.37  | 111.32      | 105.82   |
| 2   | C     | 1115 | HEC  | C2A-C1A-NA  | -3.37 | 107.08      | 110.32   |
| 2   | D     | 1107 | HEC  | C4D-ND-C1D  | 3.36  | 111.30      | 105.82   |
| 2   | C     | 1106 | HEC  | CBB-CAB-C3B | -3.33 | 120.78      | 127.43   |
| 2   | C     | 1107 | HEC  | CBC-CAC-C3C | -3.32 | 120.80      | 127.43   |
| 2   | A     | 1112 | HEC  | C4D-ND-C1D  | 3.31  | 111.22      | 105.82   |
| 2   | A     | 1106 | HEC  | C4D-ND-C1D  | 3.31  | 111.22      | 105.82   |
| 2   | A     | 1106 | HEC  | CBC-CAC-C3C | -3.30 | 120.83      | 127.43   |
| 2   | D     | 1111 | HEC  | CBB-CAB-C3B | -3.30 | 120.84      | 127.43   |
| 2   | C     | 1114 | HEC  | C4D-ND-C1D  | 3.30  | 111.19      | 105.82   |
| 2   | B     | 1107 | HEC  | CAD-CBD-CGD | -3.28 | 104.97      | 113.67   |
| 2   | C     | 1109 | HEC  | CBC-CAC-C3C | -3.27 | 120.89      | 127.43   |
| 2   | D     | 1101 | HEC  | C4D-ND-C1D  | 3.25  | 111.12      | 105.82   |
| 2   | A     | 1105 | HEC  | CBB-CAB-C3B | -3.25 | 120.94      | 127.43   |
| 2   | D     | 1112 | HEC  | C4D-ND-C1D  | 3.24  | 111.11      | 105.82   |
| 2   | B     | 1114 | HEC  | C4D-ND-C1D  | 3.24  | 111.10      | 105.82   |
| 2   | D     | 1104 | HEC  | CBB-CAB-C3B | -3.22 | 120.99      | 127.43   |
| 2   | A     | 1111 | HEC  | C4D-ND-C1D  | 3.22  | 111.07      | 105.82   |
| 2   | D     | 1105 | HEC  | C4D-ND-C1D  | 3.21  | 111.06      | 105.82   |
| 2   | A     | 1114 | HEC  | C2A-C1A-NA  | -3.21 | 107.23      | 110.32   |
| 2   | D     | 1108 | HEC  | CBB-CAB-C3B | -3.20 | 121.04      | 127.43   |
| 2   | C     | 1108 | HEC  | CBB-CAB-C3B | -3.19 | 121.05      | 127.43   |
| 2   | B     | 1104 | HEC  | C4D-ND-C1D  | 3.19  | 111.02      | 105.82   |
| 2   | B     | 1116 | HEC  | CBC-CAC-C3C | -3.19 | 121.06      | 127.43   |
| 2   | B     | 1111 | HEC  | CBC-CAC-C3C | -3.17 | 121.10      | 127.43   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | A     | 1115 | HEC  | C4D-ND-C1D  | 3.17  | 110.98      | 105.82   |
| 2   | D     | 1106 | HEC  | C4D-ND-C1D  | 3.17  | 110.98      | 105.82   |
| 2   | D     | 1110 | HEC  | C4D-ND-C1D  | 3.16  | 110.98      | 105.82   |
| 2   | D     | 1116 | HEC  | CBD-CAD-C3D | -3.16 | 103.79      | 112.53   |
| 2   | C     | 1116 | HEC  | CBC-CAC-C3C | -3.15 | 121.14      | 127.43   |
| 2   | B     | 1106 | HEC  | C4D-ND-C1D  | 3.14  | 110.94      | 105.82   |
| 2   | B     | 1103 | HEC  | CBD-CAD-C3D | -3.11 | 103.92      | 112.53   |
| 2   | A     | 1110 | HEC  | C4D-ND-C1D  | 3.11  | 110.90      | 105.82   |
| 2   | A     | 1116 | HEC  | CBB-CAB-C3B | -3.11 | 121.23      | 127.43   |
| 2   | A     | 1113 | HEC  | CBC-CAC-C3C | -3.10 | 121.23      | 127.43   |
| 2   | D     | 1111 | HEC  | C4D-ND-C1D  | 3.09  | 110.86      | 105.82   |
| 2   | A     | 1108 | HEC  | CBC-CAC-C3C | -3.07 | 121.30      | 127.43   |
| 2   | A     | 1107 | HEC  | CAA-C2A-C1A | -3.06 | 118.64      | 124.85   |
| 2   | A     | 1108 | HEC  | C4D-ND-C1D  | 3.05  | 110.79      | 105.82   |
| 2   | C     | 1101 | HEC  | CHC-C4B-NB  | 3.05  | 127.77      | 124.45   |
| 2   | C     | 1104 | HEC  | CBC-CAC-C3C | -3.03 | 121.38      | 127.43   |
| 2   | C     | 1107 | HEC  | C4D-ND-C1D  | 3.03  | 110.75      | 105.82   |
| 2   | A     | 1104 | HEC  | CBA-CAA-C2A | -3.02 | 104.18      | 112.53   |
| 2   | D     | 1103 | HEC  | CBD-CAD-C3D | -3.02 | 104.18      | 112.53   |
| 2   | C     | 1102 | HEC  | CBC-CAC-C3C | -3.01 | 121.42      | 127.43   |
| 2   | C     | 1105 | HEC  | C4D-ND-C1D  | 3.00  | 110.71      | 105.82   |
| 2   | C     | 1106 | HEC  | C4D-ND-C1D  | 2.99  | 110.70      | 105.82   |
| 2   | B     | 1110 | HEC  | C4D-ND-C1D  | 2.99  | 110.69      | 105.82   |
| 2   | B     | 1105 | HEC  | C4D-ND-C1D  | 2.98  | 110.68      | 105.82   |
| 2   | C     | 1108 | HEC  | C4D-ND-C1D  | 2.98  | 110.67      | 105.82   |
| 2   | A     | 1112 | HEC  | CBC-CAC-C3C | -2.97 | 121.49      | 127.43   |
| 2   | D     | 1103 | HEC  | C4D-ND-C1D  | 2.96  | 110.65      | 105.82   |
| 2   | C     | 1113 | HEC  | C4D-ND-C1D  | 2.92  | 110.58      | 105.82   |
| 2   | D     | 1105 | HEC  | CAA-CBA-CGA | -2.91 | 105.94      | 113.67   |
| 2   | D     | 1102 | HEC  | C4D-ND-C1D  | 2.90  | 110.55      | 105.82   |
| 2   | B     | 1106 | HEC  | CMD-C2D-C1D | 2.90  | 129.83      | 125.42   |
| 2   | C     | 1112 | HEC  | CBC-CAC-C3C | -2.88 | 121.68      | 127.43   |
| 2   | D     | 1111 | HEC  | CMD-C2D-C1D | 2.86  | 129.78      | 125.42   |
| 2   | A     | 1107 | HEC  | CHC-C4B-NB  | 2.86  | 127.56      | 124.45   |
| 2   | B     | 1114 | HEC  | CBC-CAC-C3C | -2.83 | 121.78      | 127.43   |
| 2   | C     | 1113 | HEC  | CBA-CAA-C2A | -2.83 | 104.71      | 112.53   |
| 2   | B     | 1109 | HEC  | C4D-ND-C1D  | 2.83  | 110.43      | 105.82   |
| 2   | D     | 1108 | HEC  | C3D-C4D-ND  | -2.81 | 107.03      | 110.15   |
| 2   | B     | 1107 | HEC  | CHA-C1A-NA  | 2.80  | 127.50      | 124.45   |
| 2   | C     | 1104 | HEC  | CAD-C3D-C4D | 2.80  | 130.40      | 124.94   |
| 2   | D     | 1108 | HEC  | C2A-C1A-NA  | -2.79 | 107.63      | 110.32   |
| 2   | B     | 1106 | HEC  | CAD-CBD-CGD | -2.78 | 106.28      | 113.67   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1109 | HEC  | CBC-CAC-C3C | -2.78 | 121.88      | 127.43   |
| 2   | A     | 1109 | HEC  | CHD-C4C-NC  | 2.77  | 127.47      | 124.45   |
| 2   | D     | 1104 | HEC  | C4D-ND-C1D  | 2.77  | 110.33      | 105.82   |
| 2   | B     | 1113 | HEC  | CHC-C4B-NB  | 2.76  | 127.45      | 124.45   |
| 2   | B     | 1109 | HEC  | CBC-CAC-C3C | -2.75 | 121.93      | 127.43   |
| 2   | C     | 1111 | HEC  | C4D-ND-C1D  | 2.75  | 110.31      | 105.82   |
| 2   | D     | 1109 | HEC  | C4D-ND-C1D  | 2.75  | 110.31      | 105.82   |
| 2   | D     | 1104 | HEC  | CBA-CAA-C2A | -2.75 | 104.93      | 112.53   |
| 2   | D     | 1110 | HEC  | C2A-C1A-NA  | -2.75 | 107.67      | 110.32   |
| 2   | C     | 1108 | HEC  | CBC-CAC-C3C | -2.74 | 121.96      | 127.43   |
| 2   | B     | 1102 | HEC  | CBC-CAC-C3C | -2.74 | 121.96      | 127.43   |
| 2   | C     | 1112 | HEC  | C4D-ND-C1D  | 2.74  | 110.28      | 105.82   |
| 2   | B     | 1115 | HEC  | C4D-ND-C1D  | 2.74  | 110.28      | 105.82   |
| 2   | C     | 1104 | HEC  | CAD-CBD-CGD | -2.73 | 106.41      | 113.67   |
| 2   | B     | 1106 | HEC  | CBC-CAC-C3C | -2.73 | 121.97      | 127.43   |
| 2   | A     | 1108 | HEC  | C2A-C1A-NA  | -2.73 | 107.69      | 110.32   |
| 2   | C     | 1104 | HEC  | CBA-CAA-C2A | -2.72 | 105.02      | 112.53   |
| 2   | D     | 1102 | HEC  | CBC-CAC-C3C | -2.72 | 122.00      | 127.43   |
| 2   | A     | 1106 | HEC  | CHB-C4A-NA  | 2.70  | 127.40      | 124.45   |
| 2   | C     | 1101 | HEC  | C4D-ND-C1D  | 2.70  | 110.23      | 105.82   |
| 2   | C     | 1103 | HEC  | C4D-ND-C1D  | 2.69  | 110.21      | 105.82   |
| 2   | C     | 1109 | HEC  | CBA-CAA-C2A | -2.69 | 105.10      | 112.53   |
| 2   | A     | 1107 | HEC  | C4D-ND-C1D  | 2.66  | 110.17      | 105.82   |
| 2   | A     | 1115 | HEC  | CMD-C2D-C1D | 2.66  | 129.47      | 125.42   |
| 2   | A     | 1107 | HEC  | CMB-C2B-C1B | -2.63 | 121.41      | 125.42   |
| 2   | A     | 1104 | HEC  | CHA-C1A-NA  | 2.63  | 127.32      | 124.45   |
| 2   | A     | 1115 | HEC  | CBD-CAD-C3D | -2.63 | 105.26      | 112.53   |
| 2   | D     | 1114 | HEC  | C2A-C1A-NA  | -2.63 | 107.79      | 110.32   |
| 2   | A     | 1109 | HEC  | C4D-ND-C1D  | 2.62  | 110.10      | 105.82   |
| 2   | B     | 1112 | HEC  | C4D-ND-C1D  | 2.62  | 110.09      | 105.82   |
| 2   | D     | 1113 | HEC  | C4D-ND-C1D  | 2.61  | 110.08      | 105.82   |
| 2   | A     | 1104 | HEC  | CAD-C3D-C4D | 2.60  | 130.03      | 124.94   |
| 2   | A     | 1108 | HEC  | CBB-CAB-C3B | -2.59 | 122.25      | 127.43   |
| 2   | A     | 1105 | HEC  | CBC-CAC-C3C | -2.58 | 122.29      | 127.43   |
| 2   | C     | 1106 | HEC  | CMD-C2D-C1D | 2.58  | 129.34      | 125.42   |
| 2   | C     | 1112 | HEC  | CHC-C4B-NB  | 2.57  | 127.26      | 124.45   |
| 2   | B     | 1104 | HEC  | CMD-C2D-C1D | 2.56  | 129.31      | 125.42   |
| 2   | A     | 1104 | HEC  | C4D-ND-C1D  | 2.55  | 109.99      | 105.82   |
| 2   | A     | 1103 | HEC  | C4D-ND-C1D  | 2.55  | 109.97      | 105.82   |
| 2   | C     | 1116 | HEC  | C4D-ND-C1D  | 2.53  | 109.94      | 105.82   |
| 2   | B     | 1116 | HEC  | C4D-ND-C1D  | 2.53  | 109.94      | 105.82   |
| 2   | C     | 1104 | HEC  | O1A-CGA-CBA | -2.51 | 115.12      | 123.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 1103 | HEC  | C4D-ND-C1D  | 2.51  | 109.91      | 105.82   |
| 2   | B     | 1112 | HEC  | CMD-C2D-C1D | 2.50  | 129.23      | 125.42   |
| 2   | D     | 1107 | HEC  | CBC-CAC-C3C | -2.50 | 122.43      | 127.43   |
| 2   | B     | 1103 | HEC  | CBC-CAC-C3C | -2.49 | 122.46      | 127.43   |
| 2   | C     | 1115 | HEC  | CAA-CBA-CGA | -2.48 | 107.08      | 113.67   |
| 2   | B     | 1110 | HEC  | CBD-CAD-C3D | -2.48 | 105.68      | 112.53   |
| 2   | D     | 1113 | HEC  | CHC-C4B-NB  | 2.47  | 127.14      | 124.45   |
| 2   | D     | 1106 | HEC  | CBB-CAB-C3B | -2.47 | 122.50      | 127.43   |
| 2   | B     | 1104 | HEC  | CBC-CAC-C3C | -2.47 | 122.50      | 127.43   |
| 2   | D     | 1116 | HEC  | C4D-ND-C1D  | 2.46  | 109.84      | 105.82   |
| 2   | A     | 1116 | HEC  | O1D-CGD-CBD | -2.46 | 115.28      | 123.09   |
| 2   | D     | 1116 | HEC  | C1D-C2D-C3D | -2.46 | 104.00      | 106.82   |
| 2   | A     | 1104 | HEC  | CHB-C4A-NA  | 2.45  | 127.13      | 124.45   |
| 2   | B     | 1102 | HEC  | CBA-CAA-C2A | -2.44 | 105.78      | 112.53   |
| 2   | B     | 1116 | HEC  | CBD-CAD-C3D | -2.44 | 105.79      | 112.53   |
| 2   | B     | 1116 | HEC  | C1D-C2D-C3D | -2.44 | 104.02      | 106.82   |
| 2   | A     | 1108 | HEC  | CBD-CAD-C3D | -2.44 | 105.79      | 112.53   |
| 2   | C     | 1107 | HEC  | C2A-C1A-NA  | -2.43 | 107.98      | 110.32   |
| 2   | C     | 1104 | HEC  | C4D-ND-C1D  | 2.43  | 109.78      | 105.82   |
| 2   | A     | 1108 | HEC  | O1D-CGD-CBD | -2.42 | 115.41      | 123.09   |
| 2   | B     | 1104 | HEC  | CAD-C3D-C4D | 2.42  | 129.66      | 124.94   |
| 2   | A     | 1103 | HEC  | CBC-CAC-C3C | -2.41 | 122.61      | 127.43   |
| 2   | C     | 1113 | HEC  | CAA-C2A-C3A | -2.41 | 123.35      | 127.87   |
| 2   | D     | 1102 | HEC  | CBA-CAA-C2A | -2.40 | 105.89      | 112.53   |
| 2   | A     | 1102 | HEC  | CHA-C4D-ND  | 2.40  | 128.22      | 123.86   |
| 2   | C     | 1110 | HEC  | CHD-C1D-ND  | 2.39  | 128.19      | 123.86   |
| 2   | A     | 1103 | HEC  | CAD-C3D-C4D | 2.38  | 129.59      | 124.94   |
| 2   | D     | 1102 | HEC  | CMD-C2D-C1D | 2.38  | 129.04      | 125.42   |
| 2   | D     | 1115 | HEC  | C4D-ND-C1D  | 2.38  | 109.70      | 105.82   |
| 2   | D     | 1108 | HEC  | CAD-CBD-CGD | -2.37 | 107.38      | 113.67   |
| 2   | D     | 1103 | HEC  | O1A-CGA-CBA | -2.37 | 115.58      | 123.09   |
| 2   | B     | 1107 | HEC  | C4D-ND-C1D  | 2.37  | 109.68      | 105.82   |
| 2   | A     | 1109 | HEC  | O1A-CGA-CBA | -2.37 | 115.59      | 123.09   |
| 2   | A     | 1116 | HEC  | C4D-ND-C1D  | 2.36  | 109.67      | 105.82   |
| 2   | C     | 1109 | HEC  | C4D-ND-C1D  | 2.36  | 109.66      | 105.82   |
| 2   | A     | 1107 | HEC  | CHB-C1B-NB  | 2.34  | 128.11      | 123.86   |
| 2   | C     | 1101 | HEC  | CAD-C3D-C4D | 2.34  | 129.51      | 124.94   |
| 2   | C     | 1115 | HEC  | C3D-C4D-ND  | -2.34 | 107.56      | 110.15   |
| 2   | C     | 1110 | HEC  | CHC-C4B-NB  | 2.34  | 127.00      | 124.45   |
| 2   | D     | 1109 | HEC  | O2D-CGD-CBD | 2.33  | 121.36      | 114.00   |
| 2   | D     | 1105 | HEC  | CBB-CAB-C3B | -2.32 | 122.79      | 127.43   |
| 2   | A     | 1103 | HEC  | O1A-CGA-CBA | -2.31 | 115.75      | 123.09   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 1107 | HEC  | CHC-C4B-NB  | 2.31  | 126.97      | 124.45   |
| 2   | C     | 1111 | HEC  | CAA-CBA-CGA | -2.30 | 107.56      | 113.67   |
| 2   | D     | 1112 | HEC  | CMD-C2D-C1D | 2.29  | 128.91      | 125.42   |
| 2   | A     | 1105 | HEC  | C4D-ND-C1D  | 2.28  | 109.55      | 105.82   |
| 2   | B     | 1112 | HEC  | CHB-C4A-NA  | 2.27  | 126.93      | 124.45   |
| 2   | D     | 1109 | HEC  | O1D-CGD-CBD | -2.27 | 115.91      | 123.09   |
| 2   | C     | 1101 | HEC  | C4D-C3D-C2D | -2.26 | 103.36      | 106.87   |
| 2   | A     | 1109 | HEC  | CAA-CBA-CGA | -2.26 | 107.67      | 113.67   |
| 2   | A     | 1106 | HEC  | C2A-C1A-NA  | -2.26 | 108.14      | 110.32   |
| 2   | B     | 1113 | HEC  | CHD-C1D-ND  | 2.26  | 127.96      | 123.86   |
| 2   | B     | 1106 | HEC  | CBD-CAD-C3D | -2.25 | 106.30      | 112.53   |
| 2   | C     | 1106 | HEC  | CBD-CAD-C3D | -2.25 | 106.32      | 112.53   |
| 2   | C     | 1116 | HEC  | O1D-CGD-CBD | -2.25 | 115.97      | 123.09   |
| 2   | A     | 1111 | HEC  | CBA-CAA-C2A | 2.24  | 118.73      | 112.53   |
| 2   | C     | 1105 | HEC  | CBC-CAC-C3C | -2.24 | 122.96      | 127.43   |
| 2   | B     | 1112 | HEC  | CHC-C1C-NC  | 2.23  | 127.91      | 123.86   |
| 2   | C     | 1103 | HEC  | CHB-C1B-NB  | 2.23  | 127.91      | 123.86   |
| 2   | B     | 1108 | HEC  | O2D-CGD-CBD | 2.23  | 121.05      | 114.00   |
| 2   | B     | 1115 | HEC  | CAA-CBA-CGA | -2.23 | 107.76      | 113.67   |
| 2   | D     | 1101 | HEC  | CAD-C3D-C4D | 2.22  | 129.28      | 124.94   |
| 2   | B     | 1113 | HEC  | CHA-C1A-C2A | 2.22  | 128.37      | 124.86   |
| 2   | B     | 1110 | HEC  | CBC-CAC-C3C | -2.22 | 123.00      | 127.43   |
| 2   | C     | 1102 | HEC  | CAA-CBA-CGA | -2.22 | 107.78      | 113.67   |
| 2   | D     | 1115 | HEC  | CBC-CAC-C3C | -2.22 | 123.00      | 127.43   |
| 2   | C     | 1110 | HEC  | CAD-CBD-CGD | -2.22 | 107.79      | 113.67   |
| 2   | C     | 1110 | HEC  | O1D-CGD-CBD | -2.21 | 116.08      | 123.09   |
| 2   | B     | 1105 | HEC  | CMD-C2D-C1D | 2.21  | 128.78      | 125.42   |
| 2   | C     | 1102 | HEC  | CBA-CAA-C2A | -2.21 | 106.42      | 112.53   |
| 2   | C     | 1115 | HEC  | C2C-C1C-NC  | -2.21 | 106.61      | 110.14   |
| 2   | D     | 1104 | HEC  | CHD-C4C-NC  | 2.21  | 126.85      | 124.45   |
| 2   | C     | 1108 | HEC  | CAA-CBA-CGA | -2.20 | 107.83      | 113.67   |
| 2   | B     | 1116 | HEC  | CHD-C4C-NC  | 2.20  | 126.85      | 124.45   |
| 2   | C     | 1107 | HEC  | CHC-C4B-C3B | 2.18  | 128.89      | 125.21   |
| 2   | B     | 1104 | HEC  | O2A-CGA-CBA | 2.18  | 120.88      | 114.00   |
| 2   | A     | 1115 | HEC  | O1D-CGD-CBD | -2.18 | 116.19      | 123.09   |
| 2   | A     | 1113 | HEC  | CBA-CAA-C2A | -2.17 | 106.53      | 112.53   |
| 2   | B     | 1110 | HEC  | O1D-CGD-CBD | -2.17 | 116.21      | 123.09   |
| 2   | A     | 1105 | HEC  | O2D-CGD-CBD | 2.16  | 120.84      | 114.00   |
| 2   | A     | 1116 | HEC  | CHC-C4B-NB  | 2.16  | 126.81      | 124.45   |
| 2   | C     | 1110 | HEC  | O2A-CGA-CBA | 2.16  | 120.83      | 114.00   |
| 2   | B     | 1108 | HEC  | CHA-C4D-ND  | 2.16  | 127.78      | 123.86   |
| 2   | D     | 1103 | HEC  | O2A-CGA-CBA | 2.16  | 120.82      | 114.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | D     | 1102 | HEC  | O2A-CGA-CBA | 2.15  | 120.80      | 114.00   |
| 2   | A     | 1113 | HEC  | O1A-CGA-CBA | -2.15 | 116.27      | 123.09   |
| 2   | B     | 1111 | HEC  | CMD-C2D-C1D | 2.15  | 128.69      | 125.42   |
| 2   | D     | 1115 | HEC  | CHC-C4B-NB  | 2.15  | 126.79      | 124.45   |
| 2   | B     | 1111 | HEC  | O2D-CGD-CBD | 2.14  | 120.76      | 114.00   |
| 2   | B     | 1116 | HEC  | CHC-C1C-NC  | 2.14  | 127.73      | 123.86   |
| 2   | C     | 1107 | HEC  | CAA-CBA-CGA | -2.12 | 108.03      | 113.67   |
| 2   | D     | 1108 | HEC  | CBD-CAD-C3D | -2.12 | 106.66      | 112.53   |
| 2   | D     | 1108 | HEC  | C1D-C2D-C3D | -2.12 | 104.39      | 106.82   |
| 2   | B     | 1113 | HEC  | C1D-C2D-C3D | -2.12 | 104.39      | 106.82   |
| 2   | B     | 1116 | HEC  | CMD-C2D-C1D | 2.12  | 128.64      | 125.42   |
| 2   | C     | 1114 | HEC  | CBA-CAA-C2A | -2.11 | 106.70      | 112.53   |
| 2   | D     | 1105 | HEC  | CBC-CAC-C3C | -2.11 | 123.22      | 127.43   |
| 2   | B     | 1110 | HEC  | CAA-C2A-C3A | -2.11 | 123.92      | 127.87   |
| 2   | B     | 1111 | HEC  | CAD-CBD-CGD | -2.11 | 108.08      | 113.67   |
| 2   | D     | 1104 | HEC  | CHB-C4A-NA  | 2.10  | 126.74      | 124.45   |
| 2   | B     | 1115 | HEC  | CMD-C2D-C1D | 2.09  | 128.61      | 125.42   |
| 2   | D     | 1116 | HEC  | O2D-CGD-CBD | 2.09  | 120.60      | 114.00   |
| 2   | B     | 1115 | HEC  | C2A-C1A-NA  | -2.09 | 108.31      | 110.32   |
| 2   | B     | 1107 | HEC  | O1D-CGD-CBD | -2.08 | 116.49      | 123.09   |
| 2   | D     | 1103 | HEC  | CHA-C4D-ND  | 2.08  | 127.63      | 123.86   |
| 2   | A     | 1114 | HEC  | CHA-C1A-C2A | 2.08  | 128.15      | 124.86   |
| 2   | D     | 1114 | HEC  | CBA-CAA-C2A | -2.08 | 106.78      | 112.53   |
| 2   | C     | 1105 | HEC  | CAD-C3D-C4D | 2.08  | 129.00      | 124.94   |
| 2   | D     | 1115 | HEC  | C1D-C2D-C3D | -2.08 | 104.44      | 106.82   |
| 2   | B     | 1101 | HEC  | CHA-C4D-ND  | 2.07  | 127.62      | 123.86   |
| 2   | C     | 1112 | HEC  | CMD-C2D-C1D | 2.07  | 128.57      | 125.42   |
| 2   | D     | 1116 | HEC  | O1D-CGD-CBD | -2.07 | 116.53      | 123.09   |
| 2   | B     | 1113 | HEC  | CHA-C4D-ND  | 2.07  | 127.61      | 123.86   |
| 2   | D     | 1111 | HEC  | C2A-C1A-NA  | -2.06 | 108.33      | 110.32   |
| 2   | C     | 1106 | HEC  | C1D-C2D-C3D | -2.06 | 104.46      | 106.82   |
| 2   | D     | 1104 | HEC  | C1D-C2D-C3D | -2.06 | 104.46      | 106.82   |
| 2   | B     | 1102 | HEC  | CHC-C4B-NB  | 2.06  | 126.69      | 124.45   |
| 2   | C     | 1113 | HEC  | CHA-C1A-C2A | 2.06  | 128.11      | 124.86   |
| 2   | A     | 1114 | HEC  | CHA-C4D-ND  | 2.05  | 127.58      | 123.86   |
| 2   | A     | 1111 | HEC  | O2D-CGD-CBD | 2.05  | 120.48      | 114.00   |
| 2   | C     | 1113 | HEC  | CMC-C2C-C1C | 2.05  | 128.54      | 125.42   |
| 2   | A     | 1112 | HEC  | CBD-CAD-C3D | -2.05 | 106.87      | 112.53   |
| 2   | D     | 1116 | HEC  | CMD-C2D-C1D | 2.05  | 128.54      | 125.42   |
| 2   | B     | 1115 | HEC  | CBC-CAC-C3C | -2.05 | 123.34      | 127.43   |
| 2   | C     | 1115 | HEC  | O1D-CGD-CBD | -2.04 | 116.62      | 123.09   |
| 2   | A     | 1115 | HEC  | CBA-CAA-C2A | -2.04 | 106.89      | 112.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | C     | 1105 | HEC  | CHD-C1D-ND  | 2.04  | 127.55      | 123.86   |
| 2   | D     | 1107 | HEC  | O2D-CGD-CBD | 2.03  | 120.43      | 114.00   |
| 2   | A     | 1107 | HEC  | O1D-CGD-CBD | -2.03 | 116.64      | 123.09   |
| 2   | D     | 1105 | HEC  | O1A-CGA-CBA | -2.03 | 116.65      | 123.09   |
| 2   | A     | 1116 | HEC  | O2D-CGD-CBD | 2.03  | 120.42      | 114.00   |
| 2   | C     | 1108 | HEC  | O1D-CGD-CBD | -2.03 | 116.66      | 123.09   |
| 2   | B     | 1110 | HEC  | C2A-C1A-NA  | -2.03 | 108.37      | 110.32   |
| 2   | A     | 1105 | HEC  | CHD-C4C-NC  | 2.03  | 126.66      | 124.45   |
| 2   | A     | 1101 | HEC  | CBC-CAC-C3C | -2.02 | 123.39      | 127.43   |
| 2   | B     | 1108 | HEC  | O1D-CGD-CBD | -2.02 | 116.68      | 123.09   |
| 2   | B     | 1110 | HEC  | CHA-C4D-ND  | 2.02  | 127.52      | 123.86   |
| 2   | C     | 1110 | HEC  | CHA-C4D-ND  | 2.02  | 127.52      | 123.86   |
| 2   | D     | 1108 | HEC  | CBC-CAC-C3C | -2.02 | 123.40      | 127.43   |
| 2   | D     | 1110 | HEC  | CBC-CAC-C3C | -2.02 | 123.40      | 127.43   |
| 2   | D     | 1115 | HEC  | CAD-C3D-C4D | 2.02  | 128.88      | 124.94   |
| 2   | B     | 1110 | HEC  | CHD-C1D-ND  | 2.01  | 127.51      | 123.86   |
| 2   | D     | 1108 | HEC  | CMD-C2D-C1D | 2.01  | 128.48      | 125.42   |
| 2   | B     | 1115 | HEC  | CAD-C3D-C4D | 2.01  | 128.86      | 124.94   |
| 2   | C     | 1107 | HEC  | C1D-C2D-C3D | -2.01 | 104.52      | 106.82   |
| 2   | C     | 1105 | HEC  | O1D-CGD-CBD | -2.01 | 116.73      | 123.09   |
| 2   | C     | 1113 | HEC  | CAA-CBA-CGA | -2.00 | 108.35      | 113.67   |
| 2   | A     | 1101 | HEC  | O2D-CGD-O1D | -2.00 | 118.18      | 123.33   |
| 2   | B     | 1106 | HEC  | CBB-CAB-C3B | -2.00 | 123.43      | 127.43   |
| 2   | D     | 1108 | HEC  | C4A-NA-C1A  | 2.00  | 109.08      | 105.82   |

There are no chirality outliers.

All (451) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1101 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1101 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1101 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1101 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1102 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1102 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1102 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1102 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1103 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1103 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1103 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1103 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1104 | HEC  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1104 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1104 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1104 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1105 | HEC  | C1A-C2A-CAA-CBA |
| 2   | A     | 1105 | HEC  | C3A-C2A-CAA-CBA |
| 2   | A     | 1105 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1105 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1106 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1106 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1106 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1106 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1107 | HEC  | C1A-C2A-CAA-CBA |
| 2   | A     | 1107 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1107 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1107 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1107 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1108 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1108 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1108 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1108 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1109 | HEC  | C1A-C2A-CAA-CBA |
| 2   | A     | 1109 | HEC  | C3A-C2A-CAA-CBA |
| 2   | A     | 1109 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1110 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1110 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1110 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1110 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1111 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1111 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1112 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1112 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1112 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1112 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1113 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1113 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1114 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1114 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1115 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1115 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1115 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1115 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1116 | HEC  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1116 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1116 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1116 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1101 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1101 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1102 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1102 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1102 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1102 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1103 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1103 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1103 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1104 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1104 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1104 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1104 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1105 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1105 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1105 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1105 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1106 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1106 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1106 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1106 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1107 | HEC  | C1A-C2A-CAA-CBA |
| 2   | B     | 1107 | HEC  | C3A-C2A-CAA-CBA |
| 2   | B     | 1107 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1107 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1108 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1108 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1108 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1108 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1109 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1109 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1109 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1109 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1110 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1110 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1110 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1110 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1111 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1111 | HEC  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | B     | 1111 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1111 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1112 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1112 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1113 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1113 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1113 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1114 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1114 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1114 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1115 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1115 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1115 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1115 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1116 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1116 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1116 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1101 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1101 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1101 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1101 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1102 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1102 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1103 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1103 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1103 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1103 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1104 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1104 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1105 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1105 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1105 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1106 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1106 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1106 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1106 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1107 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1107 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1107 | HEC  | C3D-CAD-CBD-CGD |
| 2   | C     | 1109 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1109 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1109 | HEC  | C2C-C3C-CAC-CBC |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | C     | 1109 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1110 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1110 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1110 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1110 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1111 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1111 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1111 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1111 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1112 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1112 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1112 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1112 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1113 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1113 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1113 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1113 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1114 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1114 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1114 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1115 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1115 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1115 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1115 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1116 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1116 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1101 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1101 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1102 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1102 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1102 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1103 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1103 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1103 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1103 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1104 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1104 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1104 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1104 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1105 | HEC  | C1A-C2A-CAA-CBA |
| 2   | D     | 1105 | HEC  | C3A-C2A-CAA-CBA |
| 2   | D     | 1105 | HEC  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | D     | 1105 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1105 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1105 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1106 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1106 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1106 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1106 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1107 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1108 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1108 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1109 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1109 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1109 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1109 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1110 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1110 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1110 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1110 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1111 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1111 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1111 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1111 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1112 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1112 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1112 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1112 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1113 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1113 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1113 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1113 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1114 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1114 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1115 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1115 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1115 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1115 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1116 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1116 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1107 | HEC  | C3A-C2A-CAA-CBA |
| 2   | C     | 1105 | HEC  | C3A-C2A-CAA-CBA |
| 2   | A     | 1111 | HEC  | C2A-CAA-CBA-CGA |
| 2   | C     | 1105 | HEC  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | C     | 1105 | HEC  | C1A-C2A-CAA-CBA |
| 2   | D     | 1109 | HEC  | C2A-CAA-CBA-CGA |
| 2   | A     | 1109 | HEC  | C2A-CAA-CBA-CGA |
| 2   | B     | 1101 | HEC  | C3D-CAD-CBD-CGD |
| 2   | C     | 1110 | HEC  | C2A-CAA-CBA-CGA |
| 2   | D     | 1109 | HEC  | C1A-C2A-CAA-CBA |
| 2   | A     | 1104 | HEC  | C2A-CAA-CBA-CGA |
| 2   | D     | 1101 | HEC  | C3D-CAD-CBD-CGD |
| 2   | D     | 1109 | HEC  | C2D-C3D-CAD-CBD |
| 2   | D     | 1109 | HEC  | C3A-C2A-CAA-CBA |
| 2   | C     | 1101 | HEC  | C3D-CAD-CBD-CGD |
| 2   | B     | 1101 | HEC  | C2A-CAA-CBA-CGA |
| 2   | B     | 1107 | HEC  | C4D-C3D-CAD-CBD |
| 2   | A     | 1101 | HEC  | C3D-CAD-CBD-CGD |
| 2   | A     | 1105 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1109 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1109 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1111 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1113 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1101 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1103 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1107 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1107 | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 1113 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1114 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1104 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1105 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1108 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1108 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1114 | HEC  | C4C-C3C-CAC-CBC |
| 2   | C     | 1116 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1101 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1102 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1107 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1108 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1114 | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 1105 | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 1109 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1111 | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 1113 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 1101 | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 1116 | HEC  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | C     | 1104 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1107 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1108 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1108 | HEC  | C2C-C3C-CAC-CBC |
| 2   | C     | 1116 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1101 | HEC  | C2B-C3B-CAB-CBB |
| 2   | D     | 1107 | HEC  | C2C-C3C-CAC-CBC |
| 2   | D     | 1108 | HEC  | C2B-C3B-CAB-CBB |
| 2   | C     | 1111 | HEC  | C1A-C2A-CAA-CBA |
| 2   | A     | 1113 | HEC  | C2A-CAA-CBA-CGA |
| 2   | C     | 1105 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1105 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1113 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1113 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1115 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1109 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1110 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1115 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1115 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1104 | HEC  | C2A-CAA-CBA-CGA |
| 2   | B     | 1116 | HEC  | C3D-CAD-CBD-CGD |
| 2   | C     | 1104 | HEC  | C2A-CAA-CBA-CGA |
| 2   | C     | 1109 | HEC  | C2A-CAA-CBA-CGA |
| 2   | D     | 1104 | HEC  | C2A-CAA-CBA-CGA |
| 2   | D     | 1108 | HEC  | C2A-CAA-CBA-CGA |
| 2   | D     | 1111 | HEC  | C3D-CAD-CBD-CGD |
| 2   | A     | 1111 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1111 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1108 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1115 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1108 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1105 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1110 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1103 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1107 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1102 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 1106 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1109 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1103 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1102 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1109 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1113 | HEC  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | C     | 1115 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1102 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 1103 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1115 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1106 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1110 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1104 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1109 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1102 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1104 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1113 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1104 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1110 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1113 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1103 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1115 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1104 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1110 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1113 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 1105 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 1105 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1109 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1115 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1109 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1105 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1105 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1105 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1105 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 1115 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1107 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1112 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1103 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 1105 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 1110 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1112 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1102 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1105 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1107 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1105 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 1109 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1105 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1105 | HEC  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | D     | 1112 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1110 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1113 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1103 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1104 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 1107 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1110 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1113 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1107 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1115 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1116 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1104 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1104 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1103 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1110 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1108 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1111 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1113 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1107 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1111 | HEC  | C3D-CAD-CBD-CGD |
| 2   | A     | 1106 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 1104 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1102 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1108 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1109 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1101 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1110 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1109 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1109 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1103 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1106 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1108 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1111 | HEC  | C3A-C2A-CAA-CBA |
| 2   | A     | 1105 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1107 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 1113 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1116 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1112 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1112 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 1112 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1115 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 1107 | HEC  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1115 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1105 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1111 | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 1107 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1112 | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 1108 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1108 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1101 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1107 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1108 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1111 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1112 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1107 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1108 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 1112 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1107 | HEC  | C2D-C3D-CAD-CBD |
| 2   | D     | 1111 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 1114 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 1106 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1102 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1101 | HEC  | CAA-CBA-CGA-O1A |
| 2   | C     | 1101 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1106 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1107 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 1102 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1112 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1112 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 1106 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1106 | HEC  | CAD-CBD-CGD-O1D |
| 2   | D     | 1109 | HEC  | C4D-C3D-CAD-CBD |
| 2   | C     | 1108 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1111 | HEC  | CAA-CBA-CGA-O2A |
| 2   | D     | 1114 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1114 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1112 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1116 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 1115 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 1112 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1109 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1116 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1108 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1116 | HEC  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 2   | A     | 1101 | HEC  | CAA-CBA-CGA-O2A |
| 2   | C     | 1111 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1108 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1115 | HEC  | CAD-CBD-CGD-O2D |
| 2   | D     | 1114 | HEC  | CAD-CBD-CGD-O1D |
| 2   | C     | 1116 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1112 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1109 | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 1114 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 1112 | HEC  | C4B-C3B-CAB-CBB |
| 2   | C     | 1107 | HEC  | C4B-C3B-CAB-CBB |
| 2   | D     | 1107 | HEC  | C4C-C3C-CAC-CBC |
| 2   | D     | 1116 | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 1101 | HEC  | CAA-CBA-CGA-O1A |
| 2   | D     | 1110 | HEC  | C2D-C3D-CAD-CBD |
| 2   | B     | 1110 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 1108 | HEC  | CAD-CBD-CGD-O2D |
| 2   | C     | 1111 | HEC  | CAD-CBD-CGD-O2D |

There are no ring outliers.

