



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:47 PM EDT

PDB ID : 4L3Y / pdb\_00004l3y  
Title : Nitrite complex of TvNiR, high dose data set (NO complex)  
Authors : Trofimov, A.A.; Polyakov, K.M.; Lazarenko, V.A.; Popov, A.N.; Tikhonova, T.V.; Tikhonov, A.V.; Popov, V.O.  
Deposited on : 2013-06-07  
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

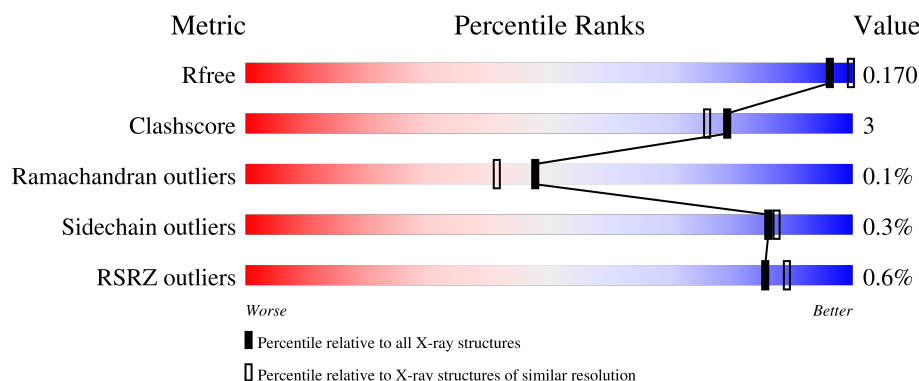
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3494 (1.96-1.96)                                      |
| Clashscore            | 190562                      | 3612 (1.96-1.96)                                      |
| Ramachandran outliers | 187476                      | 3587 (1.96-1.96)                                      |
| Sidechain outliers    | 187428                      | 3587 (1.96-1.96)                                      |
| RSRZ outliers         | 180081                      | 3495 (1.96-1.96)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                                                                                                                                                                                                    |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1   | A     | 520    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>93%</span> <span>7%</span> </div> </div> |
| 1   | B     | 520    | <div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> <span>%</span> <span>96%</span> <span>.</span> </div> </div>  |

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

| Mol | Type | Chain | Res    | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 2   | HEC  | A     | 601    | X         | -        | -       | -                |
| 2   | HEC  | A     | 602    | X         | -        | -       | -                |
| 2   | HEC  | A     | 603    | X         | -        | -       | -                |
| 2   | HEC  | A     | 604    | X         | -        | -       | -                |
| 2   | HEC  | A     | 605    | X         | -        | -       | -                |
| 2   | HEC  | A     | 606    | X         | -        | -       | -                |
| 2   | HEC  | A     | 607    | X         | -        | -       | -                |
| 2   | HEC  | A     | 608    | X         | -        | -       | -                |
| 2   | HEC  | B     | 601    | X         | -        | -       | -                |
| 2   | HEC  | B     | 602    | X         | -        | -       | -                |
| 2   | HEC  | B     | 603    | X         | -        | -       | -                |
| 2   | HEC  | B     | 604[A] | X         | -        | -       | -                |
| 2   | HEC  | B     | 604[B] | X         | -        | -       | -                |
| 2   | HEC  | B     | 605    | X         | -        | -       | -                |
| 2   | HEC  | B     | 606    | X         | -        | -       | -                |
| 2   | HEC  | B     | 607    | X         | -        | -       | -                |
| 2   | HEC  | B     | 608    | X         | -        | -       | -                |

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10324 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.

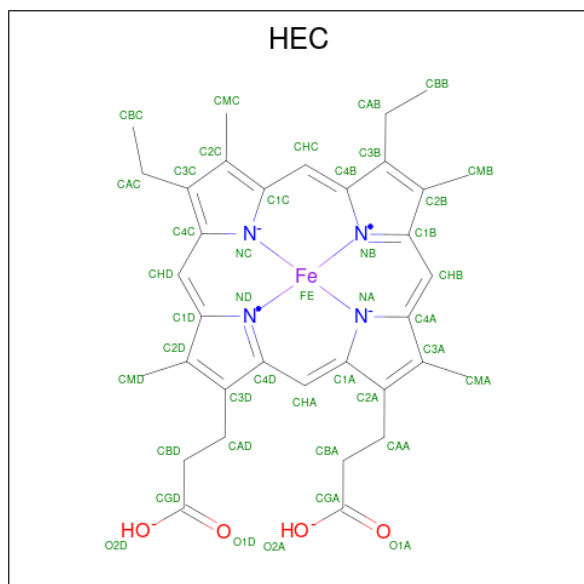
- Molecule 1 is a protein called Eight-heme nitrite reductase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 520      | Total | C    | N   | O   | S  | 0       | 17      | 0     |
|     |       |          | 4172  | 2587 | 755 | 796 | 34 |         |         |       |
| 1   | B     | 520      | Total | C    | N   | O   | S  | 0       | 16      | 0     |
|     |       |          | 4179  | 2591 | 759 | 795 | 34 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 524     | VAL      | -      | expression tag | UNP L0DSL2 |
| B     | 524     | VAL      | -      | expression tag | UNP L0DSL2 |

- Molecule 2 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{36}FeN_4O_4$ ).



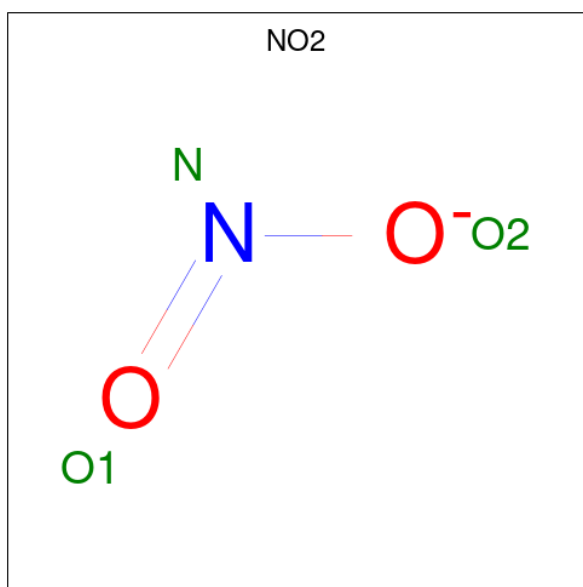
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | A     | 1        | Total | 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 |         |         |
| 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       |
|     |       |          | 38    | 31 | 1  | 4 | 2 |         |         |
| 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 |         |         |
| 2   | A     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 1       |
|     |       |          | 47    | 36 | 1  | 4 | 6 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 39    | 32 | 1  | 4 | 2 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | B     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 3 is NITRITE ION (CCD ID: NO2) (formula: NO<sub>2</sub>).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | A     | 1        | Total N O<br>2 1 1 | 0       | 0       |
| 3   | A     | 1        | Total N O<br>3 1 2 | 0       | 0       |
| 3   | A     | 1        | Total N O<br>3 1 2 | 0       | 0       |
| 3   | B     | 1        | Total N O<br>2 1 1 | 0       | 0       |
| 3   | B     | 1        | Total N O<br>3 1 2 | 0       | 0       |
| 3   | B     | 1        | Total N O<br>3 1 2 | 0       | 0       |

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

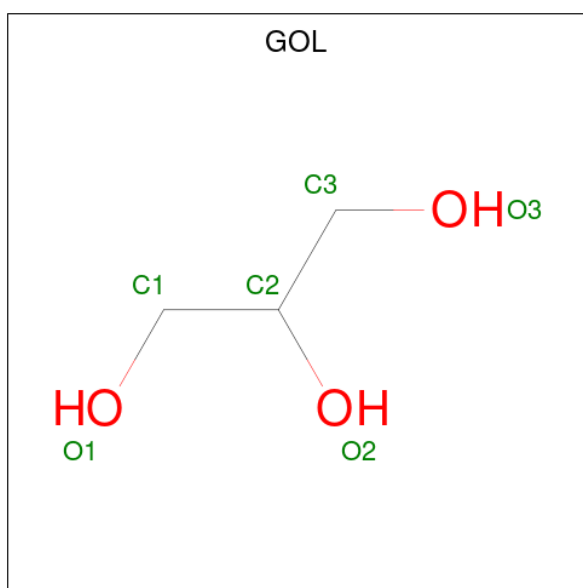
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | A     | 2        | Total Ca<br>2 2 | 0       | 0       |
| 4   | B     | 2        | Total Ca<br>2 2 | 0       | 0       |

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |
| 5   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 8     | 6 | 2 |         |         |

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



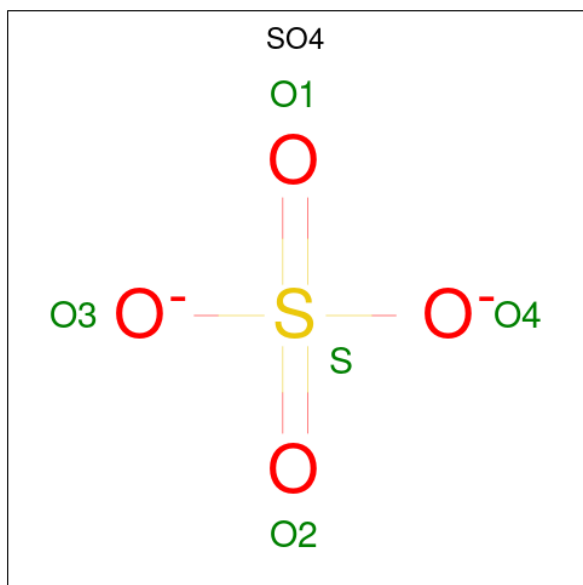
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | A     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 7     | 3 | 4 |         |         |
| 6   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6   | A     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 7     | 3 | 4 |         |         |
| 6   | B     | 1        | Total | C | O | 0       | 1       |
|     |       |          | 7     | 3 | 4 |         |         |
| 6   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 6     | 3 | 3 |         |         |

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

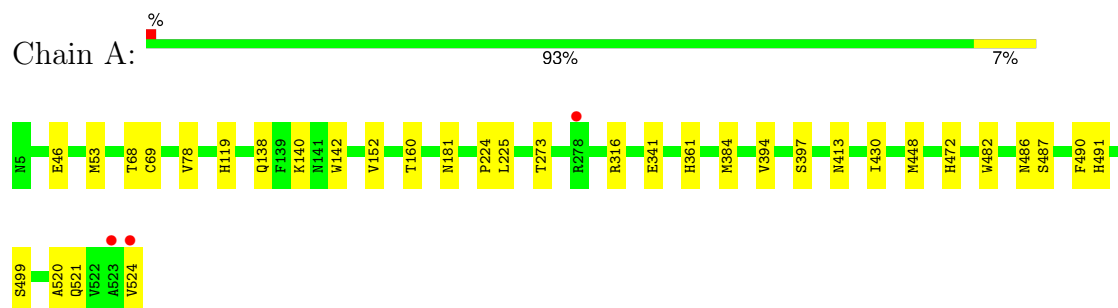
- Molecule 8 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 8   | A     | 594      | Total | O   | 0       | 0       |
|     |       |          | 594   | 594 |         |         |
| 8   | B     | 617      | Total | O   | 0       | 0       |
|     |       |          | 617   | 617 |         |         |

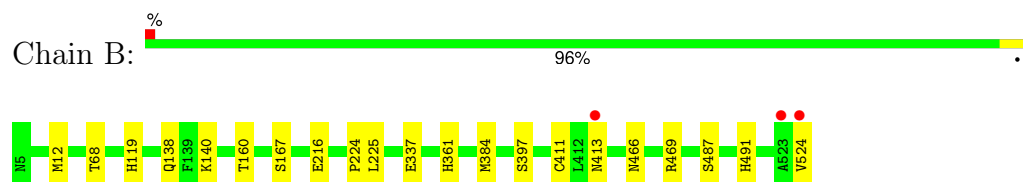
### 3 Residue-property plots [i](#)

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

- Molecule 1: Eight-heme nitrite reductase



- Molecule 1: Eight-heme nitrite reductase



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 3                                                      | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 194.98Å 194.98Å 194.98Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 29.08 – 1.95<br>29.08 – 1.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.5 (29.08-1.95)<br>99.5 (29.08-1.95)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.06 (at 1.95Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.7.0029                                             | Depositor        |
| R, $R_{free}$                                                           | 0.151 , 0.170<br>0.152 , 0.170                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 8889 reflections (4.98%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 16.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.000                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.37 , 51.0                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | 0.050 for l,-k,h                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.96                                                        | EDS              |
| Total number of atoms                                                   | 10324                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 17.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, NO2, CA, MPD, 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     | 0.91         | 0/4370      | 0.90        | 1/5930 (0.0%)  |
| 1   | B     | 0.89         | 0/4369      | 0.91        | 1/5928 (0.0%)  |
| All | All   | 0.90         | 0/8739      | 0.90        | 2/11858 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | A     | 181 | ASN  | N-CA-C  | -5.54 | 103.14      | 108.07   |
| 1   | B     | 411 | CYS  | CB-CA-C | -5.37 | 99.74       | 110.42   |

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 4172  | 0        | 3878     | 24      | 0            |
| 1   | B     | 4179  | 0        | 3892     | 17      | 0            |
| 2   | A     | 339   | 0        | 236      | 6       | 0            |
| 2   | B     | 344   | 0        | 214      | 6       | 0            |
| 3   | A     | 8     | 0        | 0        | 0       | 0            |
| 3   | B     | 8     | 0        | 0        | 1       | 0            |
| 4   | A     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 2     | 0        | 0        | 0       | 0            |
| 5   | A     | 8     | 0        | 14       | 1       | 0            |
| 5   | B     | 8     | 0        | 14       | 3       | 0            |
| 6   | A     | 20    | 0        | 18       | 0       | 0            |
| 6   | B     | 13    | 0        | 12       | 0       | 0            |
| 7   | A     | 5     | 0        | 0        | 0       | 0            |
| 7   | B     | 5     | 0        | 0        | 0       | 0            |
| 8   | A     | 594   | 0        | 0        | 5       | 0            |
| 8   | B     | 617   | 0        | 0        | 5       | 0            |
| All | All   | 10324 | 0        | 8278     | 48      | 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 3.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:B:605:HEC:HMC3    | 2:B:605:HEC:HBC3    | 1.57                     | 0.84              |
| 1:B:138[B]:GLN:NE2  | 5:B:612:MPD:H32     | 1.96                     | 0.81              |
| 1:A:413:ASN:HB2     | 8:A:1118:HOH:O      | 1.84                     | 0.76              |
| 2:A:605:HEC:HMC3    | 2:A:605:HEC:HBC3    | 1.74                     | 0.69              |
| 1:A:521:GLN:O       | 1:A:524:VAL:HG22    | 1.94                     | 0.67              |
| 1:B:413:ASN:HB2     | 8:B:1148:HOH:O      | 2.03                     | 0.58              |
| 1:B:138[B]:GLN:HE21 | 5:B:612:MPD:H32     | 1.68                     | 0.57              |
| 1:A:140:LYS:HG2     | 1:A:160[B]:THR:HG23 | 1.84                     | 0.57              |
| 1:A:140:LYS:HG2     | 1:A:160[B]:THR:CG2  | 2.39                     | 0.53              |
| 1:A:394[B]:VAL:HG12 | 8:A:950:HOH:O       | 2.10                     | 0.52              |
| 1:A:384:MET:HB2     | 1:A:397:SER:O       | 2.10                     | 0.51              |
| 1:B:138[B]:GLN:NE2  | 5:B:612:MPD:C3      | 2.70                     | 0.51              |
| 2:B:606:HEC:HHA     | 2:B:606:HEC:HBD2    | 1.93                     | 0.51              |
| 1:B:524:VAL:HG13    | 8:B:1132:HOH:O      | 2.11                     | 0.50              |
| 1:B:466:ASN:HD22    | 1:B:469:ARG:HD2     | 1.77                     | 0.47              |
| 1:A:53[B]:MET:HE2   | 2:A:608:HEC:HAD1    | 1.97                     | 0.47              |
| 1:A:273[B]:THR:HG22 | 8:A:949:HOH:O       | 2.14                     | 0.47              |
| 1:A:68[A]:THR:HG23  | 1:A:69:CYS:N        | 2.29                     | 0.47              |
| 1:B:384:MET:HB2     | 1:B:397:SER:O       | 2.15                     | 0.47              |
| 1:B:466:ASN:ND2     | 1:B:469:ARG:HH11    | 2.13                     | 0.47              |
| 1:B:413:ASN:ND2     | 8:B:1142:HOH:O      | 2.48                     | 0.46              |
| 1:B:12:MET:HE3      | 8:B:955:HOH:O       | 2.15                     | 0.46              |
| 1:A:487:SER:HB3     | 1:A:491:HIS:CE1     | 2.52                     | 0.45              |
| 1:B:140:LYS:HG2     | 1:B:160[B]:THR:HG23 | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:448:MET:HE1    | 1:A:472:HIS:CG     | 2.52                     | 0.45              |
| 1:A:520:ALA:O      | 1:A:524:VAL:HG13   | 2.17                     | 0.45              |
| 2:B:601:HEC:C4D    | 2:B:603:HEC:HMD2   | 2.47                     | 0.44              |
| 1:A:138:GLN:HG2    | 8:A:1098:HOH:O     | 2.18                     | 0.44              |
| 1:A:486:ASN:HB3    | 2:A:604:HEC:HAA1   | 2.00                     | 0.44              |
| 1:B:487:SER:HB3    | 1:B:491:HIS:CE1    | 2.52                     | 0.44              |
| 1:B:361:HIS:NE2    | 3:B:609:NO2:O2     | 2.39                     | 0.44              |
| 1:A:46:GLU:HG3     | 8:A:1232:HOH:O     | 2.18                     | 0.43              |
| 1:B:224:PRO:O      | 1:B:225:LEU:C      | 2.61                     | 0.43              |
| 1:A:448:MET:HE1    | 1:A:472:HIS:CD2    | 2.54                     | 0.42              |
| 1:A:486:ASN:HB3    | 2:A:604:HEC:CAA    | 2.49                     | 0.42              |
| 2:B:605:HEC:HMC3   | 2:B:605:HEC:CBC    | 2.40                     | 0.42              |
| 1:A:430:ILE:HG21   | 1:A:490:PHE:HA     | 2.02                     | 0.42              |
| 1:B:119:HIS:CD2    | 2:B:603:HEC:ND     | 2.88                     | 0.42              |
| 2:A:606:HEC:HMC1   | 2:A:606:HEC:HBC3   | 2.02                     | 0.41              |
| 1:A:78[A]:VAL:HG12 | 1:A:152:VAL:HG21   | 2.02                     | 0.41              |
| 1:A:119:HIS:CD2    | 2:A:603:HEC:ND     | 2.89                     | 0.41              |
| 1:A:224:PRO:O      | 1:A:225:LEU:C      | 2.64                     | 0.41              |
| 1:B:337:GLU:HG2    | 8:B:1252:HOH:O     | 2.21                     | 0.41              |
| 1:A:482:TRP:HE1    | 1:A:499:SER:CB     | 2.34                     | 0.41              |
| 1:A:142:TRP:CE3    | 5:A:612:MPD:H11    | 2.56                     | 0.40              |
| 2:B:605:HEC:HBC3   | 2:B:605:HEC:CMC    | 2.38                     | 0.40              |
| 1:B:167:SER:HB2    | 1:B:216[B]:GLU:HG2 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 535/520 (103%) | 508 (95%) | 26 (5%) | 1 (0%)   | 43          | 36  |
| 1   | B     | 534/520 (103%) | 510 (96%) | 24 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|------------------|------------|---------|----------|-------------|----|
| All | All   | 1069/1040 (103%) | 1018 (95%) | 50 (5%) | 1 (0%)   | 48          | 41 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 361 | HIS  |

### 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     | 455/439 (104%) | 453 (100%) | 2 (0%)   | 84          | 85 |
| 1   | B     | 454/439 (103%) | 452 (100%) | 2 (0%)   | 84          | 85 |
| All | All   | 909/878 (104%) | 905 (100%) | 4 (0%)   | 86          | 85 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | A     | 316   | ARG  |
| 1   | A     | 341   | GLU  |
| 1   | B     | 68[A] | THR  |
| 1   | B     | 68[B] | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 138 | GLN  |
| 1   | B     | 413 | ASN  |
| 1   | B     | 466 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 for Mogul analysis.

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

| Mol | Type | Chain | Res    | Link  | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|--------|-------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |        |       | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 6   | GOL  | A     | 615[A] | -     | 5,5,5        | 0.34 | 0           | 5,5,5       | 0.52 | 0           |
| 2   | HEC  | A     | 608    | 1     | 50,50,50     | 2.76 | 27 (54%)    | 68,82,82    | 2.35 | 26 (38%)    |
| 2   | HEC  | A     | 602    | 1     | 50,50,50     | 2.50 | 27 (54%)    | 68,82,82    | 2.56 | 29 (42%)    |
| 2   | HEC  | A     | 605    | 1     | 45,45,50     | 3.17 | 26 (57%)    | 61,75,82    | 2.49 | 25 (40%)    |
| 3   | NO2  | A     | 609    | 2     | 0,1,2        | -    | -           | -           | -    | -           |
| 6   | GOL  | B     | 613[A] | -     | 5,5,5        | 0.64 | 0           | 5,5,5       | 0.42 | 0           |
| 2   | HEC  | A     | 604    | 1     | 50,50,50     | 2.44 | 26 (52%)    | 68,82,82    | 2.45 | 26 (38%)    |
| 6   | GOL  | A     | 614    | -     | 5,5,5        | 0.67 | 0           | 5,5,5       | 0.33 | 0           |
| 2   | HEC  | B     | 604[B] | 4     | 50,50,50     | 2.45 | 21 (42%)    | 68,82,82    | 2.43 | 23 (33%)    |
| 2   | HEC  | B     | 605    | 1     | 46,46,50     | 3.05 | 24 (52%)    | 63,77,82    | 2.63 | 22 (34%)    |
| 2   | HEC  | B     | 601    | 1,3,8 | 50,50,50     | 2.44 | 24 (48%)    | 68,82,82    | 2.41 | 22 (32%)    |
| 2   | HEC  | A     | 603    | 1,4   | 50,50,50     | 2.62 | 24 (48%)    | 68,82,82    | 2.52 | 26 (38%)    |
| 2   | HEC  | A     | 601    | 1,3,8 | 50,50,50     | 2.50 | 26 (52%)    | 68,82,82    | 2.37 | 30 (44%)    |
| 3   | NO2  | B     | 617    | -     | 1,2,2        | 0.05 | 0           | 0,1,1       | -    | -           |
| 5   | MPD  | B     | 612    | -     | 7,7,7        | 0.70 | 0           | 9,10,10     | 0.99 | 0           |
| 2   | HEC  | A     | 606    | 1     | 50,50,50     | 2.69 | 28 (56%)    | 68,82,82    | 2.51 | 31 (45%)    |
| 7   | SO4  | A     | 616    | -     | 4,4,4        | 0.46 | 0           | 6,6,6       | 0.51 | 0           |
| 6   | GOL  | A     | 613[B] | -     | 5,5,5        | 0.72 | 0           | 5,5,5       | 0.82 | 0           |
| 5   | MPD  | A     | 612    | -     | 7,7,7        | 0.77 | 0           | 9,10,10     | 0.64 | 0           |
| 2   | HEC  | B     | 607    | 1     | 50,50,50     | 2.42 | 22 (44%)    | 68,82,82    | 2.43 | 30 (44%)    |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | GOL  | A     | 615[B] | -    | 5,5,5        | 0.38 | 0        | 5,5,5       | 0.51 | 0        |
| 2   | HEC  | B     | 604[A] | -    | 50,50,50     | 2.46 | 21 (42%) | 68,82,82    | 2.44 | 24 (35%) |
| 7   | SO4  | B     | 615    | -    | 4,4,4        | 0.59 | 0        | 6,6,6       | 0.51 | 0        |
| 3   | NO2  | B     | 616    | -    | 1,2,2        | 0.05 | 0        | 0,1,1       | -    | -        |
| 2   | HEC  | B     | 608    | 1    | 50,50,50     | 2.74 | 27 (54%) | 68,82,82    | 2.52 | 27 (39%) |
| 2   | HEC  | B     | 603    | 1,4  | 50,50,50     | 2.36 | 22 (44%) | 68,82,82    | 2.41 | 27 (39%) |
| 6   | GOL  | B     | 613[B] | -    | 5,5,5        | 0.66 | 0        | 5,5,5       | 0.56 | 0        |
| 2   | HEC  | B     | 602    | 1    | 50,50,50     | 2.34 | 25 (50%) | 68,82,82    | 2.52 | 28 (41%) |
| 3   | NO2  | B     | 609    | 2    | 0,1,2        | -    | -        | -           | -    | -        |
| 3   | NO2  | A     | 618    | 3    | 1,2,2        | 0.04 | 0        | 0,1,1       | -    | -        |
| 3   | NO2  | A     | 617    | 3    | 1,2,2        | 0.12 | 0        | 0,1,1       | -    | -        |
| 2   | HEC  | A     | 607    | 1    | 50,50,50     | 2.39 | 21 (42%) | 68,82,82    | 2.36 | 29 (42%) |
| 6   | GOL  | A     | 613[A] | -    | 5,5,5        | 0.69 | 0        | 5,5,5       | 0.54 | 0        |
| 2   | HEC  | B     | 606    | 1    | 50,50,50     | 2.67 | 24 (48%) | 68,82,82    | 2.45 | 30 (44%) |
| 6   | GOL  | B     | 614    | -    | 5,5,5        | 0.53 | 0        | 5,5,5       | 0.31 | 0        |