48 monomers are involved in 99 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 1111 | HEC  | 1       | 0            |
| 2   | D     | 1102 | HEC  | 3       | 0            |
| 2   | A     | 1114 | HEC  | 1       | 0            |
| 2   | C     | 1108 | HEC  | 1       | 0            |
| 2   | B     | 1107 | HEC  | 3       | 0            |
| 2   | A     | 1102 | HEC  | 2       | 0            |
| 2   | B     | 1109 | HEC  | 1       | 0            |
| 2   | B     | 1113 | HEC  | 1       | 0            |
| 2   | B     | 1116 | HEC  | 1       | 0            |
| 2   | C     | 1103 | HEC  | 1       | 0            |
| 2   | C     | 1104 | HEC  | 1       | 0            |
| 2   | A     | 1113 | HEC  | 2       | 0            |
| 2   | D     | 1109 | HEC  | 4       | 0            |
| 2   | D     | 1107 | HEC  | 2       | 0            |
| 2   | D     | 1114 | HEC  | 2       | 0            |
| 2   | C     | 1107 | HEC  | 2       | 0            |
| 2   | B     | 1102 | HEC  | 2       | 0            |
| 2   | A     | 1115 | HEC  | 1       | 0            |
| 2   | D     | 1108 | HEC  | 3       | 0            |

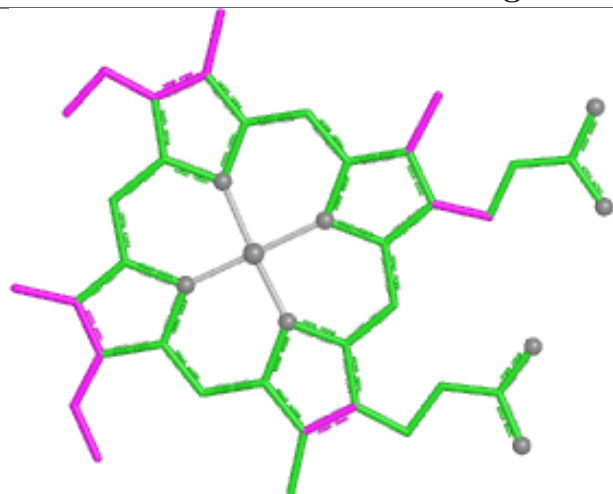
*Continued on next page...*

*Continued from previous page...*

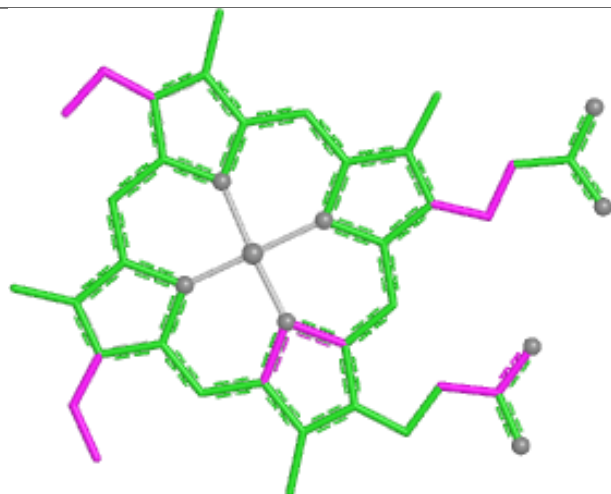
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | C     | 1109 | HEC  | 5       | 0            |
| 2   | D     | 1104 | HEC  | 7       | 0            |
| 2   | B     | 1112 | HEC  | 1       | 0            |
| 2   | D     | 1106 | HEC  | 4       | 0            |
| 2   | A     | 1112 | HEC  | 2       | 0            |
| 2   | D     | 1115 | HEC  | 1       | 0            |
| 2   | B     | 1111 | HEC  | 2       | 0            |
| 2   | B     | 1114 | HEC  | 1       | 0            |
| 2   | D     | 1103 | HEC  | 2       | 0            |
| 2   | A     | 1110 | HEC  | 2       | 0            |
| 2   | C     | 1110 | HEC  | 3       | 0            |
| 2   | B     | 1110 | HEC  | 1       | 0            |
| 2   | A     | 1109 | HEC  | 2       | 0            |
| 2   | B     | 1104 | HEC  | 1       | 0            |
| 2   | A     | 1108 | HEC  | 2       | 0            |
| 2   | C     | 1102 | HEC  | 1       | 0            |
| 2   | C     | 1106 | HEC  | 1       | 0            |
| 2   | C     | 1114 | HEC  | 2       | 0            |
| 2   | C     | 1115 | HEC  | 5       | 0            |
| 2   | B     | 1106 | HEC  | 2       | 0            |
| 2   | D     | 1111 | HEC  | 1       | 0            |
| 2   | D     | 1112 | HEC  | 2       | 0            |
| 2   | C     | 1111 | HEC  | 1       | 0            |
| 2   | A     | 1104 | HEC  | 3       | 0            |
| 2   | B     | 1115 | HEC  | 7       | 0            |
| 2   | D     | 1110 | HEC  | 4       | 0            |
| 2   | D     | 1101 | HEC  | 3       | 0            |
| 2   | D     | 1113 | HEC  | 1       | 0            |
| 2   | C     | 1101 | HEC  | 2       | 0            |