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

| Mol | Type | Chain | Res    | Link  | Chirals | Torsions   | Rings |
|-----|------|-------|--------|-------|---------|------------|-------|
| 6   | GOL  | A     | 615[A] | -     | -       | 4/4/4/4    | -     |
| 2   | HEC  | A     | 608    | 1     | 1/1/3/7 | 8/14/54/54 | -     |
| 2   | HEC  | A     | 602    | 1     | 1/1/3/7 | 6/14/54/54 | -     |
| 2   | HEC  | A     | 605    | 1     | 1/1/2/7 | 4/9/49/54  | -     |
| 6   | GOL  | B     | 613[A] | -     | -       | 0/4/4/4    | -     |
| 2   | HEC  | A     | 604    | 1     | 1/1/3/7 | 6/14/54/54 | -     |
| 6   | GOL  | A     | 614    | -     | -       | 0/4/4/4    | -     |
| 2   | HEC  | B     | 604[B] | 4     | 1/1/3/7 | 4/14/54/54 | -     |
| 2   | HEC  | B     | 605    | 1     | 1/1/2/7 | 6/9/49/54  | -     |
| 2   | HEC  | B     | 601    | 1,3,8 | 1/1/3/7 | 6/14/54/54 | -     |
| 2   | HEC  | A     | 603    | 1,4   | 1/1/3/7 | 4/14/54/54 | -     |
| 2   | HEC  | A     | 601    | 1,3,8 | 1/1/3/7 | 6/14/54/54 | -     |
| 5   | MPD  | B     | 612    | -     | -       | 0/5/5/5    | -     |
| 2   | HEC  | A     | 606    | 1     | 1/1/3/7 | 4/14/54/54 | -     |
| 6   | GOL  | A     | 613[B] | -     | -       | 0/4/4/4    | -     |
| 5   | MPD  | A     | 612    | -     | -       | 0/5/5/5    | -     |
| 2   | HEC  | B     | 607    | 1     | 1/1/3/7 | 8/14/54/54 | -     |

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| Mol | Type | Chain | Res    | Link | Chirals | Torsions   | Rings |
|-----|------|-------|--------|------|---------|------------|-------|
| 6   | GOL  | A     | 615[B] | -    | -       | 4/4/4/4    | -     |
| 2   | HEC  | B     | 604[A] | -    | 1/1/3/7 | 6/14/54/54 | -     |
| 2   | HEC  | B     | 608    | 1    | 1/1/3/7 | 7/14/54/54 | -     |
| 2   | HEC  | B     | 603    | 1,4  | 1/1/3/7 | 4/14/54/54 | -     |
| 6   | GOL  | B     | 613[B] | -    | -       | 0/4/4/4    | -     |
| 2   | HEC  | B     | 602    | 1    | 1/1/3/7 | 6/14/54/54 | -     |
| 2   | HEC  | A     | 607    | 1    | 1/1/3/7 | 4/14/54/54 | -     |
| 6   | GOL  | A     | 613[A] | -    | -       | 0/4/4/4    | -     |
| 2   | HEC  | B     | 606    | 1    | 1/1/3/7 | 7/14/54/54 | -     |
| 6   | GOL  | B     | 614    | -    | -       | 1/4/4/4    | -     |

All (415) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 2   | B     | 605    | HEC  | C3D-C2D | 6.90 | 1.50        | 1.36     |
| 2   | A     | 605    | HEC  | C3D-C2D | 6.32 | 1.50        | 1.37     |
| 2   | A     | 605    | HEC  | CHA-C1A | 6.08 | 1.50        | 1.38     |
| 2   | B     | 605    | HEC  | C2A-C3A | 5.64 | 1.48        | 1.36     |
| 2   | A     | 605    | HEC  | C2A-C3A | 5.63 | 1.48        | 1.36     |
| 2   | B     | 605    | HEC  | CHA-C1A | 5.59 | 1.49        | 1.38     |
| 2   | B     | 604[A] | HEC  | C2A-C3A | 5.45 | 1.48        | 1.36     |
| 2   | B     | 604[B] | HEC  | C2A-C3A | 5.45 | 1.48        | 1.36     |
| 2   | A     | 605    | HEC  | CHD-C1D | 5.43 | 1.49        | 1.38     |
| 2   | A     | 605    | HEC  | C3D-C4D | 5.35 | 1.51        | 1.40     |
| 2   | B     | 605    | HEC  | CHD-C1D | 5.25 | 1.49        | 1.38     |
| 2   | A     | 602    | HEC  | C3D-C2D | 5.23 | 1.48        | 1.36     |
| 2   | A     | 605    | HEC  | FE-ND   | 5.19 | 2.10        | 1.94     |
| 2   | B     | 601    | HEC  | C3B-C2B | 5.15 | 1.47        | 1.36     |
| 2   | B     | 605    | HEC  | FE-ND   | 5.14 | 2.10        | 1.94     |
| 2   | B     | 606    | HEC  | C3B-C2B | 5.07 | 1.47        | 1.36     |
| 2   | A     | 608    | HEC  | C2A-C3A | 5.06 | 1.47        | 1.36     |
| 2   | A     | 606    | HEC  | CHA-C1A | 5.05 | 1.48        | 1.38     |
| 2   | A     | 608    | HEC  | CHB-C4A | 5.05 | 1.48        | 1.38     |
| 2   | A     | 608    | HEC  | C3D-C2D | 5.02 | 1.47        | 1.36     |
| 2   | B     | 606    | HEC  | C3D-C2D | 5.00 | 1.47        | 1.36     |
| 2   | A     | 603    | HEC  | C3D-C2D | 5.00 | 1.47        | 1.36     |
| 2   | A     | 606    | HEC  | C3D-C2D | 4.99 | 1.47        | 1.36     |
| 2   | B     | 608    | HEC  | C3B-C2B | 4.97 | 1.47        | 1.36     |
| 2   | A     | 606    | HEC  | C2A-C3A | 4.93 | 1.47        | 1.36     |
| 2   | A     | 606    | HEC  | C3B-C2B | 4.93 | 1.47        | 1.36     |
| 2   | A     | 608    | HEC  | FE-NB   | 4.93 | 2.10        | 1.94     |

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| Mol | Chain | Res    | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|------|-------------|----------|
| 2   | B     | 606    | HEC  | CHB-C4A | 4.92 | 1.48        | 1.38     |
| 2   | B     | 608    | HEC  | C3D-C2D | 4.89 | 1.47        | 1.36     |
| 2   | A     | 605    | HEC  | C1D-C2D | 4.88 | 1.50        | 1.42     |
| 2   | A     | 605    | HEC  | FE-NA   | 4.88 | 2.11        | 1.95     |
| 2   | B     | 601    | HEC  | C2A-C3A | 4.86 | 1.47        | 1.36     |
| 2   | B     | 602    | HEC  | CHA-C1A | 4.84 | 1.47        | 1.38     |
| 2   | A     | 604    | HEC  | C2A-C3A | 4.81 | 1.47        | 1.36     |
| 2   | A     | 603    | HEC  | CHC-C4B | 4.81 | 1.48        | 1.38     |
| 2   | A     | 607    | HEC  | CHA-C1A | 4.80 | 1.47        | 1.38     |
| 2   | B     | 606    | HEC  | FE-ND   | 4.79 | 2.09        | 1.94     |
| 2   | B     | 601    | HEC  | C3D-C2D | 4.79 | 1.47        | 1.36     |
| 2   | B     | 603    | HEC  | C3D-C2D | 4.77 | 1.47        | 1.36     |
| 2   | B     | 604[A] | HEC  | FE-ND   | 4.75 | 2.09        | 1.94     |
| 2   | B     | 604[B] | HEC  | FE-ND   | 4.75 | 2.09        | 1.94     |
| 2   | B     | 606    | HEC  | CHA-C1A | 4.72 | 1.47        | 1.38     |
| 2   | A     | 602    | HEC  | CHD-C1D | 4.71 | 1.47        | 1.38     |
| 2   | B     | 608    | HEC  | CHA-C1A | 4.70 | 1.47        | 1.38     |
| 2   | A     | 608    | HEC  | CHA-C1A | 4.69 | 1.47        | 1.38     |
| 2   | A     | 608    | HEC  | CHC-C4B | 4.68 | 1.47        | 1.38     |
| 2   | B     | 606    | HEC  | FE-NB   | 4.66 | 2.09        | 1.94     |
| 2   | B     | 603    | HEC  | C3B-C2B | 4.65 | 1.46        | 1.36     |
| 2   | A     | 602    | HEC  | C2A-C3A | 4.63 | 1.46        | 1.36     |
| 2   | A     | 605    | HEC  | C3B-C2B | 4.63 | 1.46        | 1.36     |
| 2   | B     | 608    | HEC  | FE-NB   | 4.63 | 2.09        | 1.94     |
| 2   | A     | 608    | HEC  | FE-NC   | 4.61 | 2.10        | 1.95     |
| 2   | A     | 605    | HEC  | CHC-C4B | 4.60 | 1.47        | 1.38     |
| 2   | A     | 606    | HEC  | FE-ND   | 4.58 | 2.09        | 1.94     |
| 2   | B     | 607    | HEC  | C3B-C2B | 4.57 | 1.46        | 1.36     |
| 2   | A     | 601    | HEC  | C2A-C3A | 4.56 | 1.46        | 1.36     |
| 2   | B     | 603    | HEC  | C2A-C3A | 4.55 | 1.46        | 1.36     |
| 2   | A     | 606    | HEC  | CHC-C4B | 4.53 | 1.47        | 1.38     |
| 2   | B     | 608    | HEC  | C2A-C3A | 4.53 | 1.46        | 1.36     |
| 2   | B     | 607    | HEC  | CHA-C1A | 4.51 | 1.47        | 1.38     |
| 2   | B     | 605    | HEC  | FE-NA   | 4.49 | 2.10        | 1.95     |
| 2   | B     | 604[A] | HEC  | CHA-C1A | 4.47 | 1.47        | 1.38     |
| 2   | B     | 604[B] | HEC  | CHA-C1A | 4.47 | 1.47        | 1.38     |
| 2   | A     | 608    | HEC  | FE-ND   | 4.44 | 2.08        | 1.94     |
| 2   | A     | 602    | HEC  | C3B-C2B | 4.43 | 1.46        | 1.36     |
| 2   | B     | 608    | HEC  | FE-NC   | 4.43 | 2.09        | 1.95     |
| 2   | A     | 603    | HEC  | CHB-C4A | 4.39 | 1.47        | 1.38     |
| 2   | A     | 604    | HEC  | CHA-C1A | 4.38 | 1.47        | 1.38     |
| 2   | B     | 605    | HEC  | CHA-C4D | 4.38 | 1.49        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | A     | 608    | HEC  | C3B-C2B | 4.35  | 1.46        | 1.36     |
| 2   | A     | 603    | HEC  | C3B-C2B | 4.34  | 1.46        | 1.36     |
| 2   | A     | 601    | HEC  | C3D-C2D | 4.33  | 1.46        | 1.36     |
| 2   | A     | 606    | HEC  | FE-NB   | 4.31  | 2.08        | 1.94     |
| 2   | A     | 607    | HEC  | C2A-C3A | 4.31  | 1.46        | 1.36     |
| 2   | A     | 605    | HEC  | FE-NB   | 4.31  | 2.08        | 1.94     |
| 2   | A     | 604    | HEC  | CHB-C4A | 4.30  | 1.46        | 1.38     |
| 2   | A     | 604    | HEC  | C4B-NB  | -4.29 | 1.32        | 1.40     |
| 2   | A     | 607    | HEC  | C3B-C2B | 4.28  | 1.46        | 1.36     |
| 2   | B     | 605    | HEC  | FE-NB   | 4.24  | 2.08        | 1.94     |
| 2   | A     | 602    | HEC  | CHA-C1A | 4.24  | 1.46        | 1.38     |
| 2   | B     | 607    | HEC  | C2A-C3A | 4.23  | 1.45        | 1.36     |
| 2   | B     | 608    | HEC  | CHC-C4B | 4.22  | 1.46        | 1.38     |
| 2   | A     | 601    | HEC  | FE-NB   | 4.22  | 2.07        | 1.94     |
| 2   | B     | 604[A] | HEC  | CHB-C4A | 4.21  | 1.46        | 1.38     |
| 2   | B     | 604[B] | HEC  | CHB-C4A | 4.21  | 1.46        | 1.38     |
| 2   | B     | 605    | HEC  | CHC-C4B | 4.19  | 1.46        | 1.38     |
| 2   | B     | 605    | HEC  | CHD-C4C | 4.17  | 1.48        | 1.39     |
| 2   | B     | 602    | HEC  | C2A-C3A | 4.17  | 1.45        | 1.36     |
| 2   | B     | 604[A] | HEC  | C3D-C2D | 4.16  | 1.45        | 1.36     |
| 2   | B     | 604[B] | HEC  | C3D-C2D | 4.16  | 1.45        | 1.36     |
| 2   | A     | 604    | HEC  | FE-NB   | 4.16  | 2.07        | 1.94     |
| 2   | B     | 608    | HEC  | FE-NA   | 4.15  | 2.08        | 1.95     |
| 2   | A     | 604    | HEC  | FE-ND   | 4.14  | 2.07        | 1.94     |
| 2   | B     | 607    | HEC  | C3D-C2D | 4.14  | 1.45        | 1.36     |
| 2   | B     | 608    | HEC  | FE-ND   | 4.13  | 2.07        | 1.94     |
| 2   | A     | 606    | HEC  | CHD-C1D | 4.13  | 1.46        | 1.38     |
| 2   | A     | 606    | HEC  | FE-NA   | 4.13  | 2.08        | 1.95     |
| 2   | B     | 605    | HEC  | C3B-C2B | 4.10  | 1.45        | 1.36     |
| 2   | B     | 603    | HEC  | CHC-C4B | 4.10  | 1.46        | 1.38     |
| 2   | B     | 602    | HEC  | C3B-C2B | 4.08  | 1.45        | 1.36     |
| 2   | A     | 608    | HEC  | FE-NA   | 4.08  | 2.08        | 1.95     |
| 2   | B     | 606    | HEC  | C2A-C3A | 4.07  | 1.45        | 1.36     |
| 2   | B     | 608    | HEC  | CHD-C1D | 4.07  | 1.46        | 1.38     |
| 2   | A     | 605    | HEC  | FE-NC   | 4.06  | 2.08        | 1.95     |
| 2   | A     | 603    | HEC  | CHD-C1D | 4.05  | 1.46        | 1.38     |
| 2   | A     | 601    | HEC  | CHB-C4A | 4.05  | 1.46        | 1.38     |
| 2   | A     | 604    | HEC  | C3B-C2B | 4.04  | 1.45        | 1.36     |
| 2   | A     | 601    | HEC  | C3B-C2B | 4.04  | 1.45        | 1.36     |
| 2   | A     | 602    | HEC  | FE-NA   | 4.02  | 2.08        | 1.95     |
| 2   | A     | 603    | HEC  | CHA-C1A | 4.02  | 1.46        | 1.38     |
| 2   | A     | 604    | HEC  | C3D-C2D | 4.00  | 1.45        | 1.36     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | B     | 602    | HEC  | C3D-C2D | 3.99  | 1.45        | 1.36     |
| 2   | B     | 605    | HEC  | C4B-NB  | -3.97 | 1.33        | 1.40     |
| 2   | B     | 607    | HEC  | FE-NB   | 3.96  | 2.07        | 1.94     |
| 2   | B     | 604[A] | HEC  | C3B-C2B | 3.94  | 1.45        | 1.36     |
| 2   | B     | 604[B] | HEC  | C3B-C2B | 3.94  | 1.45        | 1.36     |
| 2   | A     | 607    | HEC  | FE-NB   | 3.92  | 2.07        | 1.94     |
| 2   | A     | 603    | HEC  | CHA-C4D | 3.91  | 1.48        | 1.39     |
| 2   | A     | 607    | HEC  | CHD-C1D | 3.91  | 1.46        | 1.38     |
| 2   | B     | 606    | HEC  | CHC-C4B | 3.90  | 1.46        | 1.38     |
| 2   | A     | 607    | HEC  | CHB-C4A | 3.89  | 1.46        | 1.38     |
| 2   | A     | 601    | HEC  | FE-NC   | 3.88  | 2.08        | 1.95     |
| 2   | A     | 603    | HEC  | FE-NC   | 3.84  | 2.07        | 1.95     |
| 2   | B     | 601    | HEC  | FE-NB   | 3.83  | 2.06        | 1.94     |
| 2   | B     | 607    | HEC  | CHC-C4B | 3.82  | 1.46        | 1.38     |
| 2   | A     | 603    | HEC  | FE-NB   | 3.81  | 2.06        | 1.94     |
| 2   | A     | 606    | HEC  | FE-NC   | 3.80  | 2.07        | 1.95     |
| 2   | B     | 605    | HEC  | CHB-C4A | 3.80  | 1.45        | 1.38     |
| 2   | A     | 608    | HEC  | CHD-C1D | 3.80  | 1.46        | 1.38     |
| 2   | B     | 605    | HEC  | FE-NC   | 3.79  | 2.07        | 1.95     |
| 2   | B     | 603    | HEC  | CHA-C4D | 3.79  | 1.47        | 1.39     |
| 2   | A     | 603    | HEC  | C2A-C3A | 3.79  | 1.44        | 1.36     |
| 2   | A     | 601    | HEC  | CHA-C1A | 3.78  | 1.45        | 1.38     |
| 2   | B     | 604[A] | HEC  | C4B-NB  | -3.77 | 1.33        | 1.40     |
| 2   | B     | 604[B] | HEC  | C4B-NB  | -3.77 | 1.33        | 1.40     |
| 2   | B     | 601    | HEC  | FE-NC   | 3.76  | 2.07        | 1.95     |
| 2   | B     | 601    | HEC  | CHA-C1A | 3.76  | 1.45        | 1.38     |
| 2   | B     | 607    | HEC  | CHB-C1B | 3.71  | 1.47        | 1.39     |
| 2   | A     | 607    | HEC  | CHC-C4B | 3.70  | 1.45        | 1.38     |
| 2   | A     | 606    | HEC  | CHB-C4A | 3.70  | 1.45        | 1.38     |
| 2   | A     | 607    | HEC  | C3D-C2D | 3.69  | 1.44        | 1.36     |
| 2   | B     | 604[A] | HEC  | FE-NB   | 3.69  | 2.06        | 1.94     |
| 2   | B     | 604[B] | HEC  | FE-NB   | 3.69  | 2.06        | 1.94     |
| 2   | B     | 603    | HEC  | CHA-C1A | 3.67  | 1.45        | 1.38     |
| 2   | A     | 601    | HEC  | C1D-ND  | -3.67 | 1.33        | 1.40     |
| 2   | B     | 607    | HEC  | CHC-C1C | 3.67  | 1.47        | 1.39     |
| 2   | A     | 607    | HEC  | FE-NC   | 3.66  | 2.07        | 1.95     |
| 2   | B     | 608    | HEC  | CHB-C4A | 3.66  | 1.45        | 1.38     |
| 2   | A     | 601    | HEC  | CHB-C1B | 3.65  | 1.47        | 1.39     |
| 2   | A     | 605    | HEC  | CHD-C4C | 3.61  | 1.47        | 1.39     |
| 2   | A     | 602    | HEC  | FE-NB   | 3.61  | 2.06        | 1.94     |
| 2   | B     | 607    | HEC  | CHB-C4A | 3.61  | 1.45        | 1.38     |
| 2   | B     | 606    | HEC  | CHB-C1B | 3.60  | 1.47        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | A     | 603    | HEC  | FE-NA   | 3.60  | 2.07        | 1.95     |
| 2   | B     | 602    | HEC  | FE-NA   | 3.60  | 2.07        | 1.95     |
| 2   | A     | 608    | HEC  | CHA-C4D | 3.59  | 1.47        | 1.39     |
| 2   | B     | 605    | HEC  | C1D-C2D | 3.57  | 1.51        | 1.44     |
| 2   | B     | 608    | HEC  | CHA-C4D | 3.57  | 1.47        | 1.39     |
| 2   | B     | 608    | HEC  | C3C-C2C | 3.56  | 1.48        | 1.38     |
| 2   | B     | 602    | HEC  | C4B-NB  | -3.55 | 1.34        | 1.40     |
| 2   | B     | 606    | HEC  | C3C-C2C | 3.55  | 1.48        | 1.38     |
| 2   | B     | 606    | HEC  | FE-NA   | 3.54  | 2.06        | 1.95     |
| 2   | B     | 603    | HEC  | FE-NA   | 3.53  | 2.06        | 1.95     |
| 2   | A     | 605    | HEC  | CHB-C1B | 3.52  | 1.47        | 1.39     |
| 2   | B     | 608    | HEC  | CHC-C1C | 3.50  | 1.47        | 1.39     |
| 2   | A     | 602    | HEC  | CHA-C4D | 3.50  | 1.47        | 1.39     |
| 2   | A     | 603    | HEC  | C1D-ND  | -3.50 | 1.34        | 1.40     |
| 2   | B     | 601    | HEC  | CHB-C4A | 3.49  | 1.45        | 1.38     |
| 2   | B     | 607    | HEC  | FE-NC   | 3.49  | 2.06        | 1.95     |
| 2   | A     | 603    | HEC  | CHB-C1B | 3.49  | 1.47        | 1.39     |
| 2   | A     | 601    | HEC  | FE-NA   | 3.47  | 2.06        | 1.95     |
| 2   | A     | 603    | HEC  | C4B-NB  | -3.47 | 1.34        | 1.40     |
| 2   | A     | 601    | HEC  | CHD-C4C | 3.47  | 1.47        | 1.39     |
| 2   | B     | 603    | HEC  | FE-NC   | 3.46  | 2.06        | 1.95     |
| 2   | A     | 601    | HEC  | C4B-NB  | -3.45 | 1.34        | 1.40     |
| 2   | B     | 606    | HEC  | C1D-ND  | -3.45 | 1.34        | 1.40     |
| 2   | A     | 607    | HEC  | CHB-C1B | 3.45  | 1.47        | 1.39     |
| 2   | A     | 603    | HEC  | C1C-NC  | -3.45 | 1.33        | 1.39     |
| 2   | A     | 605    | HEC  | C4B-NB  | -3.44 | 1.34        | 1.40     |
| 2   | B     | 605    | HEC  | CHB-C1B | 3.42  | 1.47        | 1.39     |
| 2   | A     | 601    | HEC  | FE-ND   | 3.42  | 2.05        | 1.94     |
| 2   | A     | 602    | HEC  | FE-NC   | 3.41  | 2.06        | 1.95     |
| 2   | B     | 601    | HEC  | FE-NA   | 3.39  | 2.06        | 1.95     |
| 2   | B     | 606    | HEC  | CHD-C1D | 3.39  | 1.45        | 1.38     |
| 2   | A     | 604    | HEC  | CHD-C1D | 3.39  | 1.45        | 1.38     |
| 2   | A     | 608    | HEC  | C1D-ND  | -3.38 | 1.34        | 1.40     |
| 2   | B     | 603    | HEC  | CHB-C4A | 3.38  | 1.45        | 1.38     |
| 2   | B     | 601    | HEC  | CHD-C1D | 3.38  | 1.45        | 1.38     |
| 2   | B     | 604[A] | HEC  | CHB-C1B | 3.37  | 1.46        | 1.39     |
| 2   | B     | 604[B] | HEC  | CHB-C1B | 3.37  | 1.46        | 1.39     |
| 2   | B     | 607    | HEC  | C1D-ND  | -3.36 | 1.34        | 1.40     |
| 2   | A     | 603    | HEC  | CHC-C1C | 3.35  | 1.46        | 1.39     |
| 2   | B     | 601    | HEC  | CHD-C4C | 3.35  | 1.46        | 1.39     |
| 2   | B     | 602    | HEC  | FE-NC   | 3.34  | 2.06        | 1.95     |
| 2   | B     | 607    | HEC  | CHD-C1D | 3.34  | 1.45        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | B     | 602    | HEC  | CHB-C4A | 3.34  | 1.44        | 1.38     |
| 2   | A     | 602    | HEC  | C3C-C2C | 3.33  | 1.47        | 1.38     |
| 2   | B     | 607    | HEC  | CHD-C4C | 3.33  | 1.46        | 1.39     |
| 2   | B     | 604[A] | HEC  | CHC-C1C | 3.32  | 1.46        | 1.39     |
| 2   | B     | 604[B] | HEC  | CHC-C1C | 3.32  | 1.46        | 1.39     |
| 2   | B     | 606    | HEC  | CHD-C4C | 3.31  | 1.46        | 1.39     |
| 2   | A     | 602    | HEC  | CHB-C4A | 3.30  | 1.44        | 1.38     |
| 2   | B     | 606    | HEC  | FE-NC   | 3.30  | 2.06        | 1.95     |
| 2   | B     | 604[A] | HEC  | C3C-C2C | 3.30  | 1.47        | 1.38     |
| 2   | B     | 604[B] | HEC  | C3C-C2C | 3.30  | 1.47        | 1.38     |
| 2   | B     | 601    | HEC  | C4B-NB  | -3.29 | 1.34        | 1.40     |
| 2   | A     | 608    | HEC  | CHC-C1C | 3.29  | 1.46        | 1.39     |
| 2   | A     | 603    | HEC  | C4C-NC  | -3.28 | 1.33        | 1.39     |
| 2   | A     | 607    | HEC  | FE-ND   | 3.28  | 2.05        | 1.94     |
| 2   | A     | 603    | HEC  | FE-ND   | 3.26  | 2.04        | 1.94     |
| 2   | A     | 601    | HEC  | CHD-C1D | 3.25  | 1.45        | 1.38     |
| 2   | A     | 606    | HEC  | C4C-NC  | -3.25 | 1.33        | 1.39     |
| 2   | A     | 606    | HEC  | CHC-C1C | 3.25  | 1.46        | 1.39     |
| 2   | B     | 602    | HEC  | CHC-C4B | 3.25  | 1.45        | 1.38     |
| 2   | B     | 601    | HEC  | FE-ND   | 3.23  | 2.04        | 1.94     |
| 2   | B     | 602    | HEC  | CHB-C1B | 3.21  | 1.46        | 1.39     |
| 2   | B     | 606    | HEC  | CHC-C1C | 3.21  | 1.46        | 1.39     |
| 2   | A     | 602    | HEC  | FE-ND   | 3.20  | 2.04        | 1.94     |
| 2   | A     | 601    | HEC  | CHC-C4B | 3.20  | 1.44        | 1.38     |
| 2   | A     | 606    | HEC  | C3C-C2C | 3.20  | 1.47        | 1.38     |
| 2   | A     | 607    | HEC  | FE-NA   | 3.19  | 2.05        | 1.95     |
| 2   | A     | 601    | HEC  | CHC-C1C | 3.19  | 1.46        | 1.39     |
| 2   | B     | 603    | HEC  | C3C-C2C | 3.19  | 1.47        | 1.38     |
| 2   | A     | 604    | HEC  | C4C-NC  | -3.18 | 1.33        | 1.39     |
| 2   | A     | 608    | HEC  | C3C-C2C | 3.18  | 1.47        | 1.38     |
| 2   | B     | 604[A] | HEC  | CHC-C4B | 3.18  | 1.44        | 1.38     |
| 2   | B     | 604[B] | HEC  | CHC-C4B | 3.18  | 1.44        | 1.38     |
| 2   | B     | 602    | HEC  | CHD-C1D | 3.17  | 1.44        | 1.38     |
| 2   | A     | 607    | HEC  | CHC-C1C | 3.17  | 1.46        | 1.39     |
| 2   | B     | 605    | HEC  | C3C-C2C | 3.17  | 1.47        | 1.38     |
| 2   | A     | 605    | HEC  | C1A-C2A | 3.17  | 1.50        | 1.45     |
| 2   | B     | 607    | HEC  | FE-NA   | 3.17  | 2.05        | 1.95     |
| 2   | B     | 608    | HEC  | C1A-NA  | -3.14 | 1.33        | 1.39     |
| 2   | B     | 608    | HEC  | C1D-ND  | -3.14 | 1.34        | 1.40     |
| 2   | A     | 605    | HEC  | CHB-C4A | 3.14  | 1.44        | 1.38     |
| 2   | A     | 606    | HEC  | C1C-NC  | -3.12 | 1.33        | 1.39     |
| 2   | A     | 604    | HEC  | C1D-ND  | -3.12 | 1.34        | 1.40     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | A     | 602    | HEC  | CHC-C4B | 3.12  | 1.44        | 1.38     |
| 2   | A     | 606    | HEC  | CHA-C4D | 3.11  | 1.46        | 1.39     |
| 2   | A     | 608    | HEC  | CHB-C1B | 3.09  | 1.46        | 1.39     |
| 2   | B     | 608    | HEC  | C4C-C3C | 3.09  | 1.50        | 1.44     |
| 2   | B     | 607    | HEC  | FE-ND   | 3.07  | 2.04        | 1.94     |
| 2   | A     | 604    | HEC  | C3C-C2C | 3.07  | 1.46        | 1.38     |
| 2   | B     | 602    | HEC  | CHC-C1C | 3.06  | 1.46        | 1.39     |
| 2   | A     | 605    | HEC  | C4C-C3C | 3.06  | 1.50        | 1.44     |
| 2   | A     | 602    | HEC  | CHC-C1C | 3.05  | 1.46        | 1.39     |
| 2   | A     | 602    | HEC  | O2D-CGD | -3.05 | 1.20        | 1.30     |
| 2   | A     | 603    | HEC  | C1A-NA  | -3.03 | 1.33        | 1.39     |
| 2   | B     | 602    | HEC  | CHA-C4D | 3.03  | 1.46        | 1.39     |
| 2   | A     | 601    | HEC  | C3C-C2C | 3.03  | 1.46        | 1.38     |
| 2   | B     | 607    | HEC  | CHA-C4D | 3.03  | 1.46        | 1.39     |
| 2   | B     | 604[A] | HEC  | C1D-ND  | -3.03 | 1.35        | 1.40     |
| 2   | B     | 604[B] | HEC  | C1D-ND  | -3.03 | 1.35        | 1.40     |
| 2   | B     | 602    | HEC  | C3C-C2C | 3.02  | 1.46        | 1.38     |
| 2   | B     | 603    | HEC  | CHB-C1B | 3.02  | 1.46        | 1.39     |
| 2   | B     | 603    | HEC  | CHC-C1C | 3.00  | 1.46        | 1.39     |
| 2   | B     | 603    | HEC  | FE-NB   | 2.99  | 2.04        | 1.94     |
| 2   | B     | 606    | HEC  | C4B-NB  | -2.99 | 1.35        | 1.40     |
| 2   | A     | 607    | HEC  | C1D-ND  | -2.98 | 1.35        | 1.40     |
| 2   | B     | 601    | HEC  | C3C-C2C | 2.97  | 1.46        | 1.38     |
| 2   | B     | 608    | HEC  | C4C-NC  | -2.96 | 1.34        | 1.39     |
| 2   | B     | 601    | HEC  | CHB-C1B | 2.96  | 1.45        | 1.39     |
| 2   | B     | 606    | HEC  | CHA-C4D | 2.95  | 1.45        | 1.39     |
| 2   | B     | 604[A] | HEC  | C4C-NC  | -2.95 | 1.34        | 1.39     |
| 2   | B     | 604[B] | HEC  | C4C-NC  | -2.95 | 1.34        | 1.39     |
| 2   | A     | 608    | HEC  | CHD-C4C | 2.93  | 1.46        | 1.39     |
| 2   | B     | 602    | HEC  | O2D-CGD | -2.93 | 1.21        | 1.30     |
| 2   | A     | 607    | HEC  | C4A-NA  | -2.92 | 1.34        | 1.39     |
| 2   | B     | 602    | HEC  | C4A-NA  | -2.92 | 1.34        | 1.39     |
| 2   | B     | 603    | HEC  | C1D-ND  | -2.91 | 1.35        | 1.40     |
| 2   | B     | 605    | HEC  | C4C-C3C | 2.90  | 1.50        | 1.44     |
| 2   | A     | 604    | HEC  | CHD-C4C | 2.89  | 1.45        | 1.39     |
| 2   | B     | 601    | HEC  | C4C-NC  | -2.89 | 1.34        | 1.39     |
| 2   | B     | 602    | HEC  | FE-NB   | 2.88  | 2.03        | 1.94     |
| 2   | B     | 608    | HEC  | CHB-C1B | 2.88  | 1.45        | 1.39     |
| 2   | B     | 605    | HEC  | C4D-C3D | 2.88  | 1.50        | 1.44     |
| 2   | A     | 607    | HEC  | CHD-C4C | 2.87  | 1.45        | 1.39     |
| 2   | B     | 602    | HEC  | C1A-NA  | -2.87 | 1.34        | 1.39     |
| 2   | A     | 606    | HEC  | C4A-NA  | -2.85 | 1.34        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | B     | 601    | HEC  | C1D-ND  | -2.85 | 1.35        | 1.40     |
| 2   | A     | 605    | HEC  | C3C-C2C | 2.84  | 1.46        | 1.38     |
| 2   | B     | 602    | HEC  | C4C-NC  | -2.84 | 1.34        | 1.39     |
| 2   | B     | 606    | HEC  | C1C-NC  | -2.84 | 1.34        | 1.39     |
| 2   | A     | 607    | HEC  | C4B-NB  | -2.83 | 1.35        | 1.40     |
| 2   | B     | 607    | HEC  | C1C-C2C | 2.83  | 1.49        | 1.43     |
| 2   | B     | 602    | HEC  | C1D-ND  | -2.83 | 1.35        | 1.40     |
| 2   | B     | 608    | HEC  | C1C-C2C | 2.82  | 1.49        | 1.43     |
| 2   | B     | 603    | HEC  | C1A-NA  | -2.82 | 1.34        | 1.39     |
| 2   | B     | 604[A] | HEC  | C4D-ND  | -2.80 | 1.33        | 1.38     |
| 2   | B     | 604[B] | HEC  | C4D-ND  | -2.80 | 1.33        | 1.38     |
| 2   | A     | 605    | HEC  | CHC-C1C | 2.79  | 1.45        | 1.39     |
| 2   | A     | 604    | HEC  | FE-NC   | 2.79  | 2.04        | 1.95     |
| 2   | A     | 603    | HEC  | C3C-C2C | 2.79  | 1.46        | 1.38     |
| 2   | A     | 605    | HEC  | CHA-C4D | 2.79  | 1.49        | 1.40     |
| 2   | A     | 603    | HEC  | CHD-C4C | 2.78  | 1.45        | 1.39     |
| 2   | A     | 604    | HEC  | CHB-C1B | 2.78  | 1.45        | 1.39     |
| 2   | A     | 601    | HEC  | CHA-C4D | 2.78  | 1.45        | 1.39     |
| 2   | A     | 606    | HEC  | C4B-C3B | 2.76  | 1.49        | 1.45     |
| 2   | A     | 607    | HEC  | C3C-C2C | 2.76  | 1.46        | 1.38     |
| 2   | A     | 602    | HEC  | C4A-NA  | -2.74 | 1.34        | 1.39     |
| 2   | A     | 608    | HEC  | C1B-C2B | 2.71  | 1.50        | 1.44     |
| 2   | A     | 602    | HEC  | C4B-NB  | -2.71 | 1.35        | 1.40     |
| 2   | A     | 601    | HEC  | C4C-NC  | -2.71 | 1.34        | 1.39     |
| 2   | B     | 605    | HEC  | C1A-C2A | 2.70  | 1.49        | 1.45     |
| 2   | B     | 604[A] | HEC  | FE-NC   | 2.70  | 2.04        | 1.95     |
| 2   | B     | 604[B] | HEC  | FE-NC   | 2.70  | 2.04        | 1.95     |
| 2   | B     | 601    | HEC  | CHA-C4D | 2.70  | 1.45        | 1.39     |
| 2   | B     | 608    | HEC  | CHD-C4C | 2.69  | 1.45        | 1.39     |
| 2   | A     | 602    | HEC  | CHB-C1B | 2.68  | 1.45        | 1.39     |
| 2   | A     | 607    | HEC  | C1C-C2C | 2.68  | 1.49        | 1.43     |
| 2   | B     | 608    | HEC  | C4A-NA  | -2.66 | 1.34        | 1.39     |
| 2   | A     | 608    | HEC  | C4B-C3B | 2.66  | 1.49        | 1.45     |
| 2   | B     | 603    | HEC  | FE-ND   | 2.66  | 2.03        | 1.94     |
| 2   | B     | 604[A] | HEC  | CHD-C4C | 2.63  | 1.45        | 1.39     |
| 2   | B     | 604[B] | HEC  | CHD-C4C | 2.63  | 1.45        | 1.39     |
| 2   | B     | 605    | HEC  | CHC-C1C | 2.63  | 1.45        | 1.39     |
| 2   | B     | 607    | HEC  | C3C-C2C | 2.63  | 1.45        | 1.38     |
| 2   | A     | 604    | HEC  | CHC-C1C | 2.62  | 1.45        | 1.39     |
| 2   | B     | 601    | HEC  | C4A-NA  | -2.61 | 1.34        | 1.39     |
| 2   | B     | 603    | HEC  | C4B-NB  | -2.60 | 1.35        | 1.40     |
| 2   | B     | 601    | HEC  | CHC-C4B | 2.58  | 1.43        | 1.38     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | B     | 606    | HEC  | C1A-C2A | 2.57  | 1.49        | 1.45     |
| 2   | A     | 608    | HEC  | C1A-NA  | -2.57 | 1.34        | 1.39     |
| 2   | B     | 603    | HEC  | C1C-NC  | -2.56 | 1.34        | 1.39     |
| 2   | B     | 603    | HEC  | C4A-NA  | -2.56 | 1.34        | 1.39     |
| 2   | B     | 607    | HEC  | C4B-C3B | 2.55  | 1.49        | 1.45     |
| 2   | A     | 608    | HEC  | C1C-C2C | 2.54  | 1.49        | 1.43     |
| 2   | A     | 605    | HEC  | C1B-NB  | -2.53 | 1.33        | 1.38     |
| 2   | A     | 608    | HEC  | C4C-NC  | -2.53 | 1.34        | 1.39     |
| 2   | B     | 608    | HEC  | C4B-NB  | -2.51 | 1.35        | 1.40     |
| 2   | B     | 605    | HEC  | C4A-C3A | 2.50  | 1.50        | 1.45     |
| 2   | A     | 606    | HEC  | C4D-C3D | 2.50  | 1.49        | 1.45     |
| 2   | A     | 601    | HEC  | C1B-C2B | 2.49  | 1.49        | 1.44     |
| 2   | A     | 602    | HEC  | C1A-NA  | -2.49 | 1.34        | 1.39     |
| 2   | B     | 603    | HEC  | CHD-C4C | 2.49  | 1.45        | 1.39     |
| 2   | A     | 604    | HEC  | C1C-NC  | -2.48 | 1.34        | 1.39     |
| 2   | A     | 606    | HEC  | C1D-ND  | -2.47 | 1.36        | 1.40     |
| 2   | B     | 608    | HEC  | C4D-C3D | 2.46  | 1.49        | 1.45     |
| 2   | A     | 604    | HEC  | C4D-ND  | -2.45 | 1.34        | 1.38     |
| 2   | B     | 601    | HEC  | C1B-C2B | 2.44  | 1.49        | 1.44     |
| 2   | B     | 604[A] | HEC  | CHD-C1D | 2.44  | 1.43        | 1.38     |
| 2   | B     | 604[B] | HEC  | CHD-C1D | 2.44  | 1.43        | 1.38     |
| 2   | A     | 601    | HEC  | C1A-C2A | 2.43  | 1.49        | 1.45     |
| 2   | A     | 606    | HEC  | CHB-C1B | 2.43  | 1.44        | 1.39     |
| 2   | A     | 602    | HEC  | C1D-ND  | -2.42 | 1.36        | 1.40     |
| 2   | A     | 606    | HEC  | CHD-C4C | 2.42  | 1.44        | 1.39     |
| 2   | B     | 602    | HEC  | C4D-ND  | -2.41 | 1.34        | 1.38     |
| 2   | A     | 602    | HEC  | C4D-ND  | -2.41 | 1.34        | 1.38     |
| 2   | A     | 601    | HEC  | C1B-NB  | -2.41 | 1.34        | 1.38     |
| 2   | A     | 608    | HEC  | C4C-C3C | 2.40  | 1.49        | 1.44     |
| 2   | B     | 607    | HEC  | C4A-NA  | -2.40 | 1.35        | 1.39     |
| 2   | B     | 605    | HEC  | C1D-ND  | -2.40 | 1.36        | 1.40     |
| 2   | A     | 604    | HEC  | FE-NA   | 2.40  | 2.03        | 1.95     |
| 2   | B     | 601    | HEC  | C1C-NC  | -2.40 | 1.35        | 1.39     |
| 2   | A     | 604    | HEC  | C1B-NB  | -2.40 | 1.34        | 1.38     |
| 2   | B     | 603    | HEC  | CBA-CGA | 2.39  | 1.56        | 1.50     |
| 2   | B     | 602    | HEC  | C1C-NC  | -2.39 | 1.35        | 1.39     |
| 2   | A     | 605    | HEC  | C1D-ND  | -2.36 | 1.36        | 1.40     |
| 2   | A     | 601    | HEC  | C1C-NC  | -2.35 | 1.35        | 1.39     |
| 2   | A     | 604    | HEC  | CHA-C4D | 2.35  | 1.44        | 1.39     |
| 2   | B     | 606    | HEC  | C4B-C3B | 2.35  | 1.49        | 1.45     |
| 2   | B     | 606    | HEC  | C4A-C3A | 2.34  | 1.50        | 1.45     |
| 2   | A     | 603    | HEC  | C4D-C3D | 2.34  | 1.49        | 1.45     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | A     | 608    | HEC  | C1C-NC  | -2.33 | 1.35        | 1.39     |
| 2   | B     | 608    | HEC  | C1C-NC  | -2.33 | 1.35        | 1.39     |
| 2   | B     | 607    | HEC  | C4B-NB  | -2.33 | 1.36        | 1.40     |
| 2   | A     | 606    | HEC  | C4C-C3C | 2.31  | 1.49        | 1.44     |
| 2   | A     | 604    | HEC  | C1B-C2B | 2.31  | 1.49        | 1.44     |
| 2   | A     | 602    | HEC  | C4C-NC  | -2.28 | 1.35        | 1.39     |
| 2   | A     | 608    | HEC  | C1A-C2A | 2.28  | 1.49        | 1.45     |
| 2   | A     | 608    | HEC  | C4D-ND  | -2.27 | 1.34        | 1.38     |
| 2   | B     | 604[A] | HEC  | C4B-C3B | 2.26  | 1.48        | 1.45     |
| 2   | B     | 604[B] | HEC  | C4B-C3B | 2.26  | 1.48        | 1.45     |
| 2   | B     | 601    | HEC  | C1D-C2D | 2.26  | 1.49        | 1.44     |
| 2   | B     | 603    | HEC  | CHD-C1D | 2.25  | 1.43        | 1.38     |
| 2   | B     | 601    | HEC  | C4D-ND  | -2.25 | 1.34        | 1.38     |
| 2   | B     | 608    | HEC  | C4B-C3B | 2.24  | 1.48        | 1.45     |
| 2   | A     | 603    | HEC  | C4A-NA  | -2.23 | 1.35        | 1.39     |
| 2   | A     | 601    | HEC  | C1A-NA  | -2.22 | 1.35        | 1.39     |
| 2   | A     | 608    | HEC  | C4B-NB  | -2.22 | 1.36        | 1.40     |
| 2   | A     | 602    | HEC  | C1A-C2A | 2.22  | 1.49        | 1.45     |
| 2   | A     | 607    | HEC  | CHA-C4D | 2.21  | 1.44        | 1.39     |
| 2   | A     | 602    | HEC  | C1B-NB  | -2.21 | 1.34        | 1.38     |
| 2   | A     | 604    | HEC  | C1A-NA  | -2.21 | 1.35        | 1.39     |
| 2   | A     | 601    | HEC  | C4D-ND  | -2.21 | 1.34        | 1.38     |
| 2   | B     | 604[A] | HEC  | FE-NA   | 2.21  | 2.02        | 1.95     |
| 2   | B     | 604[B] | HEC  | FE-NA   | 2.21  | 2.02        | 1.95     |
| 2   | A     | 606    | HEC  | C1C-C2C | 2.20  | 1.48        | 1.43     |
| 2   | A     | 602    | HEC  | CHD-C4C | 2.19  | 1.44        | 1.39     |
| 2   | B     | 607    | HEC  | C4C-NC  | -2.19 | 1.35        | 1.39     |
| 2   | A     | 604    | HEC  | CHC-C4B | 2.16  | 1.42        | 1.38     |
| 2   | A     | 606    | HEC  | C4A-C3A | 2.16  | 1.49        | 1.45     |
| 2   | A     | 604    | HEC  | C4A-NA  | -2.15 | 1.35        | 1.39     |
| 2   | A     | 606    | HEC  | C4B-NB  | -2.15 | 1.36        | 1.40     |
| 2   | A     | 603    | HEC  | C4B-C3B | 2.15  | 1.48        | 1.45     |
| 2   | A     | 602    | HEC  | C1C-C2C | 2.14  | 1.48        | 1.43     |
| 2   | A     | 606    | HEC  | C1A-NA  | -2.14 | 1.35        | 1.39     |
| 2   | A     | 602    | HEC  | C1C-NC  | -2.14 | 1.35        | 1.39     |
| 2   | A     | 607    | HEC  | C1C-NC  | -2.09 | 1.35        | 1.39     |
| 2   | A     | 605    | HEC  | C1C-NC  | -2.09 | 1.35        | 1.39     |
| 2   | B     | 601    | HEC  | C1B-NB  | -2.08 | 1.34        | 1.38     |
| 2   | A     | 605    | HEC  | C4A-C3A | 2.07  | 1.49        | 1.45     |
| 2   | B     | 606    | HEC  | C4A-NA  | -2.06 | 1.35        | 1.39     |
| 2   | B     | 604[A] | HEC  | C1C-C2C | 2.06  | 1.48        | 1.43     |
| 2   | B     | 604[B] | HEC  | C1C-C2C | 2.06  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 608 | HEC  | C1D-C2D | 2.05  | 1.48        | 1.44     |
| 2   | A     | 601 | HEC  | C4A-NA  | -2.04 | 1.35        | 1.39     |
| 2   | B     | 602 | HEC  | CHD-C4C | 2.04  | 1.44        | 1.39     |
| 2   | A     | 606 | HEC  | C1B-C2B | 2.04  | 1.48        | 1.44     |
| 2   | B     | 602 | HEC  | C1A-C2A | 2.03  | 1.48        | 1.45     |
| 2   | B     | 602 | HEC  | FE-ND   | 2.03  | 2.01        | 1.94     |
| 2   | A     | 605 | HEC  | C1C-C2C | 2.02  | 1.47        | 1.43     |
| 2   | B     | 605 | HEC  | C1B-NB  | -2.01 | 1.34        | 1.38     |
| 2   | A     | 604 | HEC  | C1C-C2C | 2.01  | 1.47        | 1.43     |
| 2   | B     | 606 | HEC  | C4C-C3C | 2.01  | 1.48        | 1.44     |