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

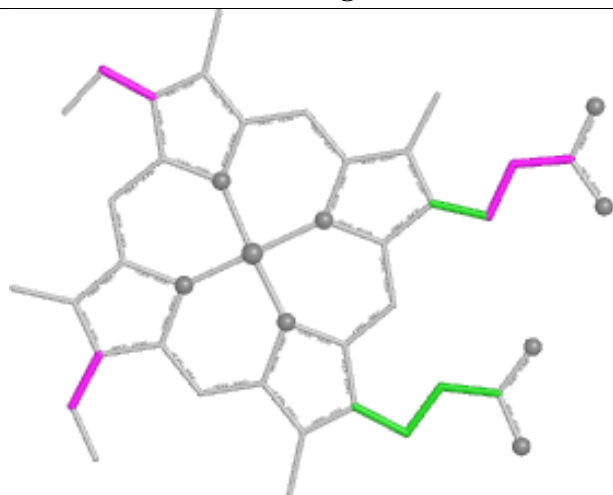
## Ligand HEC A 1111



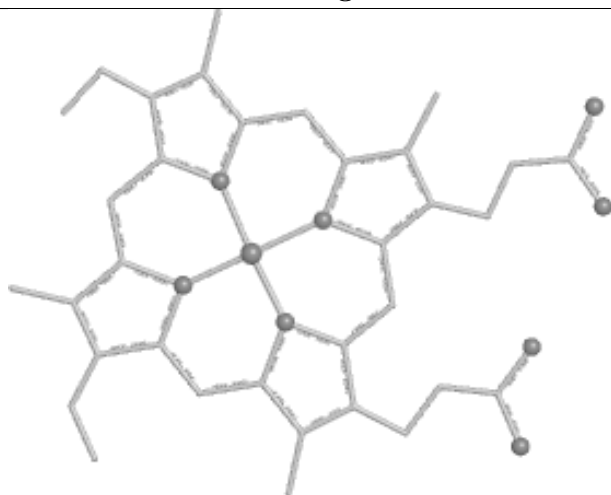
Bond lengths



Bond angles

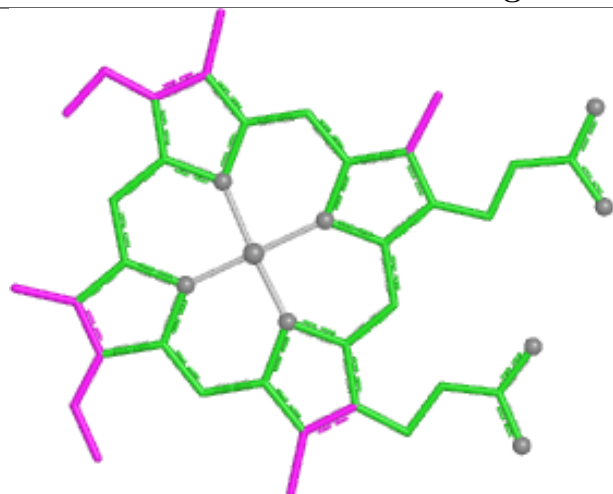


Torsions

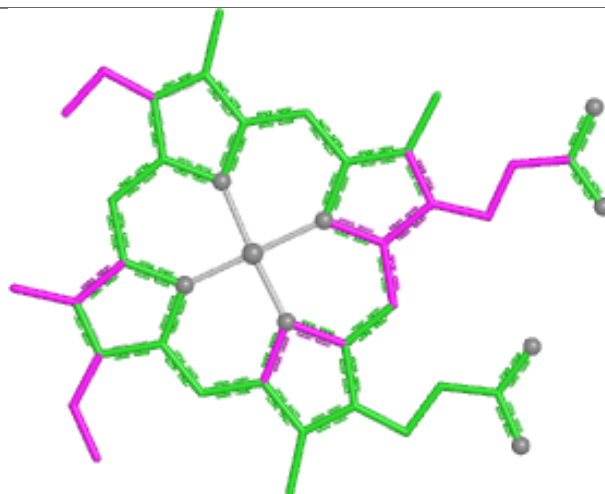


Rings

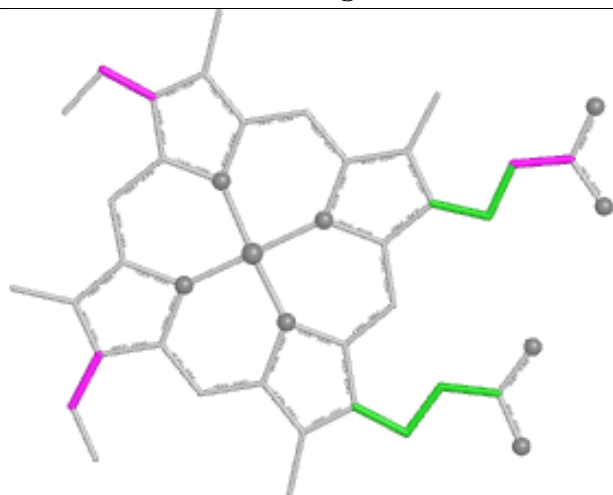
## Ligand HEC C 1113



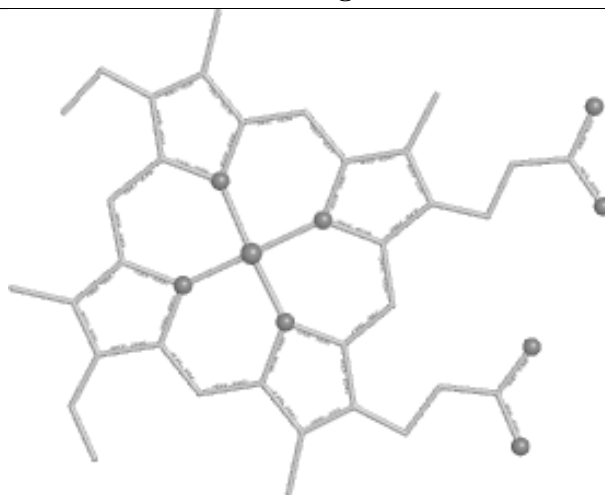
Bond lengths



Bond angles

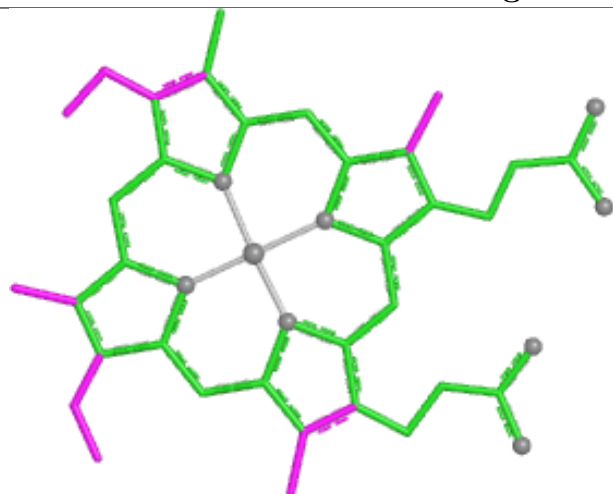


Torsions

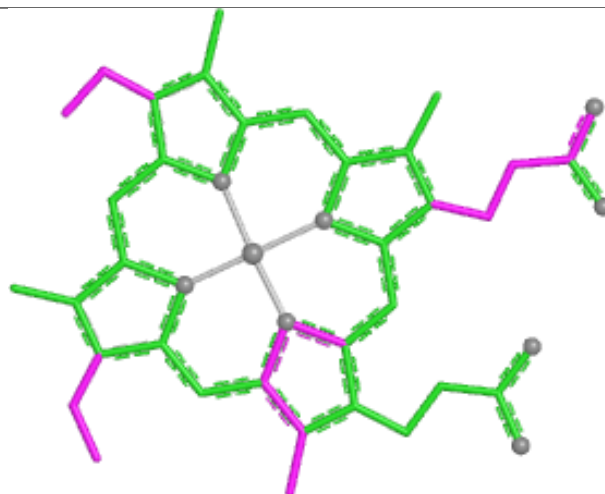


Rings

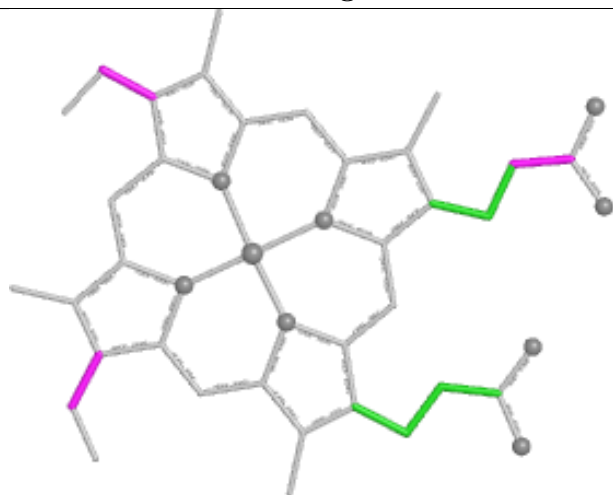
## Ligand HEC D 1102



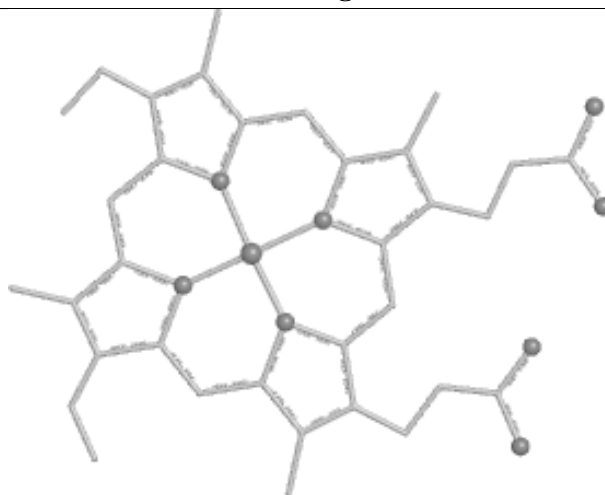
Bond lengths



Bond angles

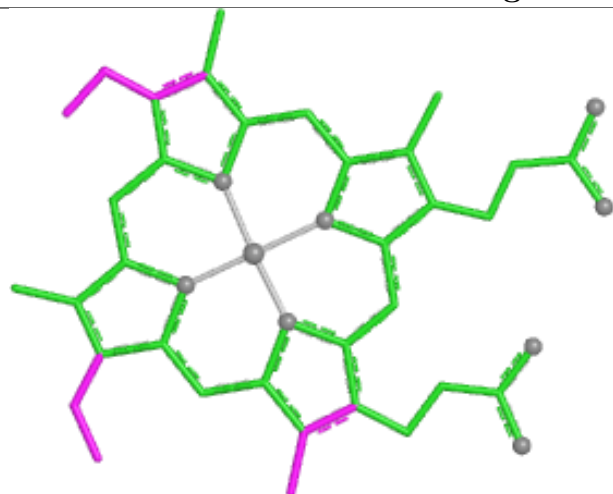


Torsions

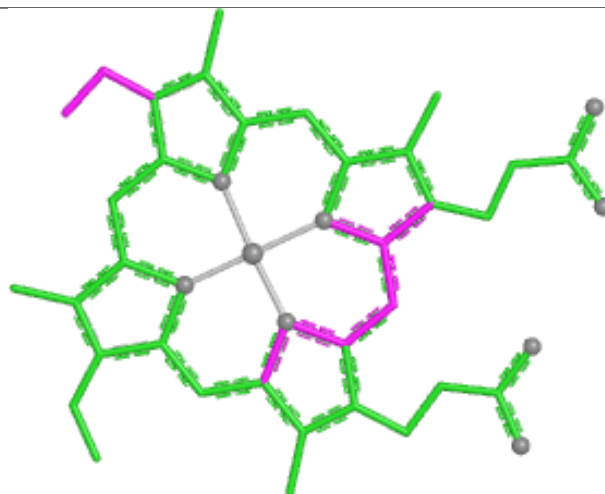


Rings

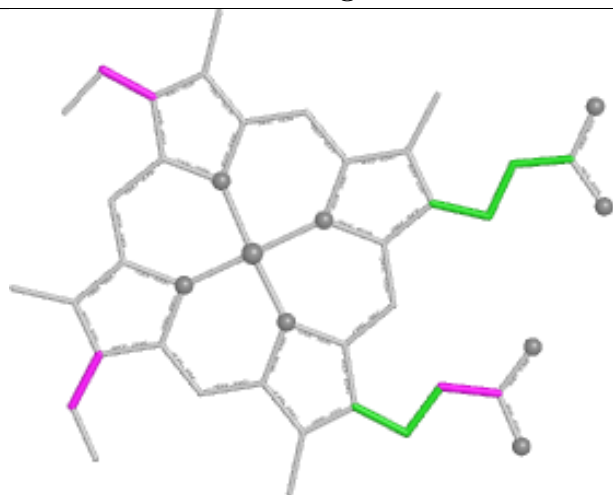
## Ligand HEC A 1114



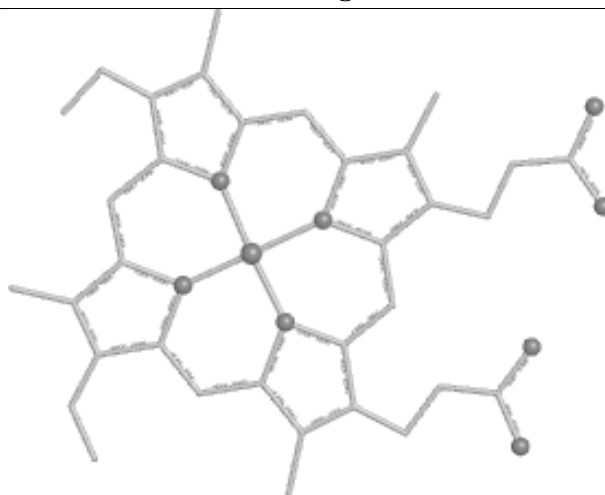
Bond lengths



Bond angles

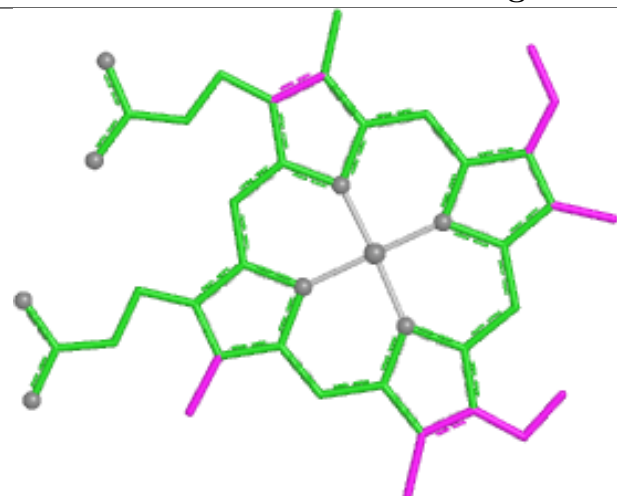


Torsions

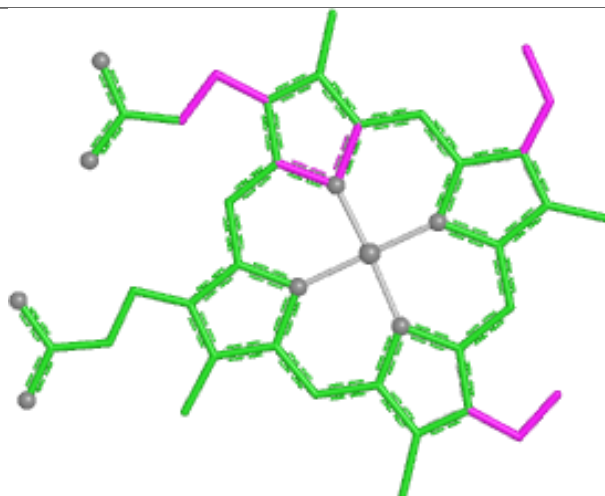


Rings

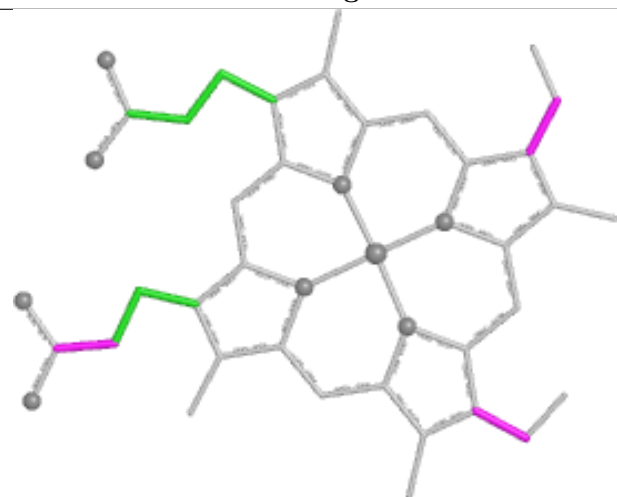
## Ligand HEC B 1103



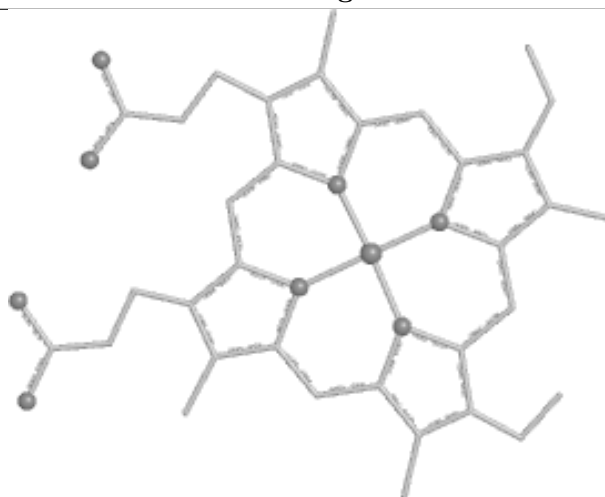
Bond lengths



Bond angles

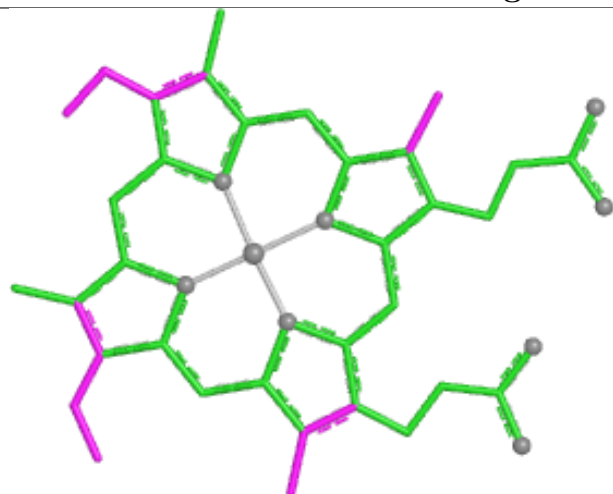


Torsions

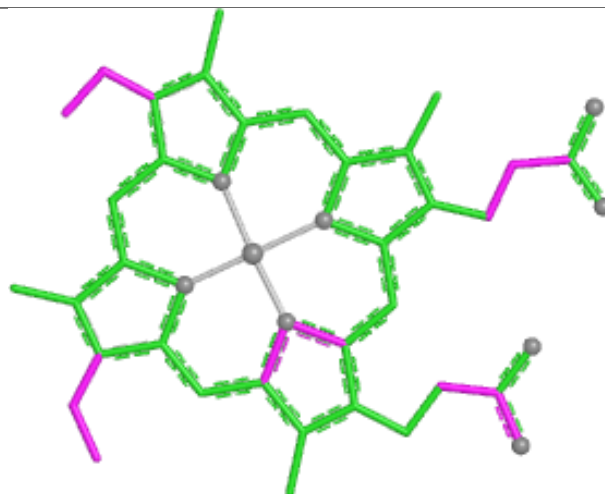


Rings

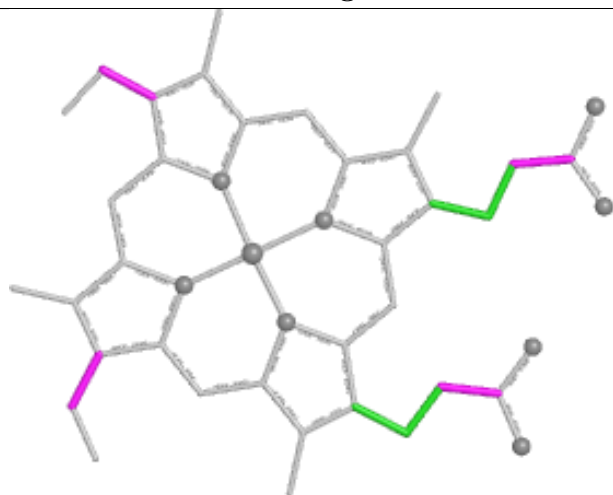
## Ligand HEC C 1108



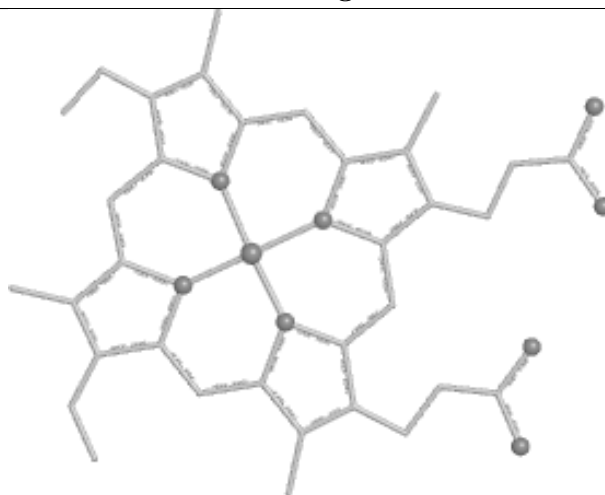
Bond lengths



Bond angles

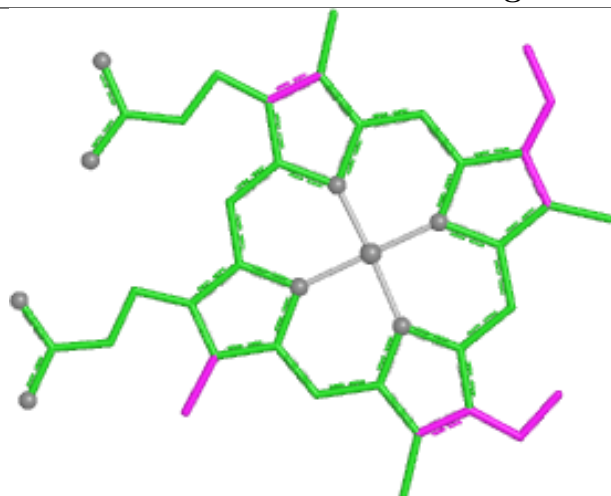


Torsions

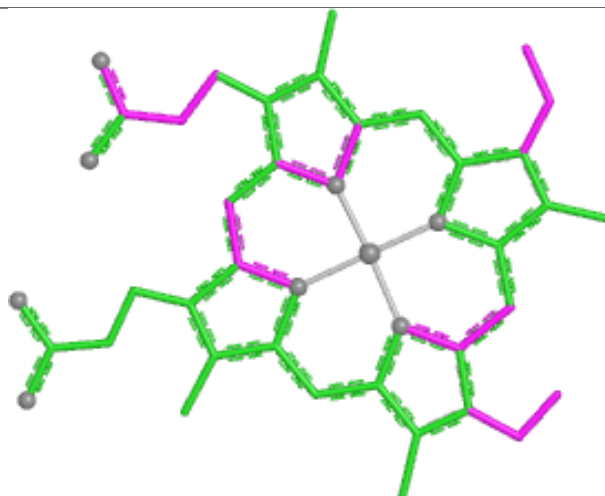


Rings

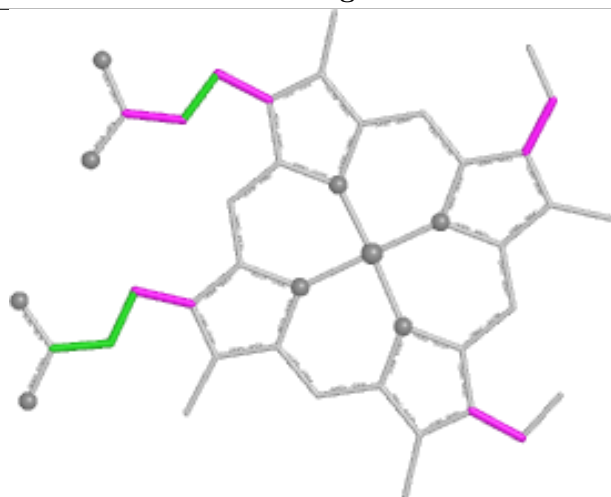
## Ligand HEC B 1107



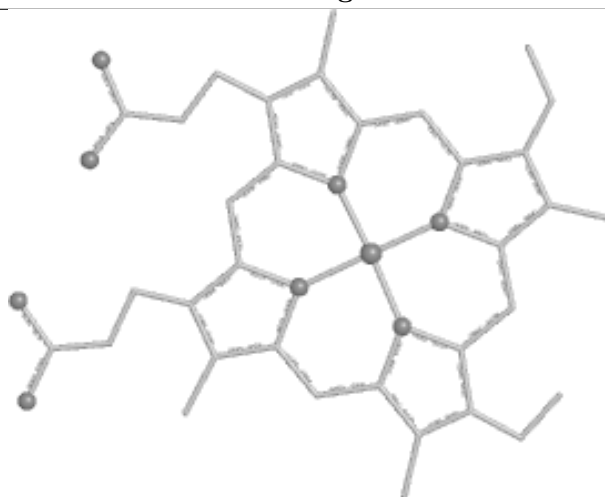
Bond lengths



Bond angles

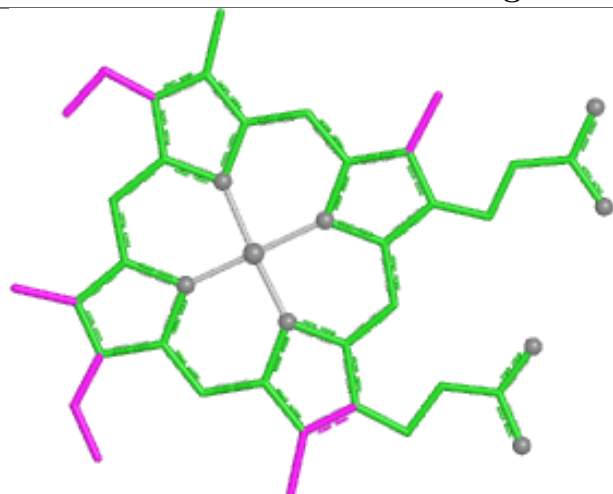


Torsions

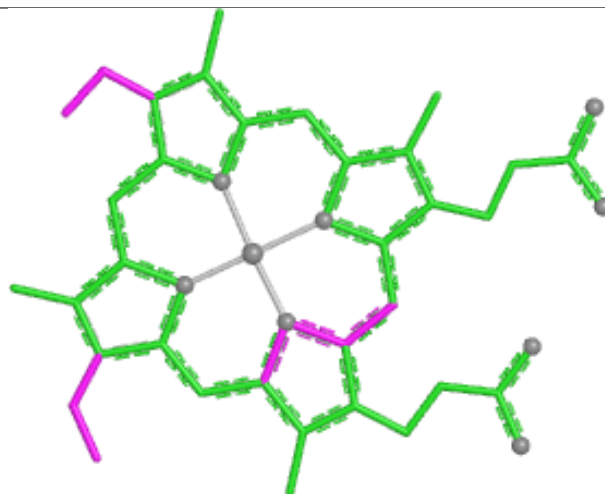


Rings

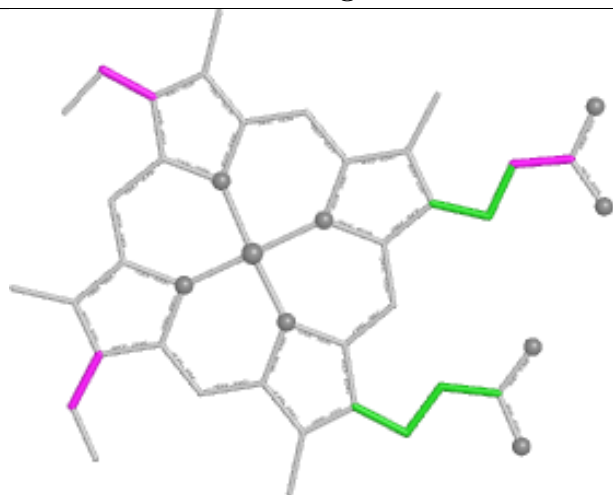
## Ligand HEC A 1102



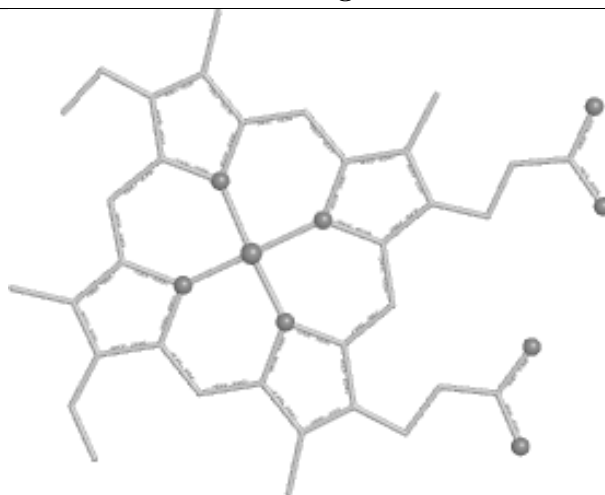
Bond lengths



Bond angles

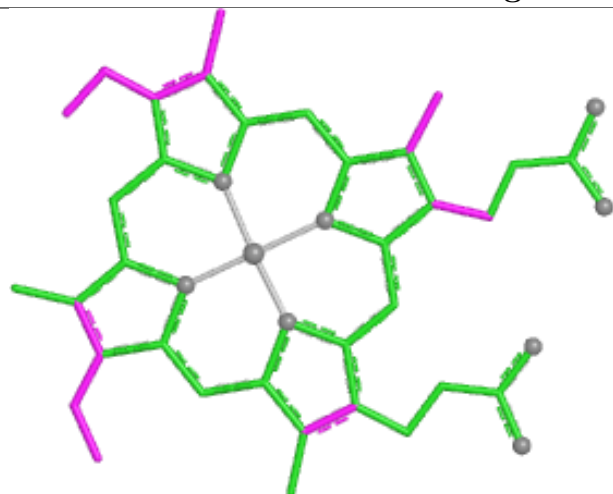


Torsions

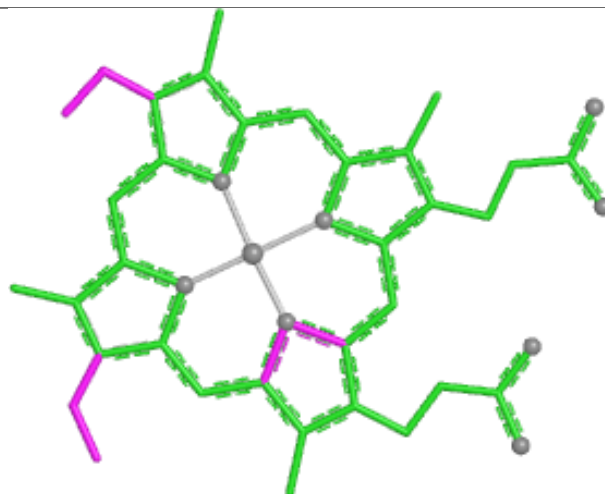


Rings

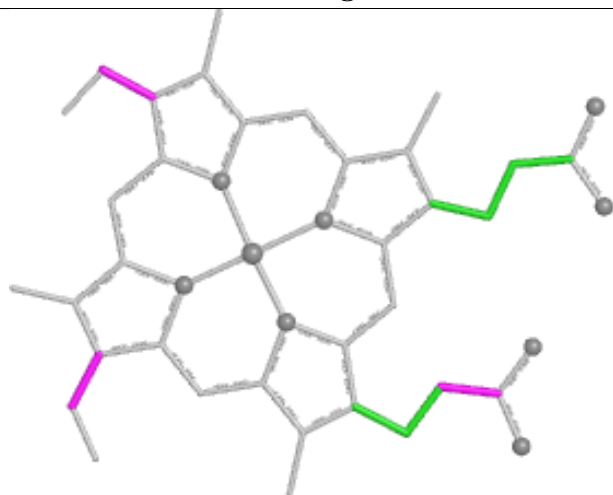
## Ligand HEC B 1109



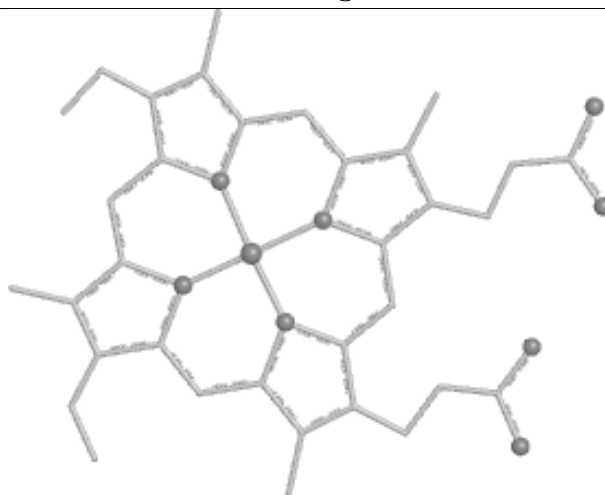
Bond lengths



Bond angles

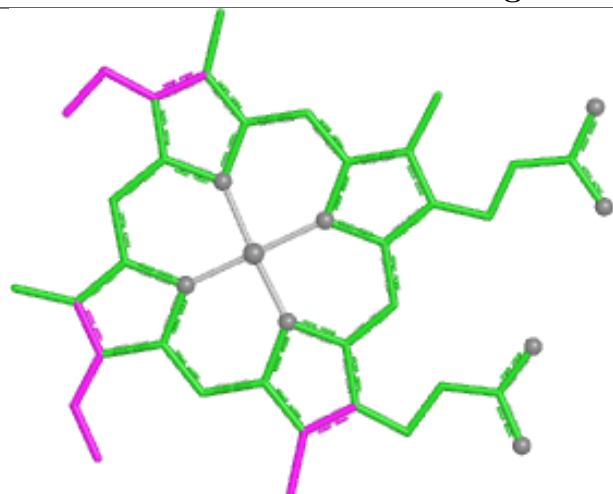


Torsions

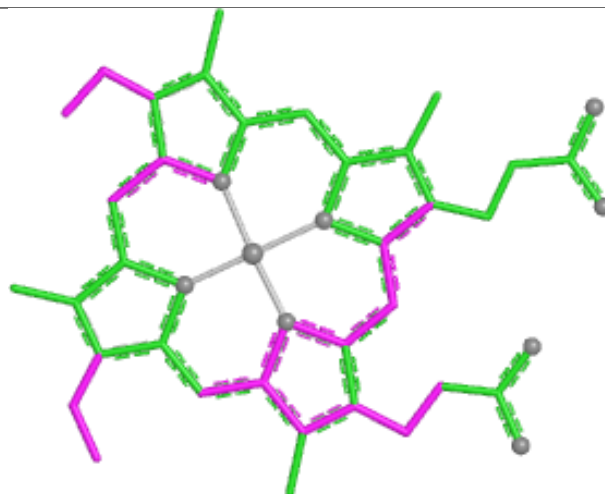


Rings

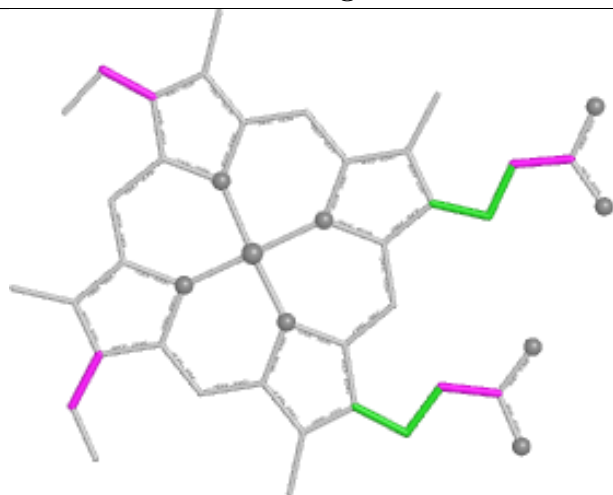
## Ligand HEC B 1113



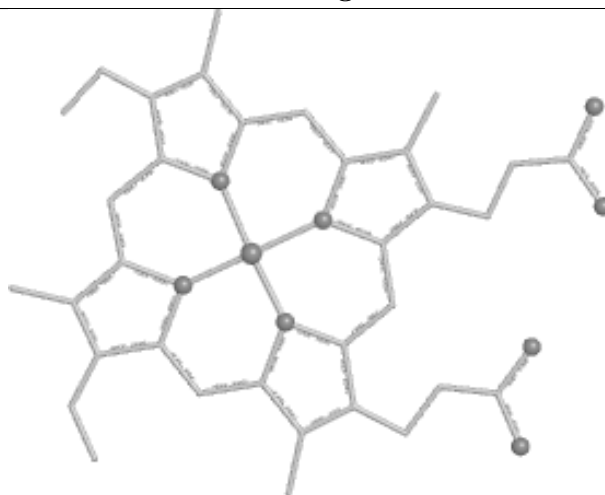
Bond lengths



Bond angles

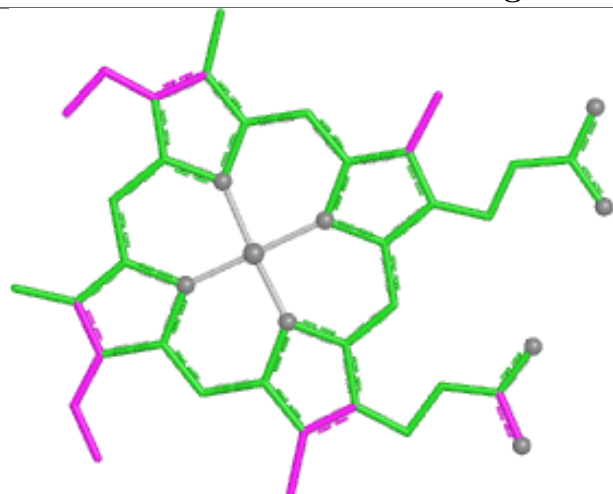


Torsions

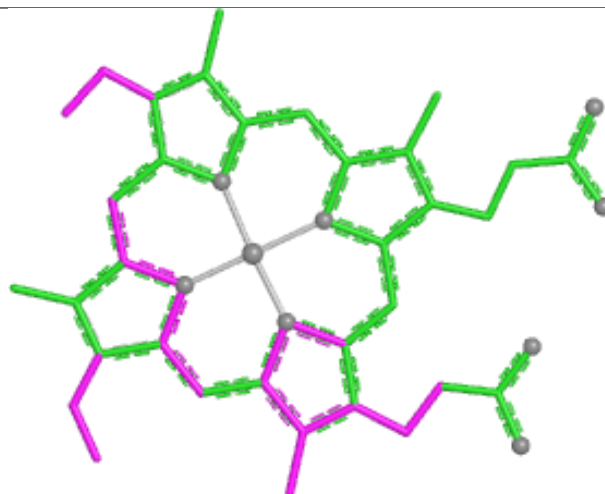


Rings

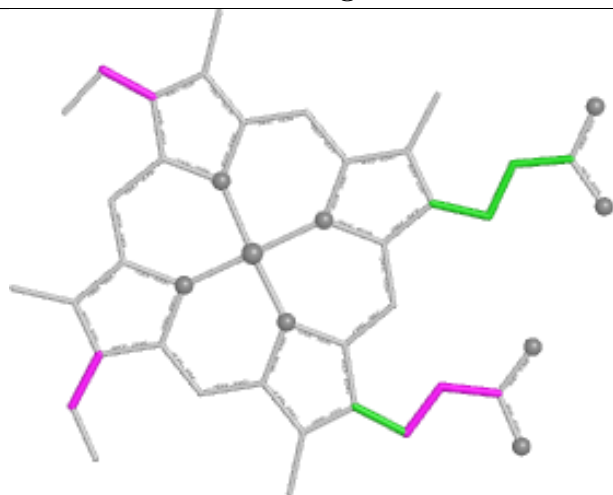
## Ligand HEC B 1116



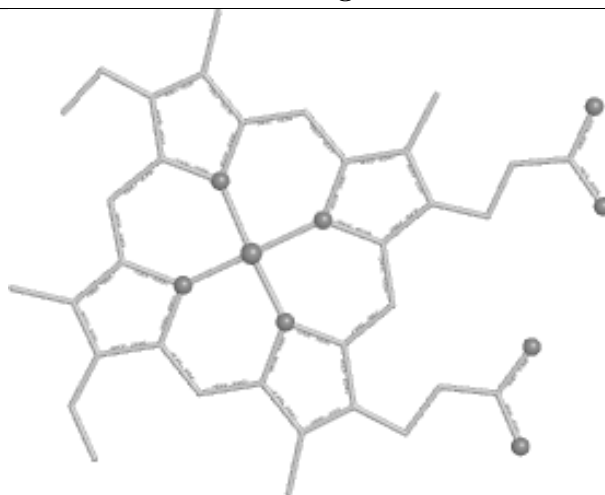
Bond lengths



Bond angles

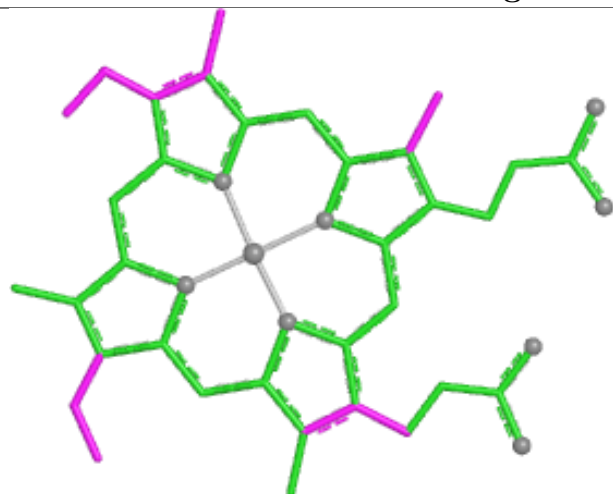


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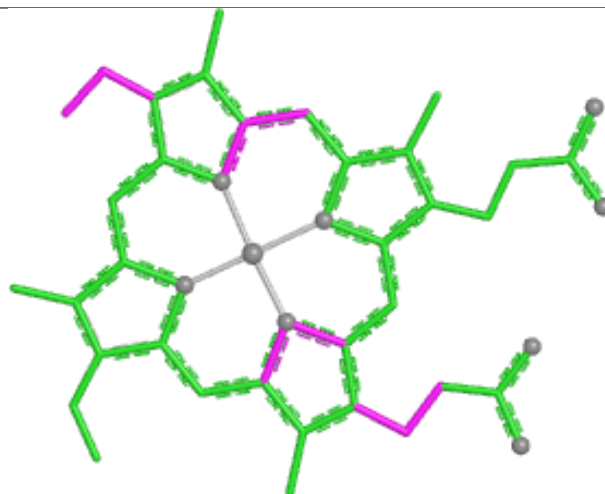