All (455) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | B     | 605    | HEC  | CAC-C3C-C4C | 6.32  | 133.61      | 124.91   |
| 2   | A     | 606    | HEC  | C2D-C1D-ND  | 6.27  | 117.05      | 109.84   |
| 2   | B     | 606    | HEC  | C3D-C4D-ND  | 6.23  | 116.37      | 110.35   |
| 2   | B     | 606    | HEC  | C2D-C1D-ND  | 6.08  | 116.83      | 109.84   |
| 2   | B     | 604[A] | HEC  | C3D-C4D-ND  | 6.07  | 116.22      | 110.35   |
| 2   | B     | 604[B] | HEC  | C3D-C4D-ND  | 6.07  | 116.22      | 110.35   |
| 2   | A     | 603    | HEC  | C2B-C1B-NB  | 5.97  | 116.81      | 109.90   |
| 2   | A     | 603    | HEC  | C1B-C2B-C3B | -5.89 | 100.78      | 106.98   |
| 2   | A     | 605    | HEC  | CAC-C3C-C4C | 5.84  | 132.95      | 124.91   |
| 2   | B     | 605    | HEC  | C1B-C2B-C3B | -5.80 | 100.88      | 106.98   |
| 2   | B     | 603    | HEC  | C2B-C1B-NB  | 5.79  | 116.60      | 109.90   |
| 2   | B     | 601    | HEC  | C1B-C2B-C3B | -5.78 | 100.90      | 106.98   |
| 2   | B     | 607    | HEC  | C1C-C2C-C3C | -5.73 | 100.25      | 106.82   |
| 2   | B     | 608    | HEC  | C2B-C1B-NB  | 5.72  | 116.52      | 109.90   |
| 2   | B     | 604[A] | HEC  | C1B-C2B-C3B | -5.71 | 100.97      | 106.98   |
| 2   | B     | 604[B] | HEC  | C1B-C2B-C3B | -5.71 | 100.97      | 106.98   |
| 2   | A     | 602    | HEC  | C2A-C1A-NA  | 5.70  | 115.82      | 110.32   |
| 2   | A     | 606    | HEC  | C3D-C4D-ND  | 5.69  | 115.85      | 110.35   |
| 2   | B     | 605    | HEC  | C1C-C2C-C3C | -5.67 | 100.32      | 106.82   |
| 2   | A     | 602    | HEC  | C1B-C2B-C3B | -5.65 | 101.03      | 106.98   |
| 2   | B     | 603    | HEC  | C2D-C1D-ND  | 5.63  | 116.32      | 109.84   |
| 2   | A     | 603    | HEC  | C2D-C1D-ND  | 5.61  | 116.29      | 109.84   |
| 2   | B     | 602    | HEC  | C1B-C2B-C3B | -5.60 | 101.08      | 106.98   |
| 2   | A     | 602    | HEC  | C2B-C1B-NB  | 5.60  | 116.38      | 109.90   |
| 2   | B     | 603    | HEC  | C1B-C2B-C3B | -5.55 | 101.15      | 106.98   |
| 2   | A     | 604    | HEC  | C3D-C4D-ND  | 5.51  | 115.68      | 110.35   |
| 2   | A     | 604    | HEC  | C1B-C2B-C3B | -5.51 | 101.18      | 106.98   |
| 2   | A     | 601    | HEC  | C1B-C2B-C3B | -5.51 | 101.19      | 106.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | A     | 605    | HEC  | C1B-C2B-C3B | -5.49 | 101.21      | 106.98   |
| 2   | B     | 605    | HEC  | C4D-C3D-C2D | -5.44 | 102.03      | 107.09   |
| 2   | A     | 608    | HEC  | C2B-C1B-NB  | 5.42  | 116.17      | 109.90   |
| 2   | A     | 606    | HEC  | C2B-C1B-NB  | 5.42  | 116.17      | 109.90   |
| 2   | B     | 602    | HEC  | C3C-C4C-NC  | 5.32  | 116.06      | 110.15   |
| 2   | A     | 601    | HEC  | C3D-C4D-ND  | 5.32  | 115.49      | 110.35   |
| 2   | B     | 601    | HEC  | C3D-C4D-ND  | 5.30  | 115.47      | 110.35   |
| 2   | B     | 608    | HEC  | C2D-C1D-ND  | 5.28  | 115.91      | 109.84   |
| 2   | B     | 601    | HEC  | C2B-C1B-NB  | 5.22  | 115.94      | 109.90   |
| 2   | A     | 601    | HEC  | C2B-C1B-NB  | 5.20  | 115.92      | 109.90   |
| 2   | B     | 607    | HEC  | C2B-C1B-NB  | 5.20  | 115.92      | 109.90   |
| 2   | B     | 604[A] | HEC  | C2B-C1B-NB  | 5.15  | 115.86      | 109.90   |
| 2   | B     | 604[B] | HEC  | C2B-C1B-NB  | 5.15  | 115.86      | 109.90   |
| 2   | B     | 601    | HEC  | C1C-C2C-C3C | -5.15 | 100.92      | 106.82   |
| 2   | B     | 608    | HEC  | C1B-C2B-C3B | -5.14 | 101.58      | 106.98   |
| 2   | B     | 604[A] | HEC  | C2D-C1D-ND  | 5.13  | 115.73      | 109.84   |
| 2   | B     | 604[B] | HEC  | C2D-C1D-ND  | 5.13  | 115.73      | 109.84   |
| 2   | B     | 608    | HEC  | C1C-C2C-C3C | -5.12 | 100.96      | 106.82   |
| 2   | B     | 601    | HEC  | C2D-C1D-ND  | 5.11  | 115.71      | 109.84   |
| 2   | A     | 601    | HEC  | C2D-C1D-ND  | 5.10  | 115.70      | 109.84   |
| 2   | A     | 607    | HEC  | C3C-C4C-NC  | 5.08  | 115.79      | 110.15   |
| 2   | B     | 607    | HEC  | C2A-C1A-NA  | 5.01  | 115.15      | 110.32   |
| 2   | B     | 608    | HEC  | C3D-C4D-ND  | 5.00  | 115.18      | 110.35   |
| 2   | B     | 602    | HEC  | C2B-C1B-NB  | 4.98  | 115.66      | 109.90   |
| 2   | B     | 601    | HEC  | C1D-C2D-C3D | -4.98 | 101.74      | 106.98   |
| 2   | B     | 602    | HEC  | C2A-C1A-NA  | 4.97  | 115.12      | 110.32   |
| 2   | B     | 608    | HEC  | C2A-C1A-NA  | 4.97  | 115.11      | 110.32   |
| 2   | A     | 607    | HEC  | C2A-C1A-NA  | 4.96  | 115.11      | 110.32   |
| 2   | B     | 607    | HEC  | C3D-C4D-ND  | 4.95  | 115.14      | 110.35   |
| 2   | A     | 604    | HEC  | C1C-C2C-C3C | -4.94 | 101.16      | 106.82   |
| 2   | A     | 608    | HEC  | C3D-C4D-ND  | 4.94  | 115.12      | 110.35   |
| 2   | A     | 602    | HEC  | C2D-C1D-ND  | 4.93  | 115.51      | 109.84   |
| 2   | B     | 602    | HEC  | C2D-C1D-ND  | 4.93  | 115.51      | 109.84   |
| 2   | A     | 604    | HEC  | C2B-C1B-NB  | 4.93  | 115.60      | 109.90   |
| 2   | B     | 605    | HEC  | C2B-C1B-NB  | 4.91  | 115.58      | 109.90   |
| 2   | B     | 607    | HEC  | CAB-C3B-C4B | 4.90  | 131.17      | 124.79   |
| 2   | B     | 604[A] | HEC  | C1C-C2C-C3C | -4.90 | 101.21      | 106.82   |
| 2   | B     | 604[B] | HEC  | C1C-C2C-C3C | -4.90 | 101.21      | 106.82   |
| 2   | A     | 603    | HEC  | C3D-C4D-ND  | 4.89  | 115.08      | 110.35   |
| 2   | B     | 606    | HEC  | C2A-C1A-NA  | 4.86  | 115.01      | 110.32   |
| 2   | A     | 605    | HEC  | C1C-C2C-C3C | -4.80 | 101.32      | 106.82   |
| 2   | B     | 602    | HEC  | C3D-C4D-ND  | 4.80  | 114.99      | 110.35   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | A     | 602    | HEC  | C1D-C2D-C3D | -4.78 | 101.96      | 106.98   |
| 2   | A     | 603    | HEC  | C1C-C2C-C3C | -4.76 | 101.37      | 106.82   |
| 2   | A     | 602    | HEC  | C3C-C4C-NC  | 4.74  | 115.41      | 110.15   |
| 2   | B     | 602    | HEC  | C3B-C4B-NB  | 4.73  | 115.36      | 110.17   |
| 2   | B     | 603    | HEC  | C3D-C4D-ND  | 4.71  | 114.90      | 110.35   |
| 2   | B     | 602    | HEC  | C1D-C2D-C3D | -4.70 | 102.03      | 106.98   |
| 2   | B     | 606    | HEC  | C2B-C1B-NB  | 4.70  | 115.33      | 109.90   |
| 2   | A     | 607    | HEC  | C3D-C4D-ND  | 4.67  | 114.87      | 110.35   |
| 2   | A     | 607    | HEC  | C1B-C2B-C3B | -4.66 | 102.08      | 106.98   |
| 2   | A     | 602    | HEC  | CAD-CBD-CGD | -4.63 | 101.39      | 113.67   |
| 2   | A     | 608    | HEC  | C1C-C2C-C3C | -4.63 | 101.52      | 106.82   |
| 2   | B     | 603    | HEC  | C1D-C2D-C3D | -4.62 | 102.12      | 106.98   |
| 2   | A     | 604    | HEC  | CBA-CAA-C2A | -4.61 | 99.78       | 112.53   |
| 2   | A     | 608    | HEC  | C1B-C2B-C3B | -4.61 | 102.13      | 106.98   |
| 2   | A     | 603    | HEC  | CAB-C3B-C4B | 4.61  | 130.79      | 124.79   |
| 2   | B     | 604[A] | HEC  | C1D-C2D-C3D | -4.58 | 102.16      | 106.98   |
| 2   | B     | 604[B] | HEC  | C1D-C2D-C3D | -4.58 | 102.16      | 106.98   |
| 2   | B     | 606    | HEC  | CAB-C3B-C4B | 4.57  | 130.73      | 124.79   |
| 2   | A     | 608    | HEC  | C3B-C4B-NB  | 4.55  | 115.16      | 110.17   |
| 2   | A     | 602    | HEC  | C3B-C4B-NB  | 4.54  | 115.15      | 110.17   |
| 2   | B     | 606    | HEC  | CAA-CBA-CGA | -4.53 | 101.66      | 113.67   |
| 2   | A     | 604    | HEC  | C3B-C4B-NB  | 4.52  | 115.13      | 110.17   |
| 2   | B     | 607    | HEC  | C1B-C2B-C3B | -4.49 | 102.26      | 106.98   |
| 2   | A     | 605    | HEC  | C4A-C3A-C2A | -4.47 | 100.33      | 106.97   |
| 2   | A     | 604    | HEC  | C2D-C1D-ND  | 4.47  | 114.98      | 109.84   |
| 2   | A     | 606    | HEC  | C1B-C2B-C3B | -4.44 | 102.31      | 106.98   |
| 2   | A     | 606    | HEC  | C1C-C2C-C3C | -4.44 | 101.73      | 106.82   |
| 2   | B     | 605    | HEC  | C2A-C1A-NA  | 4.43  | 114.60      | 110.32   |
| 2   | A     | 607    | HEC  | C2B-C1B-NB  | 4.42  | 115.01      | 109.90   |
| 2   | B     | 604[A] | HEC  | C2A-C1A-NA  | 4.41  | 114.58      | 110.32   |
| 2   | B     | 604[B] | HEC  | C2A-C1A-NA  | 4.41  | 114.58      | 110.32   |
| 2   | B     | 605    | HEC  | C2C-C1C-NC  | 4.40  | 117.19      | 110.14   |
| 2   | B     | 606    | HEC  | C1D-C2D-C3D | -4.39 | 102.37      | 106.98   |
| 2   | B     | 605    | HEC  | CBA-CAA-C2A | -4.38 | 100.41      | 112.53   |
| 2   | B     | 606    | HEC  | C1B-C2B-C3B | -4.37 | 102.38      | 106.98   |
| 2   | B     | 601    | HEC  | C2A-C1A-NA  | 4.36  | 114.53      | 110.32   |
| 2   | A     | 601    | HEC  | C2A-C1A-NA  | 4.35  | 114.53      | 110.32   |
| 2   | A     | 606    | HEC  | C1D-C2D-C3D | -4.35 | 102.40      | 106.98   |
| 2   | A     | 608    | HEC  | C2D-C1D-ND  | 4.34  | 114.82      | 109.84   |
| 2   | B     | 605    | HEC  | CAC-C3C-C2C | -4.33 | 120.05      | 126.89   |
| 2   | A     | 605    | HEC  | C2B-C1B-NB  | 4.32  | 114.90      | 109.90   |
| 2   | A     | 601    | HEC  | C3C-C4C-NC  | 4.31  | 114.94      | 110.15   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | A     | 606    | HEC  | CAB-C3B-C4B | 4.28  | 130.35      | 124.79   |
| 2   | A     | 607    | HEC  | CAB-C3B-C4B | 4.27  | 130.35      | 124.79   |
| 2   | A     | 606    | HEC  | C2A-C1A-NA  | 4.27  | 114.44      | 110.32   |
| 2   | A     | 608    | HEC  | C1D-C2D-C3D | -4.27 | 102.49      | 106.98   |
| 2   | A     | 603    | HEC  | C3C-C4C-NC  | 4.26  | 114.88      | 110.15   |
| 2   | A     | 603    | HEC  | C3B-C4B-NB  | 4.24  | 114.82      | 110.17   |
| 2   | B     | 605    | HEC  | CHB-C1B-C2B | -4.22 | 118.37      | 125.03   |
| 2   | A     | 605    | HEC  | C2C-C1C-NC  | 4.20  | 116.88      | 110.14   |
| 2   | A     | 602    | HEC  | C3D-C4D-ND  | 4.20  | 114.41      | 110.35   |
| 2   | B     | 608    | HEC  | C1D-C2D-C3D | -4.16 | 102.60      | 106.98   |
| 2   | B     | 601    | HEC  | C2C-C1C-NC  | 4.12  | 116.75      | 110.14   |
| 2   | B     | 605    | HEC  | C3D-C4D-ND  | 4.11  | 114.66      | 109.90   |
| 2   | A     | 603    | HEC  | C2A-C1A-NA  | 4.09  | 114.27      | 110.32   |
| 2   | B     | 607    | HEC  | C2C-C1C-NC  | 4.09  | 116.70      | 110.14   |
| 2   | B     | 605    | HEC  | C4A-C3A-C2A | -4.09 | 100.90      | 106.97   |
| 2   | B     | 607    | HEC  | C3C-C4C-NC  | 4.08  | 114.68      | 110.15   |
| 2   | A     | 603    | HEC  | C2C-C1C-NC  | 4.06  | 116.65      | 110.14   |
| 2   | A     | 604    | HEC  | C3C-C4C-NC  | 4.06  | 114.66      | 110.15   |
| 2   | B     | 601    | HEC  | C3B-C4B-NB  | 4.06  | 114.62      | 110.17   |
| 2   | B     | 602    | HEC  | CAC-C3C-C4C | 4.06  | 130.50      | 124.91   |
| 2   | B     | 604[A] | HEC  | C3C-C4C-NC  | 4.05  | 114.65      | 110.15   |
| 2   | B     | 604[B] | HEC  | C3C-C4C-NC  | 4.05  | 114.65      | 110.15   |
| 2   | A     | 606    | HEC  | CAA-CBA-CGA | -4.05 | 102.93      | 113.67   |
| 2   | B     | 608    | HEC  | C3B-C4B-NB  | 4.04  | 114.61      | 110.17   |
| 2   | A     | 607    | HEC  | CMD-C2D-C1D | 4.03  | 131.33      | 125.03   |
| 2   | B     | 601    | HEC  | C3C-C4C-NC  | 4.02  | 114.61      | 110.15   |
| 2   | A     | 601    | HEC  | C1C-C2C-C3C | -4.02 | 102.22      | 106.82   |
| 2   | A     | 607    | HEC  | C2D-C1D-ND  | 4.01  | 114.45      | 109.84   |
| 2   | B     | 608    | HEC  | CAB-C3B-C4B | 4.01  | 130.01      | 124.79   |
| 2   | A     | 605    | HEC  | CHB-C1B-C2B | -4.00 | 118.71      | 125.03   |
| 2   | A     | 607    | HEC  | C1C-C2C-C3C | -4.00 | 102.24      | 106.82   |
| 2   | A     | 602    | HEC  | CHA-C1A-NA  | -3.99 | 120.11      | 124.45   |
| 2   | A     | 606    | HEC  | C3B-C4B-NB  | 3.99  | 114.54      | 110.17   |
| 2   | A     | 605    | HEC  | C3A-C4A-NA  | 3.94  | 116.92      | 109.64   |
| 2   | A     | 601    | HEC  | C3B-C4B-NB  | 3.90  | 114.45      | 110.17   |
| 2   | A     | 605    | HEC  | CBA-CAA-C2A | -3.90 | 101.76      | 112.53   |
| 2   | A     | 602    | HEC  | C1C-C2C-C3C | -3.88 | 102.37      | 106.82   |
| 2   | A     | 604    | HEC  | C1D-C2D-C3D | -3.86 | 102.92      | 106.98   |
| 2   | A     | 603    | HEC  | C1D-C2D-C3D | -3.86 | 102.92      | 106.98   |
| 2   | A     | 608    | HEC  | C3C-C4C-NC  | 3.85  | 114.43      | 110.15   |
| 2   | A     | 601    | HEC  | C1D-C2D-C3D | -3.84 | 102.94      | 106.98   |
| 2   | B     | 605    | HEC  | C3A-C4A-NA  | 3.84  | 116.74      | 109.64   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | B     | 608    | HEC  | C2C-C1C-NC  | 3.84  | 116.29      | 110.14   |
| 2   | B     | 603    | HEC  | C3A-C4A-NA  | 3.79  | 116.66      | 109.64   |
| 2   | B     | 603    | HEC  | C4A-C3A-C2A | -3.78 | 101.36      | 106.97   |
| 2   | B     | 603    | HEC  | C3C-C4C-NC  | 3.74  | 114.30      | 110.15   |
| 2   | A     | 608    | HEC  | C2C-C1C-NC  | 3.72  | 116.11      | 110.14   |
| 2   | A     | 608    | HEC  | CMA-C3A-C4A | 3.72  | 131.28      | 124.73   |
| 2   | A     | 604    | HEC  | C2C-C1C-NC  | 3.70  | 116.08      | 110.14   |
| 2   | A     | 608    | HEC  | CMC-C2C-C3C | 3.70  | 133.47      | 125.62   |
| 2   | B     | 606    | HEC  | C1C-C2C-C3C | -3.69 | 102.59      | 106.82   |
| 2   | B     | 604[A] | HEC  | C2C-C1C-NC  | 3.68  | 116.03      | 110.14   |
| 2   | B     | 604[B] | HEC  | C2C-C1C-NC  | 3.68  | 116.03      | 110.14   |
| 2   | B     | 603    | HEC  | C1C-C2C-C3C | -3.65 | 102.64      | 106.82   |
| 2   | B     | 605    | HEC  | CMA-C3A-C4A | 3.65  | 131.15      | 124.73   |
| 2   | B     | 604[A] | HEC  | CBA-CAA-C2A | -3.65 | 102.45      | 112.53   |
| 2   | B     | 603    | HEC  | C3B-C4B-NB  | 3.63  | 114.15      | 110.17   |
| 2   | A     | 602    | HEC  | C3A-C4A-NA  | 3.63  | 116.35      | 109.64   |
| 2   | A     | 607    | HEC  | C2C-C1C-NC  | 3.60  | 115.91      | 110.14   |
| 2   | A     | 607    | HEC  | CBA-CAA-C2A | -3.59 | 102.61      | 112.53   |
| 2   | A     | 605    | HEC  | C4D-C3D-C2D | -3.58 | 101.92      | 109.27   |
| 2   | B     | 607    | HEC  | C3B-C4B-NB  | 3.58  | 114.09      | 110.17   |
| 2   | B     | 603    | HEC  | CAC-C3C-C4C | 3.55  | 129.80      | 124.91   |
| 2   | B     | 602    | HEC  | C3A-C4A-NA  | 3.54  | 116.19      | 109.64   |
| 2   | B     | 604[A] | HEC  | CBD-CAD-C3D | -3.54 | 102.75      | 112.53   |
| 2   | B     | 604[B] | HEC  | CBD-CAD-C3D | -3.54 | 102.75      | 112.53   |
| 2   | B     | 606    | HEC  | C3B-C4B-NB  | 3.51  | 114.02      | 110.17   |
| 2   | A     | 605    | HEC  | C3D-C4D-ND  | 3.51  | 114.41      | 110.22   |
| 2   | B     | 604[B] | HEC  | CBA-CAA-C2A | -3.50 | 102.84      | 112.53   |
| 2   | B     | 607    | HEC  | C2D-C1D-ND  | 3.50  | 113.87      | 109.84   |
| 2   | A     | 607    | HEC  | C1D-C2D-C3D | -3.50 | 103.30      | 106.98   |
| 2   | B     | 608    | HEC  | C3C-C4C-NC  | 3.50  | 114.04      | 110.15   |
| 2   | A     | 604    | HEC  | C4A-C3A-C2A | -3.50 | 101.78      | 106.97   |
| 2   | B     | 608    | HEC  | CBD-CAD-C3D | -3.48 | 102.92      | 112.53   |
| 2   | B     | 608    | HEC  | CMC-C2C-C3C | 3.45  | 132.95      | 125.62   |
| 2   | A     | 605    | HEC  | CAB-C3B-C4B | 3.45  | 129.28      | 124.79   |
| 2   | A     | 606    | HEC  | CAC-C3C-C4C | 3.43  | 129.63      | 124.91   |
| 2   | A     | 604    | HEC  | CAD-C3D-C4D | 3.42  | 130.66      | 124.70   |
| 2   | B     | 603    | HEC  | C2A-C1A-NA  | 3.41  | 113.61      | 110.32   |
| 2   | B     | 602    | HEC  | CHA-C1A-NA  | -3.40 | 120.75      | 124.45   |
| 2   | A     | 605    | HEC  | CAC-C3C-C2C | -3.40 | 121.51      | 126.89   |
| 2   | A     | 602    | HEC  | C1A-C2A-C3A | -3.40 | 102.63      | 107.11   |
| 2   | A     | 607    | HEC  | CAD-CBD-CGD | -3.37 | 104.72      | 113.67   |
| 2   | B     | 608    | HEC  | C4A-C3A-C2A | -3.35 | 102.00      | 106.97   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | A     | 601    | HEC  | C3A-C4A-NA  | 3.35  | 115.84      | 109.64   |
| 2   | B     | 606    | HEC  | C1A-C2A-C3A | -3.35 | 102.70      | 107.11   |
| 2   | A     | 602    | HEC  | C2C-C1C-NC  | 3.34  | 115.50      | 110.14   |
| 2   | B     | 602    | HEC  | C1C-C2C-C3C | -3.33 | 103.00      | 106.82   |
| 2   | A     | 604    | HEC  | C2A-C1A-NA  | 3.33  | 113.53      | 110.32   |
| 2   | A     | 608    | HEC  | CAB-C3B-C4B | 3.32  | 129.12      | 124.79   |
| 2   | B     | 607    | HEC  | CBC-CAC-C3C | 3.32  | 121.41      | 112.42   |
| 2   | A     | 601    | HEC  | C4A-C3A-C2A | -3.29 | 102.09      | 106.97   |
| 2   | A     | 602    | HEC  | C4A-C3A-C2A | -3.29 | 102.09      | 106.97   |
| 2   | A     | 604    | HEC  | CBD-CAD-C3D | -3.29 | 103.44      | 112.53   |
| 2   | B     | 608    | HEC  | CBA-CAA-C2A | -3.29 | 103.44      | 112.53   |
| 2   | B     | 606    | HEC  | C4D-C3D-C2D | -3.27 | 102.12      | 106.89   |
| 2   | A     | 601    | HEC  | C2C-C1C-NC  | 3.27  | 115.38      | 110.14   |
| 2   | B     | 606    | HEC  | C2C-C1C-NC  | 3.27  | 115.38      | 110.14   |
| 2   | A     | 606    | HEC  | CHC-C4B-NB  | -3.26 | 120.34      | 124.37   |
| 2   | A     | 608    | HEC  | C2A-C1A-NA  | 3.26  | 113.47      | 110.32   |
| 2   | B     | 605    | HEC  | CHB-C4A-NA  | -3.26 | 120.91      | 124.45   |
| 2   | B     | 602    | HEC  | C1A-C2A-C3A | -3.26 | 102.82      | 107.11   |
| 2   | B     | 604[A] | HEC  | CHA-C4D-ND  | -3.23 | 120.95      | 124.42   |
| 2   | B     | 604[B] | HEC  | CHA-C4D-ND  | -3.23 | 120.95      | 124.42   |
| 2   | A     | 608    | HEC  | C4A-C3A-C2A | -3.22 | 102.19      | 106.97   |
| 2   | B     | 602    | HEC  | CMD-C2D-C1D | 3.21  | 130.05      | 125.03   |
| 2   | A     | 606    | HEC  | C2C-C1C-NC  | 3.21  | 115.29      | 110.14   |
| 2   | B     | 607    | HEC  | CAD-CBD-CGD | -3.21 | 105.15      | 113.67   |
| 2   | B     | 606    | HEC  | CAD-C3D-C4D | 3.21  | 130.28      | 124.70   |
| 2   | B     | 603    | HEC  | C2C-C1C-NC  | 3.20  | 115.28      | 110.14   |
| 2   | A     | 606    | HEC  | CMA-C3A-C4A | 3.20  | 130.37      | 124.73   |
| 2   | B     | 602    | HEC  | CAD-CBD-CGD | -3.19 | 105.19      | 113.67   |
| 2   | B     | 607    | HEC  | CBA-CAA-C2A | -3.19 | 103.70      | 112.53   |
| 2   | A     | 607    | HEC  | C1A-C2A-C3A | -3.19 | 102.90      | 107.11   |
| 2   | B     | 606    | HEC  | CAC-C3C-C4C | 3.19  | 129.30      | 124.91   |
| 2   | A     | 603    | HEC  | CBA-CAA-C2A | -3.19 | 103.71      | 112.53   |
| 2   | A     | 603    | HEC  | C4D-C3D-C2D | -3.18 | 102.26      | 106.89   |
| 2   | B     | 607    | HEC  | C1A-C2A-C3A | -3.16 | 102.95      | 107.11   |
| 2   | B     | 606    | HEC  | C3C-C4C-NC  | 3.16  | 113.66      | 110.15   |
| 2   | B     | 608    | HEC  | C3A-C4A-NA  | 3.15  | 115.47      | 109.64   |
| 2   | B     | 603    | HEC  | CMC-C2C-C3C | 3.14  | 132.28      | 125.62   |
| 2   | A     | 602    | HEC  | CAC-C3C-C4C | 3.14  | 129.23      | 124.91   |
| 2   | A     | 604    | HEC  | CMD-C2D-C1D | 3.13  | 129.93      | 125.03   |
| 2   | A     | 605    | HEC  | C2D-C1D-ND  | 3.13  | 113.59      | 109.90   |
| 2   | A     | 605    | HEC  | CHD-C1D-C2D | -3.12 | 123.11      | 129.94   |
| 2   | A     | 607    | HEC  | C3A-C4A-NA  | 3.12  | 115.40      | 109.64   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | B     | 602    | HEC  | C4A-C3A-C2A | -3.11 | 102.35      | 106.97   |
| 2   | A     | 608    | HEC  | CAC-C3C-C4C | 3.11  | 129.19      | 124.91   |
| 2   | B     | 605    | HEC  | CHC-C1C-C2C | -3.11 | 118.39      | 127.43   |
| 2   | B     | 605    | HEC  | C1D-C2D-C3D | -3.11 | 104.20      | 107.09   |
| 2   | A     | 601    | HEC  | C4D-C3D-C2D | -3.10 | 102.38      | 106.89   |
| 2   | B     | 602    | HEC  | CAA-CBA-CGA | -3.10 | 105.45      | 113.67   |
| 2   | A     | 605    | HEC  | CHB-C4A-NA  | -3.09 | 121.09      | 124.45   |
| 2   | A     | 608    | HEC  | CAD-CBD-CGD | -3.09 | 105.47      | 113.67   |
| 2   | A     | 604    | HEC  | C3A-C4A-NA  | 3.09  | 115.35      | 109.64   |
| 2   | A     | 602    | HEC  | CAA-CBA-CGA | -3.07 | 105.53      | 113.67   |
| 2   | B     | 607    | HEC  | C1D-C2D-C3D | -3.06 | 103.76      | 106.98   |
| 2   | B     | 603    | HEC  | CBA-CAA-C2A | -3.05 | 104.09      | 112.53   |
| 2   | B     | 607    | HEC  | C3A-C4A-NA  | 3.05  | 115.27      | 109.64   |
| 2   | B     | 601    | HEC  | C1A-C2A-C3A | -3.04 | 103.10      | 107.11   |
| 2   | B     | 601    | HEC  | C3A-C4A-NA  | 3.03  | 115.24      | 109.64   |
| 2   | A     | 606    | HEC  | C4D-C3D-C2D | -3.03 | 102.48      | 106.89   |
| 2   | B     | 608    | HEC  | CHB-C1B-C2B | -3.03 | 120.25      | 125.03   |
| 2   | A     | 603    | HEC  | CMC-C2C-C3C | 3.03  | 132.04      | 125.62   |
| 2   | A     | 606    | HEC  | C3C-C4C-NC  | 3.03  | 113.51      | 110.15   |
| 2   | B     | 602    | HEC  | CHB-C4A-C3A | -3.02 | 119.20      | 125.49   |
| 2   | B     | 604[A] | HEC  | C3A-C4A-NA  | 3.01  | 115.21      | 109.64   |
| 2   | B     | 604[B] | HEC  | C3A-C4A-NA  | 3.01  | 115.21      | 109.64   |
| 2   | A     | 605    | HEC  | CMA-C3A-C4A | 3.01  | 130.03      | 124.73   |
| 2   | B     | 604[A] | HEC  | C4A-C3A-C2A | -3.01 | 102.51      | 106.97   |
| 2   | B     | 604[B] | HEC  | C4A-C3A-C2A | -3.01 | 102.51      | 106.97   |
| 2   | B     | 603    | HEC  | CAB-C3B-C4B | 3.01  | 128.71      | 124.79   |
| 2   | B     | 607    | HEC  | CHA-C4D-C3D | -3.01 | 120.39      | 124.77   |
| 2   | A     | 603    | HEC  | C3A-C4A-NA  | 2.98  | 115.15      | 109.64   |
| 2   | B     | 604[A] | HEC  | CHD-C1D-ND  | -2.97 | 120.69      | 124.37   |
| 2   | B     | 604[B] | HEC  | CHD-C1D-ND  | -2.97 | 120.69      | 124.37   |
| 2   | B     | 603    | HEC  | CHB-C1B-C2B | -2.97 | 120.34      | 125.03   |
| 2   | A     | 606    | HEC  | CMC-C2C-C3C | 2.95  | 131.88      | 125.62   |
| 2   | B     | 601    | HEC  | CHB-C1B-NB  | -2.94 | 121.25      | 124.42   |
| 2   | B     | 608    | HEC  | CAC-C3C-C4C | 2.94  | 128.96      | 124.91   |
| 2   | B     | 603    | HEC  | CBD-CAD-C3D | -2.93 | 104.42      | 112.53   |
| 2   | B     | 608    | HEC  | C1A-C2A-C3A | -2.93 | 103.25      | 107.11   |
| 2   | A     | 606    | HEC  | C1A-C2A-C3A | -2.92 | 103.26      | 107.11   |
| 2   | B     | 602    | HEC  | C4C-C3C-C2C | -2.91 | 102.36      | 106.87   |
| 2   | A     | 607    | HEC  | C3B-C4B-NB  | 2.90  | 113.35      | 110.17   |
| 2   | B     | 602    | HEC  | C2C-C1C-NC  | 2.89  | 114.78      | 110.14   |
| 2   | B     | 608    | HEC  | C4D-C3D-C2D | -2.88 | 102.70      | 106.89   |
| 2   | A     | 601    | HEC  | CAC-C3C-C4C | 2.85  | 128.84      | 124.91   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | A     | 603    | HEC  | CAC-C3C-C4C | 2.85  | 128.83      | 124.91   |
| 2   | B     | 605    | HEC  | C2D-C1D-ND  | 2.85  | 113.11      | 109.84   |
| 2   | A     | 601    | HEC  | CMB-C2B-C1B | 2.85  | 129.48      | 125.03   |
| 2   | A     | 605    | HEC  | C2A-C1A-NA  | 2.84  | 113.07      | 110.32   |
| 2   | B     | 606    | HEC  | CHB-C1B-C2B | -2.84 | 120.54      | 125.03   |
| 2   | A     | 603    | HEC  | C1A-C2A-C3A | -2.84 | 103.37      | 107.11   |
| 2   | A     | 602    | HEC  | CHB-C1B-NB  | -2.83 | 121.38      | 124.42   |
| 2   | A     | 604    | HEC  | C4D-C3D-C2D | -2.82 | 102.78      | 106.89   |
| 2   | A     | 604    | HEC  | CHA-C4D-ND  | -2.82 | 121.39      | 124.42   |
| 2   | A     | 605    | HEC  | O1A-CGA-CBA | -2.82 | 114.16      | 123.09   |
| 2   | A     | 606    | HEC  | CMD-C2D-C1D | 2.80  | 129.42      | 125.03   |
| 2   | A     | 608    | HEC  | CAA-CBA-CGA | -2.79 | 106.28      | 113.67   |
| 2   | A     | 606    | HEC  | C4A-C3A-C2A | -2.79 | 102.84      | 106.97   |
| 2   | A     | 601    | HEC  | CAD-C3D-C4D | 2.78  | 129.54      | 124.70   |
| 2   | A     | 601    | HEC  | CMD-C2D-C1D | 2.77  | 129.36      | 125.03   |
| 2   | B     | 603    | HEC  | CHD-C1D-C2D | -2.77 | 119.09      | 126.95   |
| 2   | A     | 607    | HEC  | C4A-C3A-C2A | -2.75 | 102.89      | 106.97   |
| 2   | B     | 607    | HEC  | CMD-C2D-C1D | 2.75  | 129.34      | 125.03   |
| 2   | A     | 606    | HEC  | CHB-C1B-C2B | -2.75 | 120.68      | 125.03   |
| 2   | B     | 601    | HEC  | CHA-C4D-C3D | -2.74 | 120.78      | 124.77   |
| 2   | B     | 607    | HEC  | CHB-C1B-C2B | -2.74 | 120.71      | 125.03   |
| 2   | A     | 607    | HEC  | CHA-C4D-C3D | -2.74 | 120.78      | 124.77   |
| 2   | A     | 607    | HEC  | CAC-C3C-C4C | 2.73  | 128.67      | 124.91   |
| 2   | A     | 605    | HEC  | CHC-C1C-C2C | -2.73 | 119.49      | 127.43   |
| 2   | B     | 604[A] | HEC  | C1A-C2A-C3A | -2.73 | 103.51      | 107.11   |
| 2   | B     | 604[B] | HEC  | C1A-C2A-C3A | -2.73 | 103.51      | 107.11   |
| 2   | A     | 608    | HEC  | C4D-C3D-C2D | -2.73 | 102.92      | 106.89   |
| 2   | B     | 605    | HEC  | CMB-C2B-C3B | 2.73  | 133.52      | 126.15   |
| 2   | B     | 604[A] | HEC  | C4D-C3D-C2D | -2.72 | 102.93      | 106.89   |
| 2   | B     | 604[B] | HEC  | C4D-C3D-C2D | -2.72 | 102.93      | 106.89   |
| 2   | A     | 604    | HEC  | CAC-C3C-C4C | 2.72  | 128.66      | 124.91   |
| 2   | B     | 607    | HEC  | C4D-C3D-C2D | -2.71 | 102.94      | 106.89   |
| 2   | A     | 606    | HEC  | CHC-C1C-C2C | -2.70 | 119.58      | 127.43   |
| 2   | B     | 604[A] | HEC  | CAC-C3C-C4C | 2.69  | 128.61      | 124.91   |
| 2   | B     | 604[B] | HEC  | CAC-C3C-C4C | 2.69  | 128.61      | 124.91   |
| 2   | B     | 605    | HEC  | CMC-C2C-C3C | 2.68  | 131.32      | 125.62   |
| 2   | A     | 608    | HEC  | C3A-C4A-NA  | 2.67  | 114.58      | 109.64   |
| 2   | A     | 601    | HEC  | CHB-C1B-NB  | -2.67 | 121.55      | 124.42   |
| 2   | A     | 601    | HEC  | CMA-C3A-C4A | 2.66  | 129.42      | 124.73   |
| 2   | B     | 604[A] | HEC  | CMC-C2C-C3C | 2.66  | 131.27      | 125.62   |
| 2   | B     | 604[B] | HEC  | CMC-C2C-C3C | 2.66  | 131.27      | 125.62   |
| 2   | A     | 608    | HEC  | CHC-C1C-C2C | -2.66 | 119.70      | 127.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 601 | HEC  | CBC-CAC-C3C | 2.66  | 119.63      | 112.42   |
| 2   | A     | 603 | HEC  | C4A-C3A-C2A | -2.66 | 103.03      | 106.97   |
| 2   | B     | 602 | HEC  | CBB-CAB-C3B | -2.65 | 105.22      | 112.42   |
| 2   | A     | 605 | HEC  | CHA-C4D-ND  | -2.65 | 121.60      | 124.78   |
| 2   | B     | 602 | HEC  | CMC-C2C-C3C | 2.64  | 131.22      | 125.62   |
| 2   | B     | 606 | HEC  | CMC-C2C-C3C | 2.63  | 131.21      | 125.62   |
| 2   | A     | 606 | HEC  | CBA-CAA-C2A | -2.63 | 105.26      | 112.53   |
| 2   | B     | 601 | HEC  | C4A-C3A-C2A | -2.63 | 103.08      | 106.97   |
| 2   | B     | 602 | HEC  | CHC-C4B-C3B | -2.62 | 120.40      | 125.23   |
| 2   | A     | 604 | HEC  | CMA-C3A-C4A | 2.62  | 129.34      | 124.73   |
| 2   | A     | 601 | HEC  | CHA-C4D-C3D | -2.61 | 120.96      | 124.77   |
| 2   | A     | 604 | HEC  | CBC-CAC-C3C | 2.61  | 119.50      | 112.42   |
| 2   | A     | 608 | HEC  | CMD-C2D-C1D | 2.61  | 129.11      | 125.03   |
| 2   | B     | 606 | HEC  | CHC-C1C-C2C | -2.61 | 119.86      | 127.43   |
| 2   | B     | 606 | HEC  | CMD-C2D-C1D | 2.60  | 129.10      | 125.03   |
| 2   | A     | 603 | HEC  | CAD-C3D-C4D | 2.59  | 129.22      | 124.70   |
| 2   | A     | 604 | HEC  | CMC-C2C-C1C | 2.59  | 129.36      | 125.42   |
| 2   | A     | 607 | HEC  | CAD-C3D-C4D | 2.58  | 129.19      | 124.70   |
| 2   | B     | 608 | HEC  | CHC-C1C-C2C | -2.56 | 119.99      | 127.43   |
| 2   | A     | 601 | HEC  | C1A-C2A-C3A | -2.56 | 103.74      | 107.11   |
| 2   | A     | 606 | HEC  | C1D-ND-C4D  | -2.53 | 102.21      | 105.21   |
| 2   | B     | 607 | HEC  | CMC-C2C-C3C | 2.53  | 130.98      | 125.62   |
| 2   | A     | 604 | HEC  | CAB-C3B-C4B | 2.52  | 128.07      | 124.79   |
| 2   | A     | 606 | HEC  | CAD-C3D-C4D | 2.52  | 129.09      | 124.70   |
| 2   | A     | 602 | HEC  | C4C-C3C-C2C | -2.52 | 102.97      | 106.87   |
| 2   | A     | 603 | HEC  | CBD-CAD-C3D | -2.52 | 105.57      | 112.53   |
| 2   | B     | 606 | HEC  | C3A-C4A-NA  | 2.51  | 114.28      | 109.64   |
| 2   | B     | 608 | HEC  | CHA-C4D-ND  | -2.51 | 121.72      | 124.42   |
| 2   | B     | 605 | HEC  | O1A-CGA-CBA | -2.51 | 115.14      | 123.09   |
| 2   | A     | 605 | HEC  | CMC-C2C-C3C | 2.51  | 130.94      | 125.62   |
| 2   | A     | 603 | HEC  | CHC-C1C-C2C | -2.49 | 120.19      | 127.43   |
| 2   | A     | 606 | HEC  | CHA-C1A-C2A | -2.49 | 120.94      | 124.86   |
| 2   | A     | 606 | HEC  | CHA-C4D-ND  | -2.47 | 121.76      | 124.42   |
| 2   | A     | 606 | HEC  | C4B-C3B-C2B | -2.47 | 103.30      | 106.89   |
| 2   | B     | 606 | HEC  | C1D-ND-C4D  | -2.47 | 102.28      | 105.21   |
| 2   | A     | 605 | HEC  | CMB-C2B-C3B | 2.46  | 132.82      | 126.15   |
| 2   | B     | 607 | HEC  | CAD-C3D-C4D | 2.46  | 128.99      | 124.70   |
| 2   | B     | 606 | HEC  | CHA-C4D-ND  | -2.46 | 121.78      | 124.42   |
| 2   | B     | 607 | HEC  | C4A-C3A-C2A | -2.45 | 103.34      | 106.97   |
| 2   | A     | 603 | HEC  | CHB-C1B-C2B | -2.45 | 121.16      | 125.03   |
| 2   | B     | 608 | HEC  | CMD-C2D-C1D | 2.44  | 128.85      | 125.03   |
| 2   | A     | 602 | HEC  | CHB-C4A-C3A | -2.43 | 120.44      | 125.49   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | A     | 606    | HEC  | C3A-C4A-NA  | 2.41  | 114.10      | 109.64   |
| 2   | B     | 608    | HEC  | CAD-C3D-C4D | 2.39  | 128.86      | 124.70   |
| 2   | A     | 601    | HEC  | CHC-C4B-C3B | -2.39 | 120.82      | 125.23   |
| 2   | B     | 602    | HEC  | CHA-C4D-C3D | -2.38 | 121.31      | 124.77   |
| 2   | B     | 601    | HEC  | CMC-C2C-C3C | 2.37  | 130.65      | 125.62   |
| 2   | B     | 601    | HEC  | C4D-C3D-C2D | -2.37 | 103.45      | 106.89   |
| 2   | A     | 602    | HEC  | CAB-C3B-C4B | 2.36  | 127.86      | 124.79   |
| 2   | B     | 604[A] | HEC  | CMB-C2B-C1B | 2.35  | 128.71      | 125.03   |
| 2   | B     | 604[B] | HEC  | CMB-C2B-C1B | 2.35  | 128.71      | 125.03   |
| 2   | A     | 608    | HEC  | CBD-CAD-C3D | -2.35 | 106.03      | 112.53   |
| 2   | B     | 604[A] | HEC  | C3B-C4B-NB  | 2.34  | 112.74      | 110.17   |
| 2   | B     | 604[B] | HEC  | C3B-C4B-NB  | 2.34  | 112.74      | 110.17   |
| 2   | B     | 603    | HEC  | CMB-C2B-C3B | 2.34  | 132.48      | 126.15   |
| 2   | A     | 607    | HEC  | C4D-C3D-C2D | -2.34 | 103.49      | 106.89   |
| 2   | A     | 608    | HEC  | CHB-C1B-C2B | -2.33 | 121.35      | 125.03   |
| 2   | B     | 601    | HEC  | CHD-C1D-C2D | -2.33 | 120.33      | 126.95   |
| 2   | B     | 603    | HEC  | C4D-C3D-C2D | -2.32 | 103.52      | 106.89   |
| 2   | B     | 606    | HEC  | C4C-C3C-C2C | -2.31 | 103.30      | 106.87   |
| 2   | A     | 608    | HEC  | C4B-C3B-C2B | -2.30 | 103.54      | 106.89   |
| 2   | A     | 602    | HEC  | CMC-C2C-C3C | 2.30  | 130.50      | 125.62   |
| 2   | B     | 607    | HEC  | CHC-C1C-C2C | -2.30 | 120.75      | 127.43   |
| 2   | B     | 603    | HEC  | CAD-C3D-C4D | 2.29  | 128.70      | 124.70   |
| 2   | A     | 603    | HEC  | C4C-C3C-C2C | -2.29 | 103.33      | 106.87   |
| 2   | A     | 607    | HEC  | CBD-CAD-C3D | -2.29 | 106.20      | 112.53   |
| 2   | B     | 603    | HEC  | CHC-C1C-C2C | -2.29 | 120.79      | 127.43   |
| 2   | B     | 602    | HEC  | CHB-C1B-C2B | -2.28 | 121.43      | 125.03   |
| 2   | B     | 601    | HEC  | CAB-C3B-C4B | 2.27  | 127.75      | 124.79   |
| 2   | B     | 607    | HEC  | CHA-C1A-C2A | -2.27 | 121.28      | 124.86   |
| 2   | B     | 606    | HEC  | CHD-C1D-C2D | -2.27 | 120.51      | 126.95   |
| 2   | A     | 608    | HEC  | CHA-C4D-C3D | -2.26 | 121.48      | 124.77   |
| 2   | B     | 606    | HEC  | CHA-C1A-C2A | -2.25 | 121.31      | 124.86   |
| 2   | A     | 603    | HEC  | CHB-C1B-NB  | -2.25 | 122.00      | 124.42   |
| 2   | A     | 606    | HEC  | CHD-C1D-ND  | -2.25 | 121.59      | 124.37   |
| 2   | B     | 604[A] | HEC  | CMD-C2D-C1D | 2.24  | 128.54      | 125.03   |
| 2   | B     | 604[B] | HEC  | CMD-C2D-C1D | 2.24  | 128.54      | 125.03   |
| 2   | B     | 603    | HEC  | CMD-C2D-C1D | 2.24  | 128.53      | 125.03   |
| 2   | B     | 606    | HEC  | C4B-C3B-C2B | -2.23 | 103.64      | 106.89   |
| 2   | A     | 601    | HEC  | CMC-C2C-C3C | 2.23  | 130.35      | 125.62   |
| 2   | A     | 602    | HEC  | C4D-C3D-C2D | -2.22 | 103.66      | 106.89   |
| 2   | B     | 606    | HEC  | CBA-CAA-C2A | -2.22 | 106.41      | 112.53   |
| 2   | B     | 603    | HEC  | C4C-C3C-C2C | -2.22 | 103.44      | 106.87   |
| 2   | A     | 604    | HEC  | CHB-C1B-NB  | -2.21 | 122.05      | 124.42   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | B     | 603    | HEC  | CHB-C4A-C3A | -2.20 | 120.91      | 125.49   |
| 2   | A     | 607    | HEC  | C4C-C3C-C2C | -2.20 | 103.47      | 106.87   |
| 2   | B     | 604[A] | HEC  | CHB-C1B-C2B | -2.19 | 121.57      | 125.03   |
| 2   | B     | 604[B] | HEC  | CHB-C1B-C2B | -2.19 | 121.57      | 125.03   |
| 2   | B     | 607    | HEC  | CMC-C2C-C1C | 2.19  | 128.75      | 125.42   |
| 2   | B     | 607    | HEC  | O2A-CGA-CBA | 2.19  | 120.92      | 114.00   |
| 2   | B     | 607    | HEC  | O1A-CGA-CBA | -2.19 | 116.16      | 123.09   |
| 2   | A     | 602    | HEC  | CHD-C1D-ND  | -2.19 | 121.66      | 124.37   |
| 2   | A     | 602    | HEC  | CMB-C2B-C1B | 2.18  | 128.44      | 125.03   |
| 2   | B     | 602    | HEC  | CMA-C3A-C2A | 2.18  | 132.04      | 126.15   |
| 2   | B     | 603    | HEC  | C1A-C2A-C3A | -2.17 | 104.25      | 107.11   |
| 2   | A     | 602    | HEC  | CHA-C4D-C3D | -2.16 | 121.62      | 124.77   |
| 2   | B     | 601    | HEC  | CHB-C4A-NA  | -2.16 | 122.10      | 124.45   |
| 2   | A     | 607    | HEC  | CHB-C1B-C2B | -2.16 | 121.62      | 125.03   |
| 2   | A     | 601    | HEC  | C4C-C3C-C2C | -2.15 | 103.54      | 106.87   |
| 2   | B     | 604[A] | HEC  | O2A-CGA-CBA | 2.14  | 120.78      | 114.00   |
| 2   | A     | 607    | HEC  | CMB-C2B-C1B | 2.14  | 128.38      | 125.03   |
| 2   | A     | 608    | HEC  | C1A-C2A-C3A | -2.14 | 104.29      | 107.11   |
| 2   | B     | 608    | HEC  | CHC-C4B-NB  | -2.14 | 121.72      | 124.37   |
| 2   | A     | 601    | HEC  | CHA-C1A-NA  | -2.13 | 122.13      | 124.45   |
| 2   | B     | 605    | HEC  | C1A-C2A-C3A | -2.12 | 104.31      | 107.11   |
| 2   | A     | 607    | HEC  | CHB-C4A-C3A | -2.12 | 121.09      | 125.49   |
| 2   | A     | 604    | HEC  | CHC-C1C-C2C | -2.11 | 121.29      | 127.43   |
| 2   | A     | 603    | HEC  | CAA-CBA-CGA | -2.11 | 108.07      | 113.67   |
| 2   | A     | 602    | HEC  | CHC-C1C-C2C | -2.11 | 121.31      | 127.43   |
| 2   | A     | 602    | HEC  | C4B-NB-C1B  | -2.10 | 102.72      | 105.21   |
| 2   | B     | 602    | HEC  | C4B-NB-C1B  | -2.09 | 102.73      | 105.21   |
| 2   | A     | 601    | HEC  | CAA-C2A-C1A | 2.08  | 129.09      | 124.85   |
| 2   | A     | 603    | HEC  | CMB-C2B-C1B | 2.07  | 128.27      | 125.03   |
| 2   | A     | 604    | HEC  | CHB-C4A-C3A | -2.07 | 121.18      | 125.49   |
| 2   | B     | 606    | HEC  | C4A-C3A-C2A | -2.06 | 103.91      | 106.97   |
| 2   | B     | 607    | HEC  | C4B-C3B-C2B | -2.06 | 103.89      | 106.89   |
| 2   | A     | 605    | HEC  | C3D-C2D-C1D | -2.06 | 104.27      | 106.20   |
| 2   | A     | 602    | HEC  | CHB-C1B-C2B | -2.06 | 121.78      | 125.03   |
| 2   | A     | 607    | HEC  | CHA-C1A-C2A | -2.06 | 121.62      | 124.86   |
| 2   | A     | 607    | HEC  | CAA-C2A-C1A | 2.05  | 129.03      | 124.85   |
| 2   | B     | 602    | HEC  | CHC-C1C-C2C | -2.05 | 121.48      | 127.43   |
| 2   | B     | 608    | HEC  | C4B-C3B-C2B | -2.05 | 103.91      | 106.89   |
| 2   | A     | 607    | HEC  | C4C-NC-C1C  | -2.05 | 102.48      | 105.82   |
| 2   | B     | 608    | HEC  | CHB-C4A-C3A | -2.04 | 121.24      | 125.49   |
| 2   | A     | 601    | HEC  | CBC-CAC-C3C | 2.04  | 117.95      | 112.42   |
| 2   | A     | 605    | HEC  | CHC-C4B-NB  | -2.02 | 121.86      | 124.37   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 601 | HEC  | CHD-C1D-C2D | -2.02 | 121.21      | 126.95   |
| 2   | A     | 601 | HEC  | CHB-C4A-C3A | -2.02 | 121.29      | 125.49   |
| 2   | A     | 606 | HEC  | C4C-C3C-C2C | -2.02 | 103.75      | 106.87   |
| 2   | B     | 601 | HEC  | CMB-C2B-C3B | 2.01  | 131.59      | 126.15   |
| 2   | B     | 606 | HEC  | CHA-C4D-C3D | -2.01 | 121.84      | 124.77   |
| 2   | B     | 607 | HEC  | CHB-C4A-C3A | -2.00 | 121.32      | 125.49   |
| 2   | A     | 601 | HEC  | CBA-CAA-C2A | -2.00 | 107.00      | 112.53   |

All (17) chirality outliers are listed below:

| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 2   | A     | 601    | HEC  | NA   |
| 2   | A     | 602    | HEC  | NA   |
| 2   | A     | 603    | HEC  | NA   |
| 2   | A     | 604    | HEC  | NA   |
| 2   | A     | 605    | HEC  | NA   |
| 2   | A     | 606    | HEC  | NA   |
| 2   | A     | 607    | HEC  | NA   |
| 2   | A     | 608    | HEC  | NA   |
| 2   | B     | 601    | HEC  | NA   |
| 2   | B     | 602    | HEC  | NA   |
| 2   | B     | 603    | HEC  | NA   |
| 2   | B     | 604[A] | HEC  | NA   |
| 2   | B     | 604[B] | HEC  | NA   |
| 2   | B     | 605    | HEC  | NA   |
| 2   | B     | 606    | HEC  | NA   |
| 2   | B     | 607    | HEC  | NA   |
| 2   | B     | 608    | HEC  | NA   |

All (105) torsion outliers are listed below:

| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 2   | B     | 606    | HEC  | C2C-C3C-CAC-CBC |
| 6   | A     | 615[A] | GOL  | C1-C2-C3-O3     |
| 2   | A     | 606    | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 606    | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 605    | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 606    | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 605    | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 605    | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 605    | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 604[A] | HEC  | C4C-C3C-CAC-CBC |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 2   | B     | 604[B] | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 608    | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 607    | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 607    | HEC  | C4C-C3C-CAC-CBC |
| 6   | A     | 615[A] | GOL  | O1-C1-C2-O2     |
| 6   | A     | 615[B] | GOL  | O1-C1-C2-O2     |
| 2   | B     | 604[A] | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 604[B] | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 601    | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 602    | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 601    | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 602    | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 607    | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 608    | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 608    | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 604    | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 602    | HEC  | C4C-C3C-CAC-CBC |
| 6   | A     | 615[A] | GOL  | O1-C1-C2-C3     |
| 6   | A     | 615[B] | GOL  | O1-C1-C2-C3     |
| 6   | A     | 615[B] | GOL  | C1-C2-C3-O3     |
| 2   | B     | 601    | HEC  | C4C-C3C-CAC-CBC |
| 6   | A     | 615[B] | GOL  | O2-C2-C3-O3     |
| 2   | A     | 608    | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 601    | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 603    | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 604    | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 601    | HEC  | C2C-C3C-CAC-CBC |
| 6   | A     | 615[A] | GOL  | O2-C2-C3-O3     |
| 2   | B     | 601    | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 604    | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 607    | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 602    | HEC  | C2C-C3C-CAC-CBC |
| 2   | A     | 601    | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 604[A] | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 604[B] | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 604    | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 603    | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 608    | HEC  | C2B-C3B-CAB-CBB |
| 2   | A     | 603    | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 604[A] | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 604[B] | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 605    | HEC  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 2   | A     | 603    | HEC  | C2B-C3B-CAB-CBB |
| 6   | B     | 614    | GOL  | C1-C2-C3-O3     |
| 2   | B     | 607    | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 603    | HEC  | C4C-C3C-CAC-CBC |
| 2   | A     | 601    | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 603    | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 608    | HEC  | C4C-C3C-CAC-CBC |
| 2   | B     | 608    | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 602    | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 606    | HEC  | C4D-C3D-CAD-CBD |
| 2   | A     | 602    | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 601    | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 601    | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 606    | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 602    | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 601    | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 606    | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 604[A] | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 605    | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 601    | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 602    | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 604    | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 606    | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 606    | HEC  | CAA-CBA-CGA-O2A |
| 2   | A     | 608    | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 604    | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 604[A] | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 608    | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 608    | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 607    | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 602    | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 607    | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 608    | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 608    | HEC  | CAD-CBD-CGD-O1D |
| 2   | A     | 602    | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 607    | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 603    | HEC  | C2C-C3C-CAC-CBC |
| 2   | B     | 607    | HEC  | C4B-C3B-CAB-CBB |
| 2   | A     | 605    | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 605    | HEC  | CAA-CBA-CGA-O2A |
| 2   | B     | 606    | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 607    | HEC  | CAA-CBA-CGA-O2A |