Rings

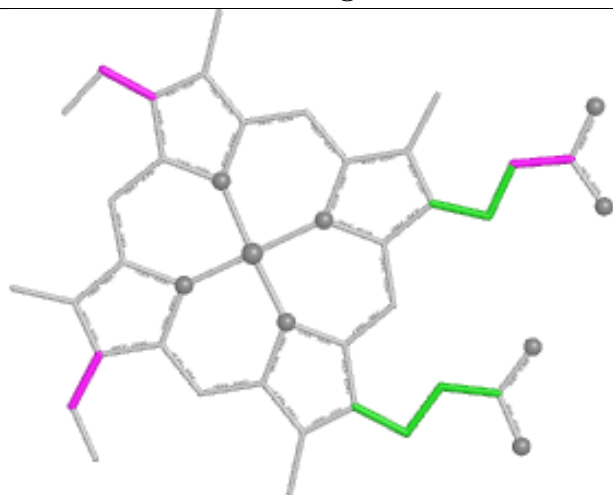
## Ligand HEC C 1103



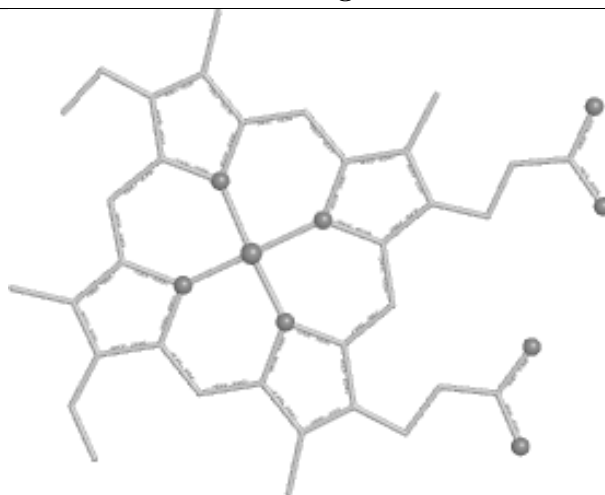
Bond lengths



Bond angles

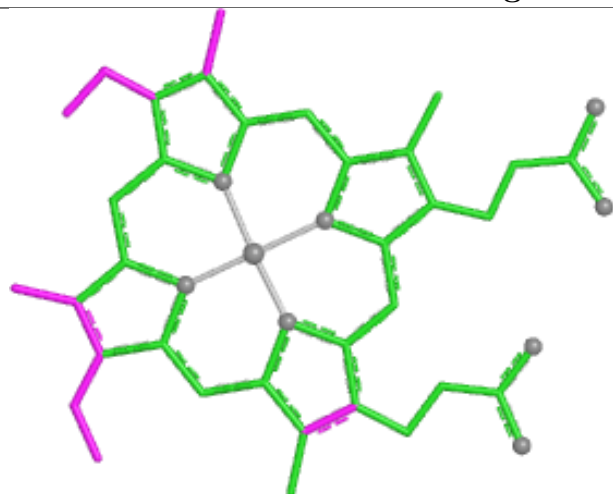


Torsions

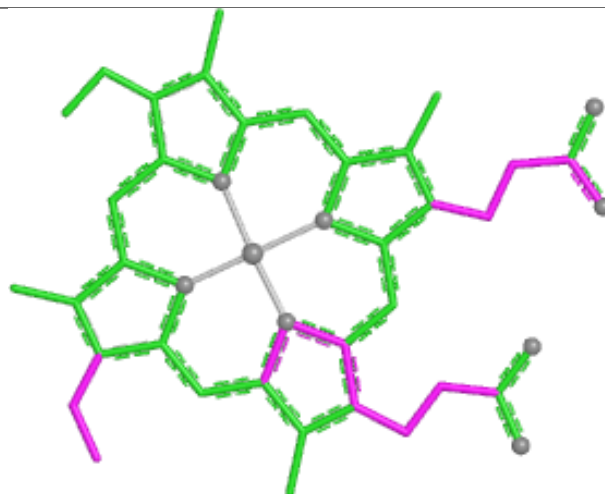


Rings

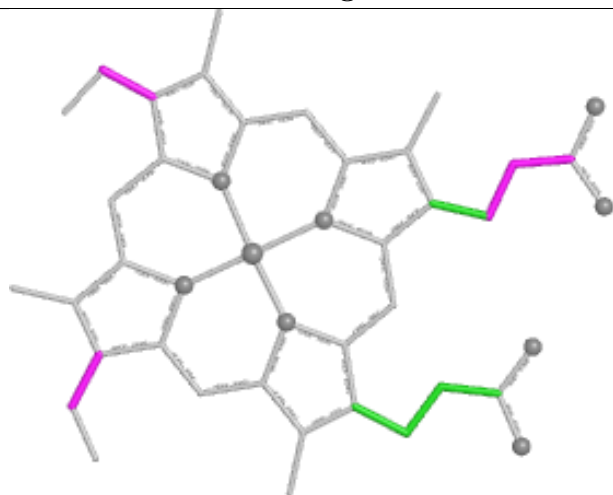
## Ligand HEC C 1104



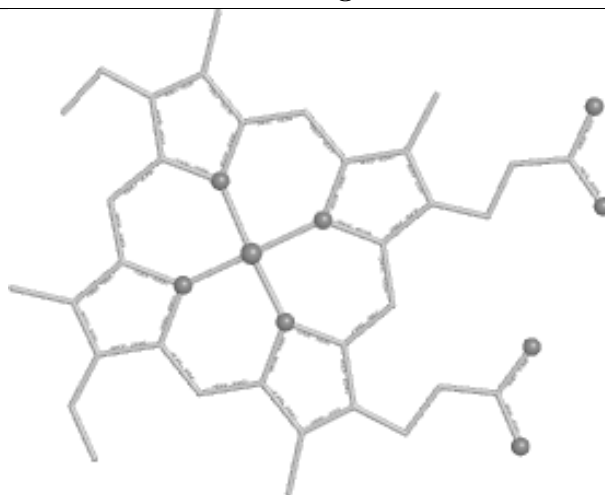
Bond lengths



Bond angles

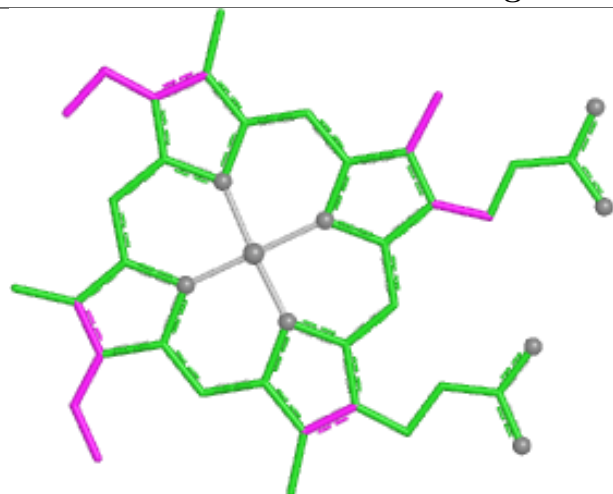


Torsions

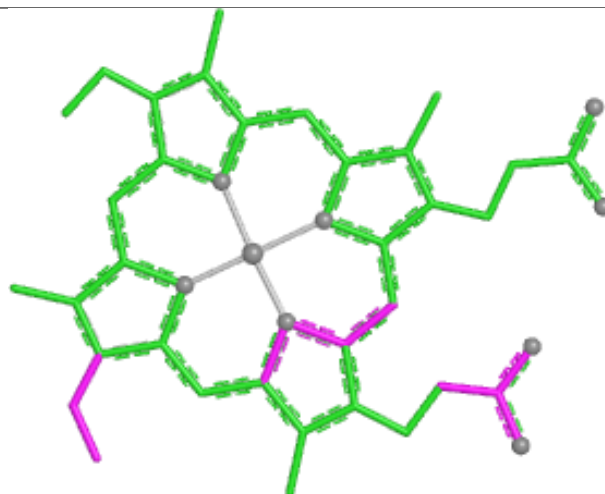


Rings

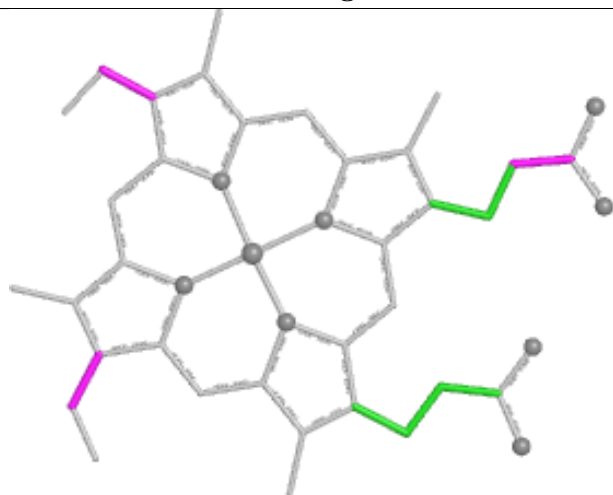
## Ligand HEC B 1108



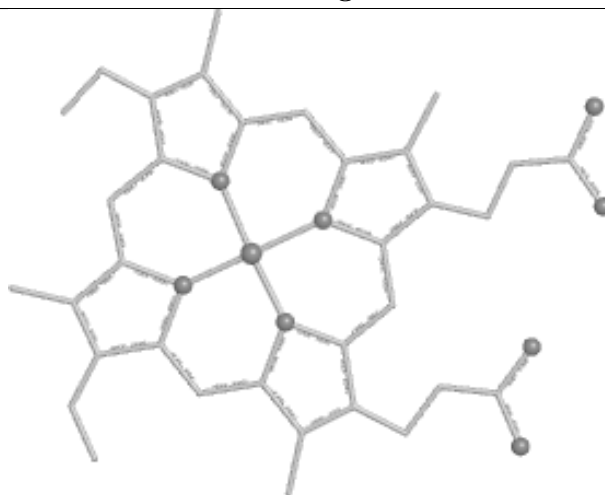
Bond lengths



Bond angles

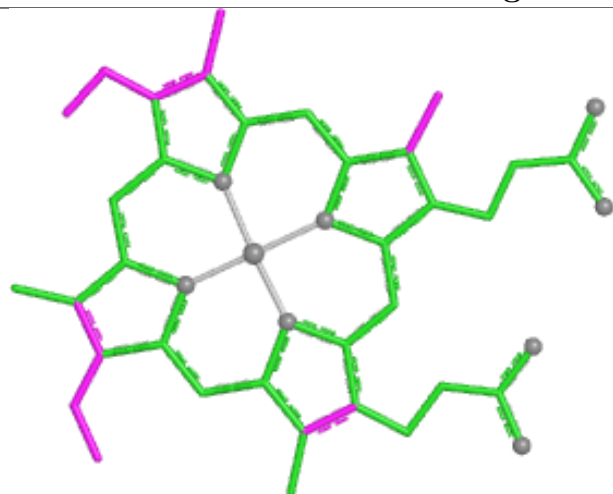


Torsions

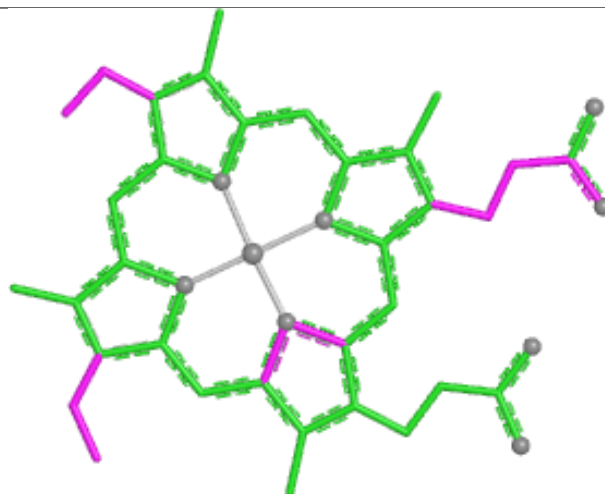


Rings

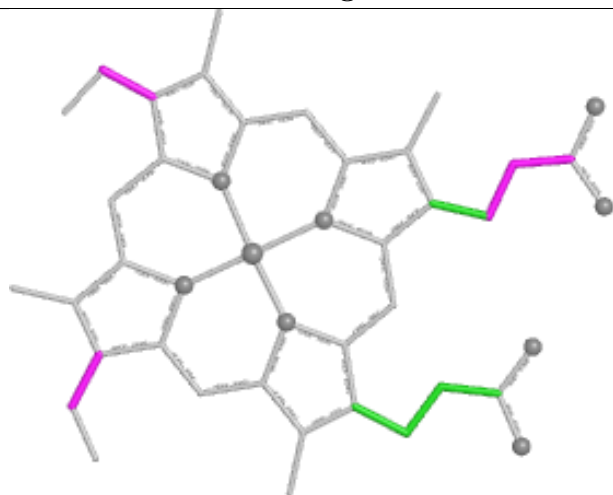
## Ligand HEC A 1113



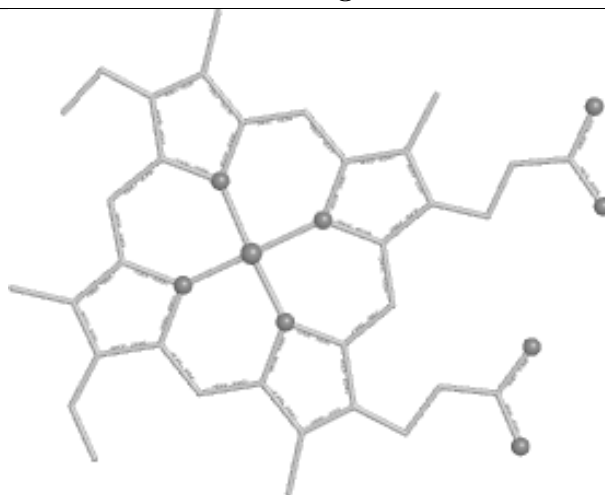
Bond lengths



Bond angles

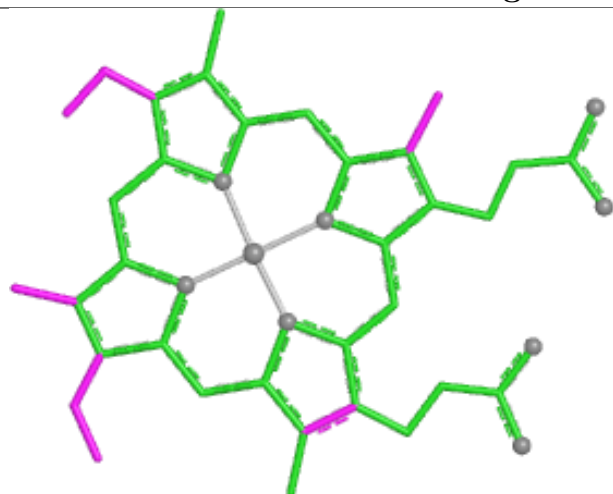


Torsions

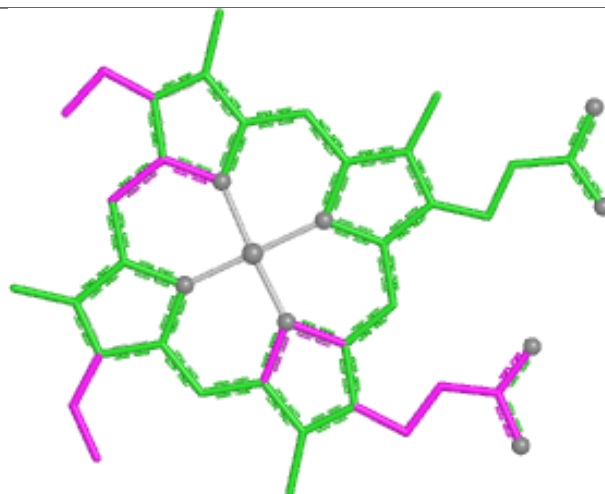


Rings

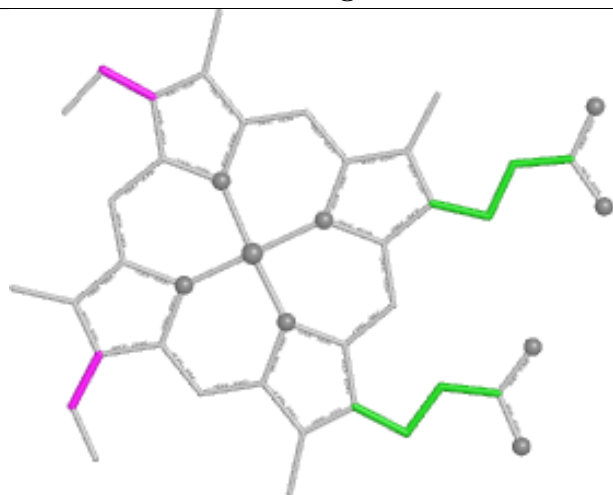
## Ligand HEC A 1116



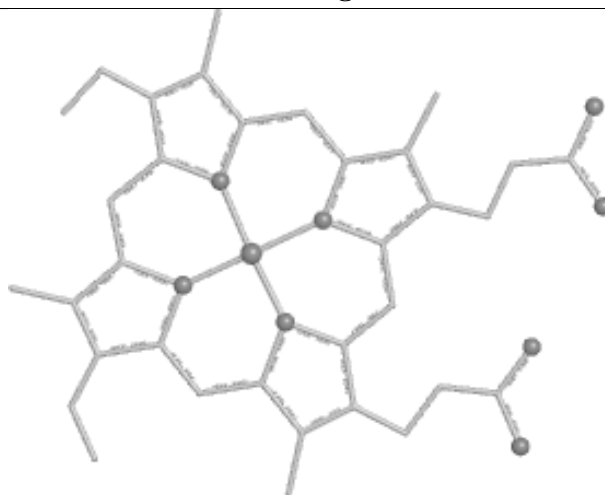
Bond lengths



Bond angles

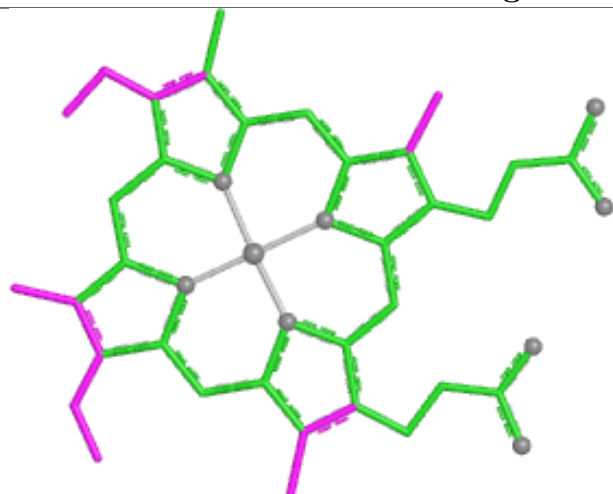


Torsions

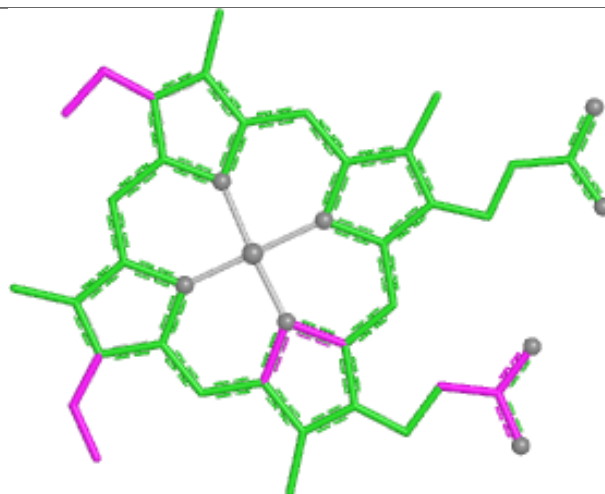


Rings

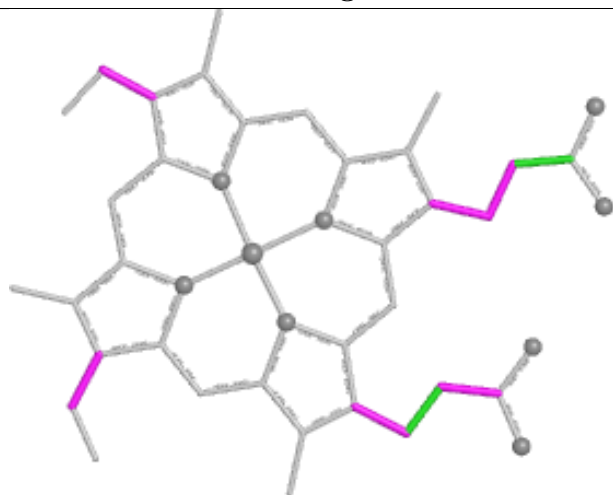
## Ligand HEC D 1109



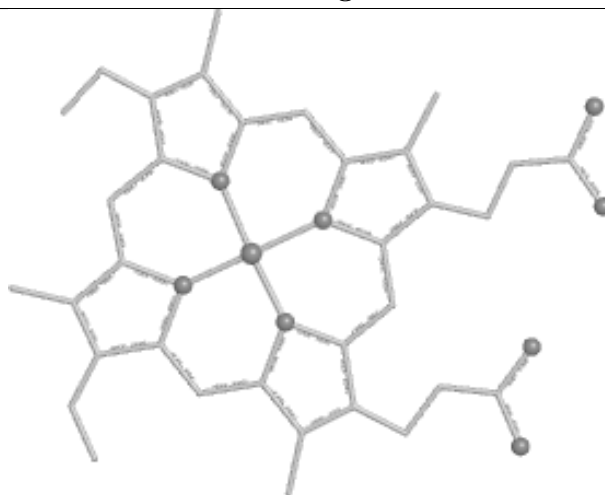
Bond lengths



Bond angles

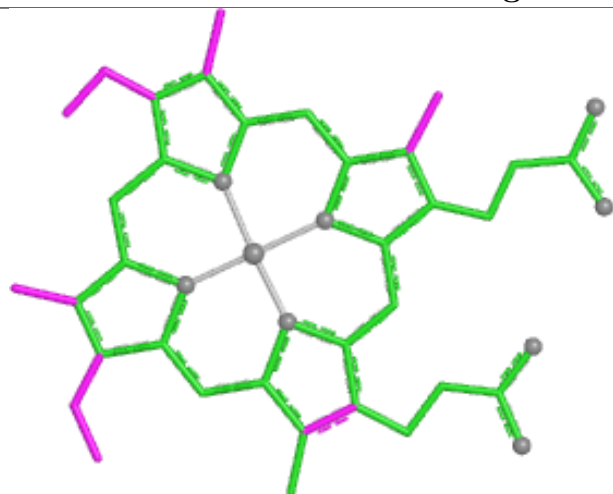


Torsions

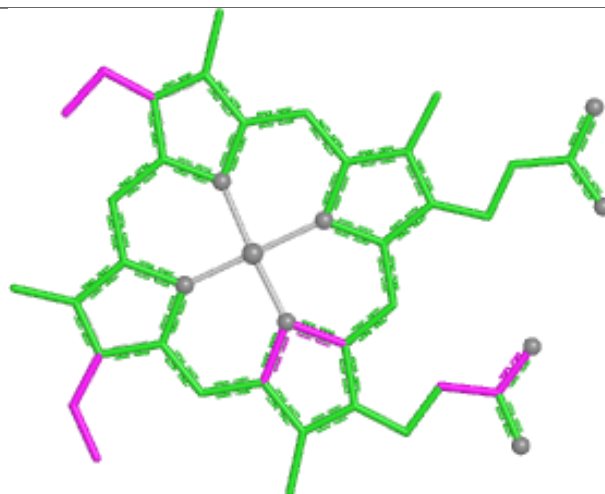


Rings

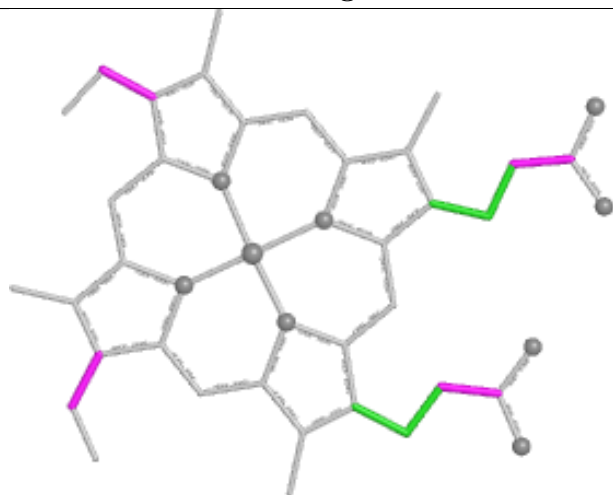
## Ligand HEC D 1107



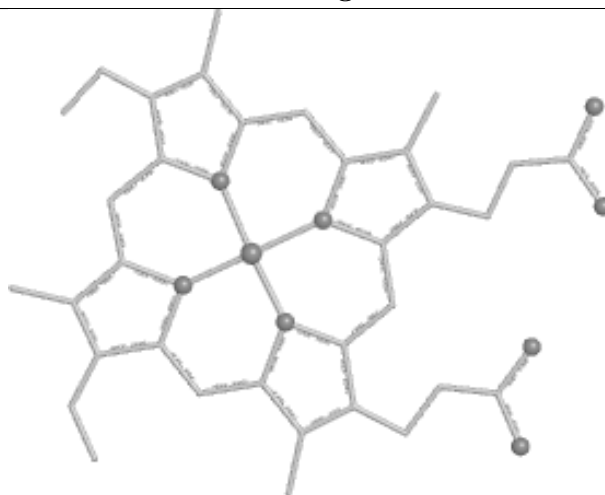
Bond lengths



Bond angles

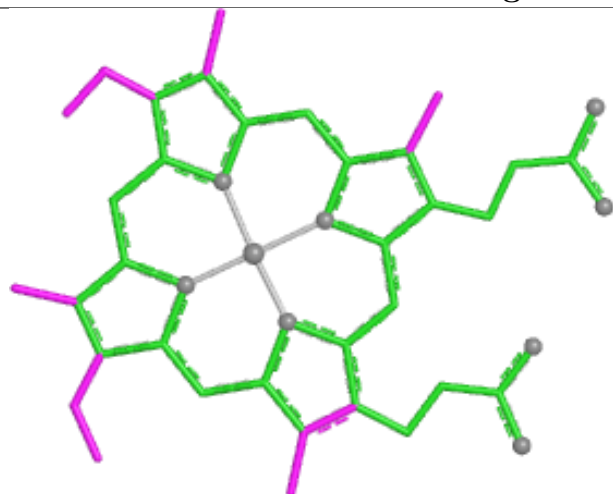


Torsions

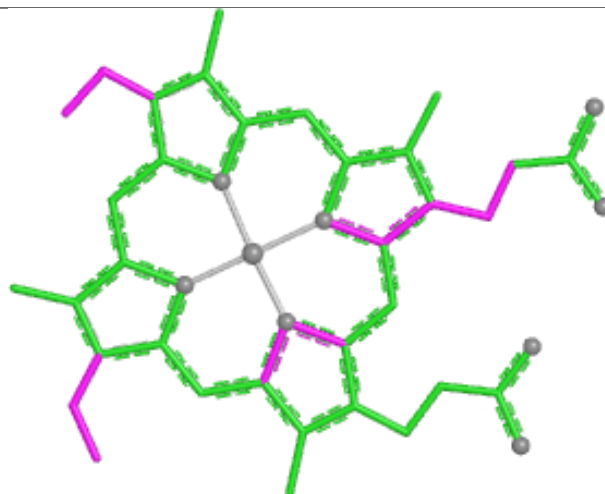


Rings

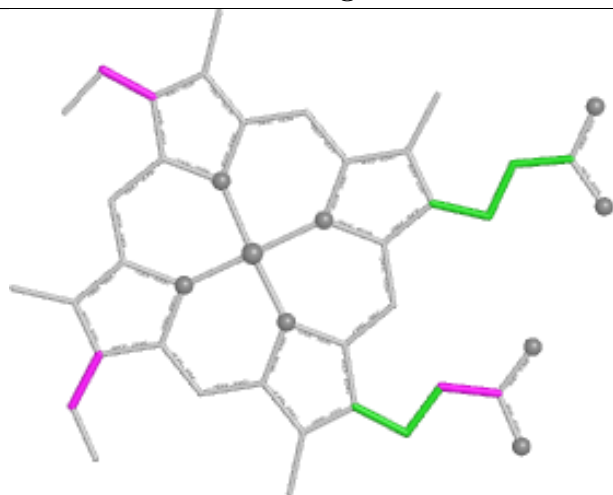
## Ligand HEC D 1114



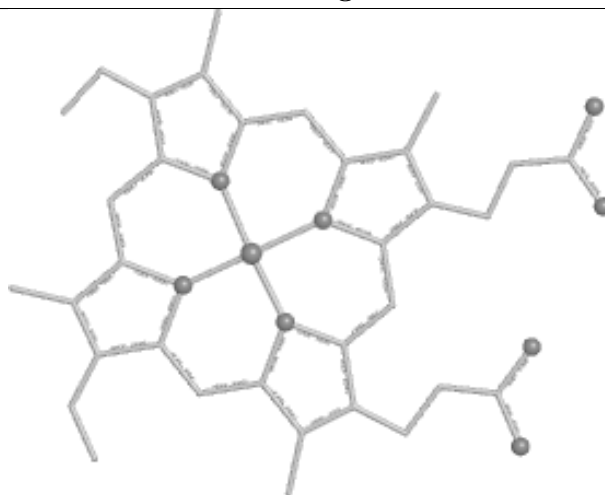
Bond lengths



Bond angles

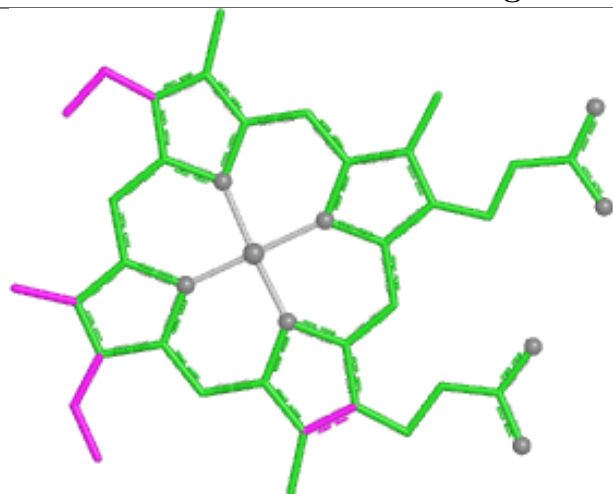


Torsions

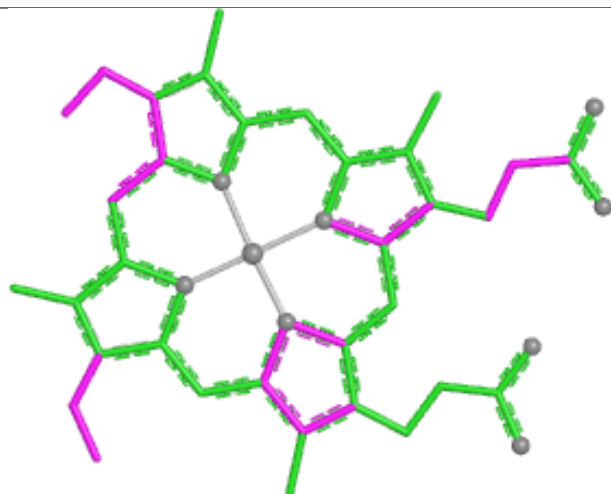


Rings

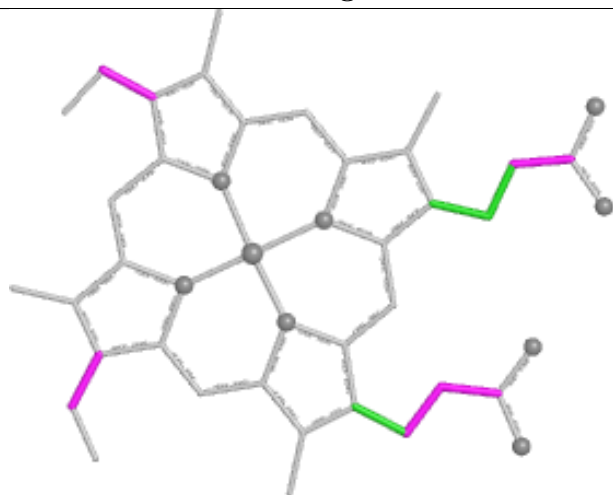
## Ligand HEC C 1107



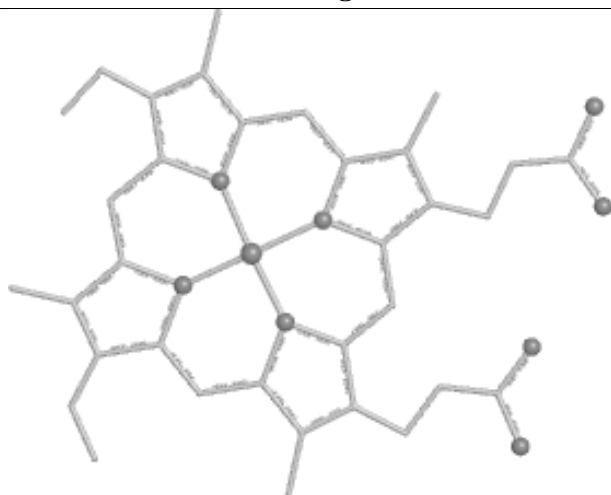
Bond lengths



Bond angles

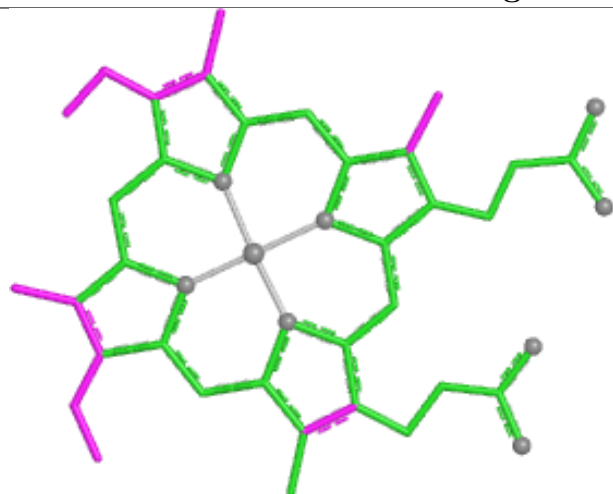


Torsions

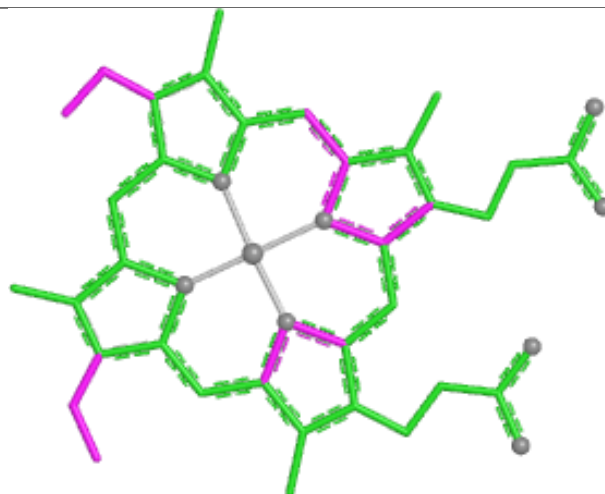


Rings

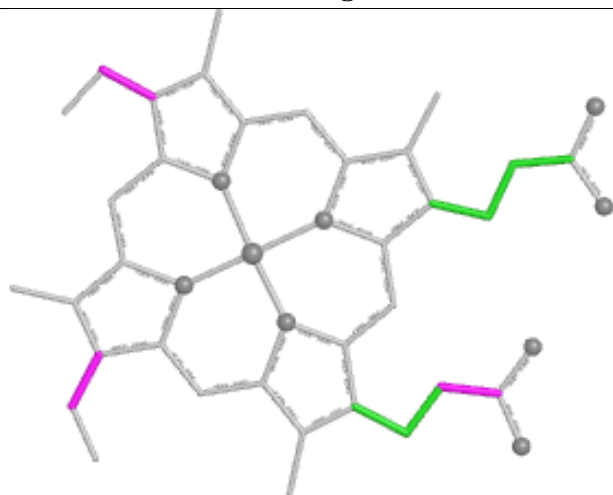
## Ligand HEC A 1106



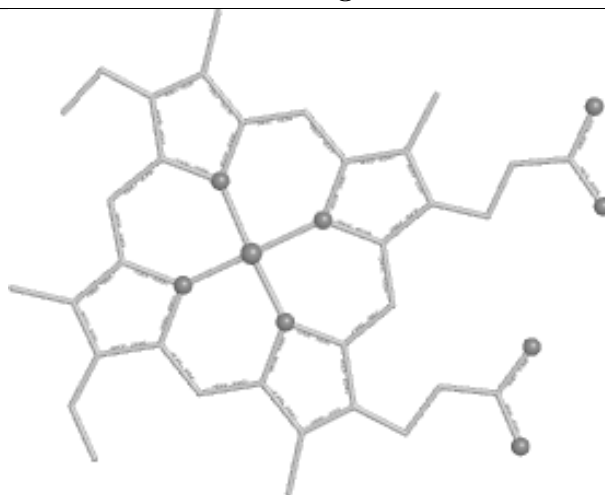
Bond lengths



Bond angles

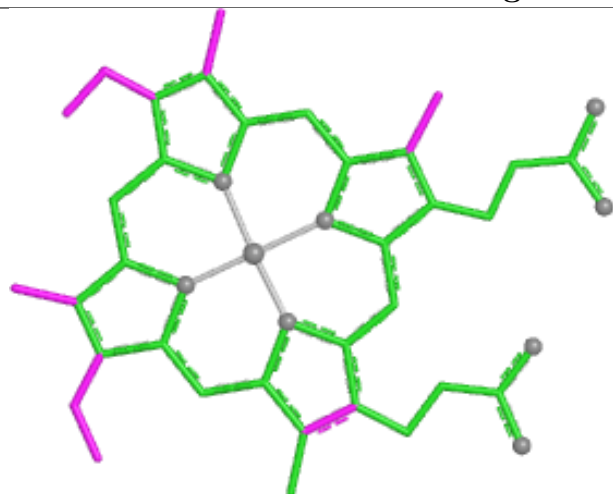


Torsions

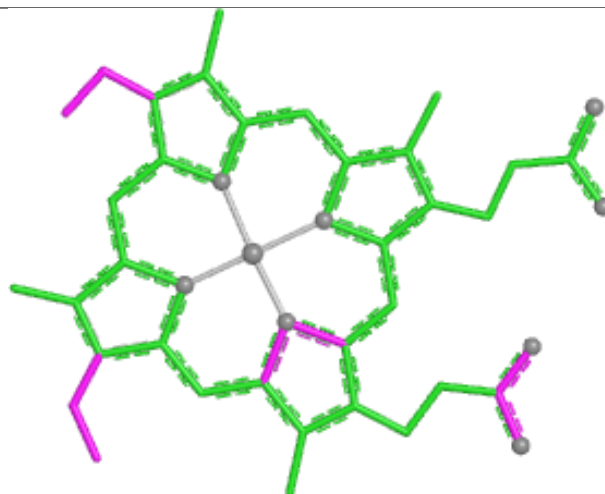


Rings

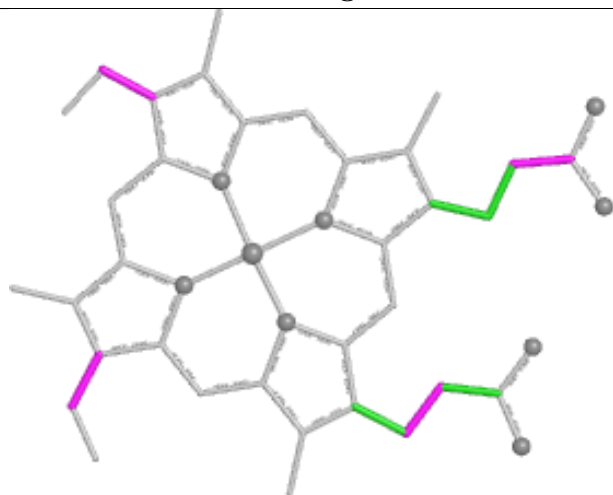
## Ligand HEC A 1101



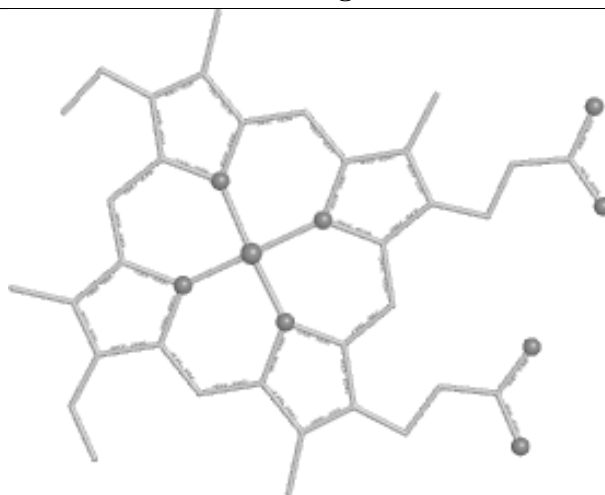
Bond lengths



Bond angles

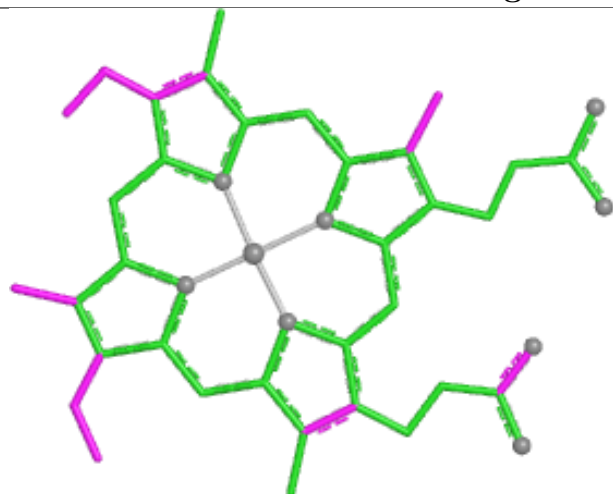


Torsions

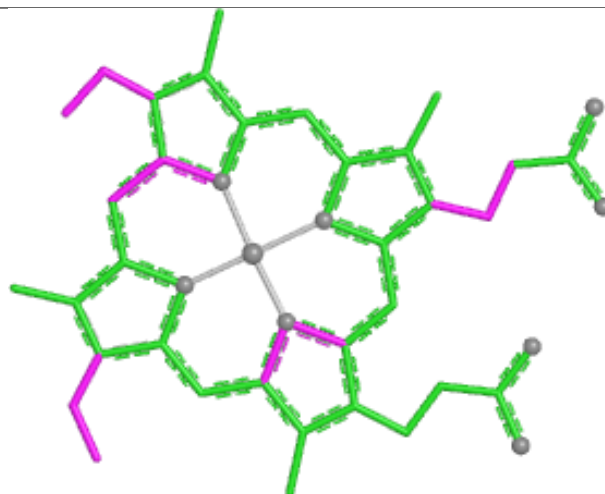


Rings

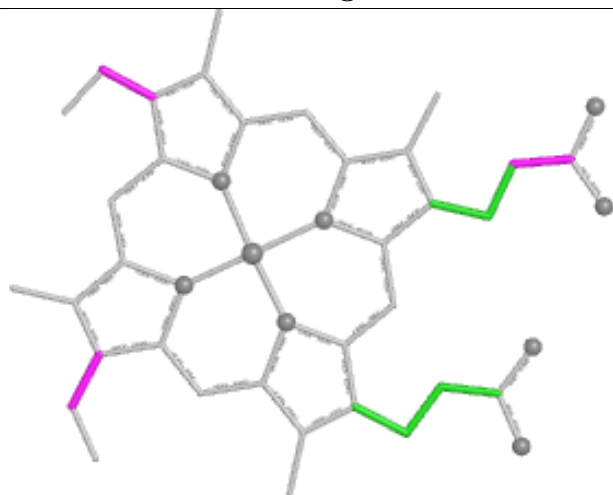
## Ligand HEC B 1102



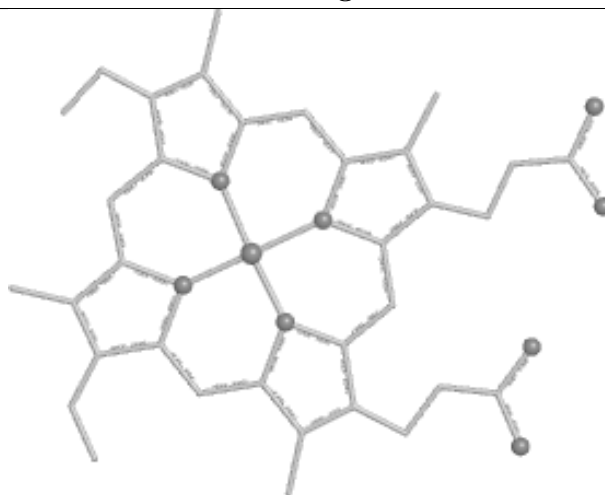
Bond lengths



Bond angles

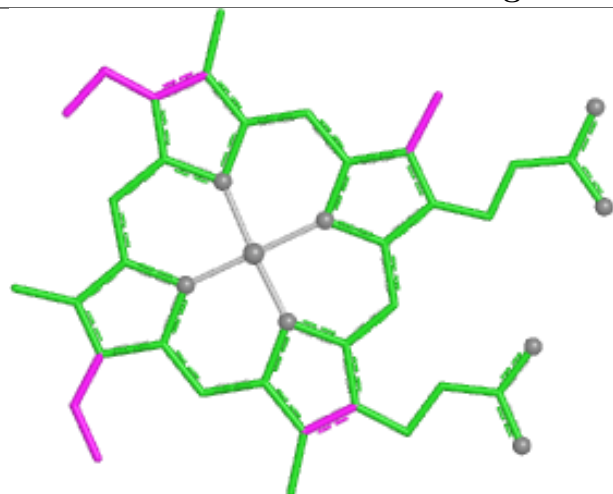


Torsions

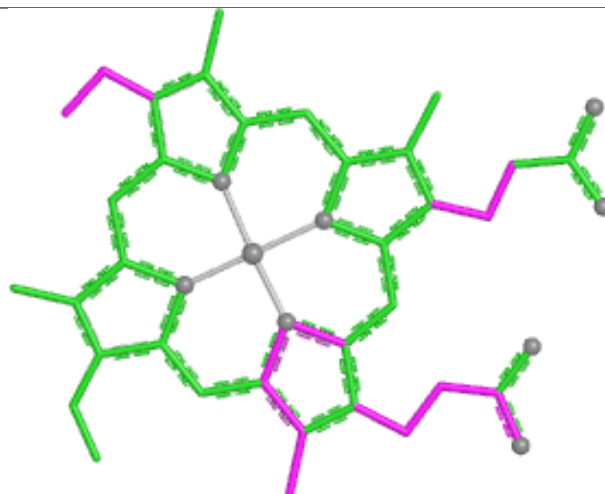


Rings

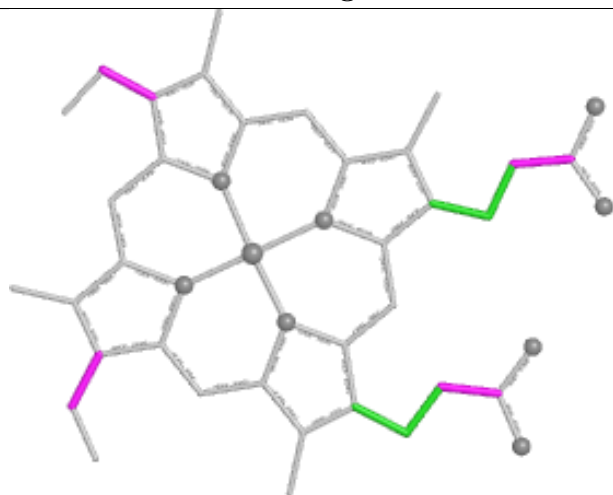
## Ligand HEC A 1115



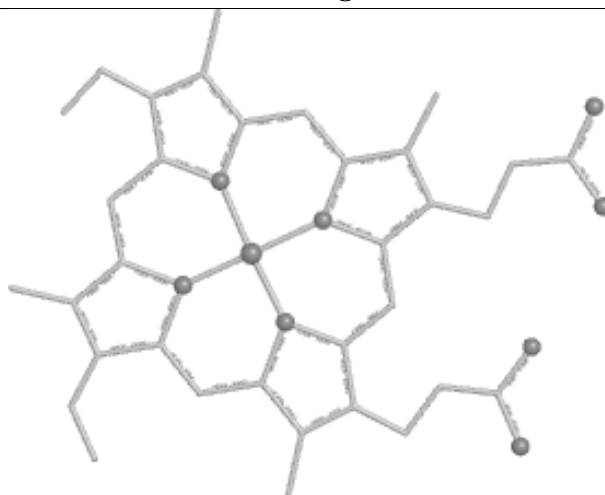
Bond lengths



Bond angles

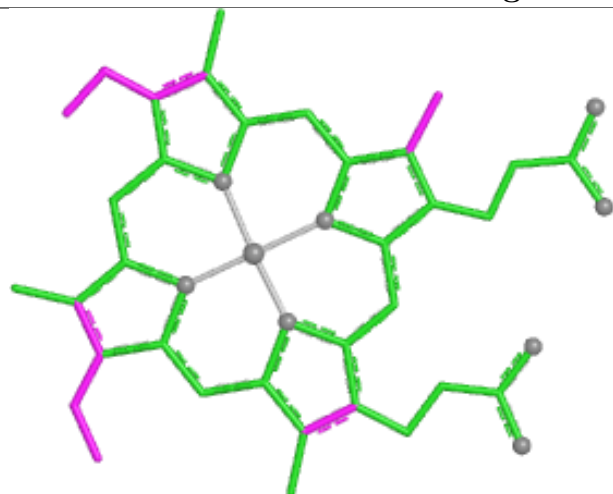


Torsions

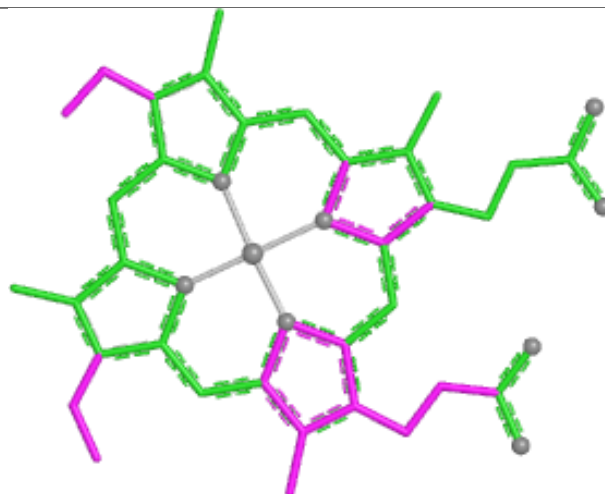


Rings

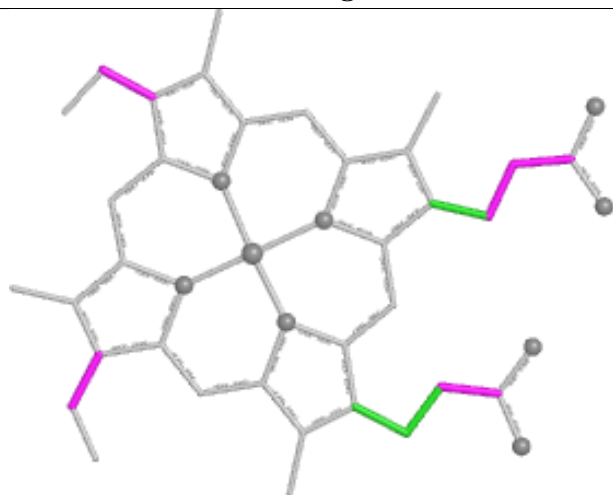
## Ligand HEC D 1108



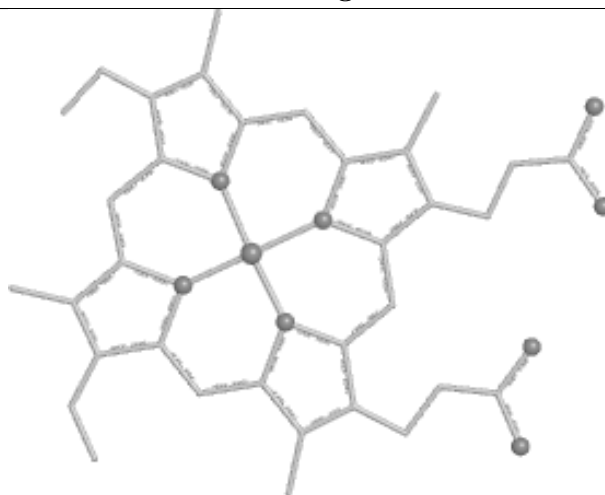
Bond lengths



Bond angles

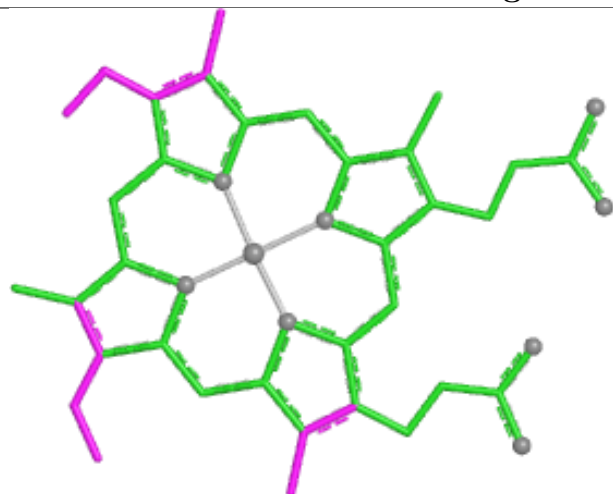


Torsions

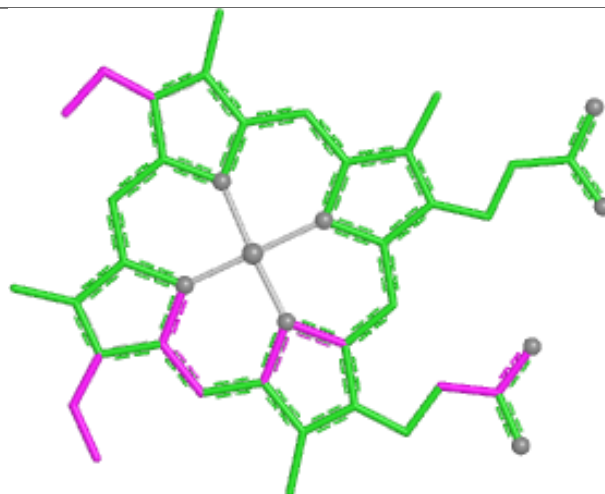


Rings

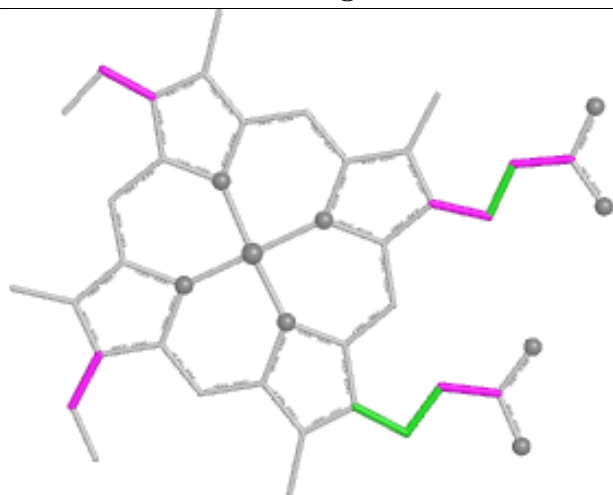
## Ligand HEC A 1105



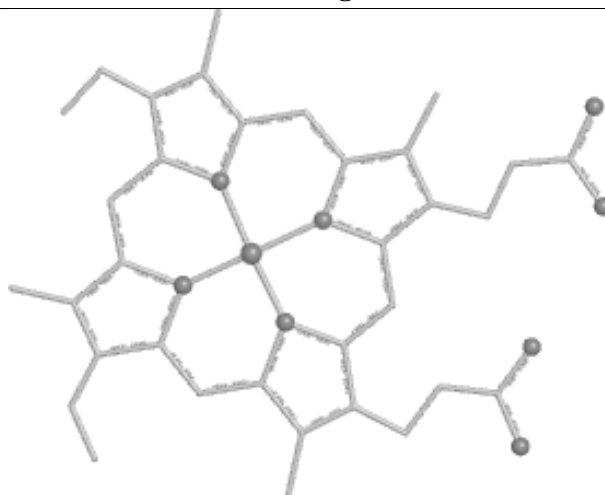
Bond lengths



Bond angles

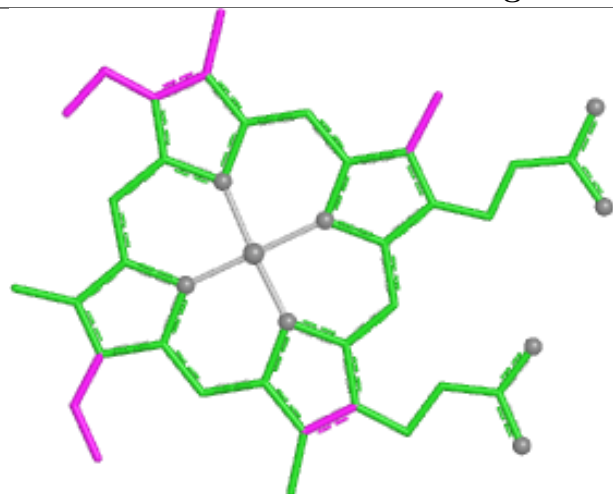


Torsions

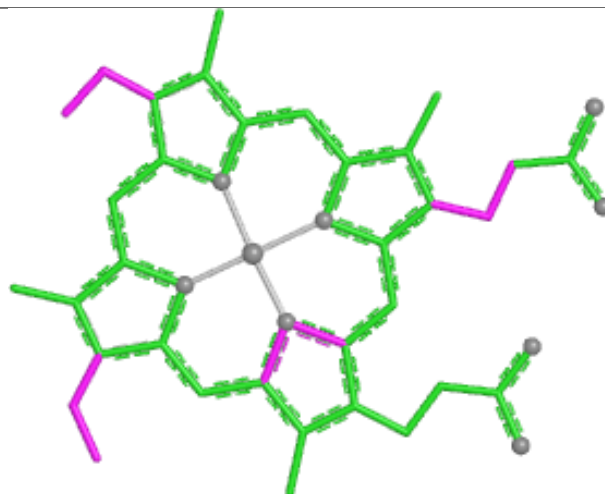


Rings

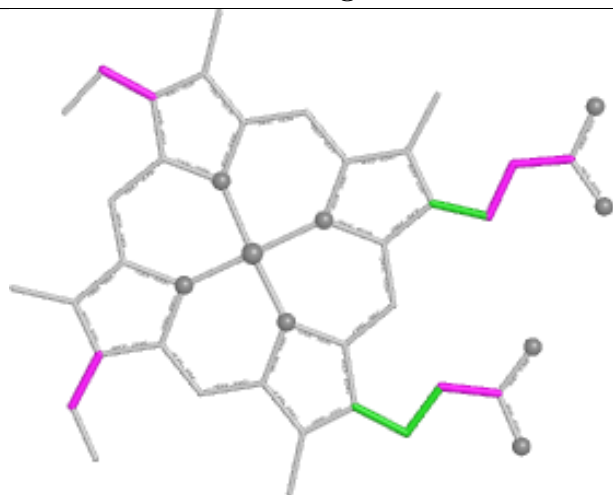
## Ligand HEC C 1109



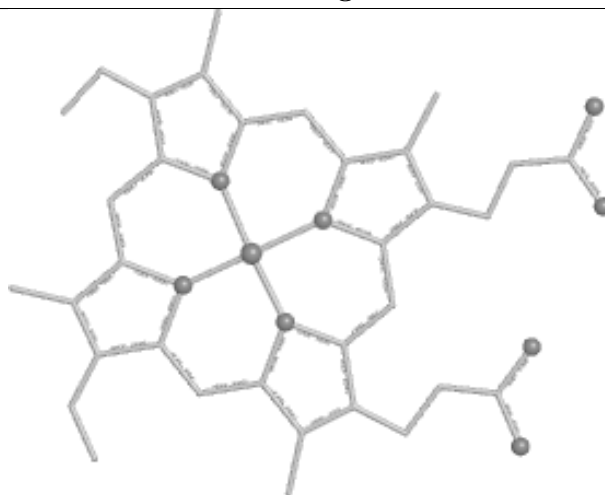
Bond lengths



Bond angles

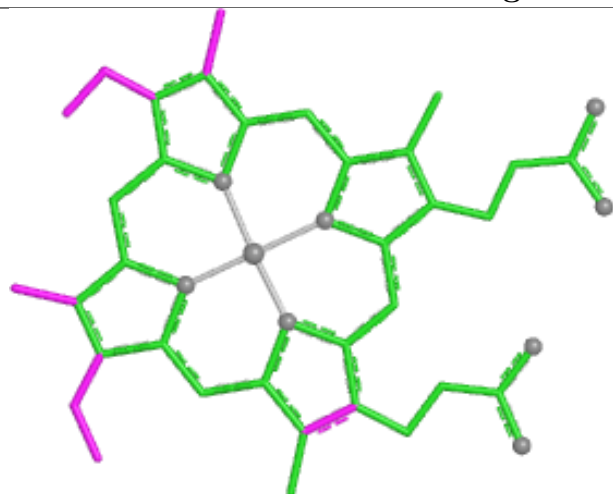


Torsions

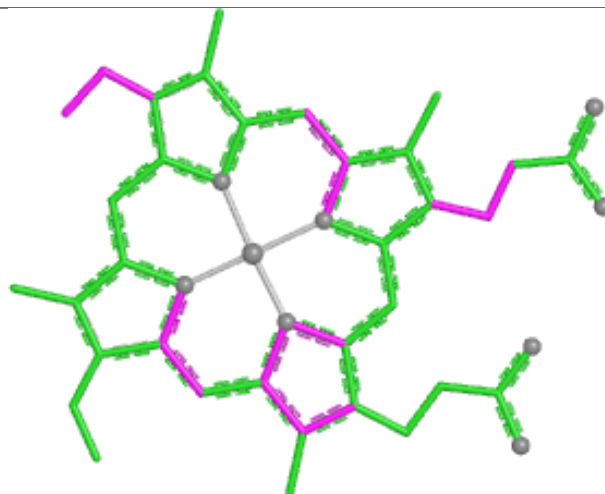


Rings

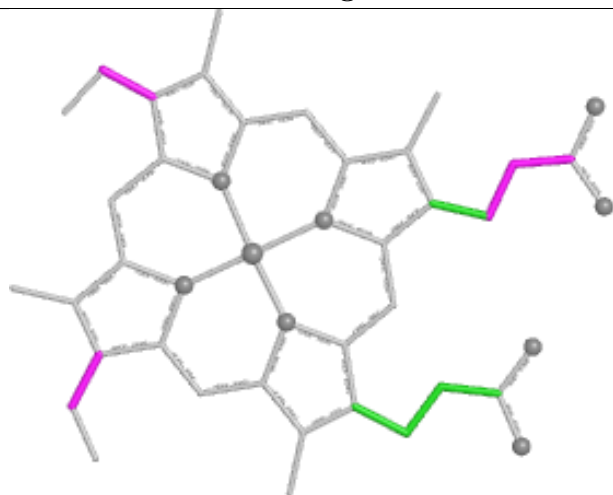
## Ligand HEC D 1104



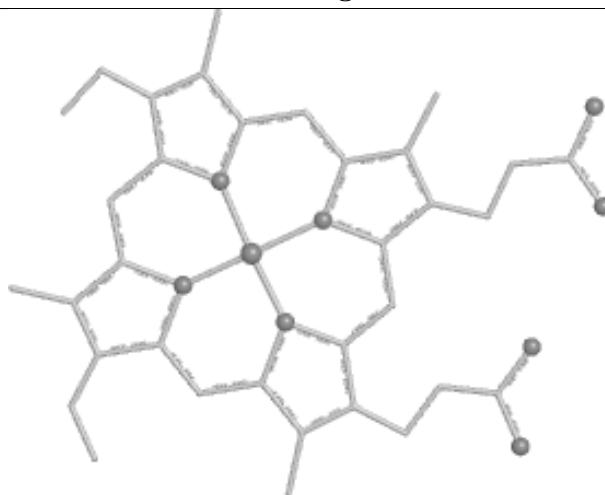
Bond lengths



Bond angles

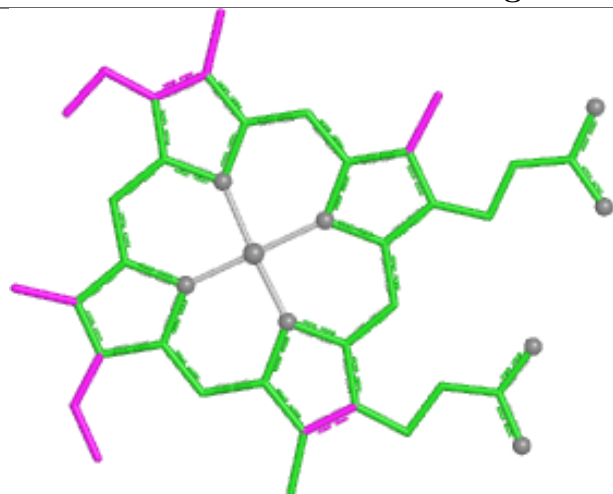


Torsions

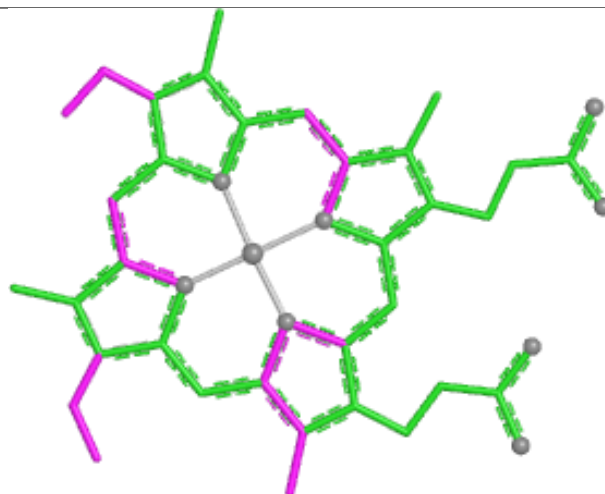


Rings

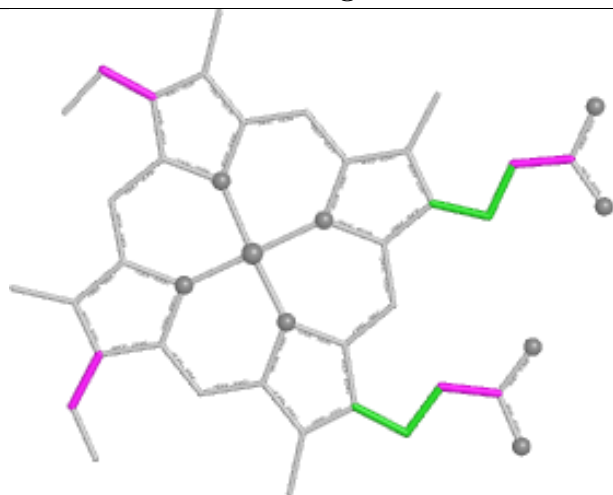
## Ligand HEC B 1112



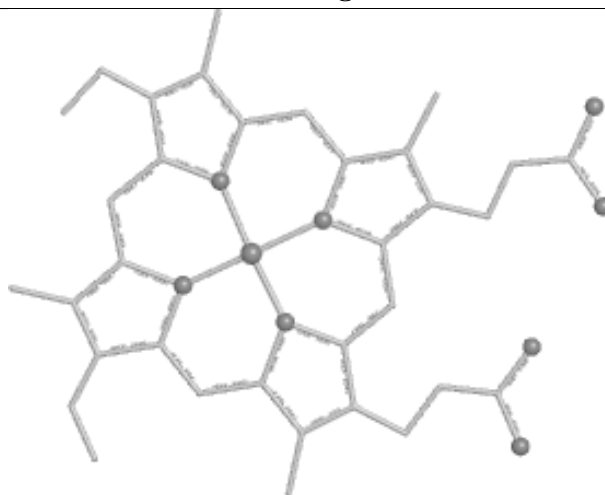
Bond lengths



Bond angles

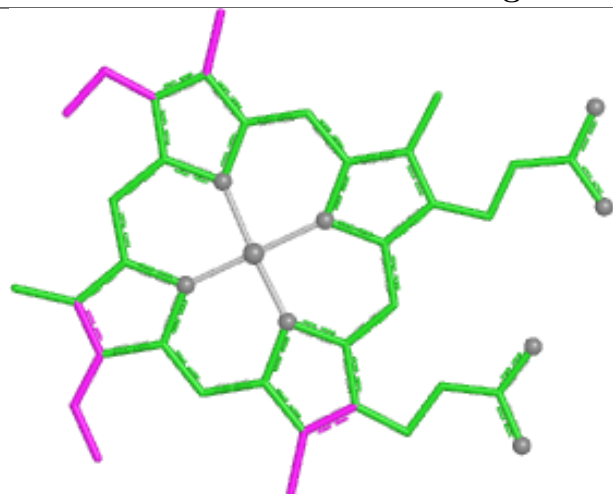


Torsions

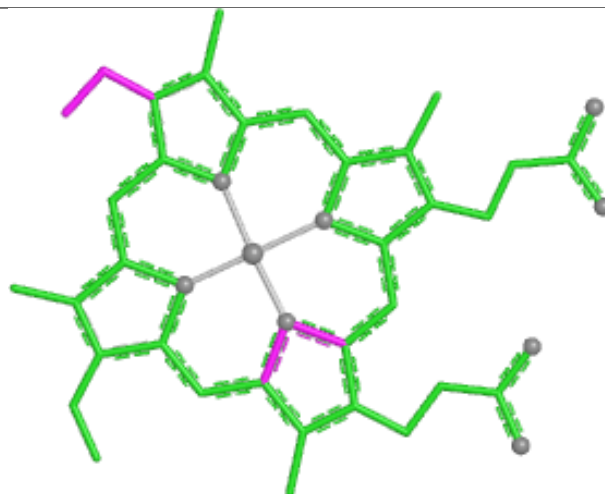


Rings

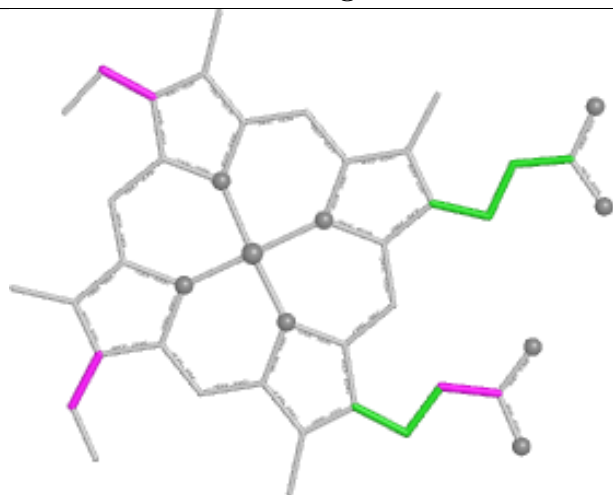
## Ligand HEC D 1106



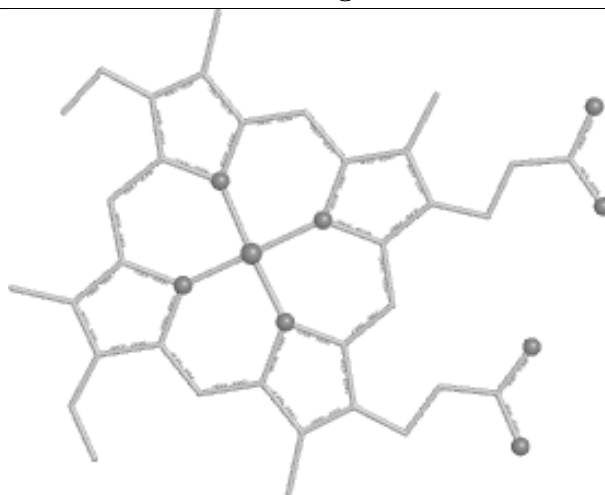
Bond lengths



Bond angles

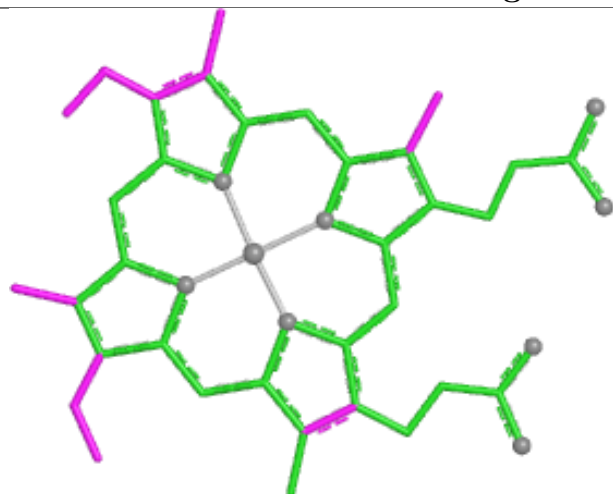


Torsions

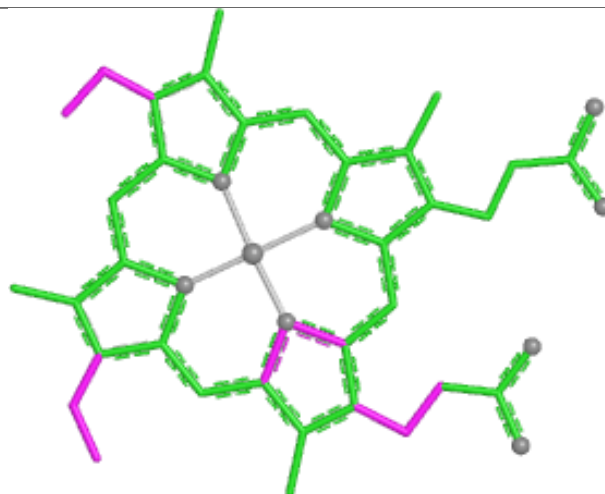


Rings

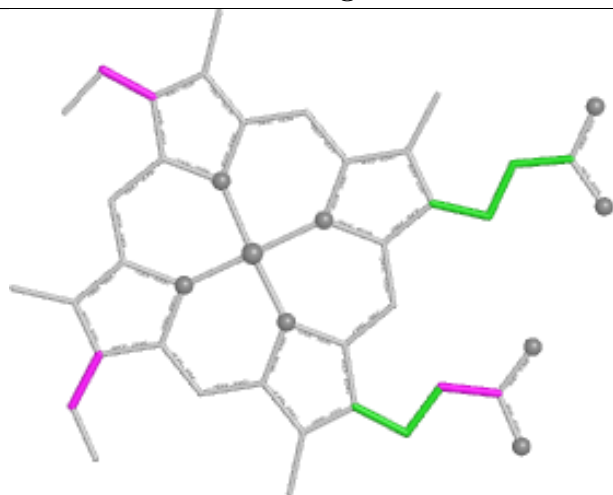
## Ligand HEC A 1112



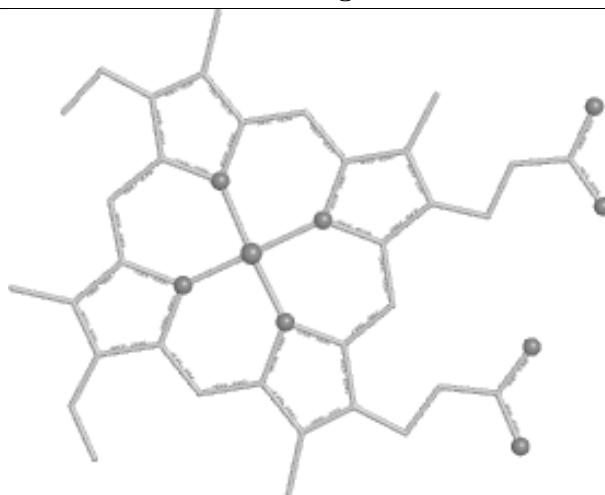
Bond lengths



Bond angles

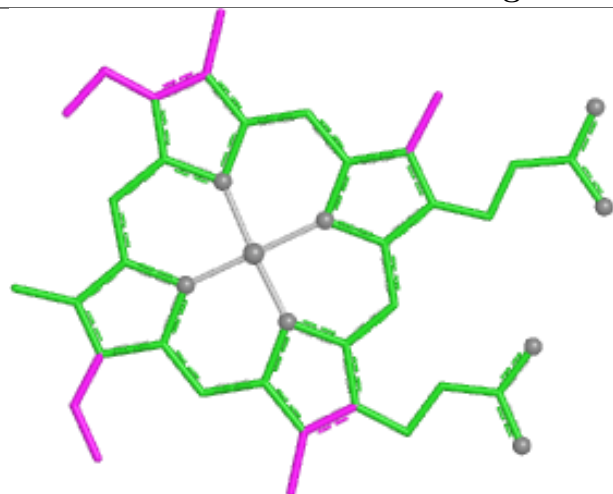


Torsions

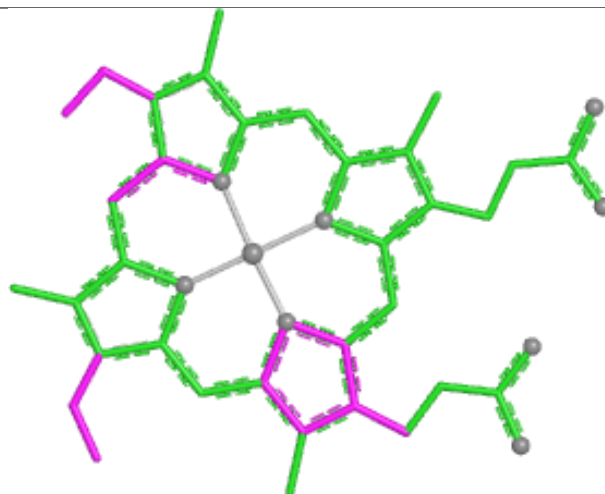


Rings

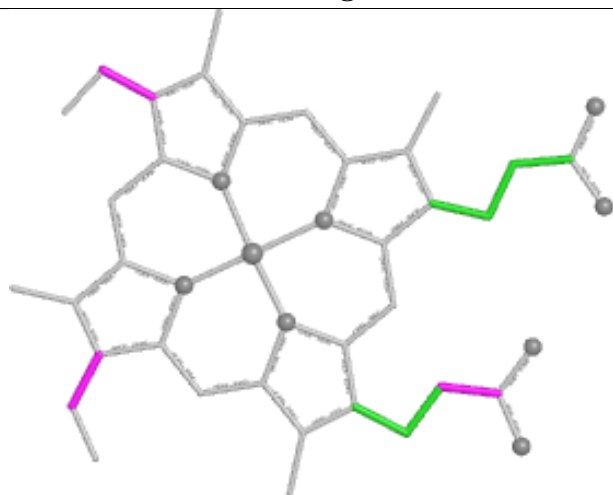
## Ligand HEC D 1115



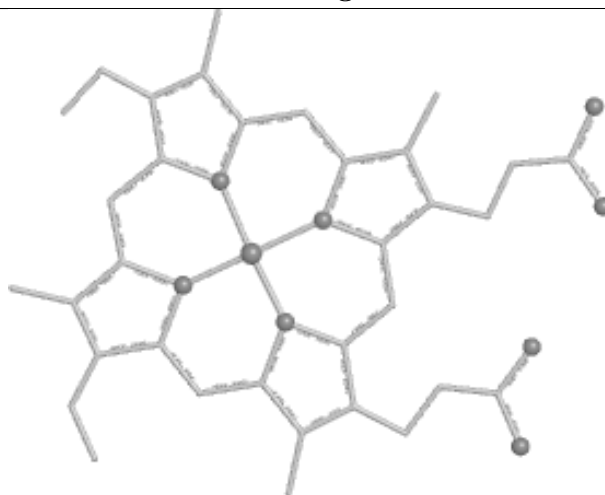
Bond lengths



Bond angles

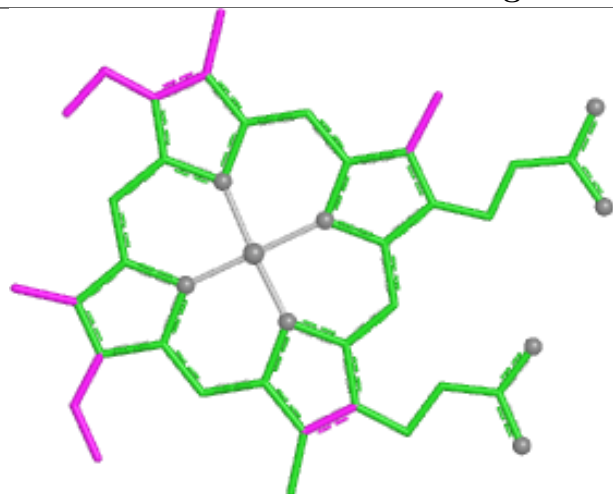


Torsions

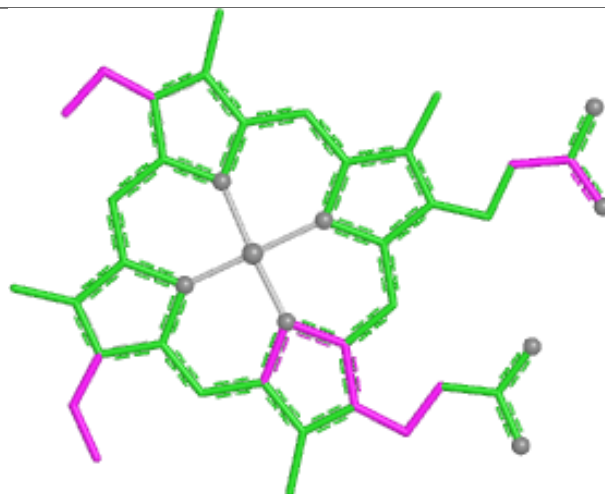


Rings

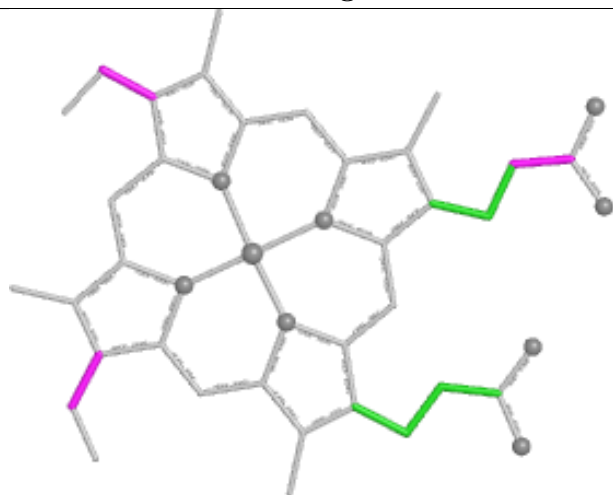
## Ligand HEC A 1103



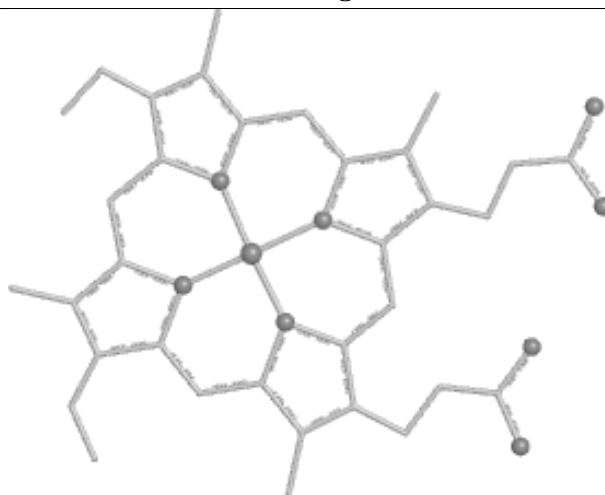
Bond lengths



Bond angles

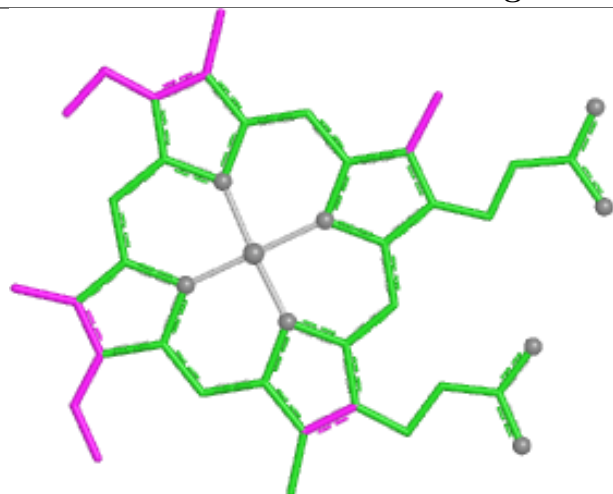


Torsions

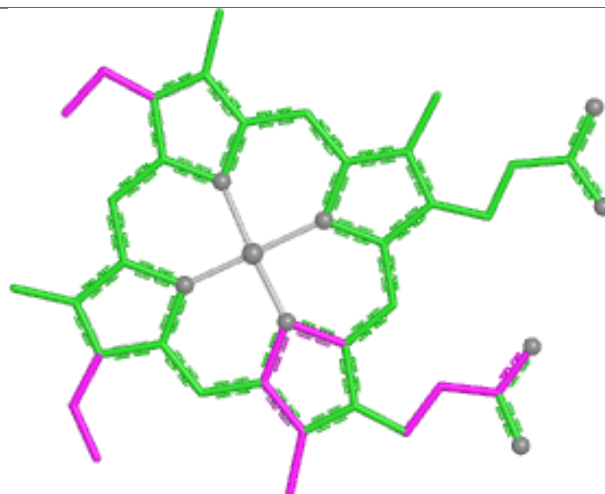


Rings

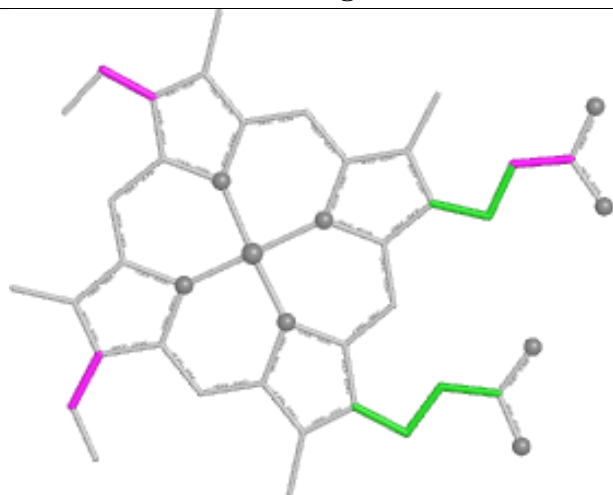
## Ligand HEC B 1111



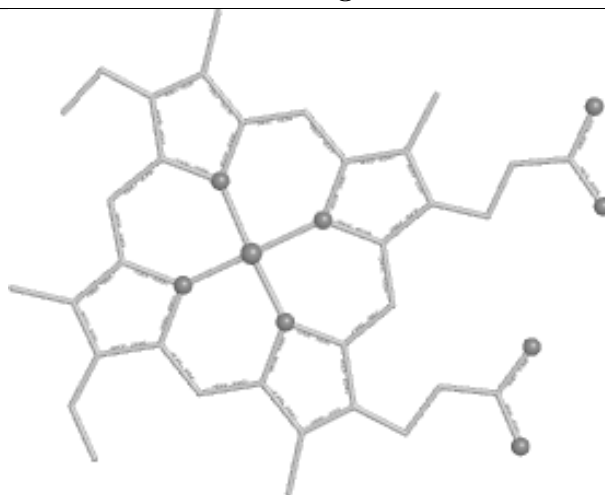
Bond lengths



Bond angles

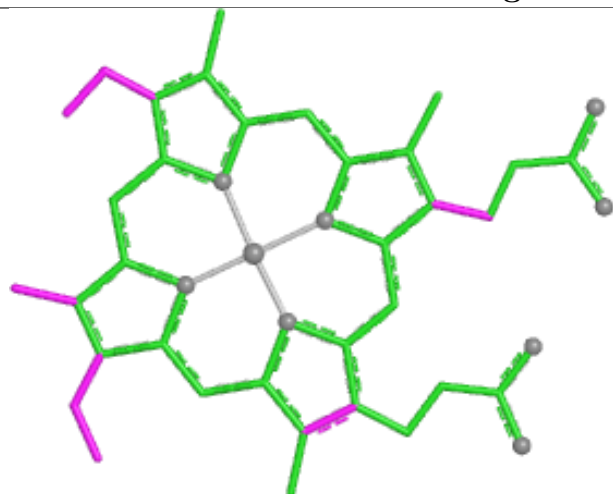


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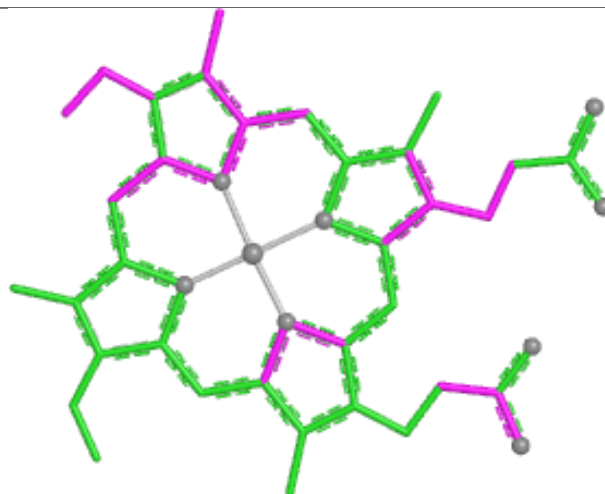


Rings

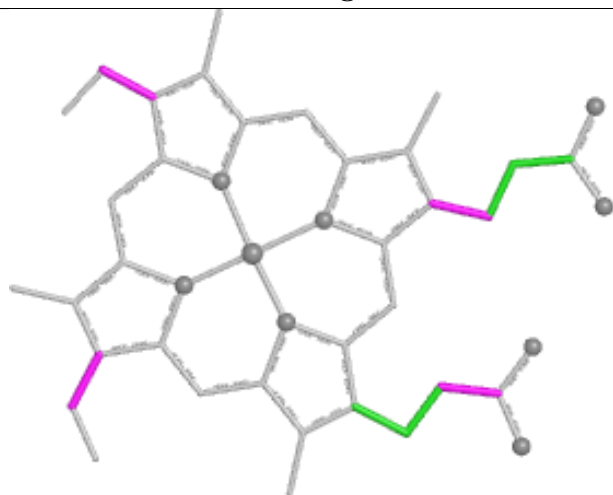
## Ligand HEC A 1107



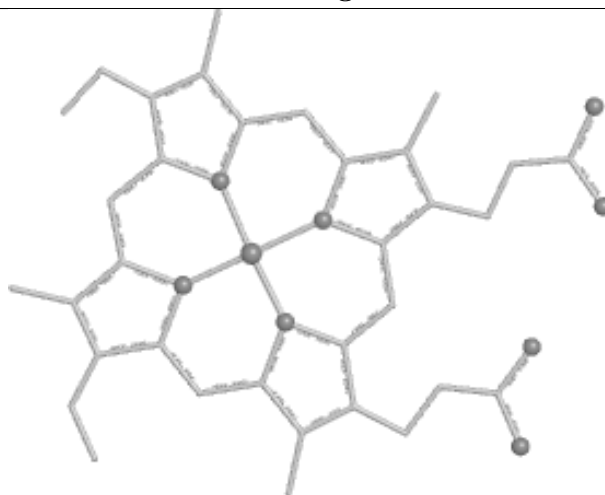
Bond lengths



Bond angles

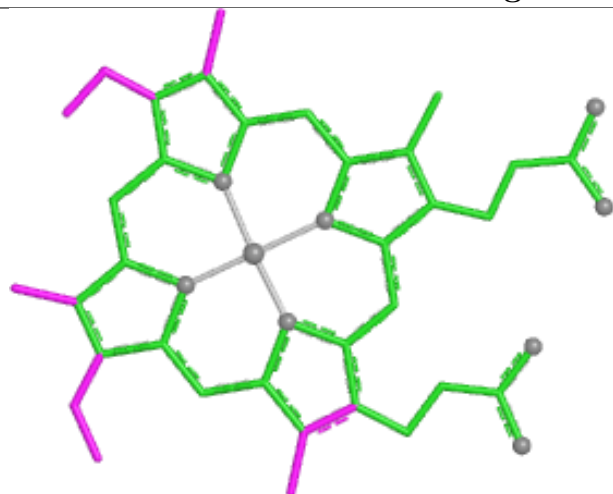


Torsions

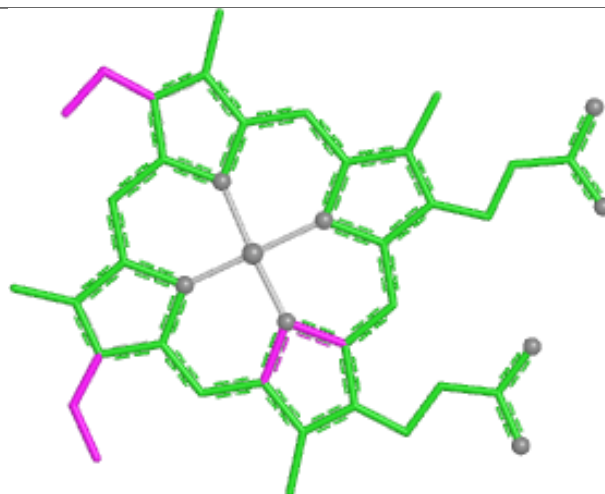


Rings

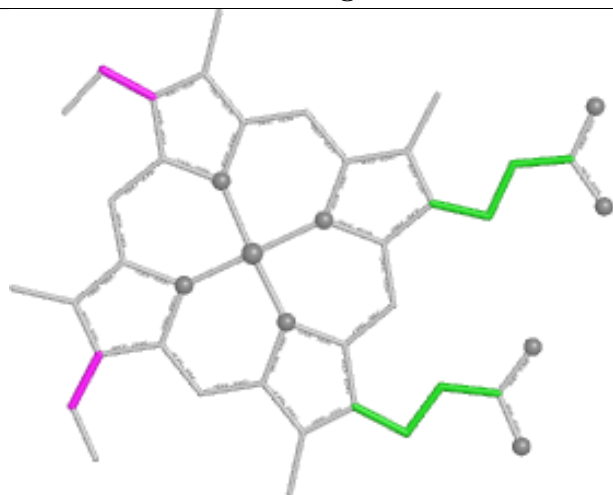
## Ligand HEC B 1114



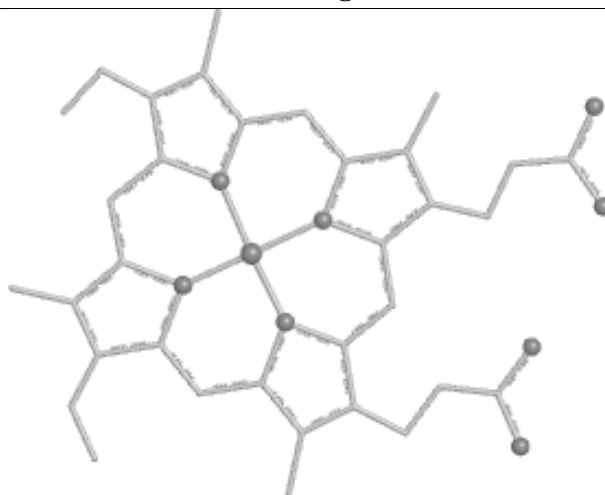
Bond lengths



Bond angles

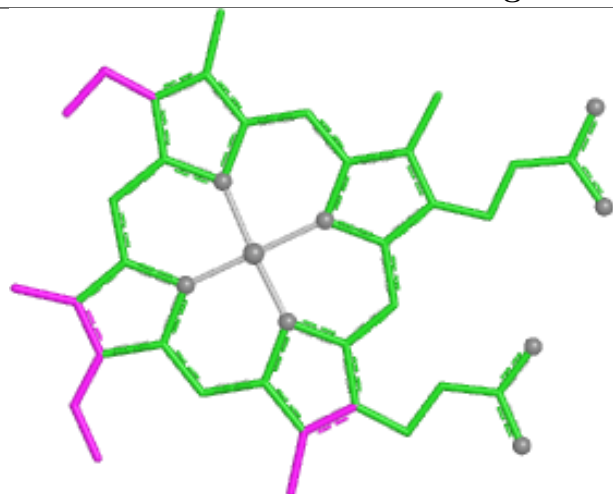


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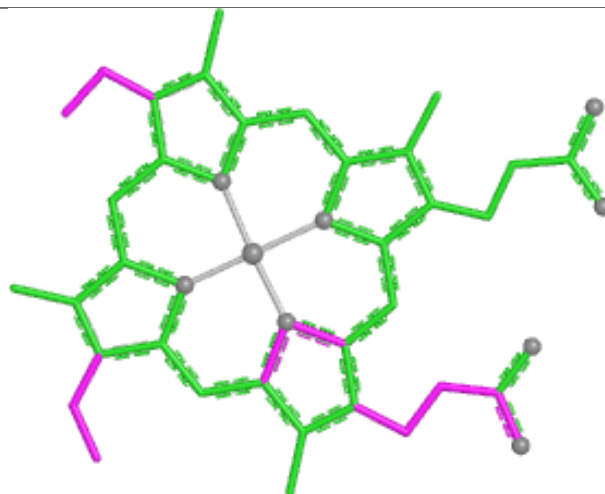