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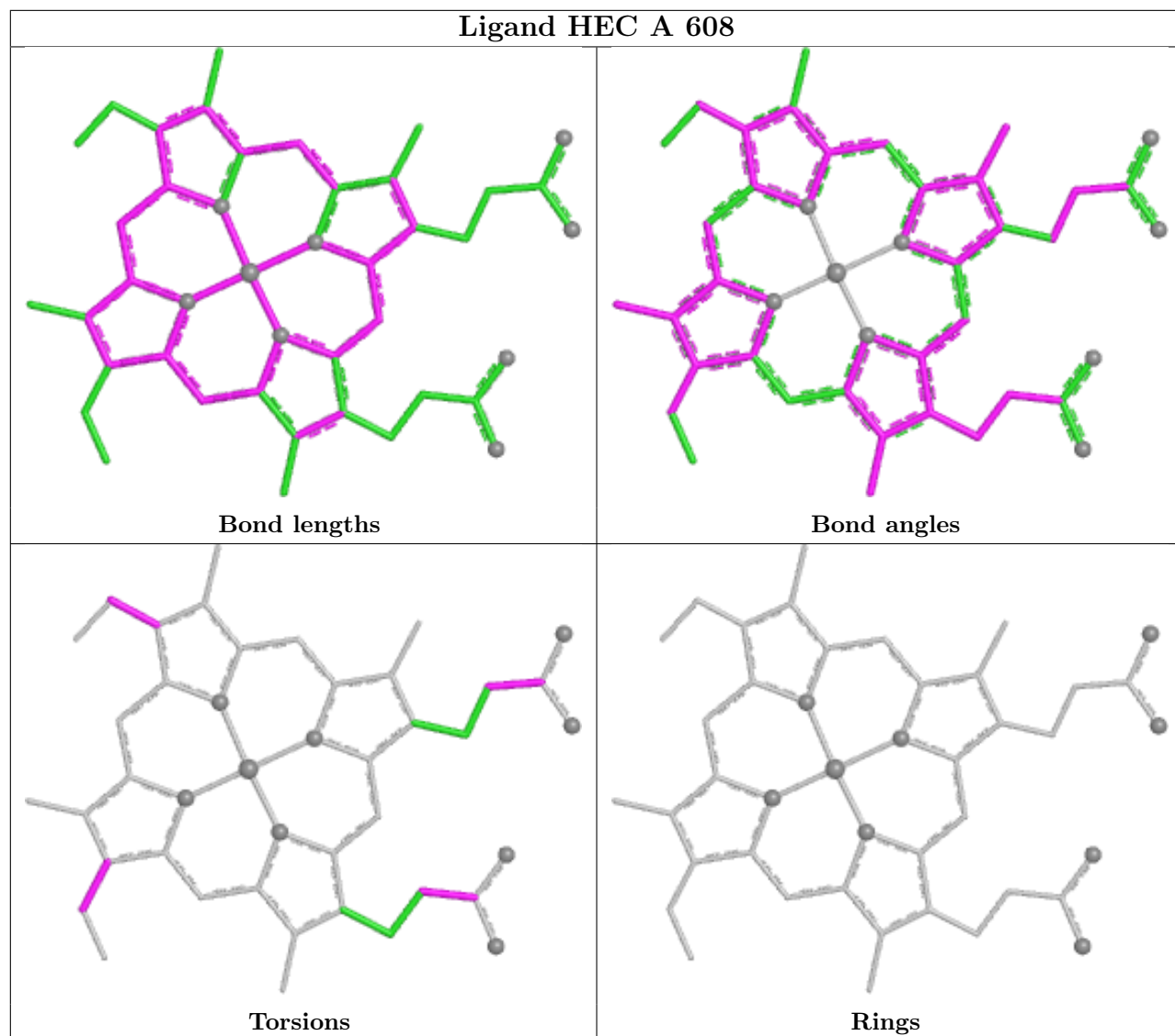
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | A     | 605 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 608 | HEC  | CAD-CBD-CGD-O2D |
| 2   | B     | 607 | HEC  | CAA-CBA-CGA-O1A |
| 2   | A     | 607 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 602 | HEC  | CAD-CBD-CGD-O2D |
| 2   | A     | 603 | HEC  | C4B-C3B-CAB-CBB |
| 2   | B     | 605 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 608 | HEC  | CAA-CBA-CGA-O1A |
| 2   | B     | 602 | HEC  | CAD-CBD-CGD-O1D |
| 2   | B     | 606 | HEC  | C2B-C3B-CAB-CBB |
| 2   | B     | 608 | HEC  | CAA-CBA-CGA-O2A |

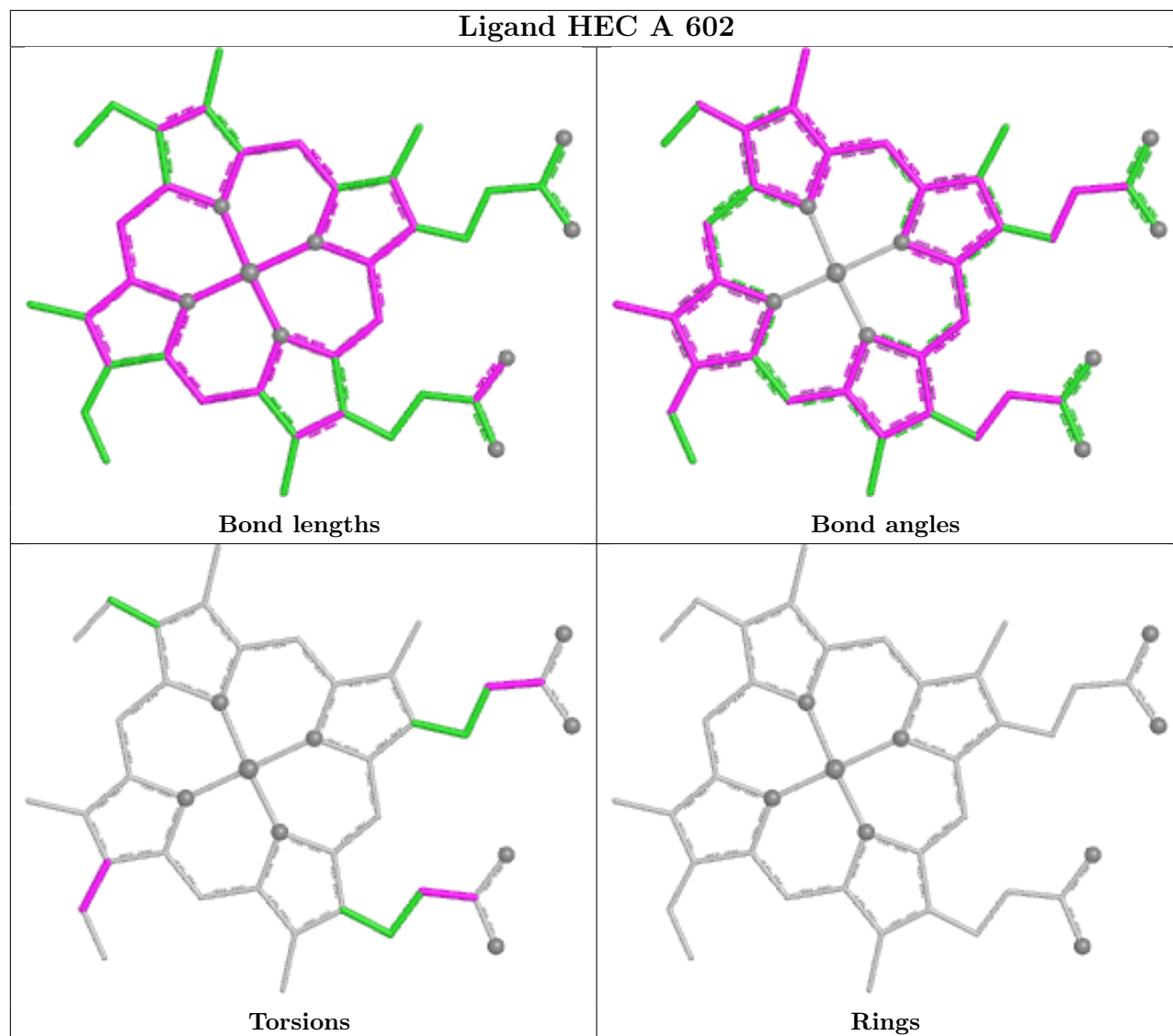
There are no ring outliers.

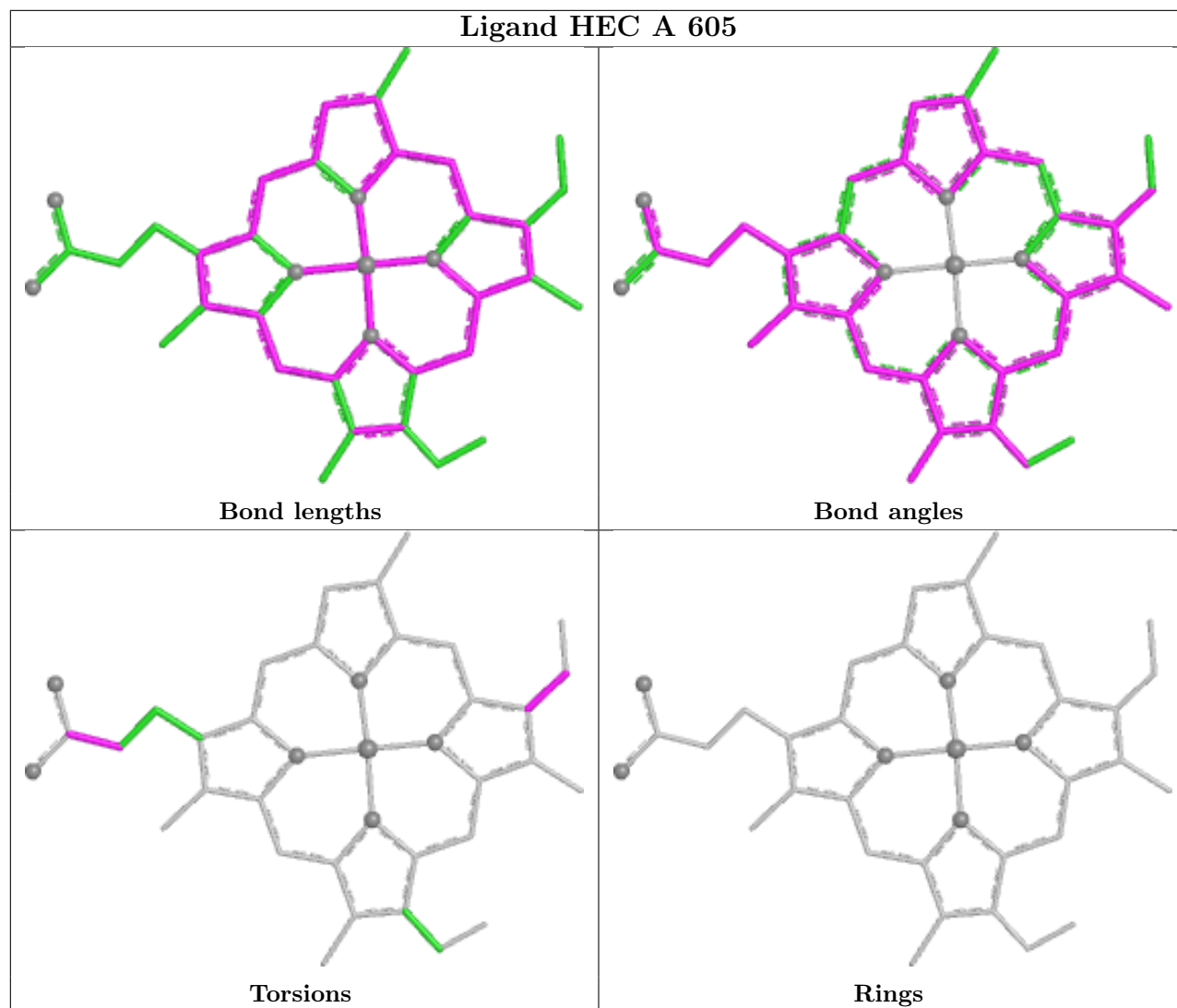
12 monomers are involved in 17 short contacts:

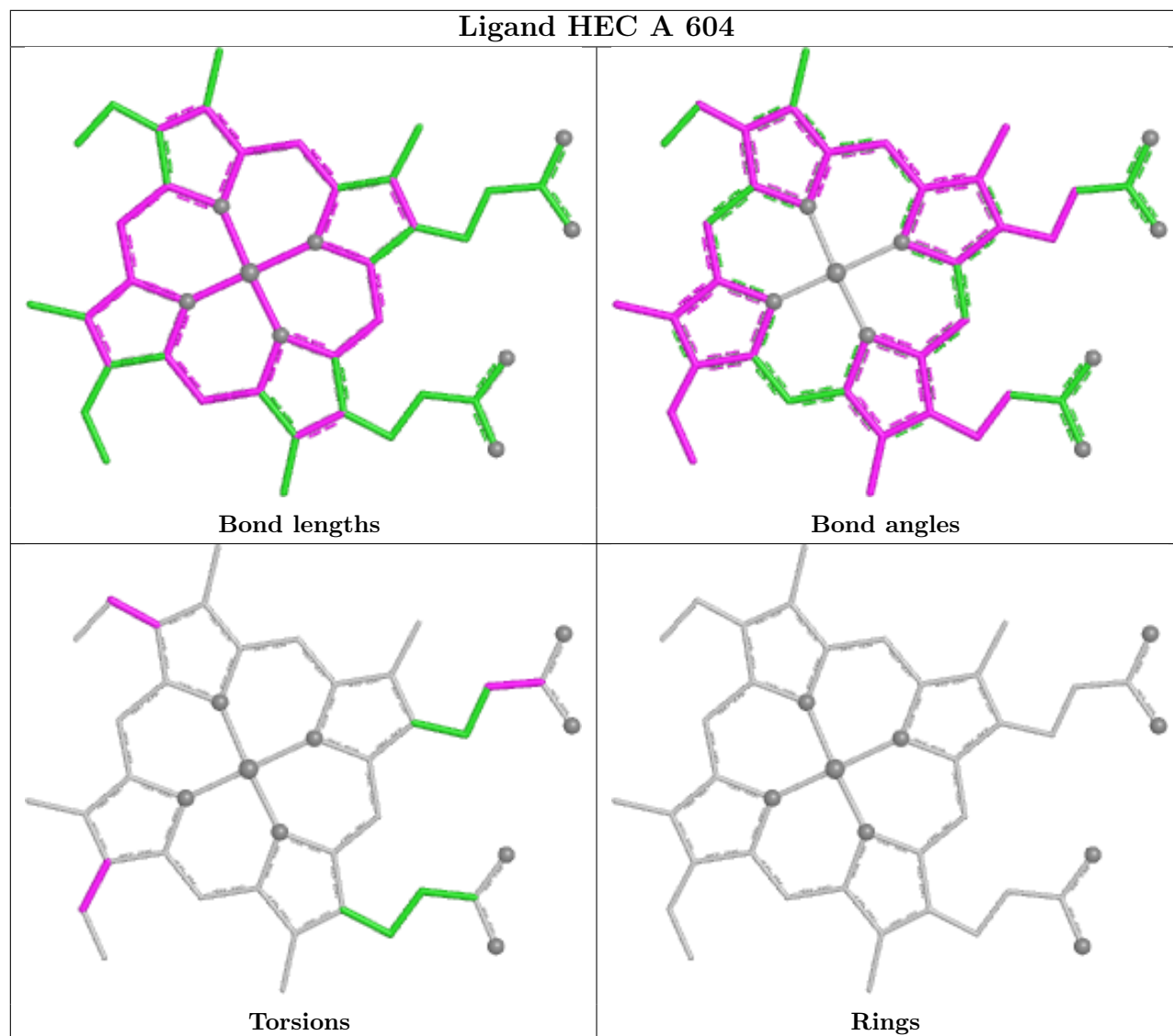
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 608 | HEC  | 1       | 0            |
| 2   | A     | 605 | HEC  | 1       | 0            |
| 2   | A     | 604 | HEC  | 2       | 0            |
| 2   | B     | 605 | HEC  | 3       | 0            |
| 2   | B     | 601 | HEC  | 1       | 0            |
| 2   | A     | 603 | HEC  | 1       | 0            |
| 5   | B     | 612 | MPD  | 3       | 0            |
| 2   | A     | 606 | HEC  | 1       | 0            |
| 5   | A     | 612 | MPD  | 1       | 0            |
| 2   | B     | 603 | HEC  | 2       | 0            |
| 3   | B     | 609 | NO2  | 1       | 0            |
| 2   | B     | 606 | HEC  | 1       | 0            |

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

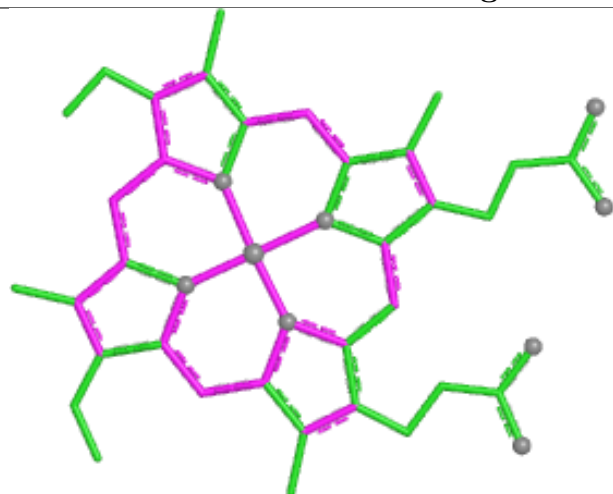




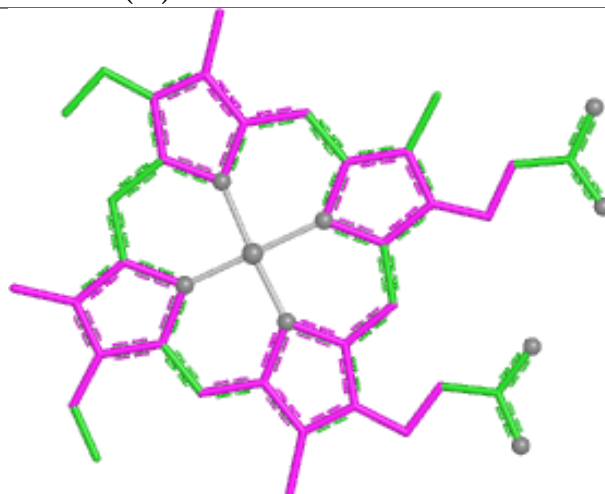




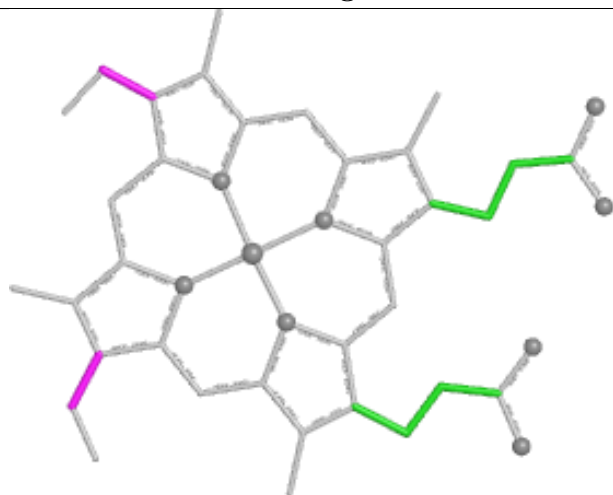
## Ligand HEC B 604 (B)