Rings

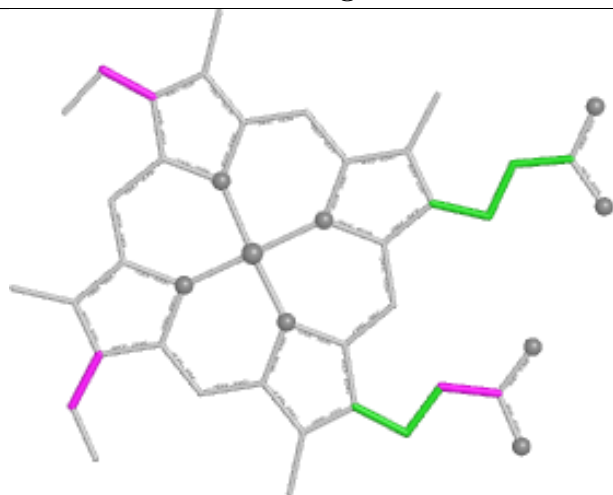
## Ligand HEC C 1116



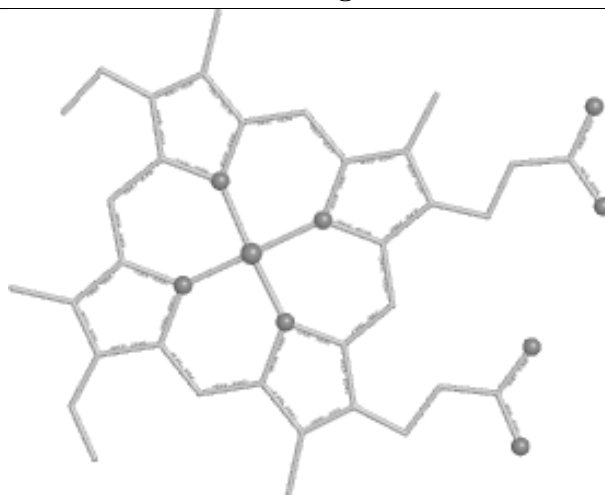
Bond lengths



Bond angles

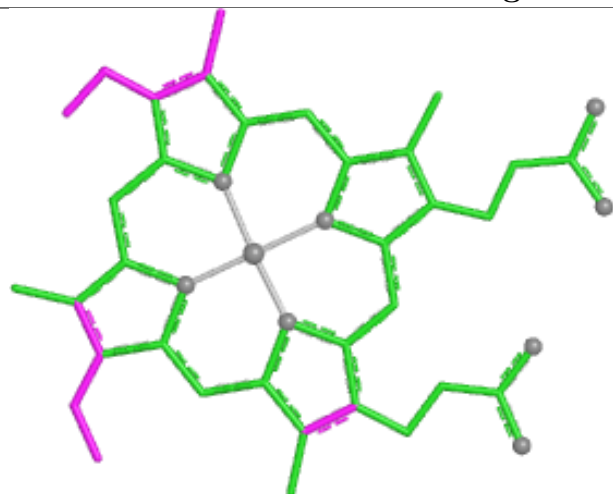


Torsions

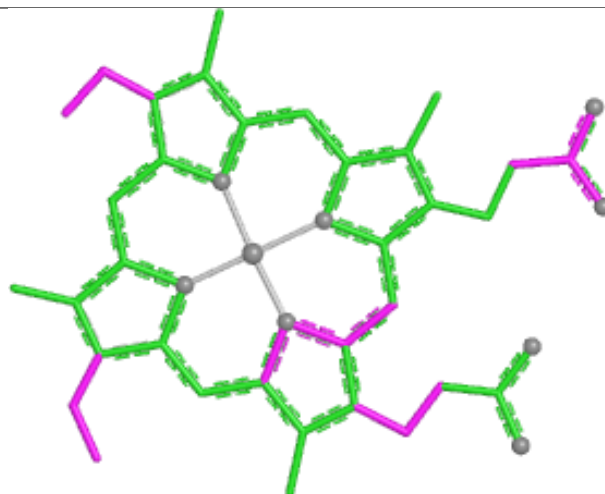


Rings

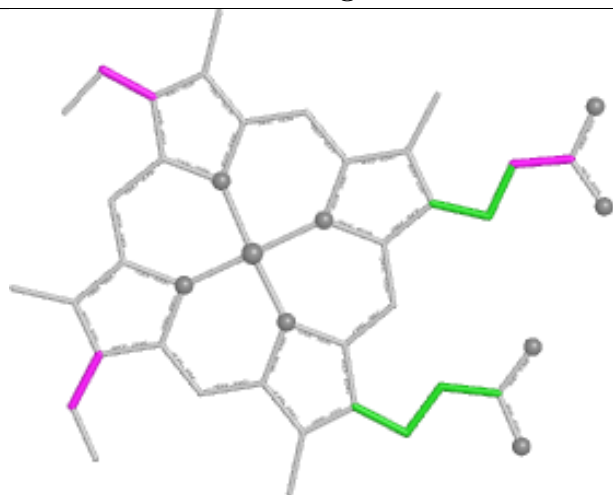
## Ligand HEC D 1103



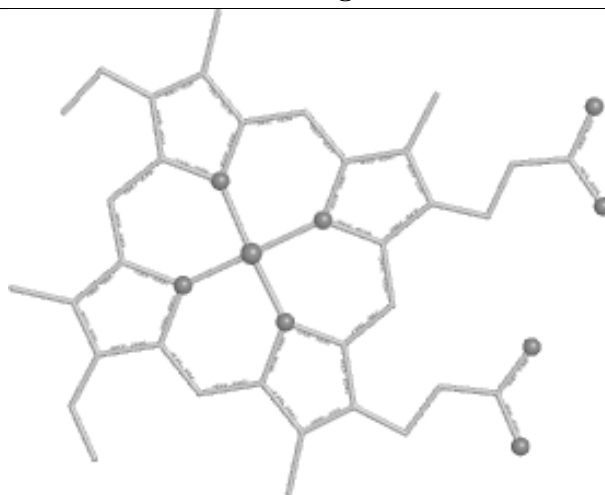
Bond lengths



Bond angles

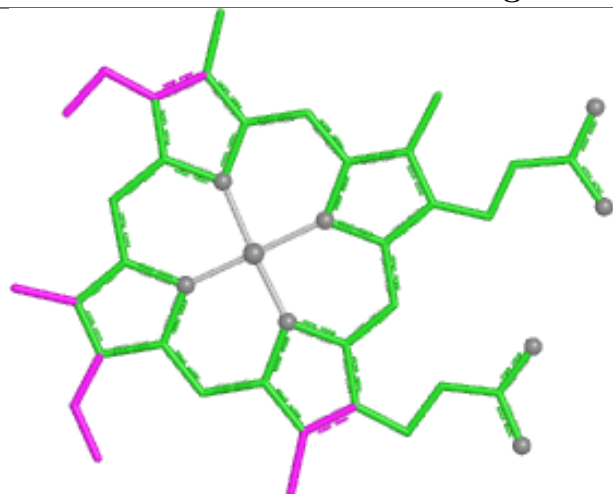


Torsions

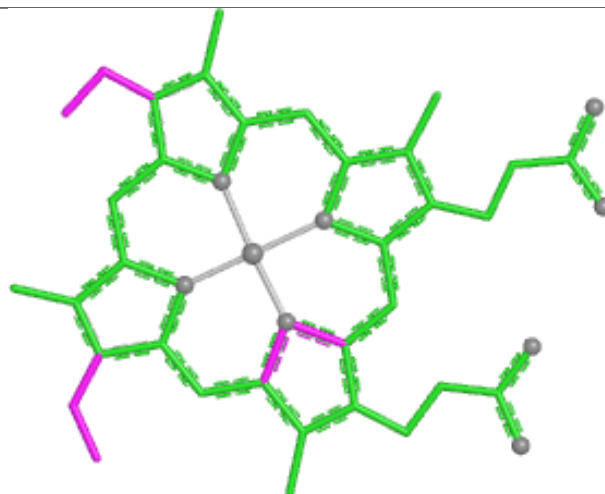


Rings

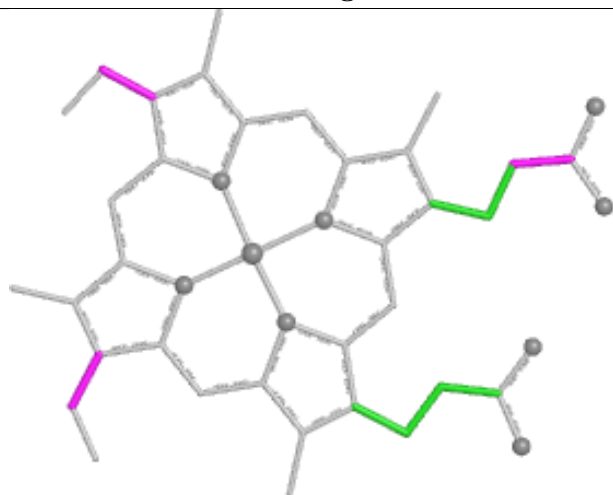
## Ligand HEC A 1110



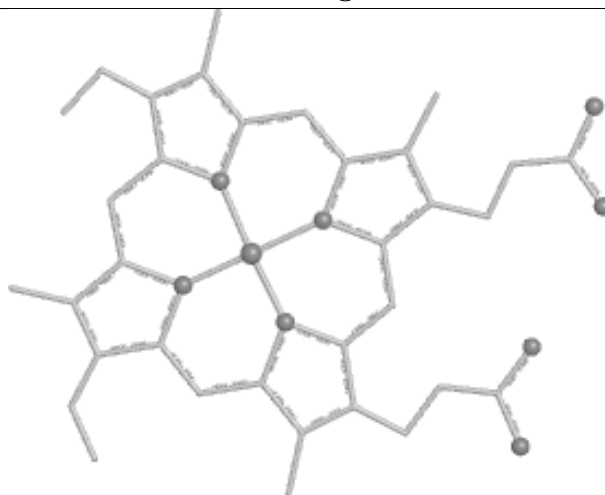
Bond lengths



Bond angles

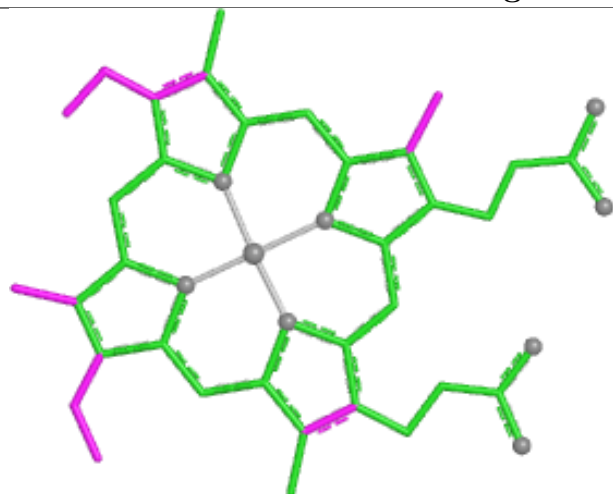


Torsions

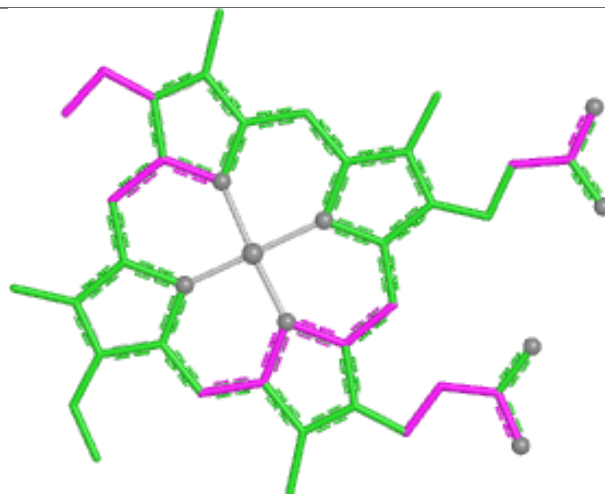


Rings

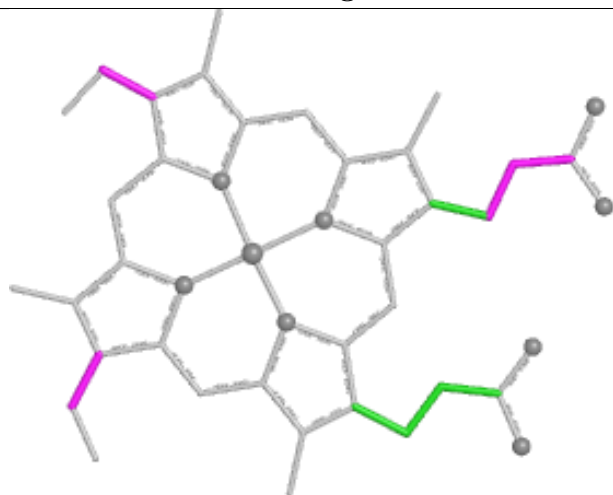
## Ligand HEC C 1110



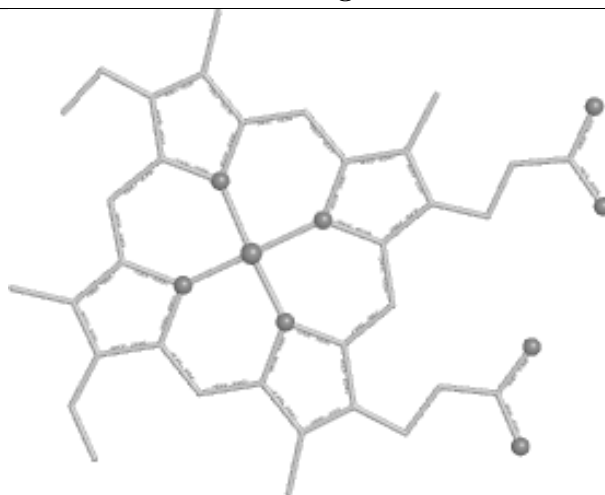
Bond lengths



Bond angles

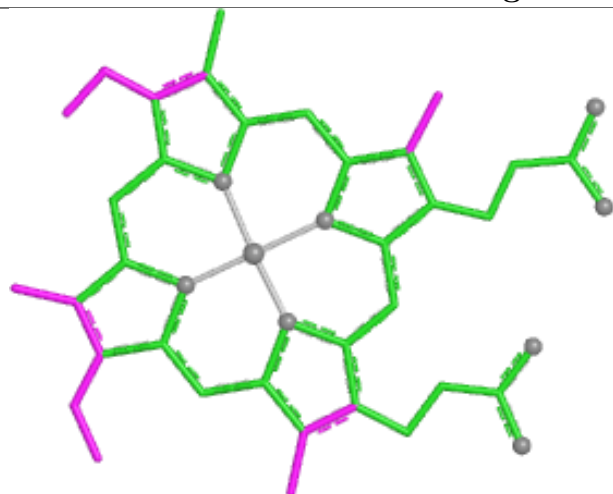


Torsions

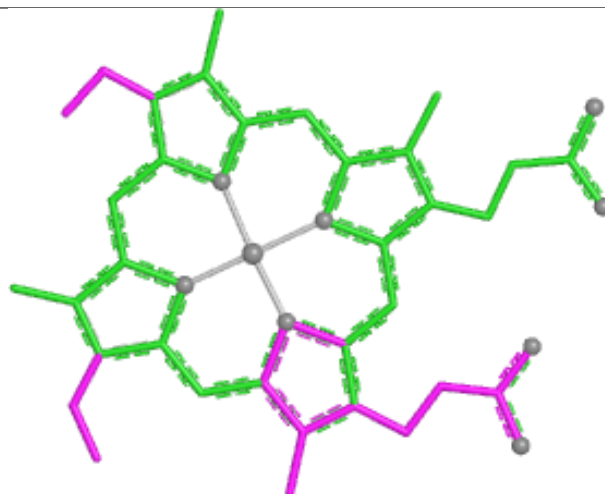


Rings

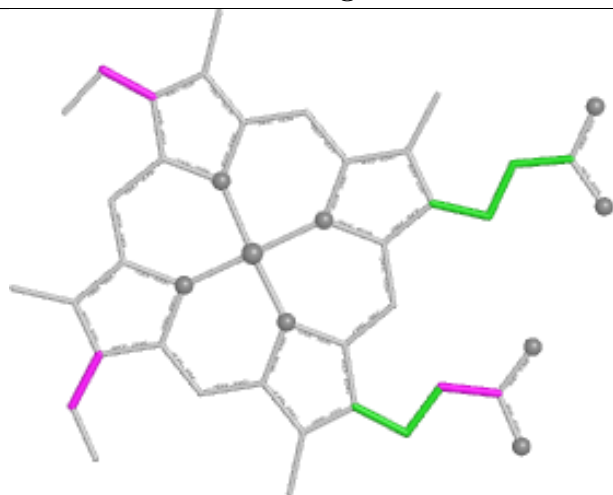
## Ligand HEC D 1116



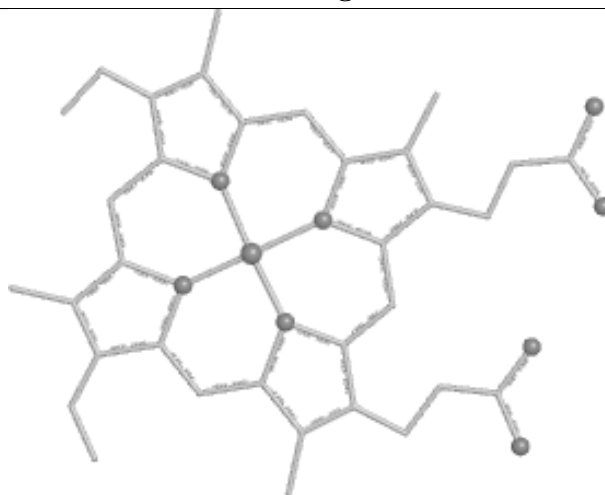
Bond lengths



Bond angles

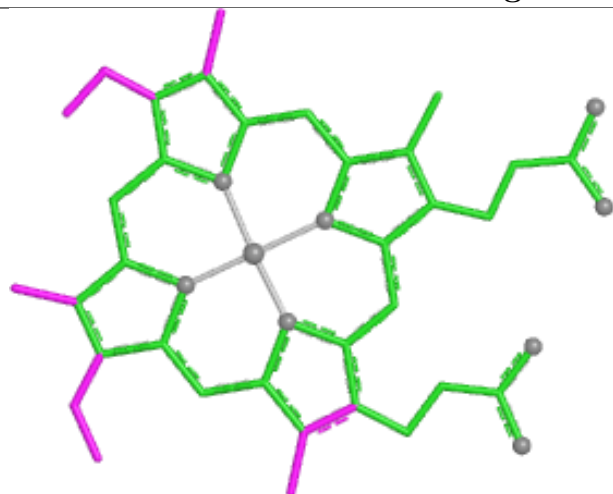


Torsions

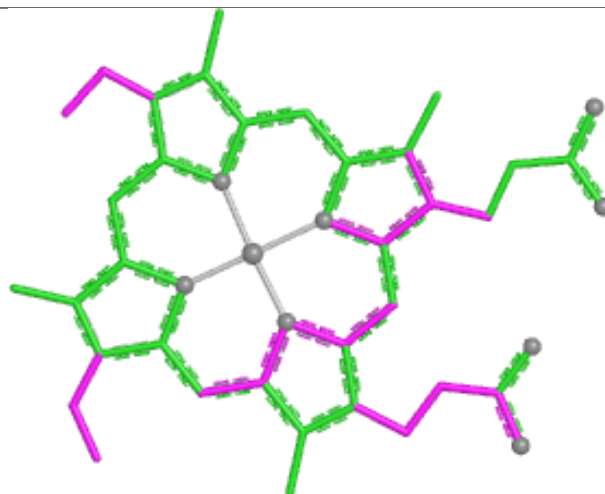


Rings

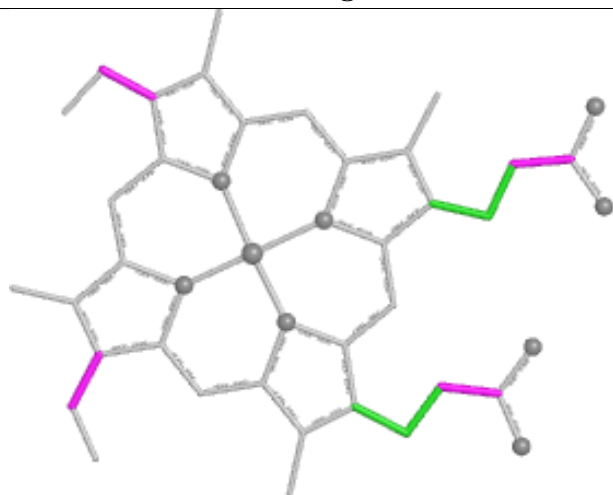
## Ligand HEC B 1110



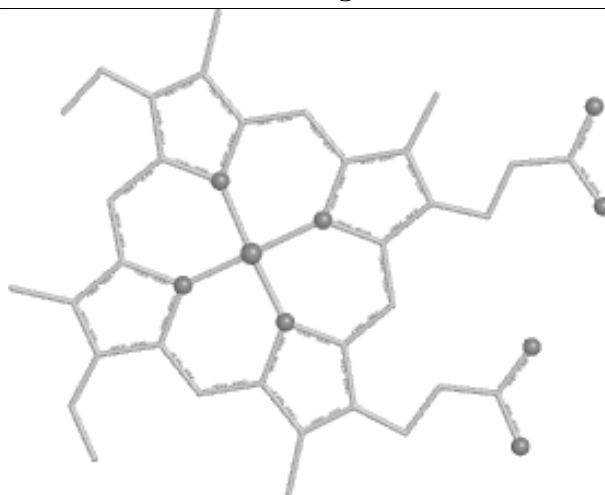
Bond lengths



Bond angles

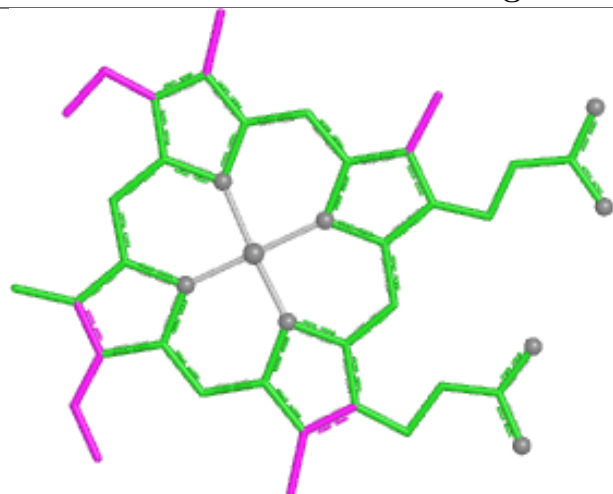


Torsions

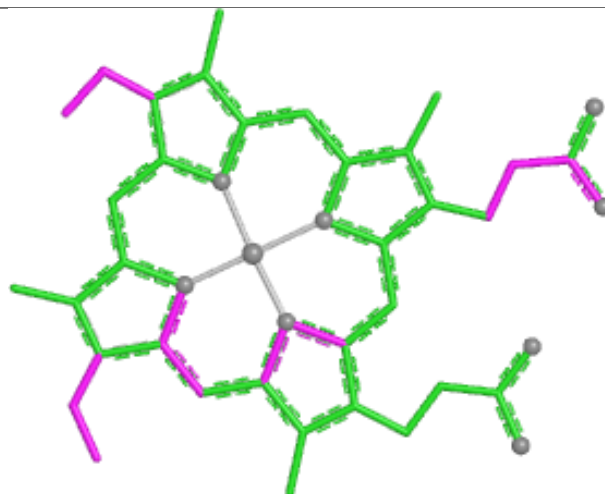


Rings

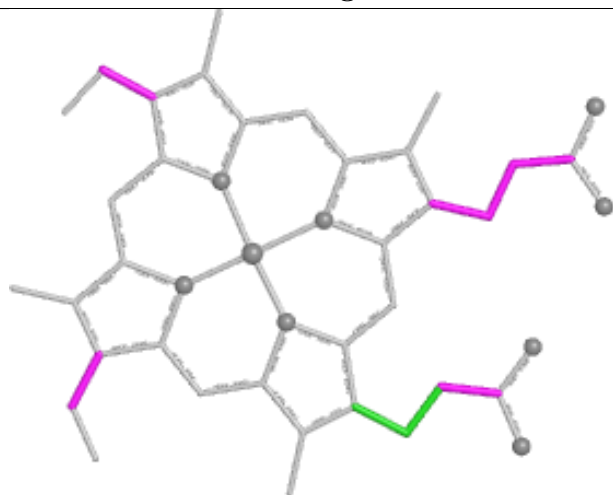
## Ligand HEC A 1109



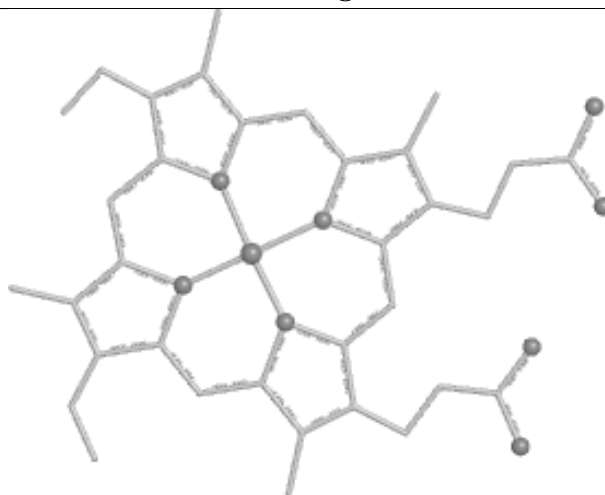
Bond lengths



Bond angles

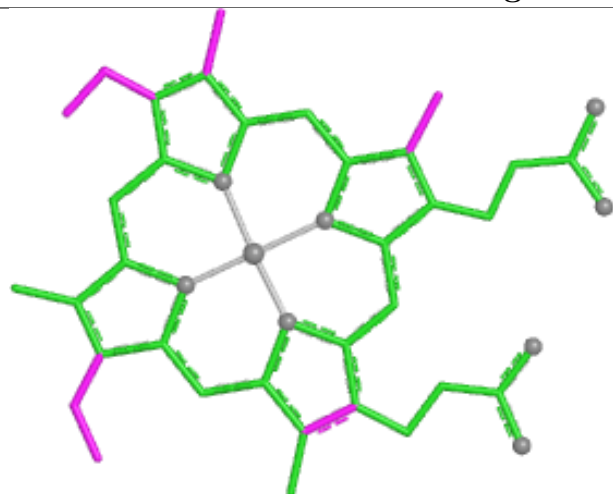


Torsions

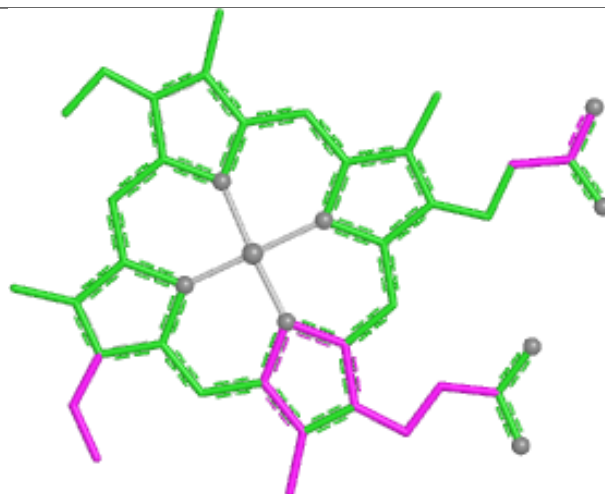


Rings

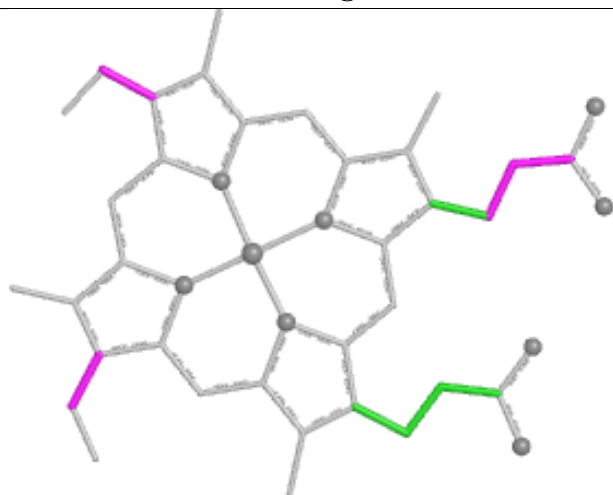
## Ligand HEC B 1104



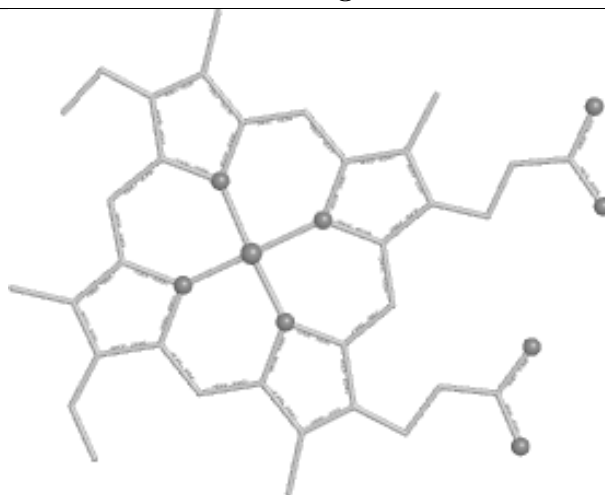
Bond lengths



Bond angles

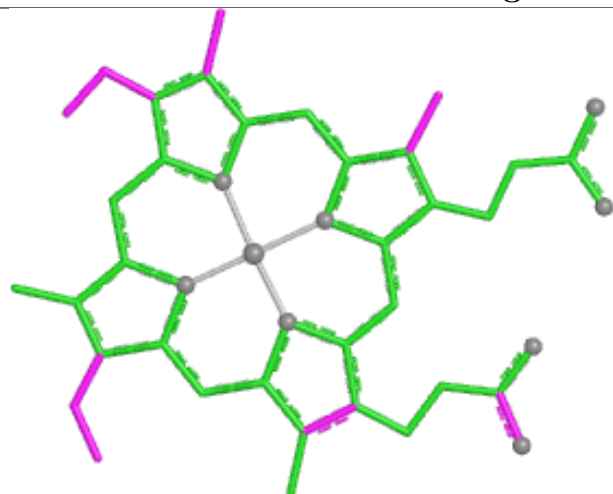


Torsions

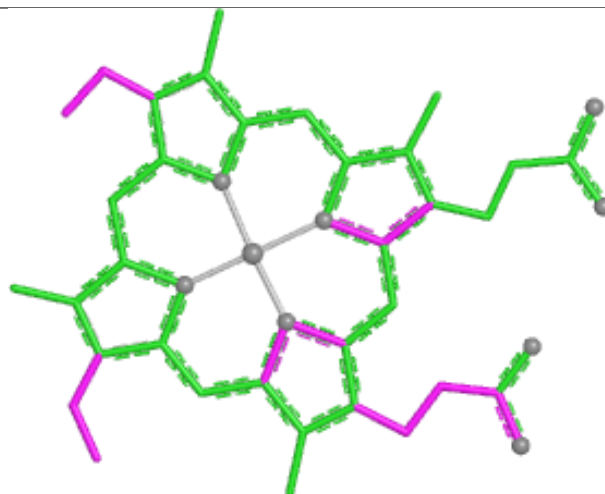


Rings

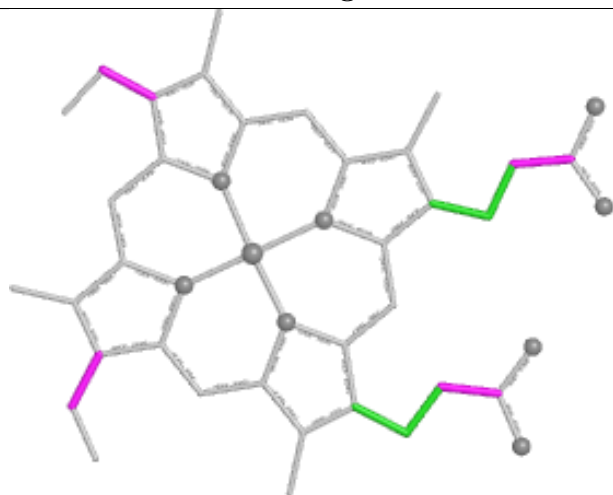
## Ligand HEC A 1108



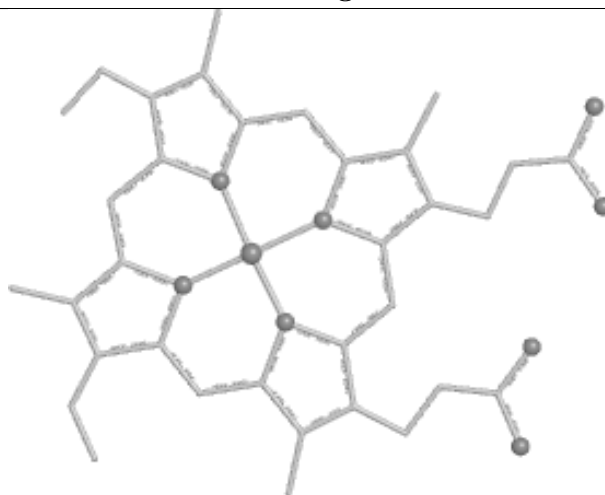
Bond lengths



Bond angles

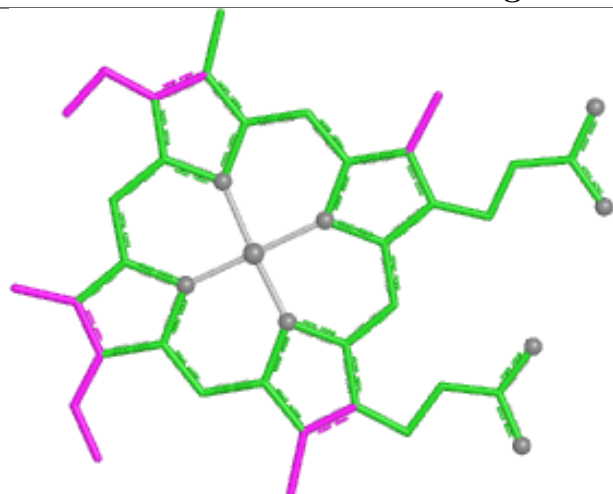


Torsions

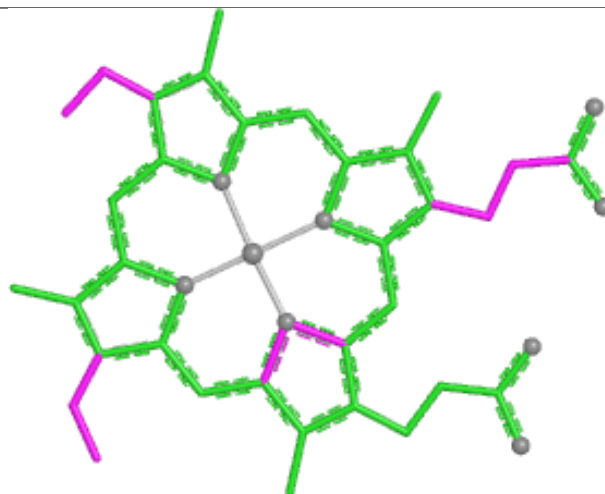


Rings

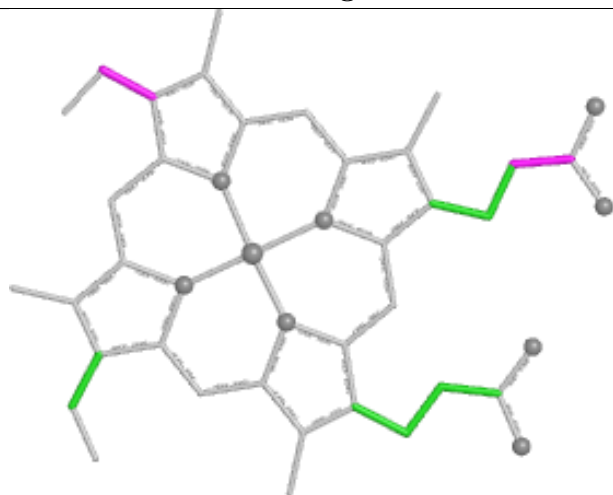
## Ligand HEC C 1102



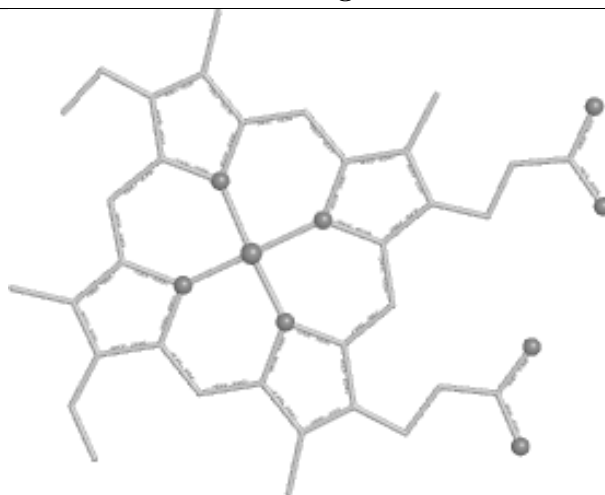
Bond lengths



Bond angles

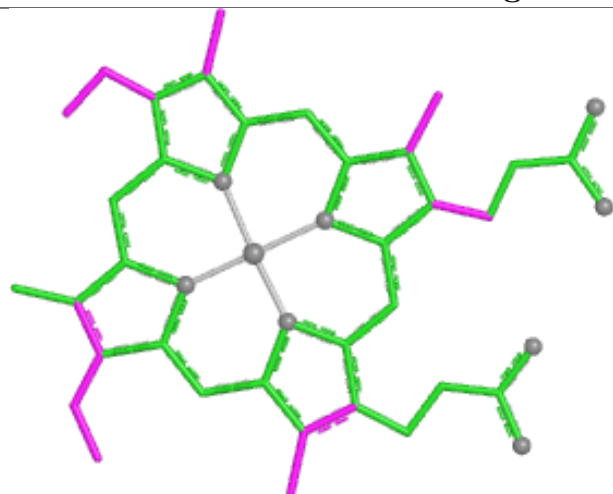


Torsions

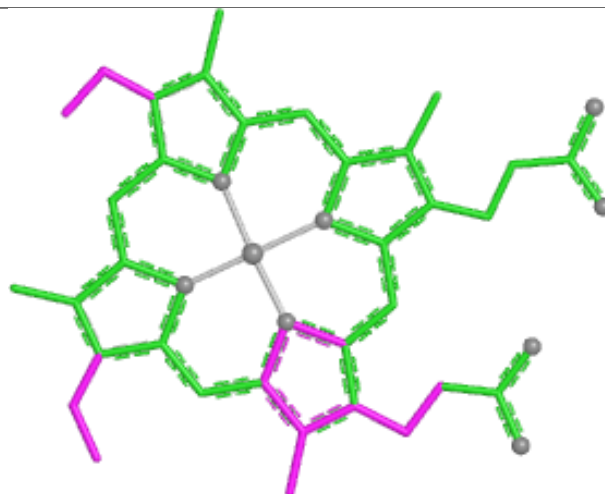


Rings

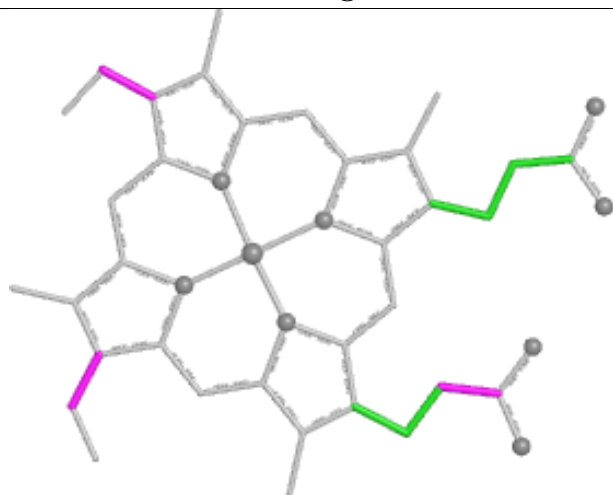
## Ligand HEC C 1106



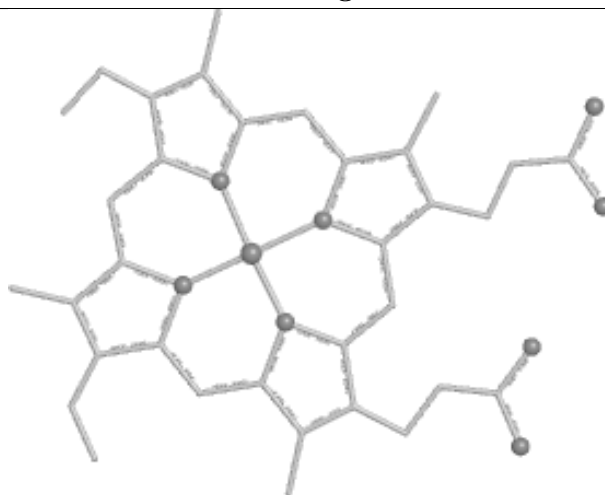
Bond lengths



Bond angles

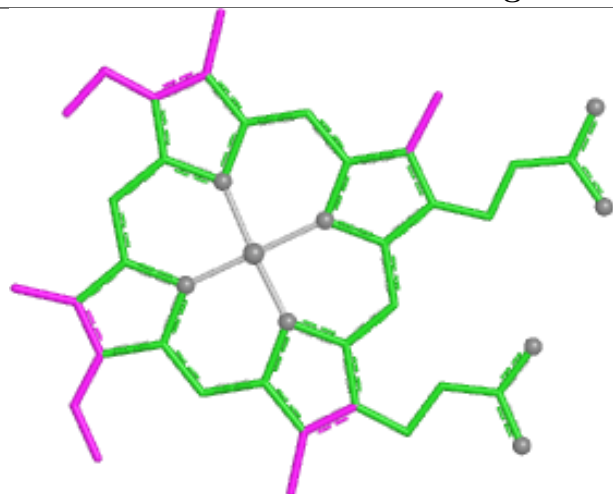


Torsions

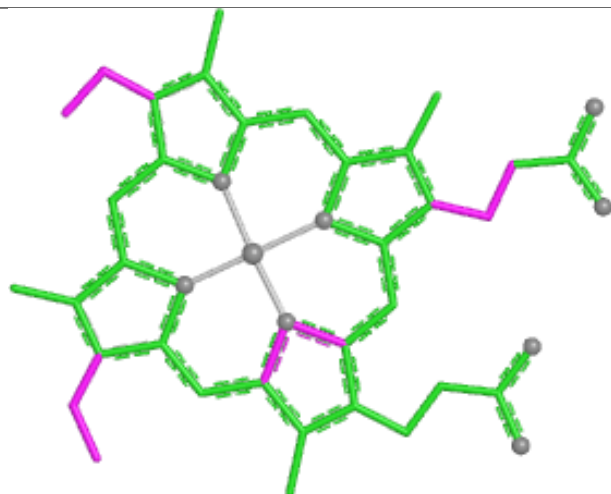


Rings

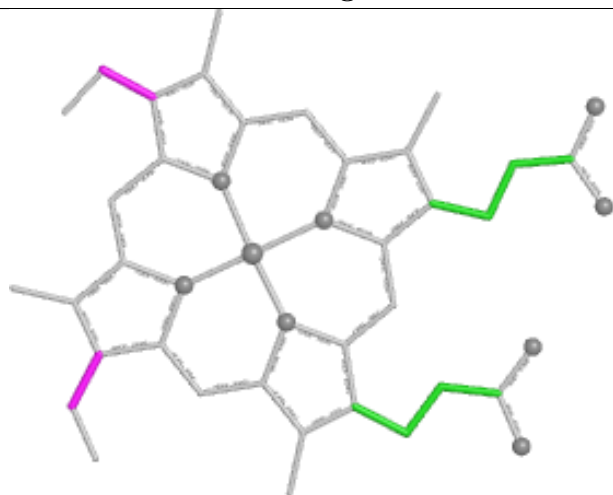
## Ligand HEC C 1114



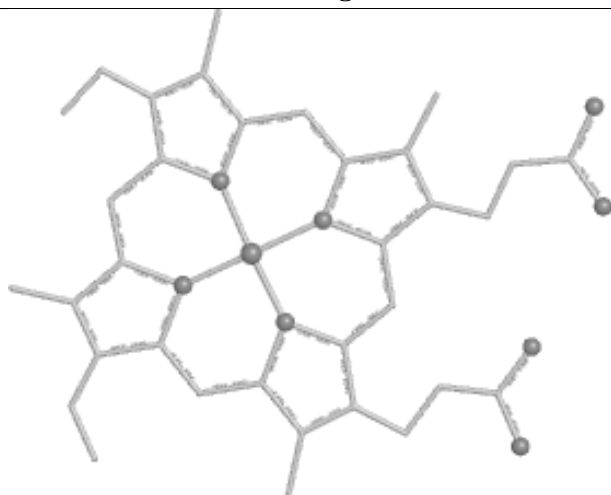
Bond lengths



Bond angles

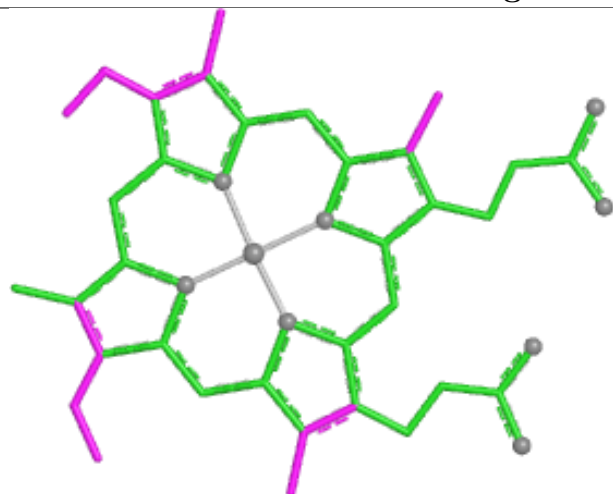


Torsions

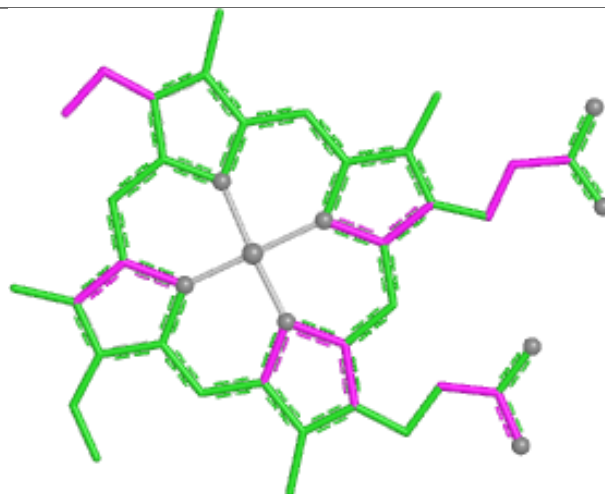


Rings

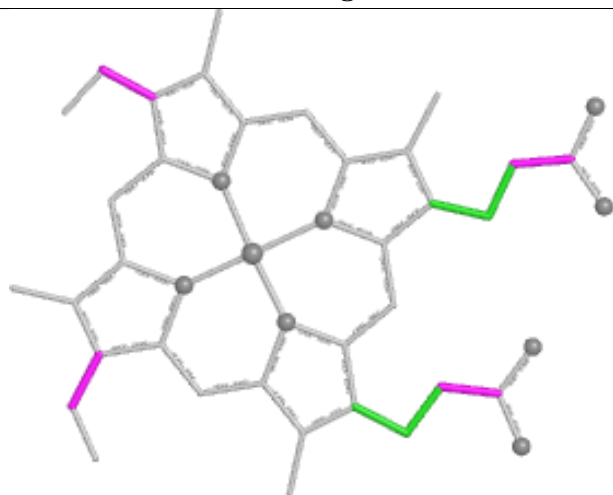
## Ligand HEC C 1115



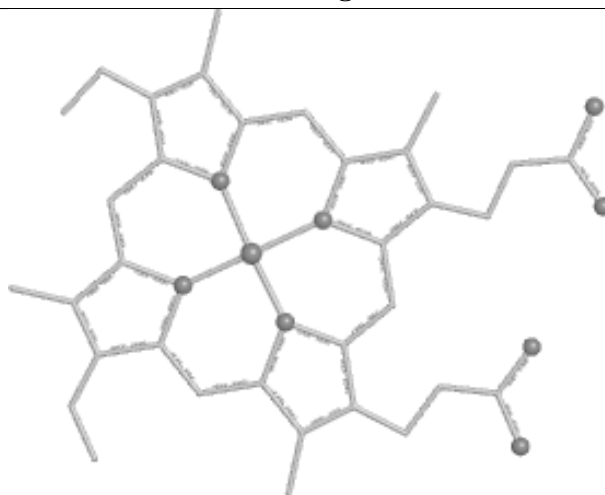
Bond lengths



Bond angles

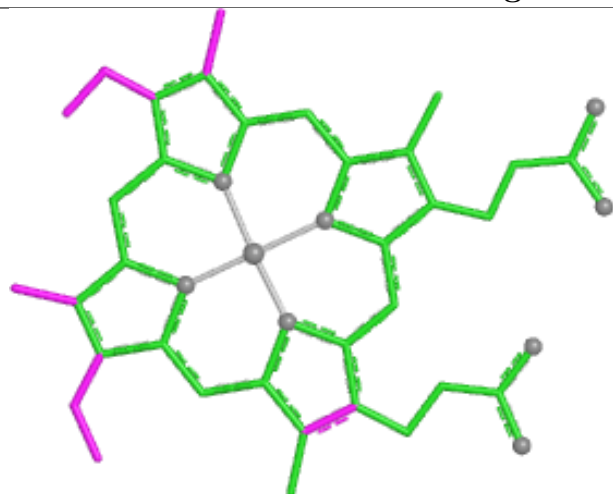


Torsions

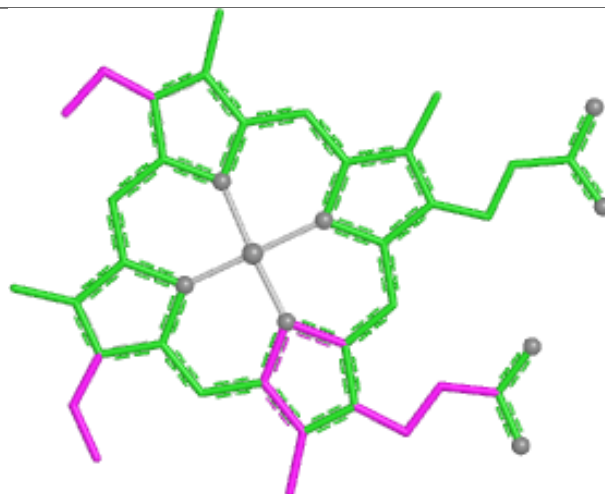


Rings

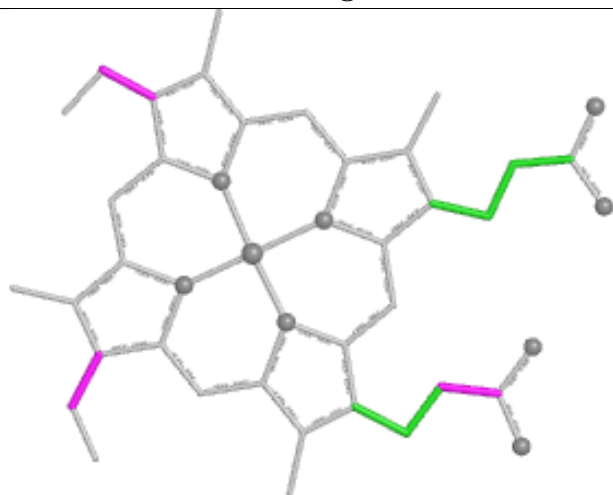
## Ligand HEC B 1106



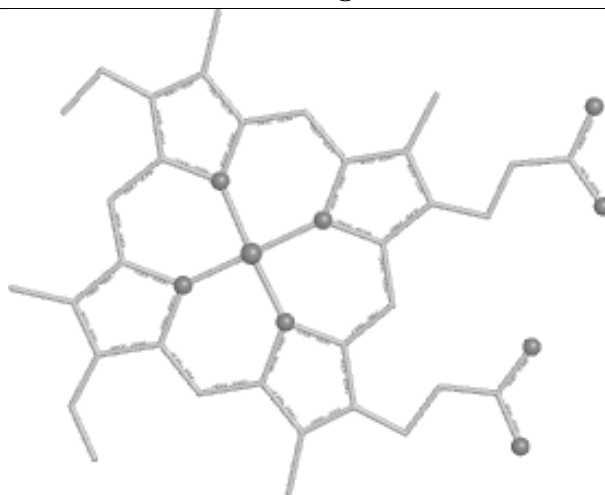
Bond lengths



Bond angles

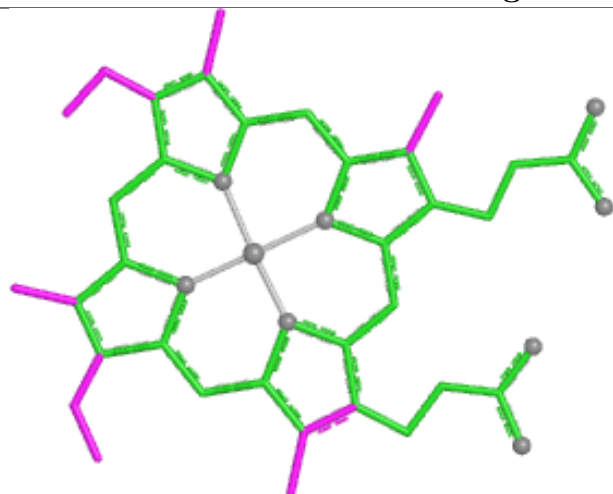


Torsions

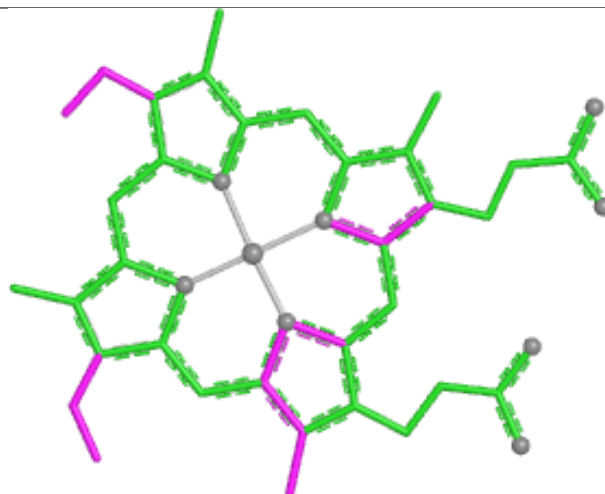


Rings

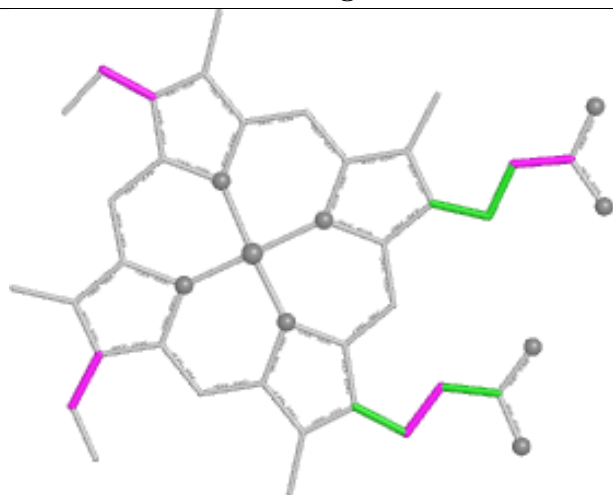
## Ligand HEC D 1111



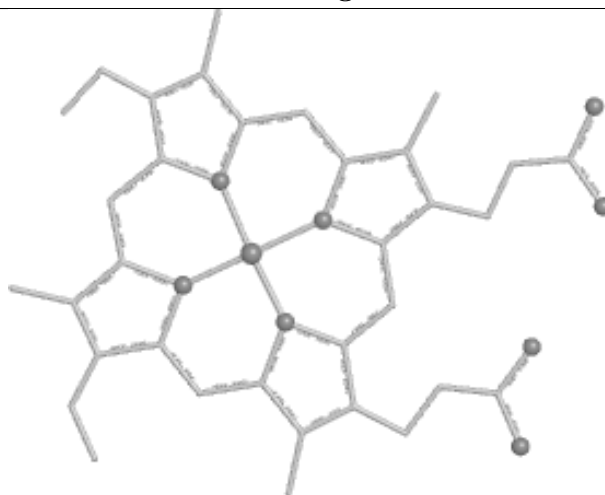
Bond lengths



Bond angles

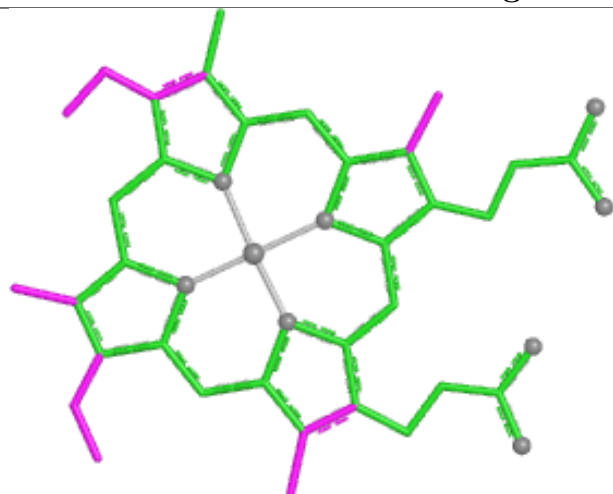


Torsions

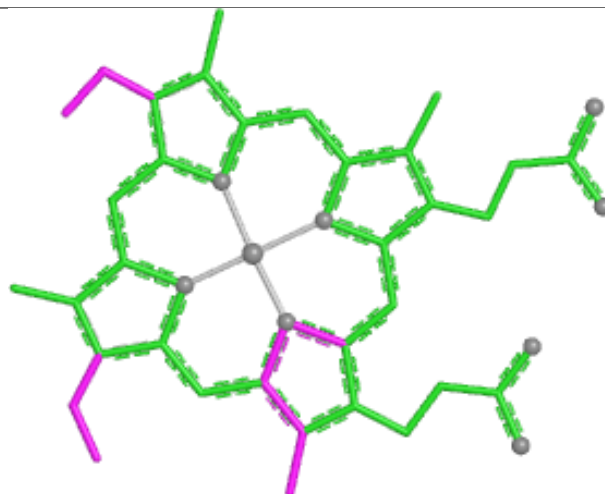


Rings

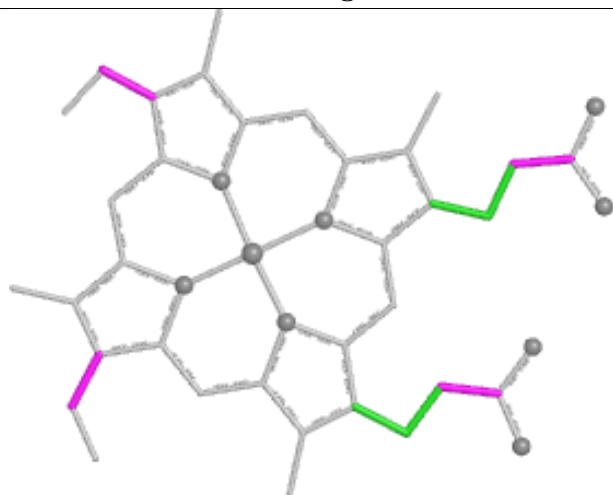
## Ligand HEC D 1112



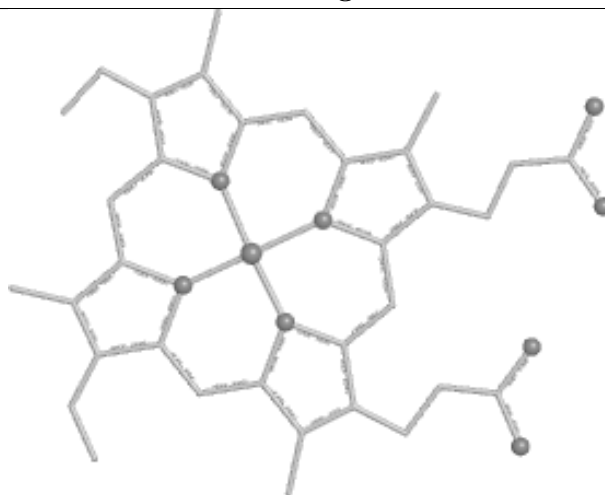
Bond lengths



Bond angles

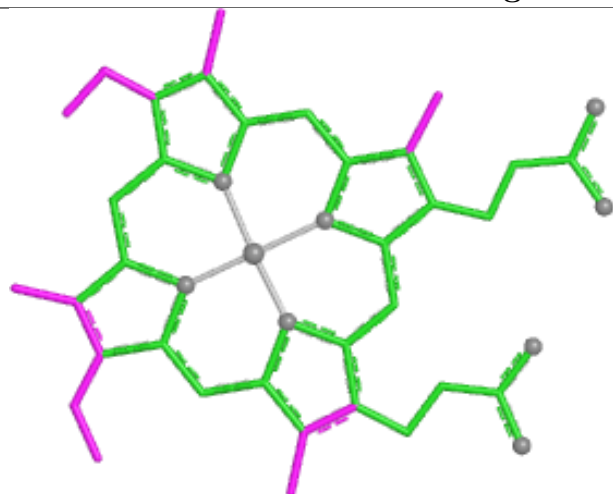


Torsions

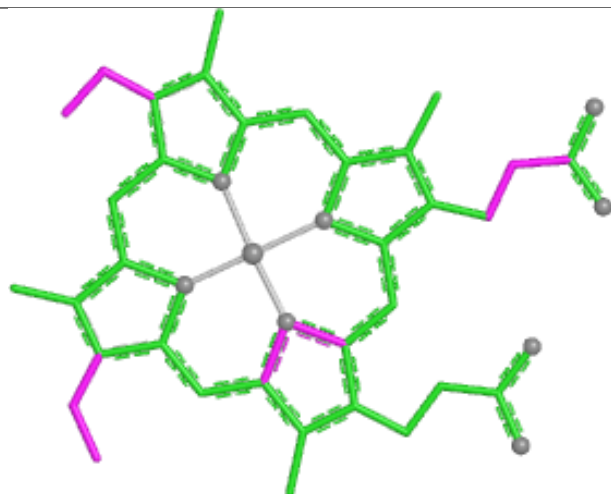


Rings

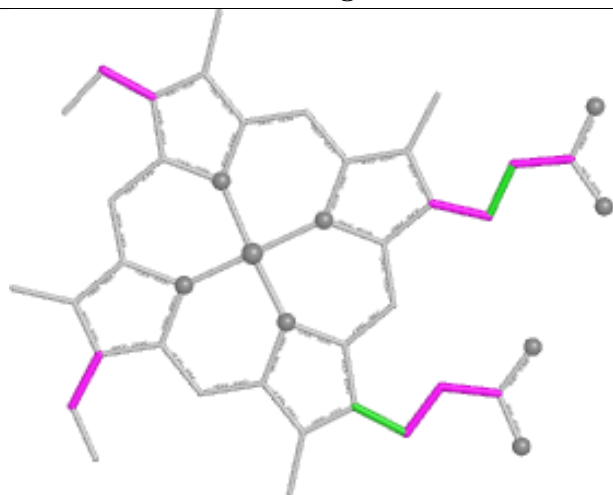
## Ligand HEC C 1111



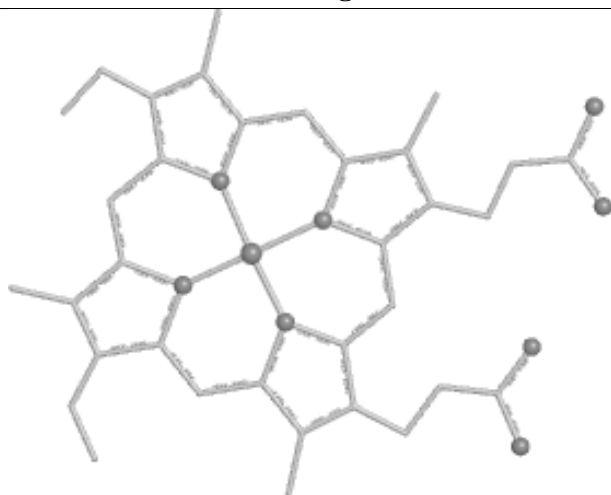
Bond lengths



Bond angles

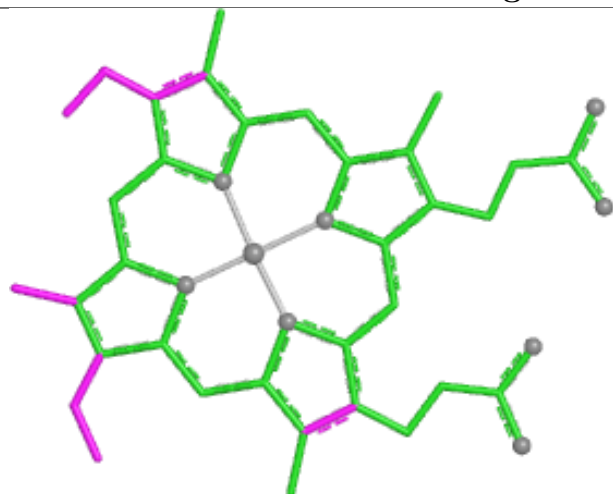


Torsions

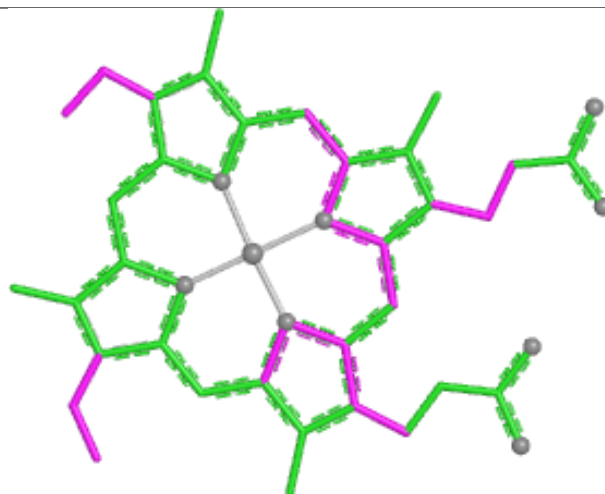


Rings

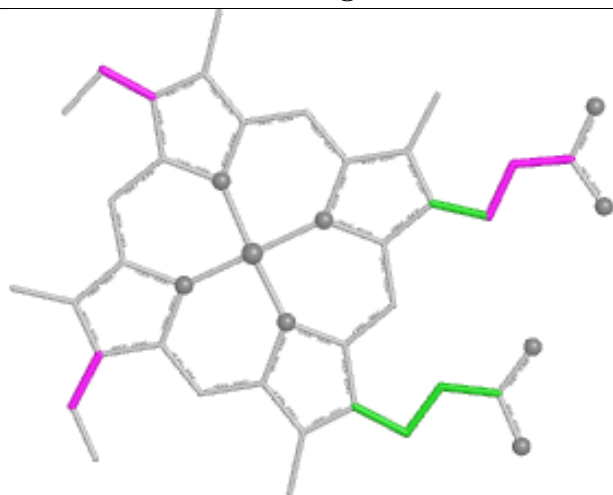
## Ligand HEC A 1104



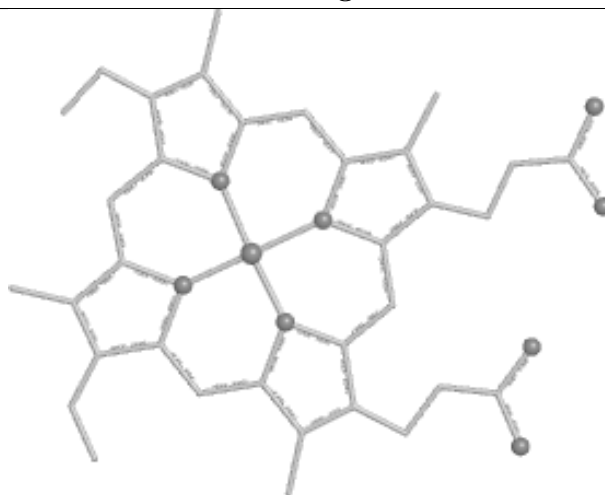
Bond lengths



Bond angles

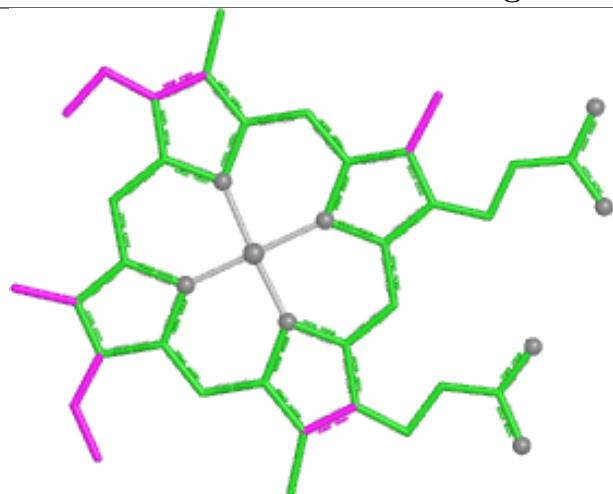


Torsions

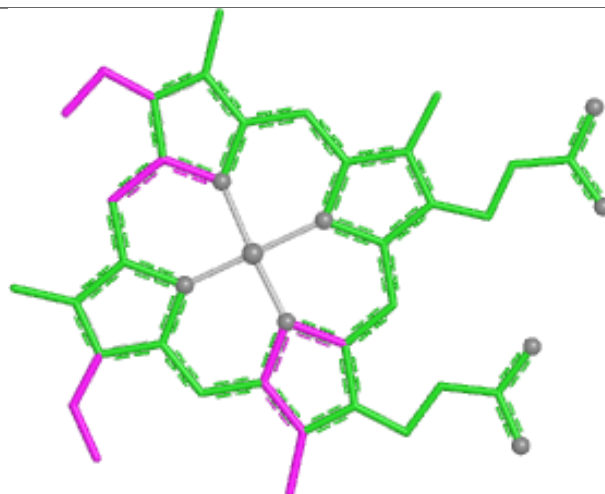


Rings