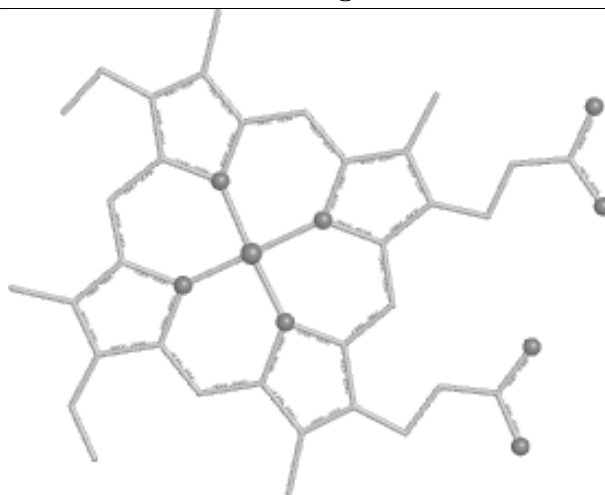
Bond lengths



Bond angles

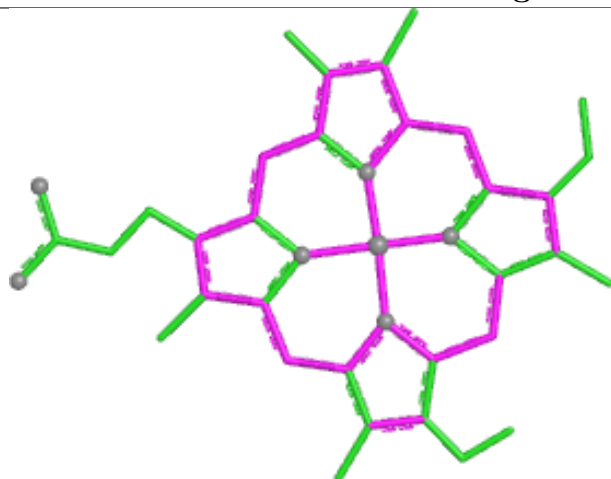


Torsions

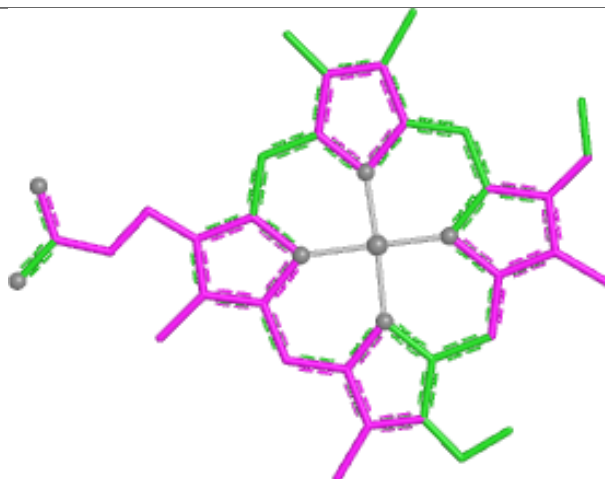


Rings

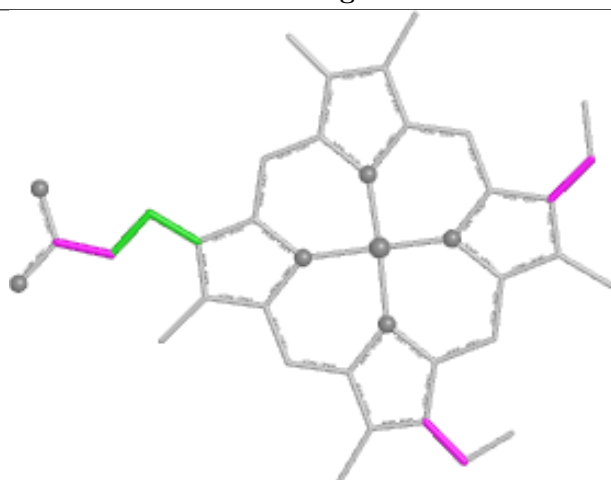
## Ligand HEC B 605



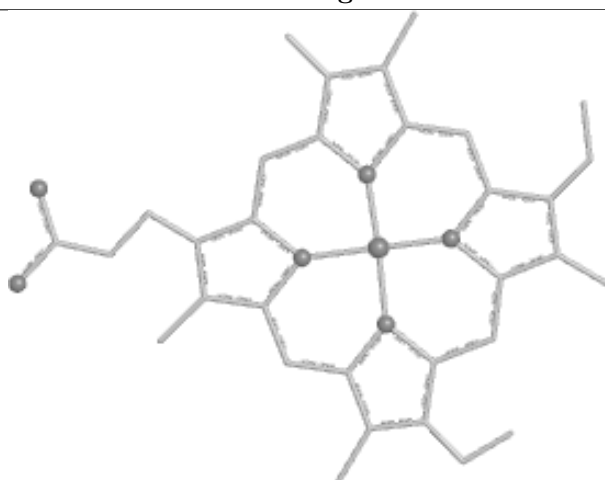
Bond lengths



Bond angles

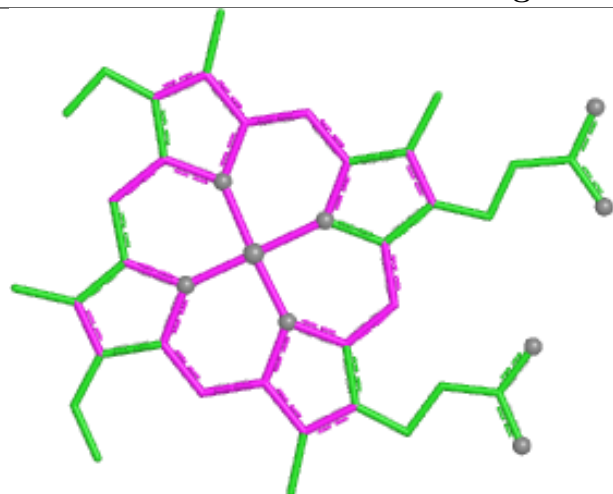


Torsions

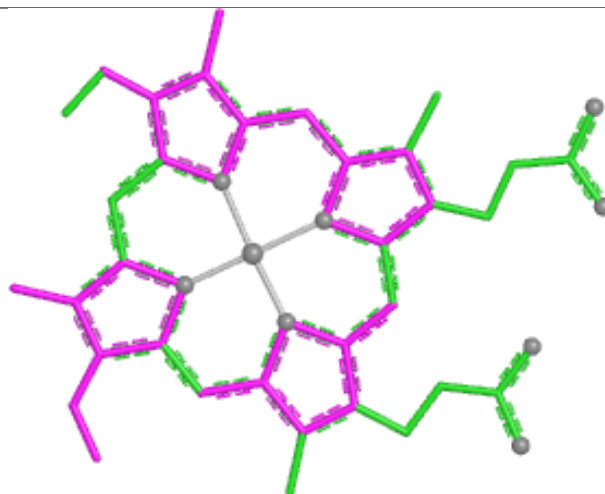


Rings

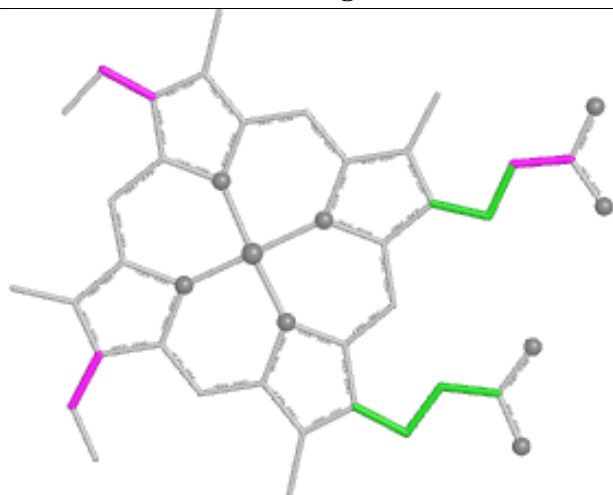
## Ligand HEC B 601



Bond lengths



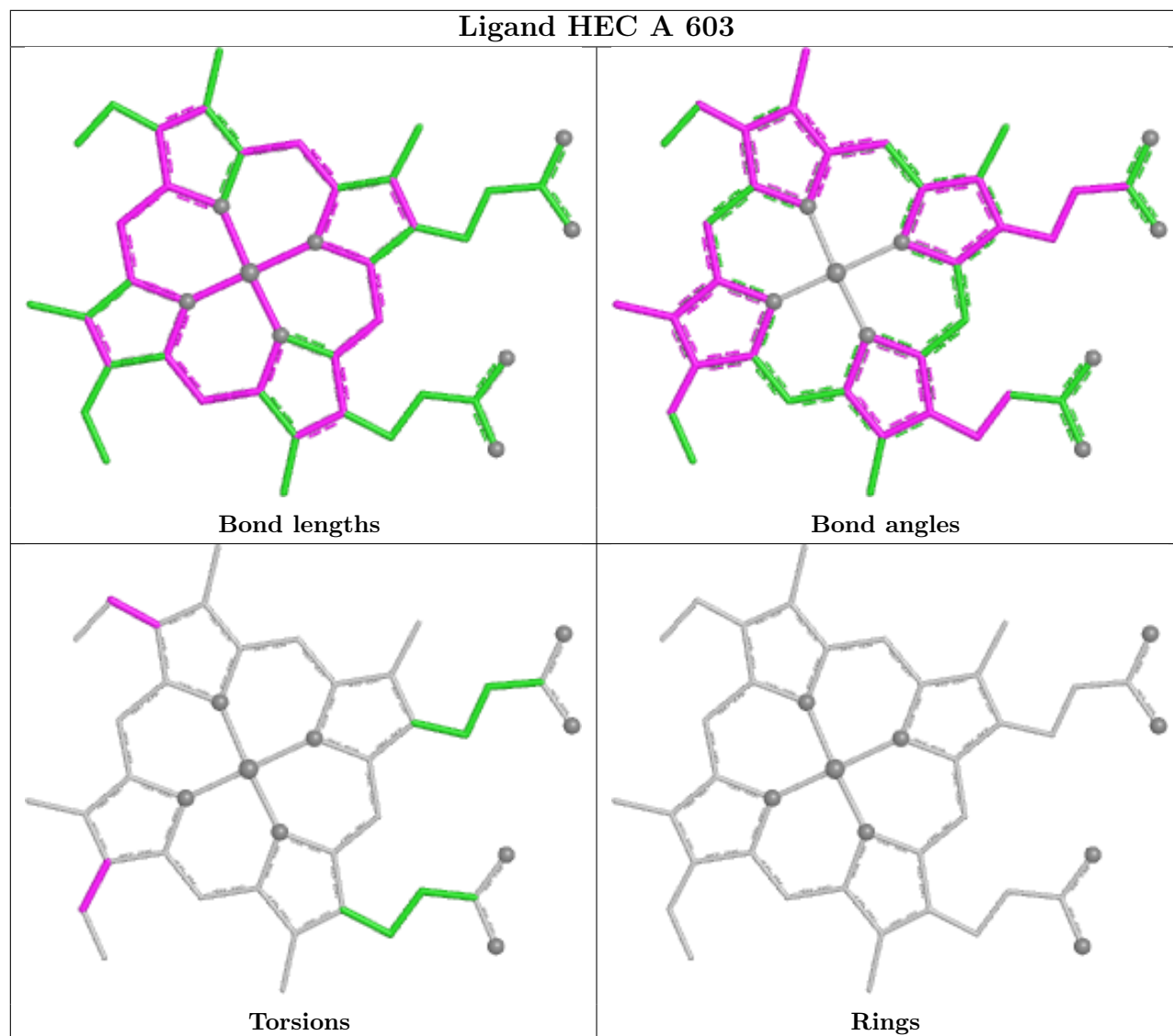
Bond angles

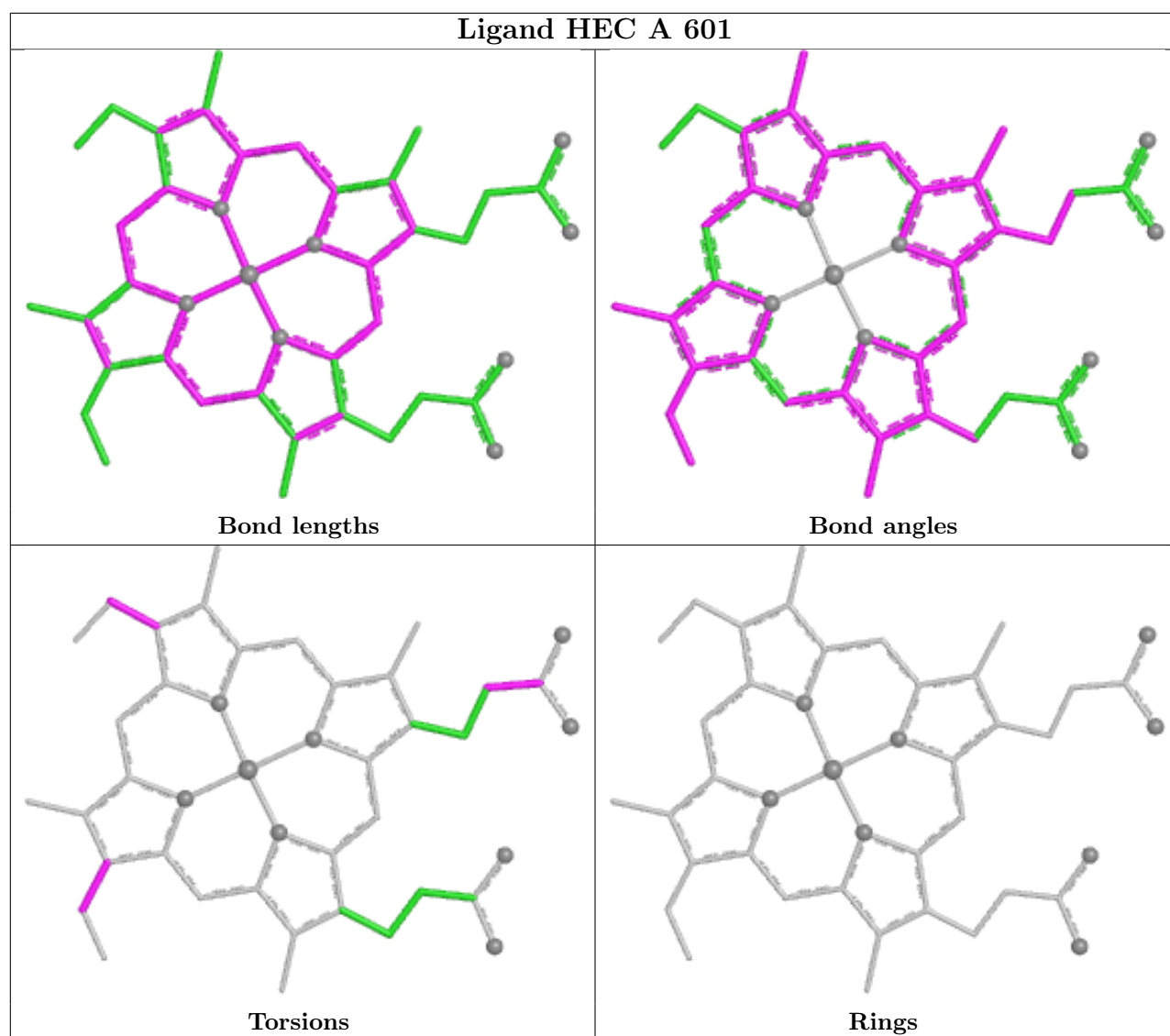


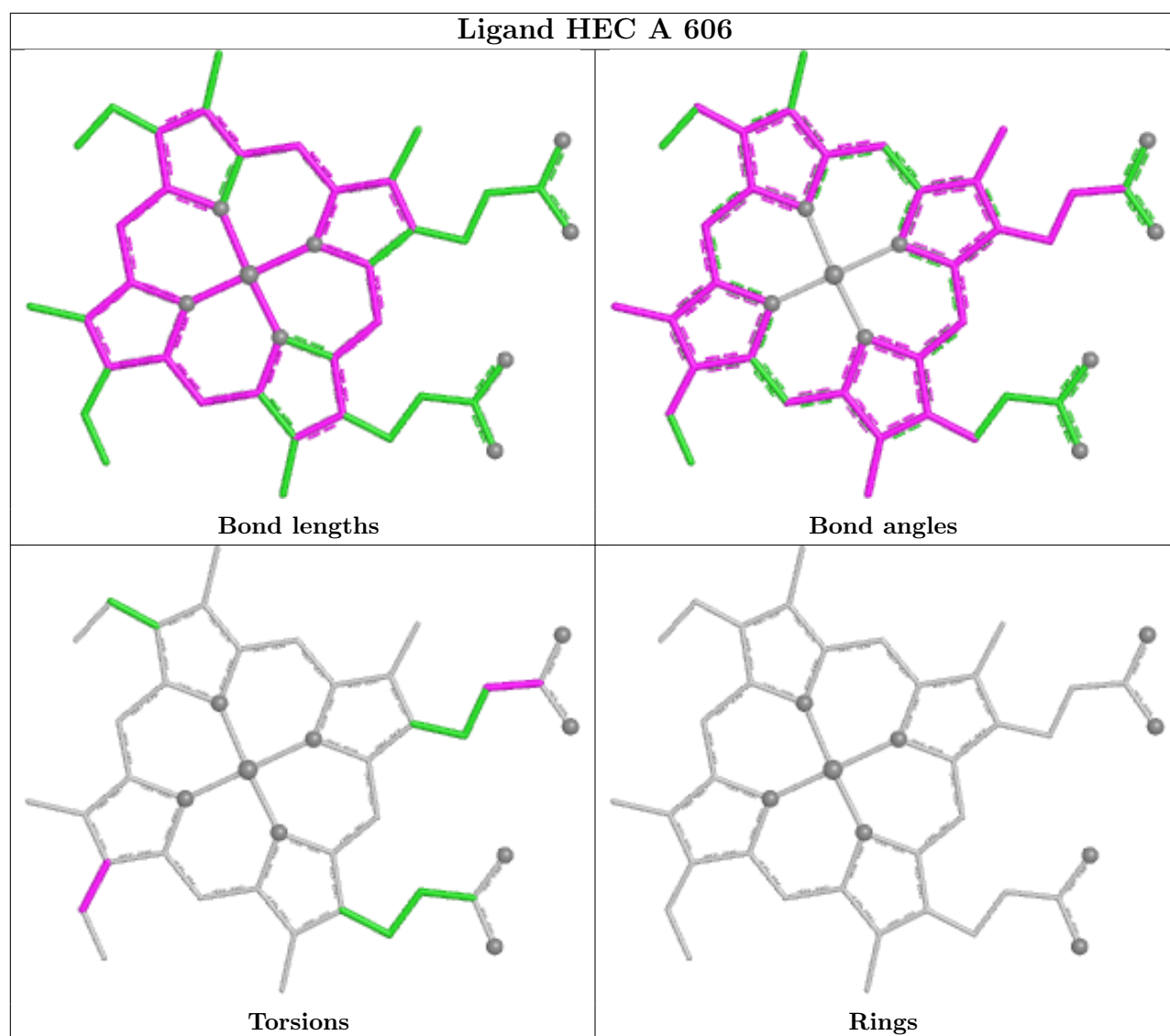
Torsions



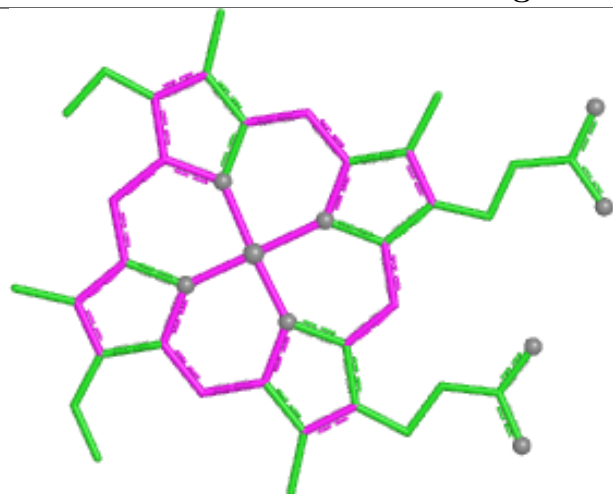
Rings



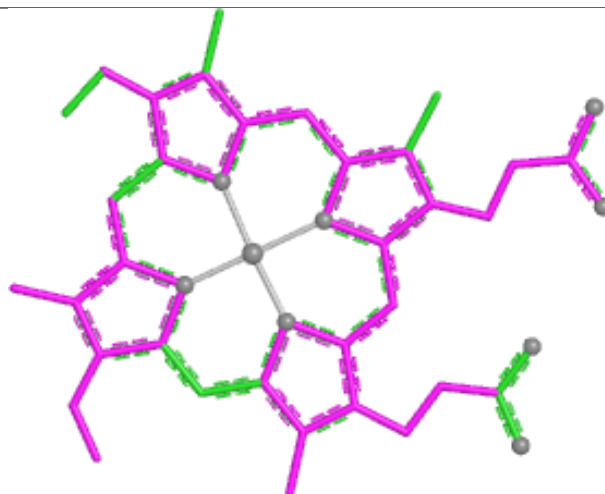




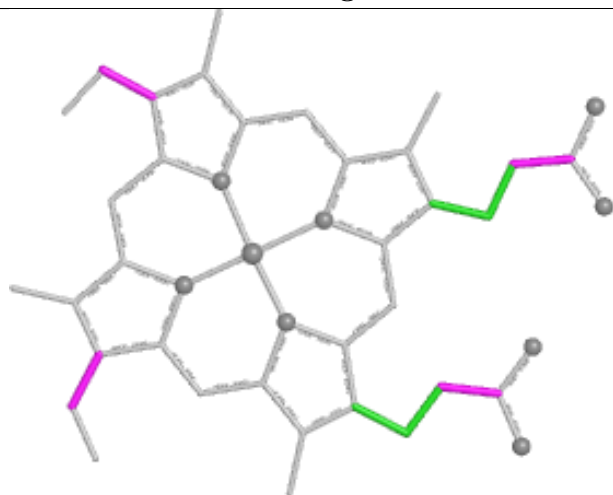
## Ligand HEC B 607



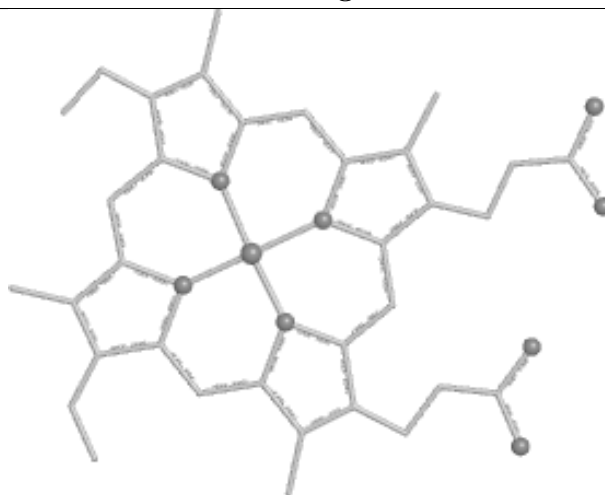
Bond lengths



Bond angles

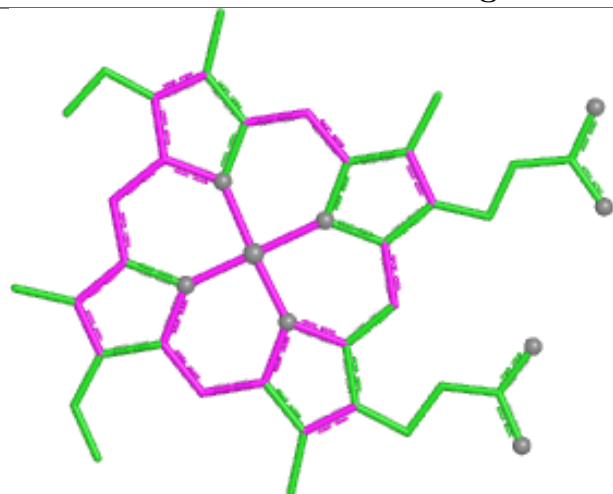


Torsions

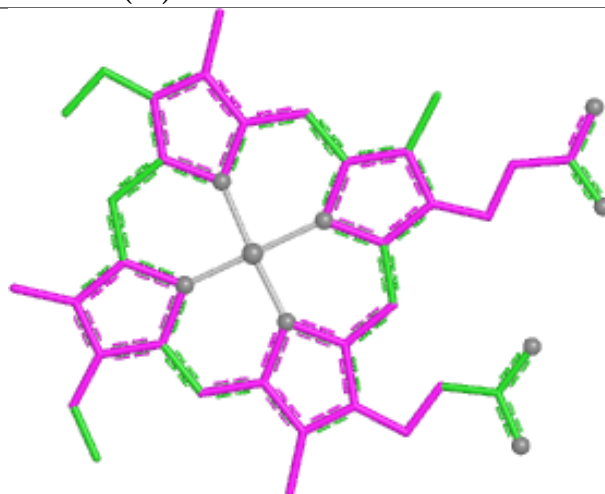


Rings

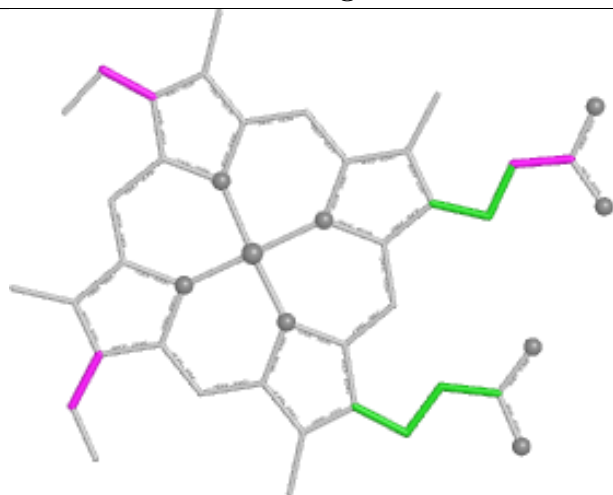
## Ligand HEC B 604 (A)