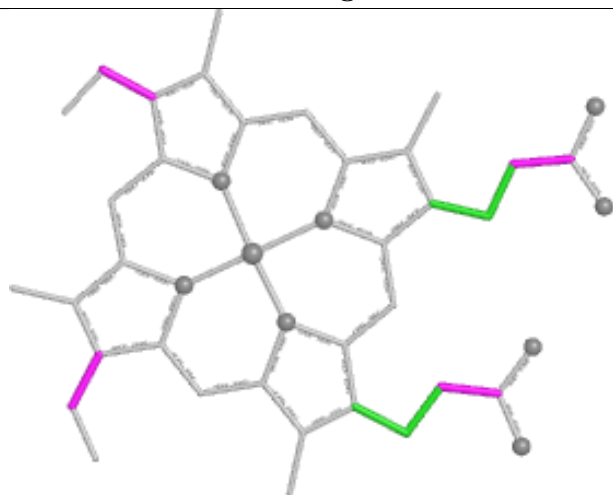
## Ligand HEC C 1112



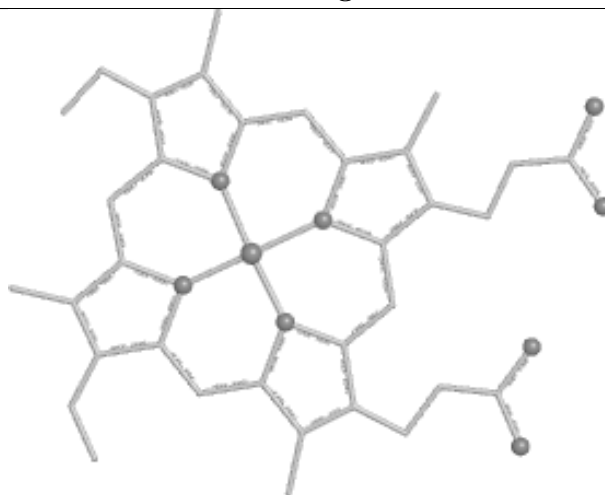
Bond lengths



Bond angles

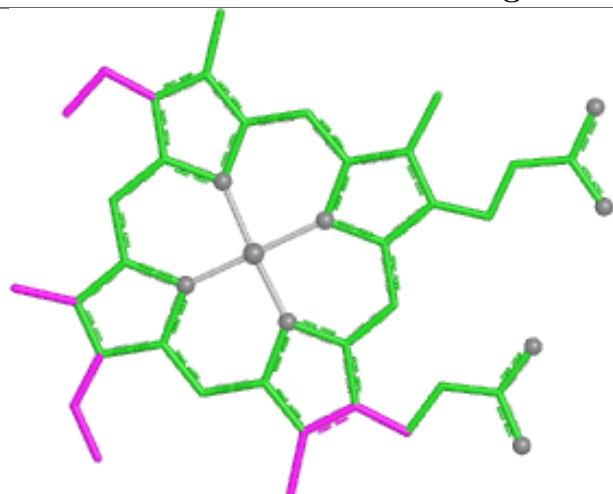


Torsions

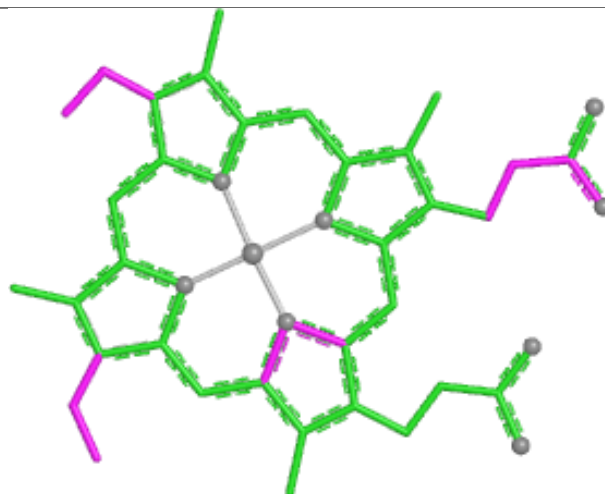


Rings

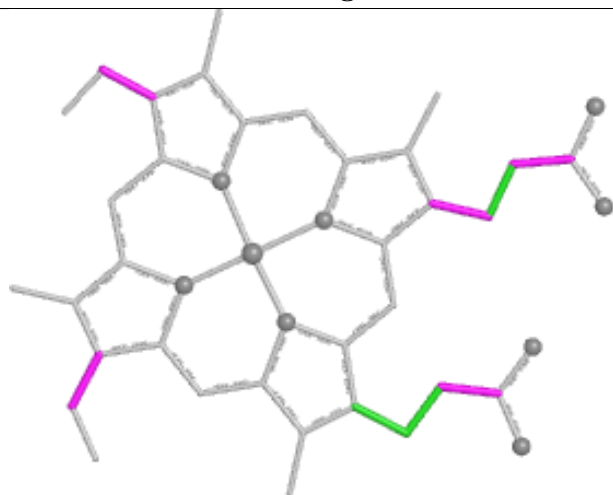
## Ligand HEC D 1105



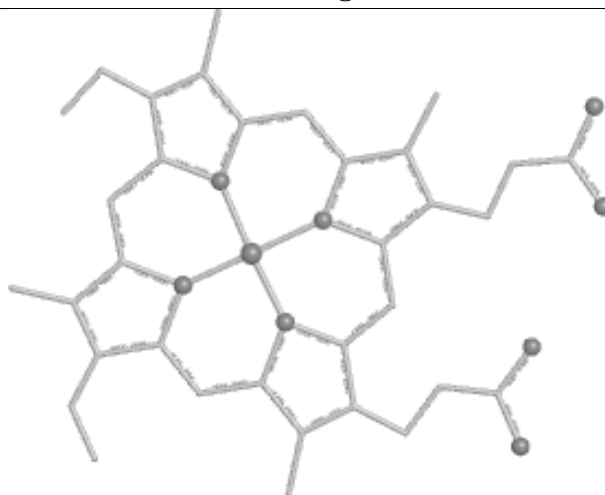
Bond lengths



Bond angles

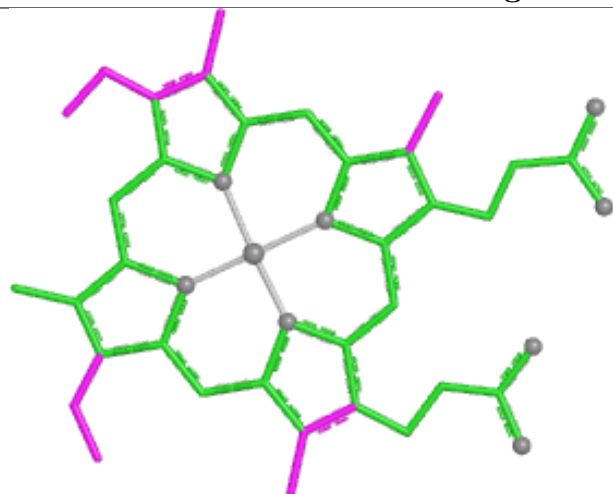


Torsions

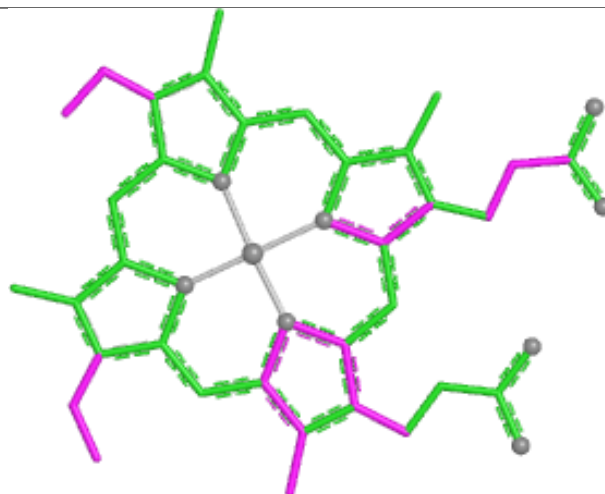


Rings

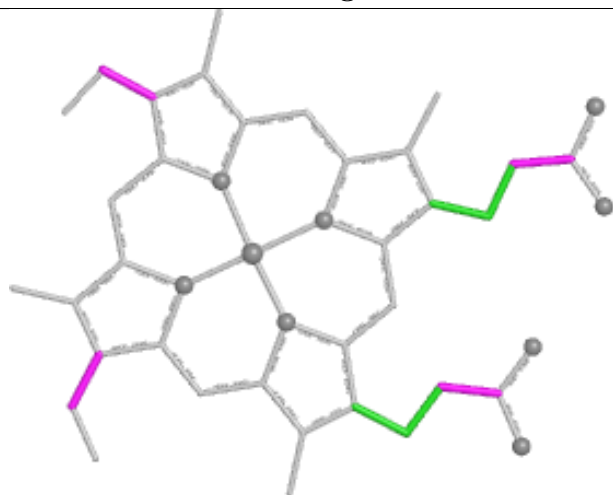
## Ligand HEC B 1115



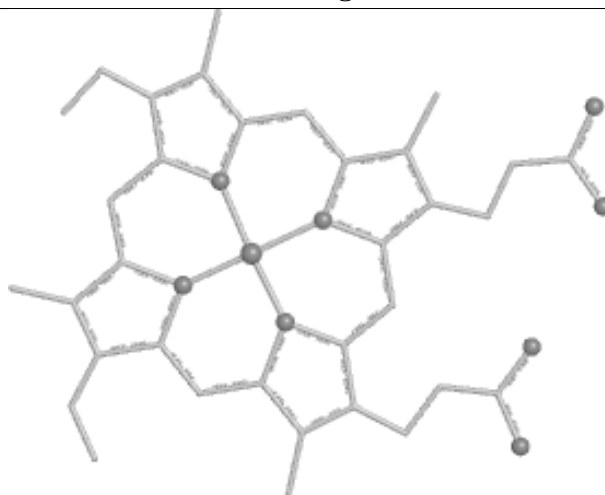
Bond lengths



Bond angles

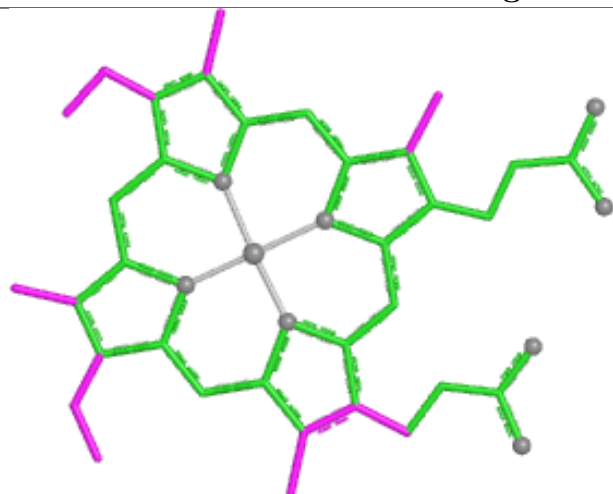


Torsions

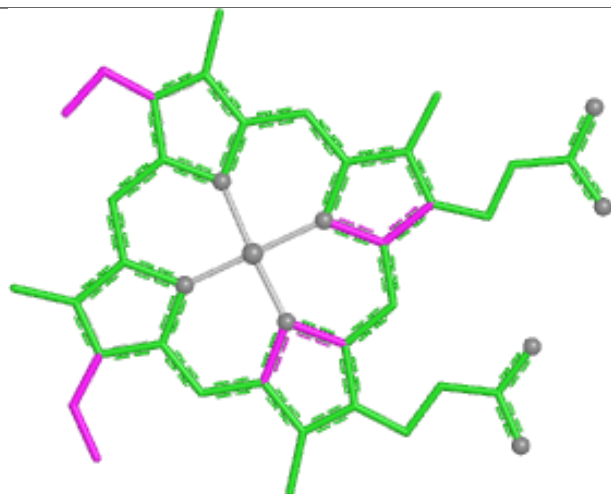


Rings

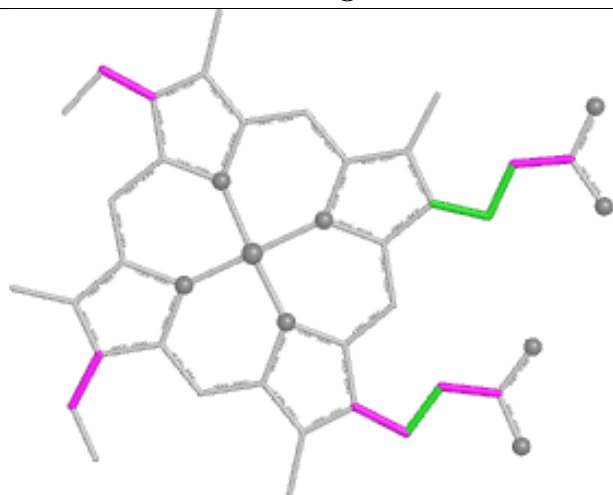
## Ligand HEC D 1110



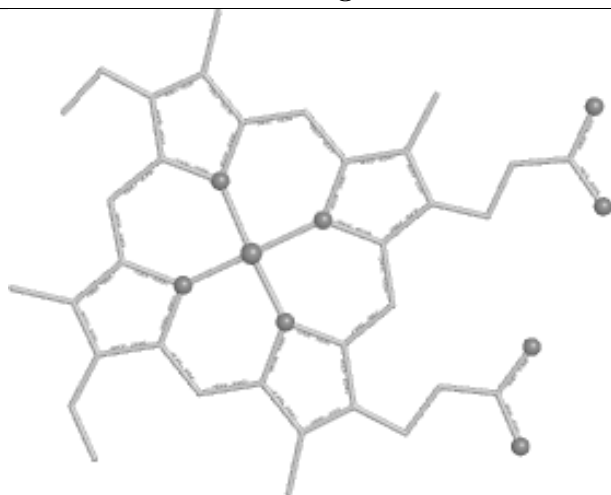
Bond lengths



Bond angles

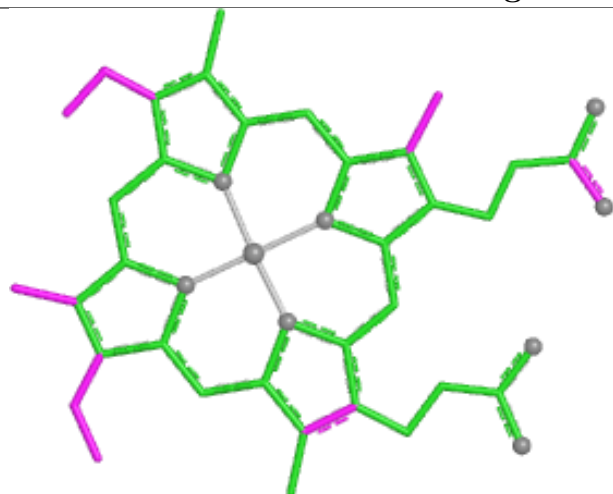


Torsions

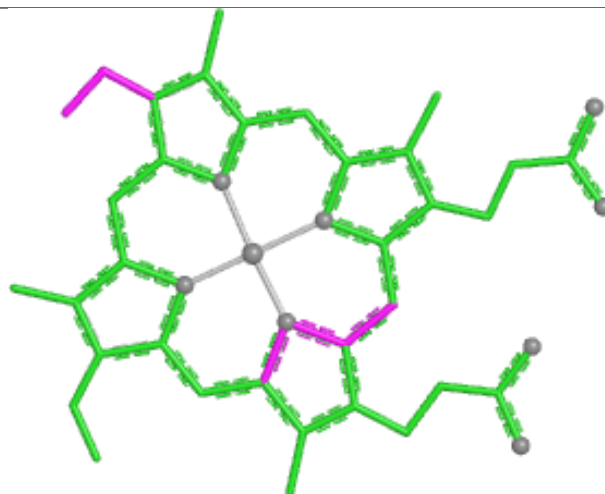


Rings

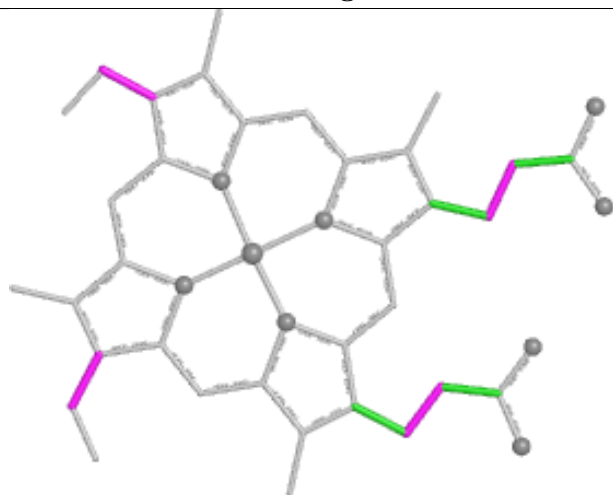
## Ligand HEC B 1101



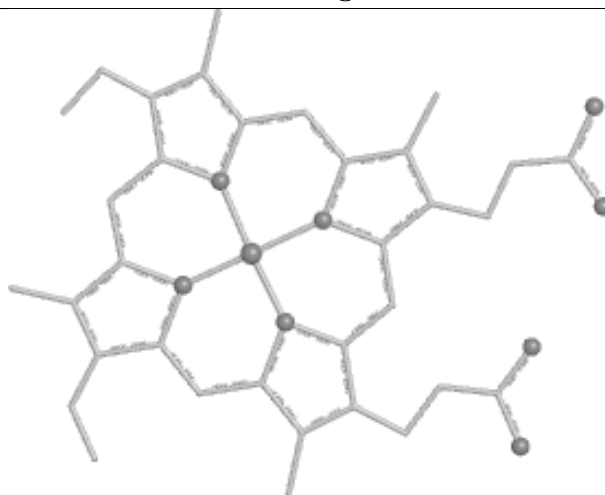
Bond lengths



Bond angles

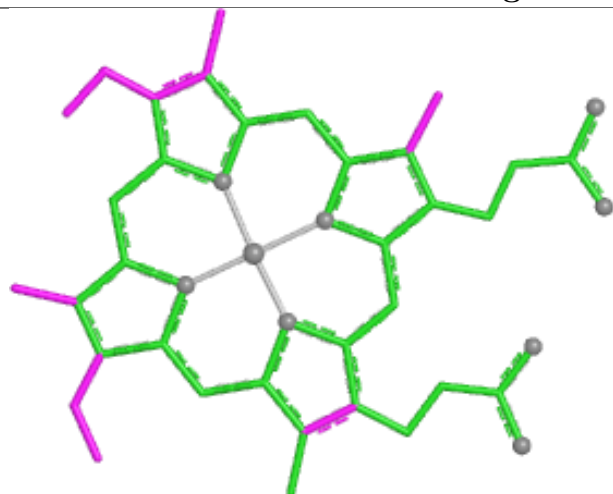


Torsions

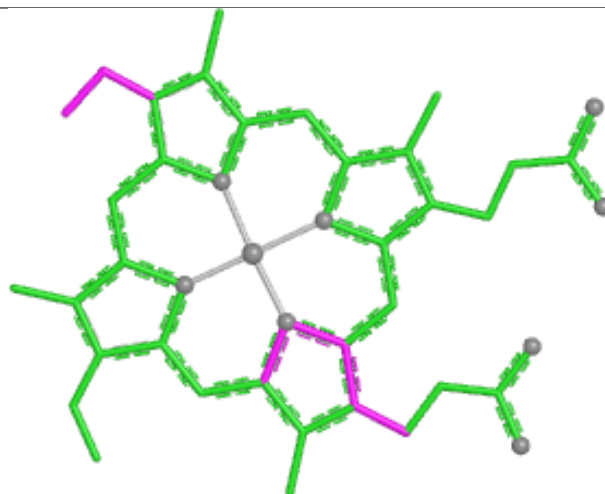


Rings

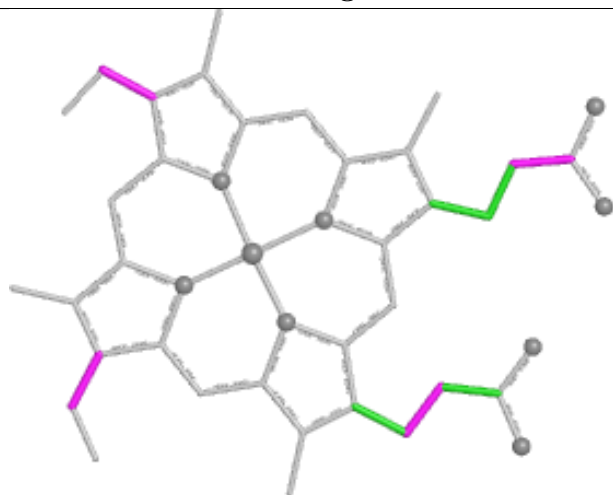
## Ligand HEC D 1101



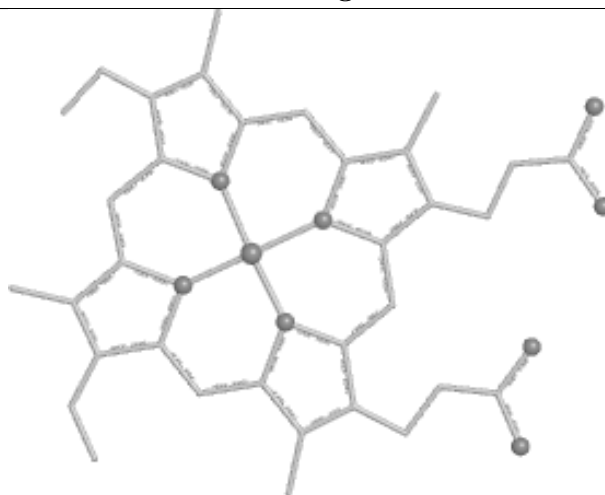
Bond lengths



Bond angles

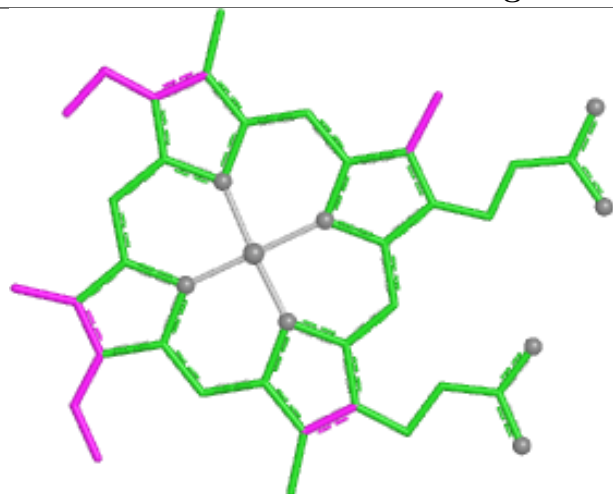


Torsions

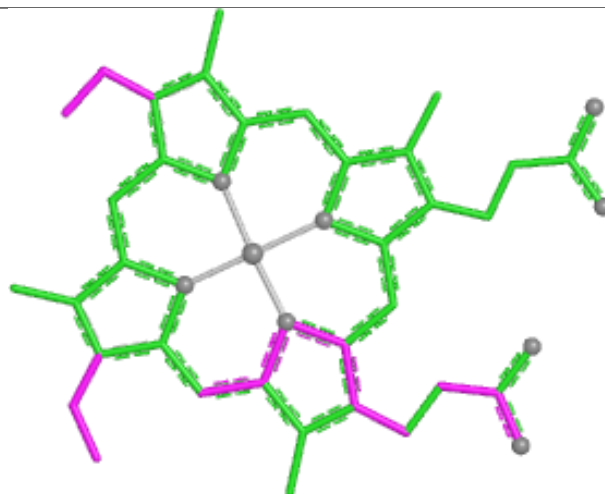


Rings

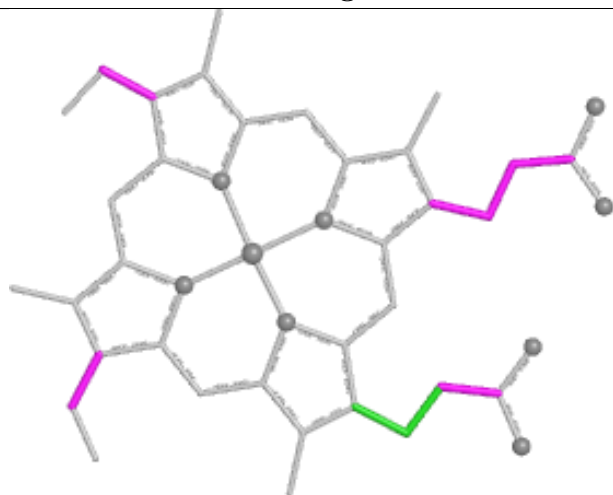
## Ligand HEC C 1105



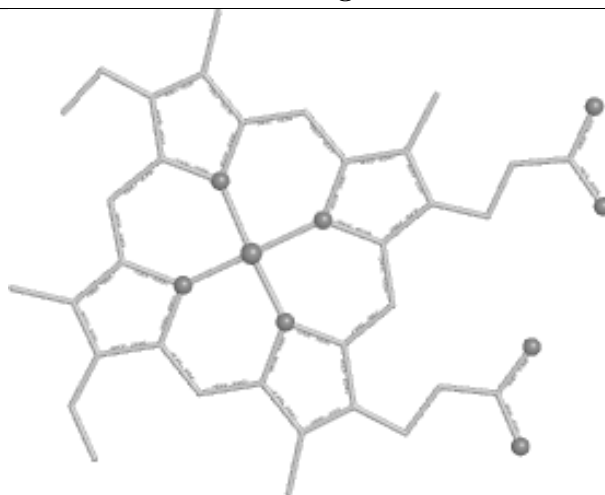
Bond lengths



Bond angles

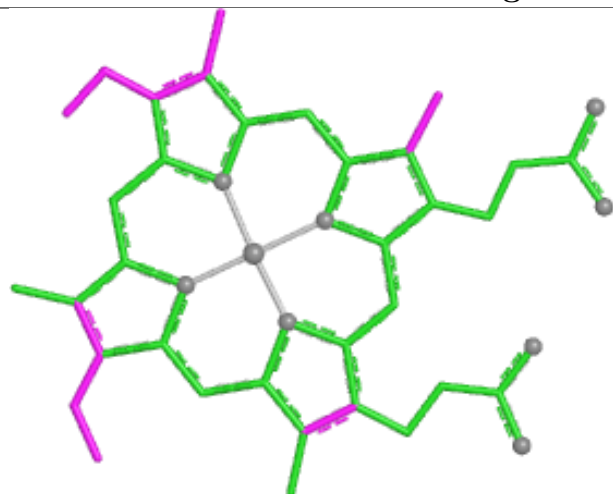


Torsions

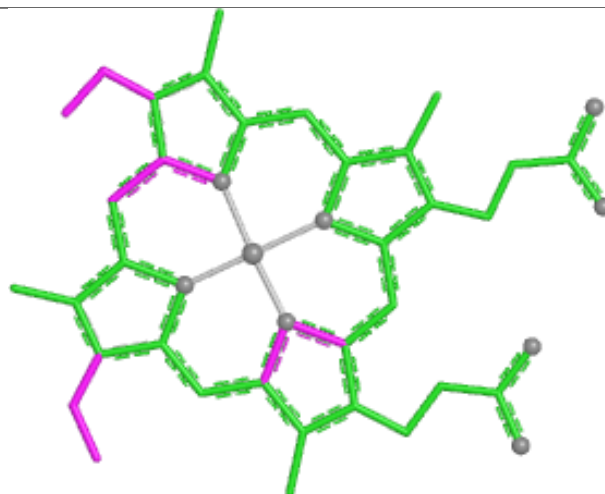


Rings

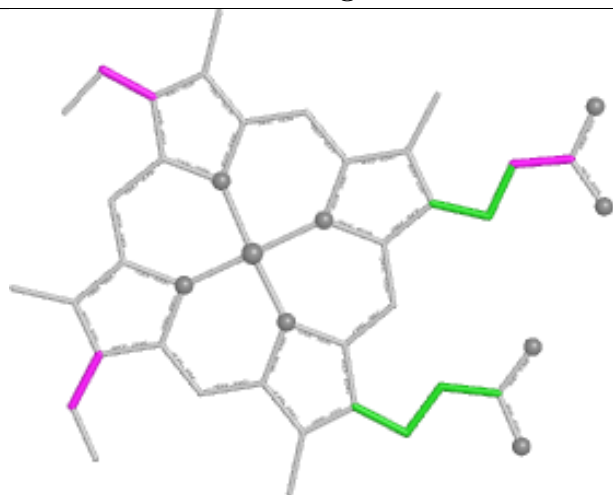
## Ligand HEC D 1113



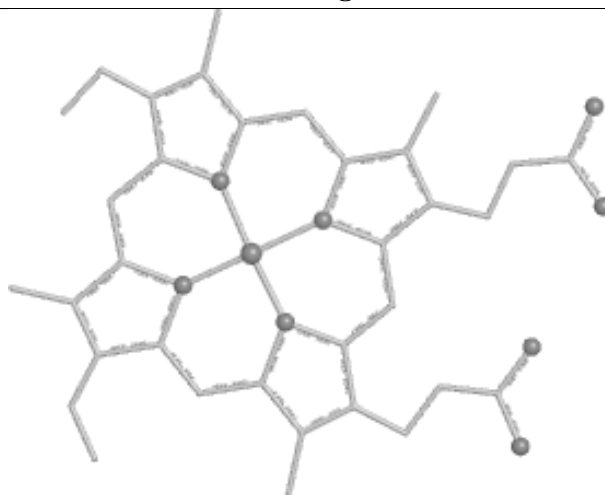
Bond lengths



Bond angles

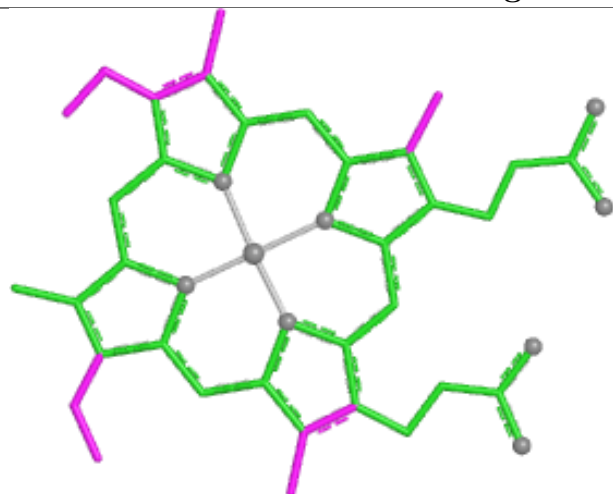


Torsions

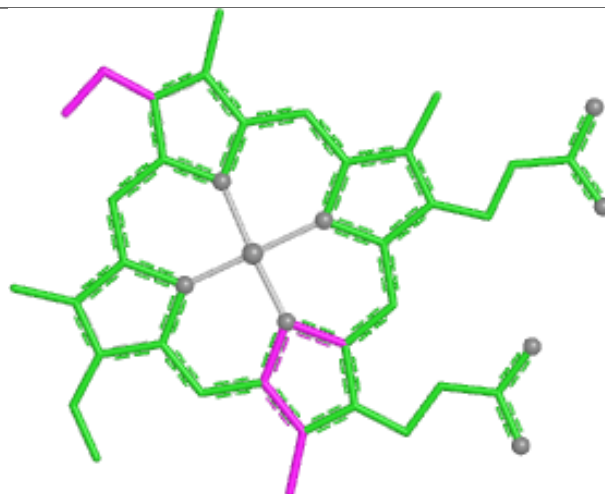


Rings

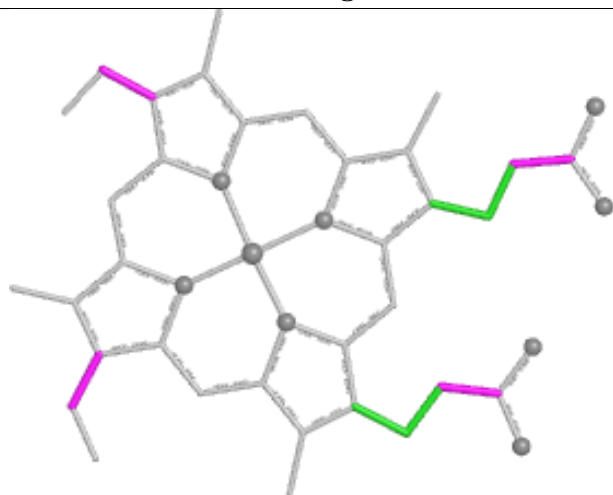
## Ligand HEC B 1105



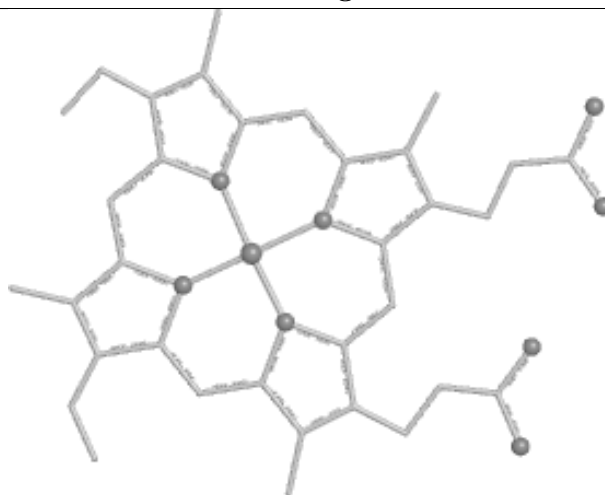
Bond lengths



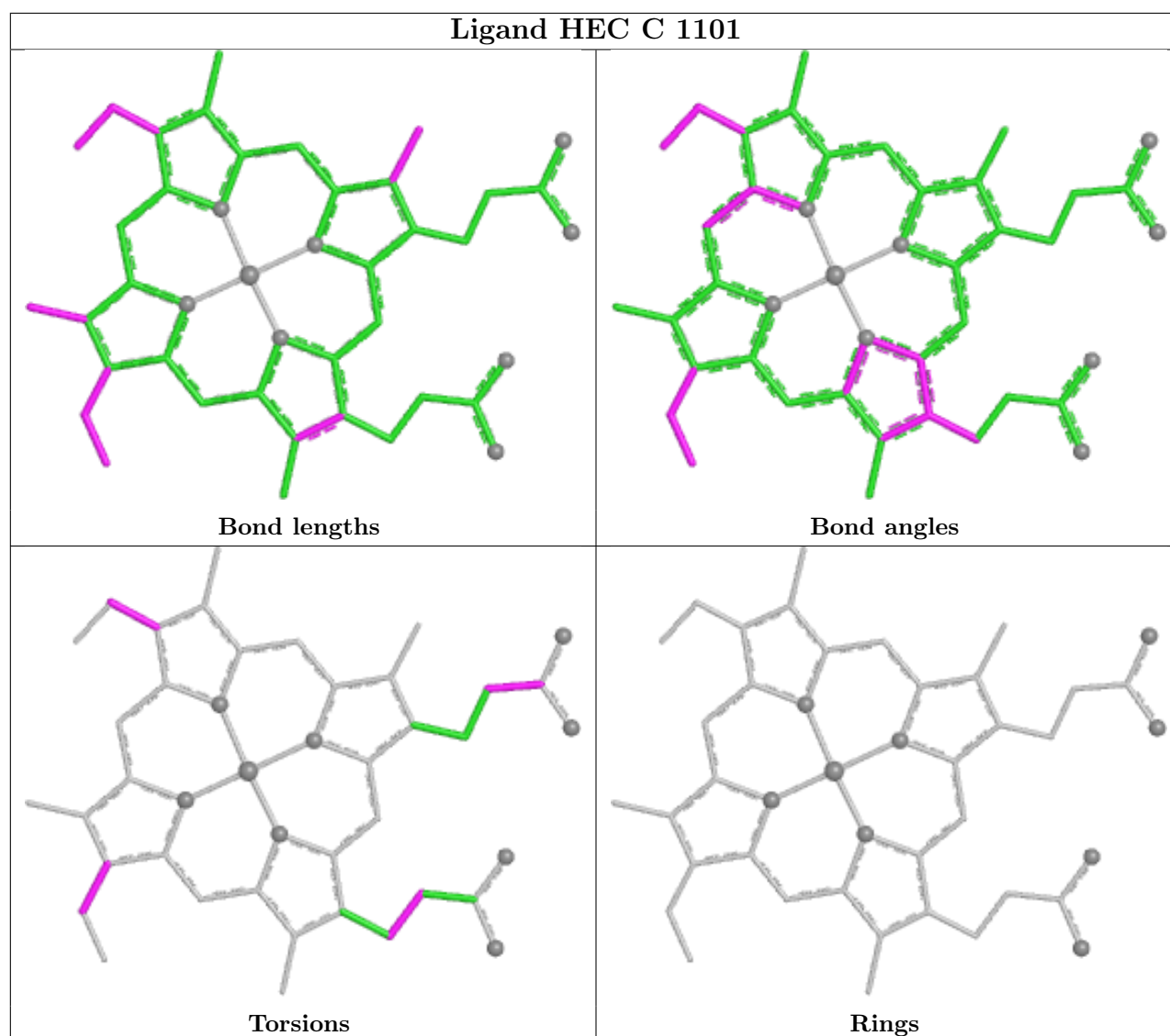
Bond angles



Torsions



Rings



## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.