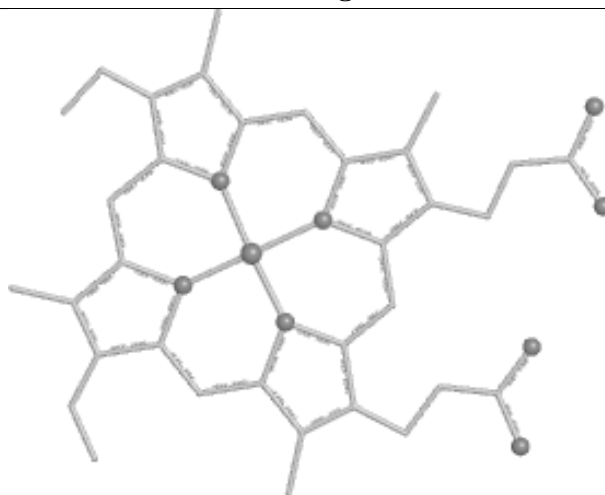
Bond lengths



Bond angles

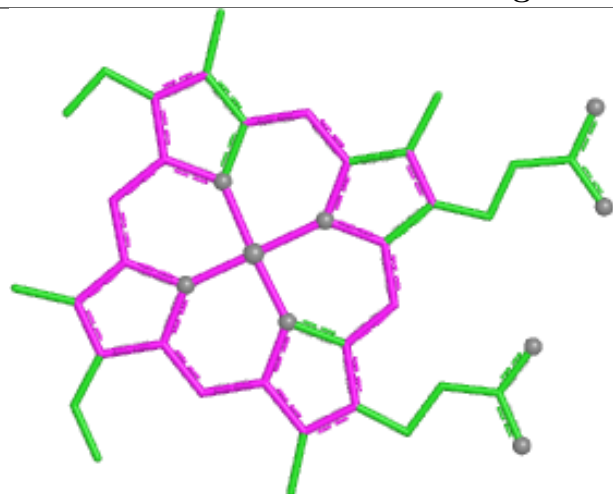


Torsions

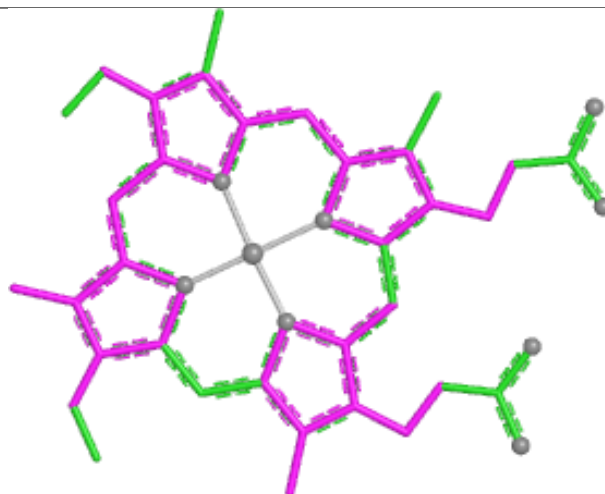


Rings

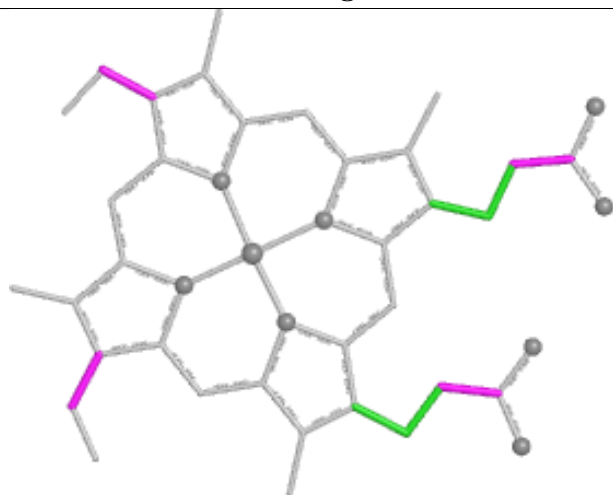
## Ligand HEC B 608



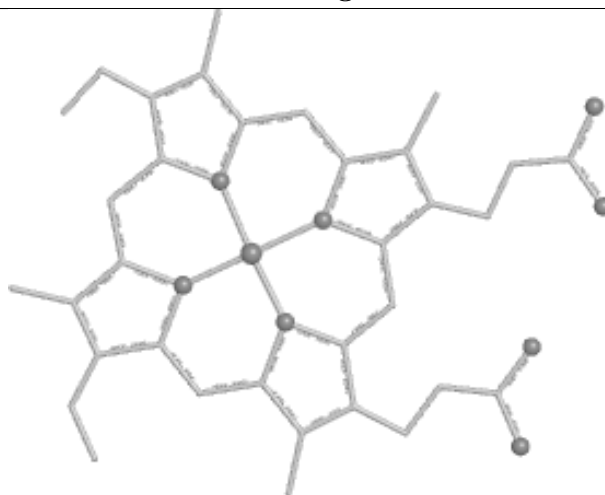
Bond lengths



Bond angles

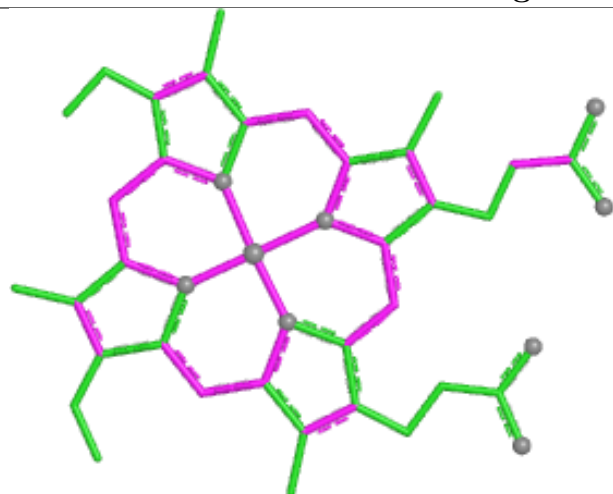


Torsions

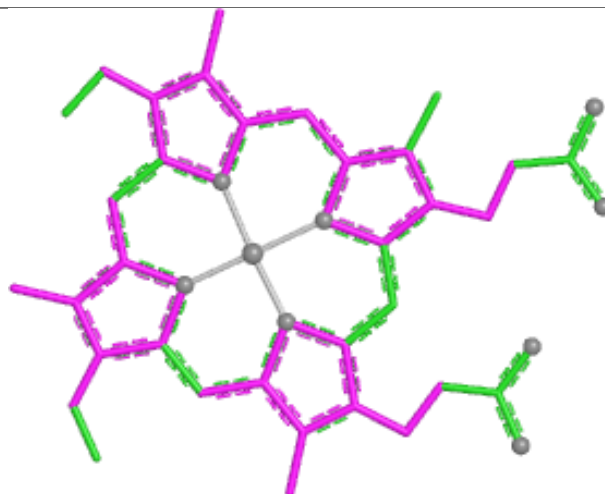


Rings

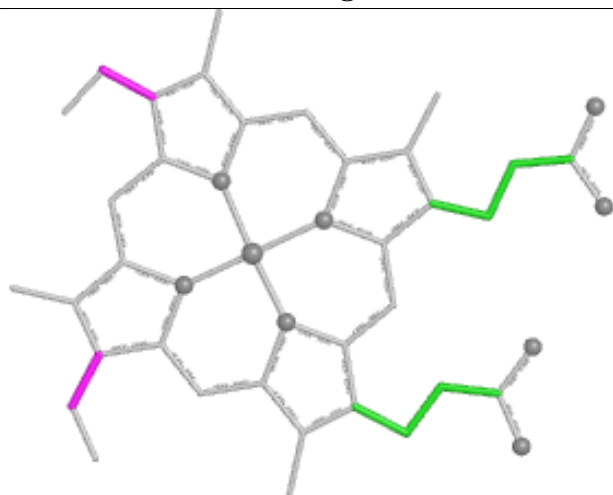
## Ligand HEC B 603



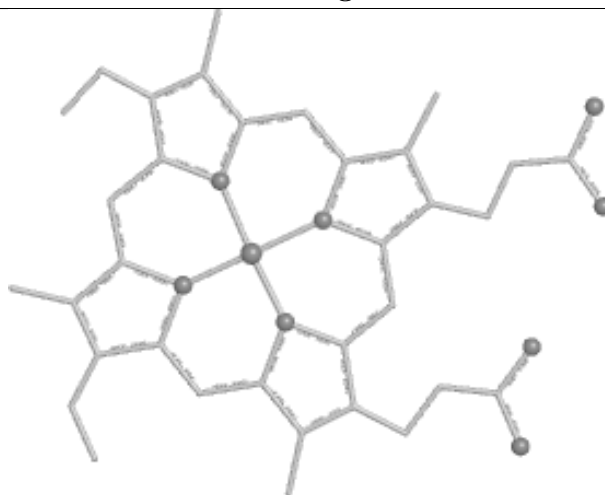
Bond lengths



Bond angles

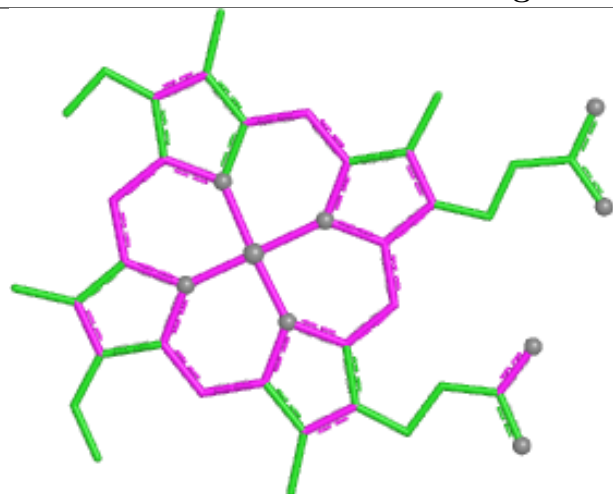


Torsions

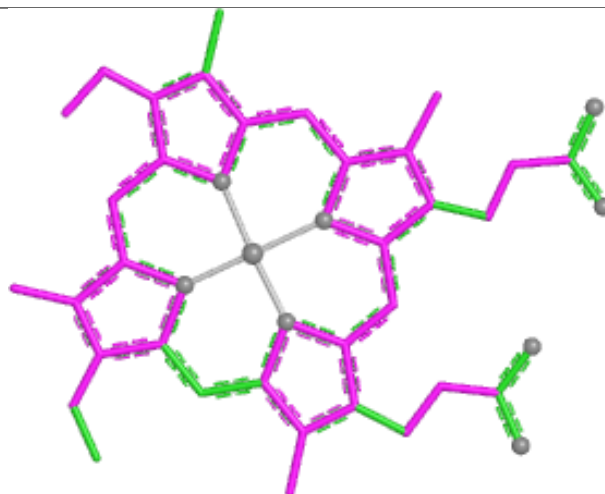


Rings

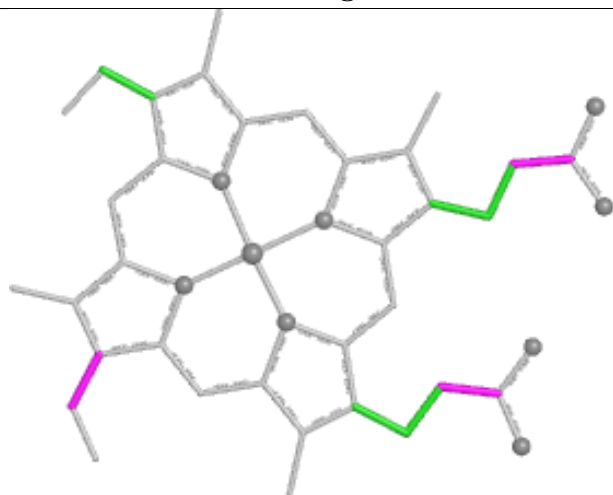
## Ligand HEC B 602



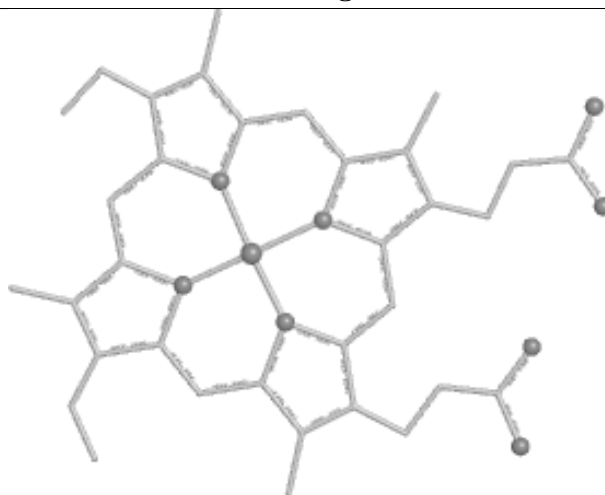
Bond lengths



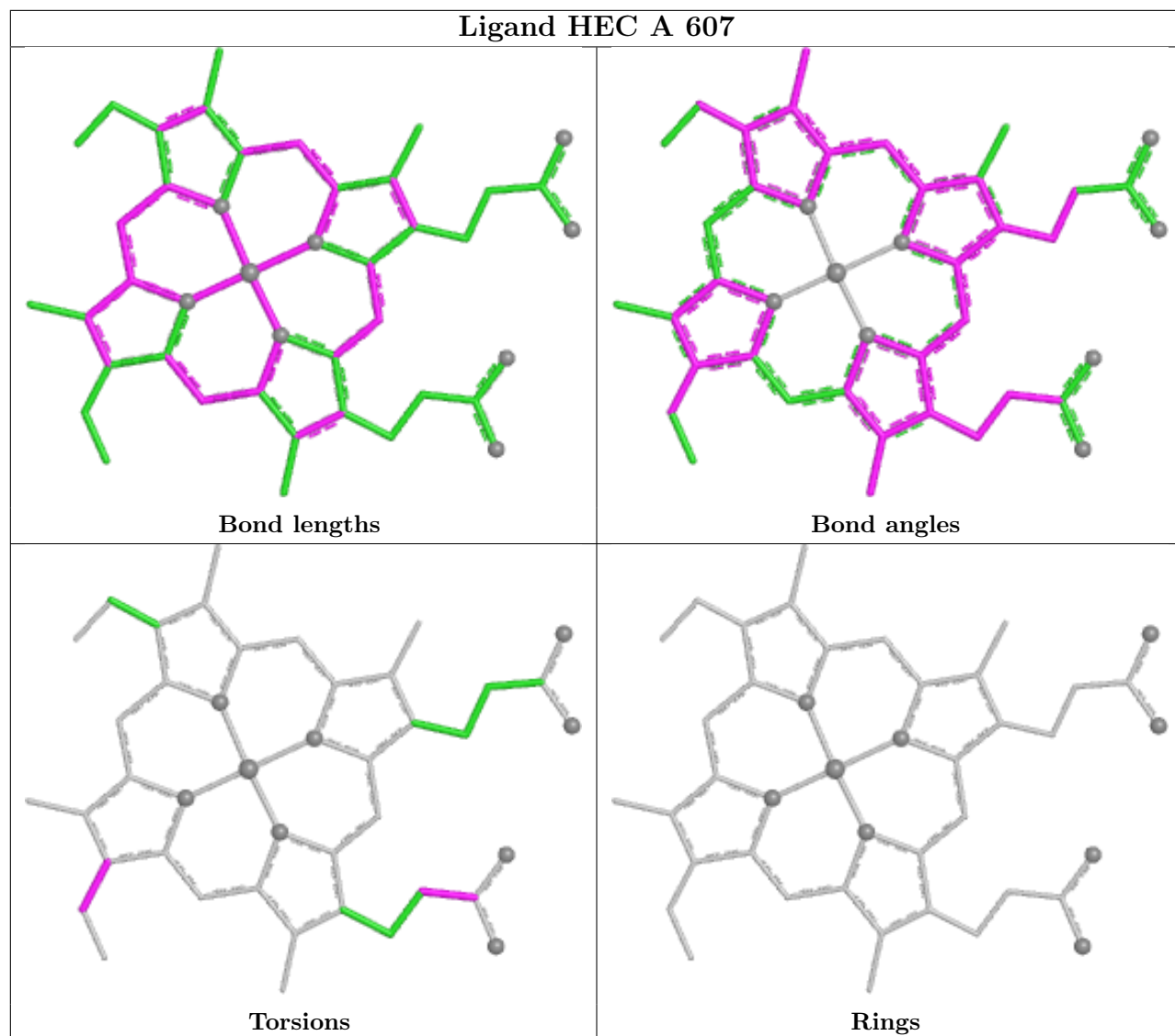
Bond angles

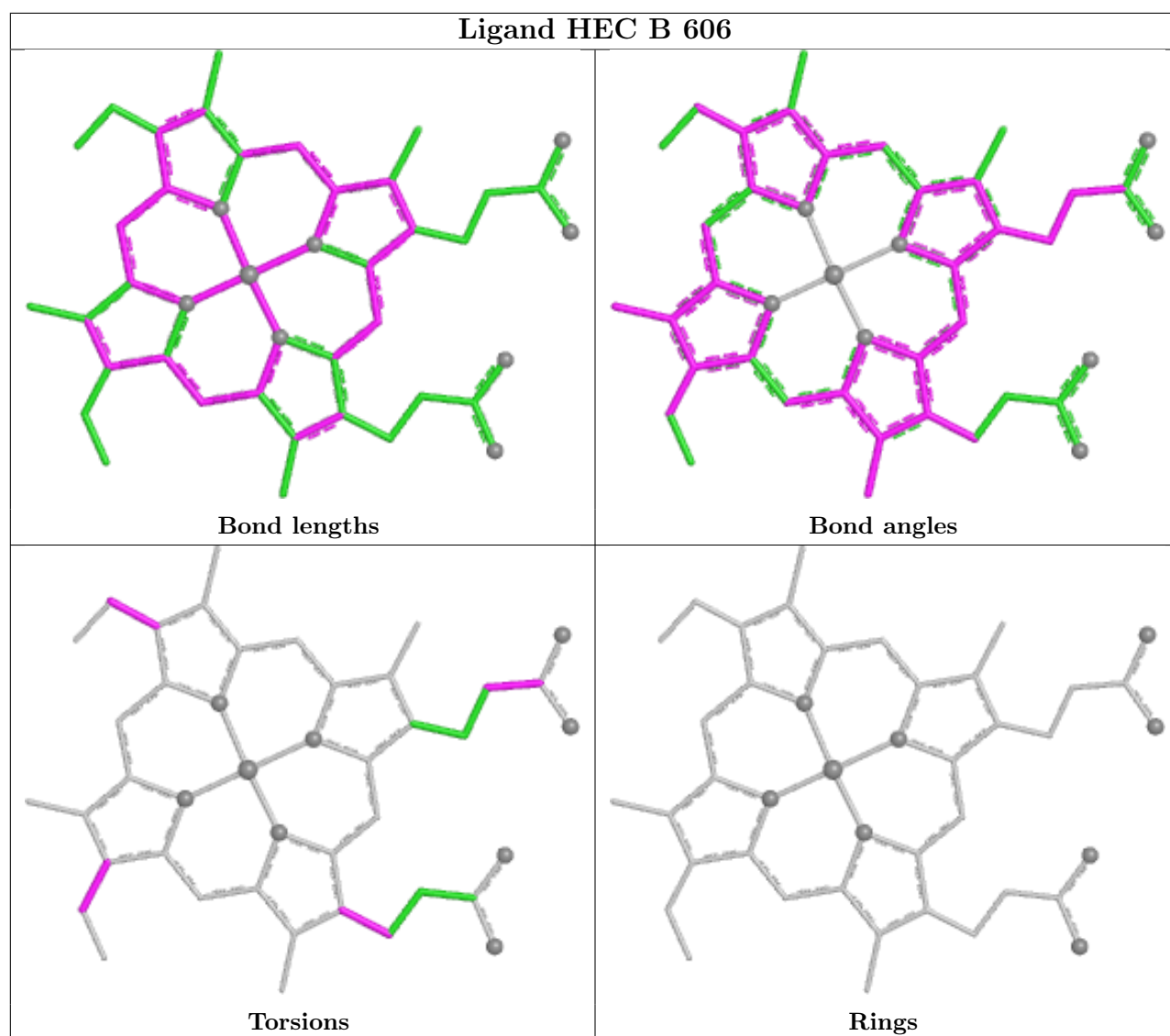


Torsions



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 [i](#)

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

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9   |
|-----|-------|------------------|--------|--------------|-----------------------|---------|
| 1   | A     | 520/520 (100%)   | -0.62  | 3 (0%) 85 89 | 10, 15, 29, 55        | 18 (3%) |
| 1   | B     | 520/520 (100%)   | -0.72  | 3 (0%) 85 89 | 8, 13, 27, 50         | 16 (3%) |
| All | All   | 1040/1040 (100%) | -0.67  | 6 (0%) 85 89 | 8, 14, 28, 55         | 34 (3%) |

All (6) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 524 | VAL  | 3.9  |
| 1   | B     | 524 | VAL  | 3.5  |
| 1   | B     | 523 | ALA  | 2.6  |
| 1   | A     | 523 | ALA  | 2.5  |
| 1   | B     | 413 | ASN  | 2.2  |
| 1   | A     | 278 | ARG  | 2.2  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

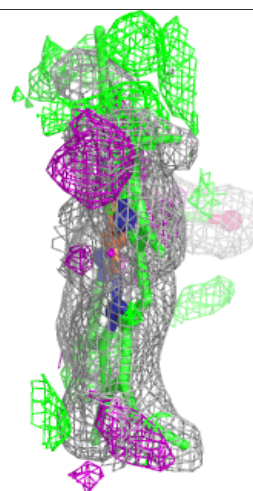
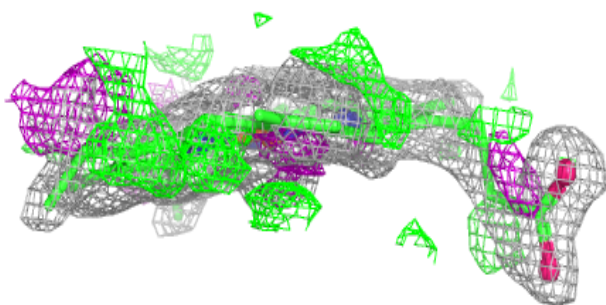
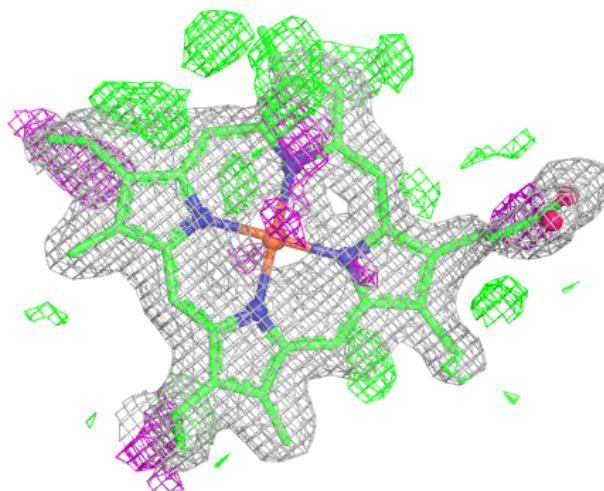
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|-----------------------------|-------|
| 6   | GOL  | A     | 615[A] | 6/6   | 0.71 | 0.24 | 36,48,56,56                 | 1     |
| 6   | GOL  | A     | 615[B] | 6/6   | 0.71 | 0.24 | 37,48,56,56                 | 1     |
| 7   | SO4  | A     | 616    | 5/5   | 0.86 | 0.15 | 26,27,29,30                 | 5     |
| 5   | MPD  | A     | 612    | 8/8   | 0.90 | 0.14 | 21,26,27,28                 | 0     |
| 5   | MPD  | B     | 612    | 8/8   | 0.93 | 0.11 | 18,21,22,22                 | 0     |
| 7   | SO4  | B     | 615    | 5/5   | 0.93 | 0.11 | 21,21,22,23                 | 5     |
| 6   | GOL  | B     | 613[A] | 6/6   | 0.95 | 0.08 | 12,15,16,16                 | 1     |
| 6   | GOL  | B     | 613[B] | 6/6   | 0.95 | 0.08 | 13,15,16,17                 | 1     |
| 3   | NO2  | A     | 617    | 3/3   | 0.95 | 0.09 | 23,23,24,25                 | 3     |
| 6   | GOL  | A     | 614    | 6/6   | 0.95 | 0.11 | 20,25,26,28                 | 0     |
| 6   | GOL  | A     | 613[B] | 6/6   | 0.96 | 0.08 | 15,16,17,18                 | 1     |
| 2   | HEC  | A     | 605    | 38/43 | 0.96 | 0.13 | 21,29,44,47                 | 0     |
| 3   | NO2  | A     | 618    | 3/3   | 0.96 | 0.06 | 17,17,17,18                 | 3     |
| 6   | GOL  | A     | 613[A] | 6/6   | 0.96 | 0.08 | 14,16,17,18                 | 1     |
| 4   | CA   | B     | 611    | 1/1   | 0.97 | 0.04 | 12,12,12,12                 | 1     |
| 6   | GOL  | B     | 614    | 6/6   | 0.97 | 0.09 | 19,23,24,28                 | 0     |
| 2   | HEC  | B     | 605    | 39/43 | 0.97 | 0.12 | 19,26,44,50                 | 0     |
| 3   | NO2  | B     | 616    | 3/3   | 0.97 | 0.06 | 21,21,22,23                 | 3     |
| 3   | NO2  | B     | 617    | 3/3   | 0.98 | 0.05 | 13,13,13,14                 | 3     |
| 4   | CA   | A     | 611    | 1/1   | 0.98 | 0.03 | 14,14,14,14                 | 1     |
| 3   | NO2  | A     | 609    | 2/3   | 0.98 | 0.08 | 13,13,13,14                 | 2     |
| 2   | HEC  | A     | 607    | 43/43 | 0.99 | 0.06 | 9,11,23,34                  | 0     |
| 4   | CA   | A     | 610    | 1/1   | 0.99 | 0.06 | 17,17,17,17                 | 0     |
| 2   | HEC  | A     | 608    | 43/43 | 0.99 | 0.04 | 11,13,17,22                 | 0     |
| 2   | HEC  | B     | 601    | 43/43 | 0.99 | 0.04 | 7,9,10,11                   | 0     |
| 2   | HEC  | B     | 602    | 43/43 | 0.99 | 0.05 | 8,9,16,21                   | 0     |
| 2   | HEC  | B     | 603    | 43/43 | 0.99 | 0.04 | 7,7,9,11                    | 0     |
| 2   | HEC  | B     | 604[A] | 43/43 | 0.99 | 0.05 | 8,8,9,10                    | 4     |
| 2   | HEC  | B     | 604[B] | 43/43 | 0.99 | 0.05 | 8,8,10,13                   | 4     |
| 2   | HEC  | A     | 602    | 43/43 | 0.99 | 0.05 | 9,11,17,21                  | 0     |
| 2   | HEC  | B     | 606    | 43/43 | 0.99 | 0.04 | 9,11,13,14                  | 0     |
| 2   | HEC  | B     | 607    | 43/43 | 0.99 | 0.06 | 9,10,22,29                  | 0     |
| 2   | HEC  | B     | 608    | 43/43 | 0.99 | 0.05 | 12,16,18,22                 | 0     |
| 2   | HEC  | A     | 603    | 43/43 | 0.99 | 0.04 | 8,9,10,12                   | 0     |
| 2   | HEC  | A     | 604    | 43/43 | 0.99 | 0.05 | 9,10,13,19                  | 0     |
| 2   | HEC  | A     | 601    | 43/43 | 0.99 | 0.05 | 9,11,12,13                  | 0     |
| 2   | HEC  | A     | 606    | 43/43 | 0.99 | 0.04 | 11,12,14,14                 | 0     |
| 4   | CA   | B     | 610    | 1/1   | 1.00 | 0.05 | 16,16,16,16                 | 0     |
| 3   | NO2  | B     | 609    | 2/3   | 1.00 | 0.03 | 10,10,10,10                 | 2     |

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

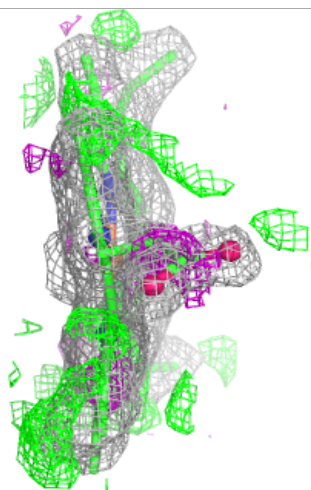
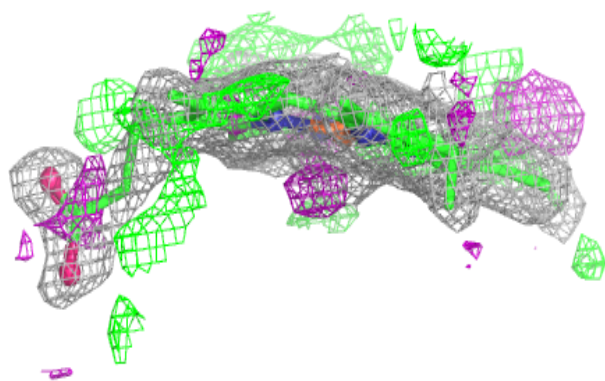
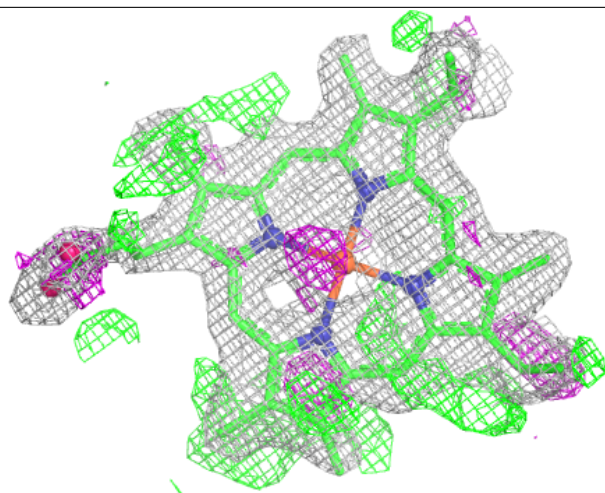
**Electron density around HEC A 605:**

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



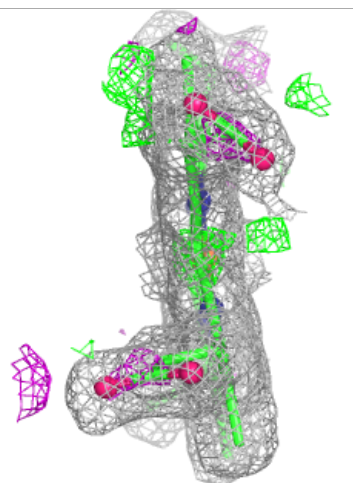
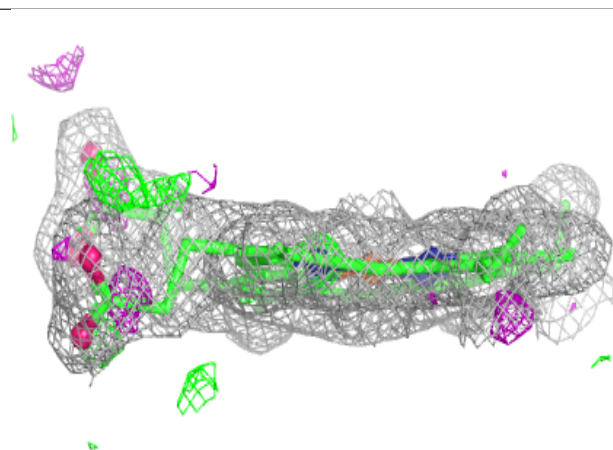
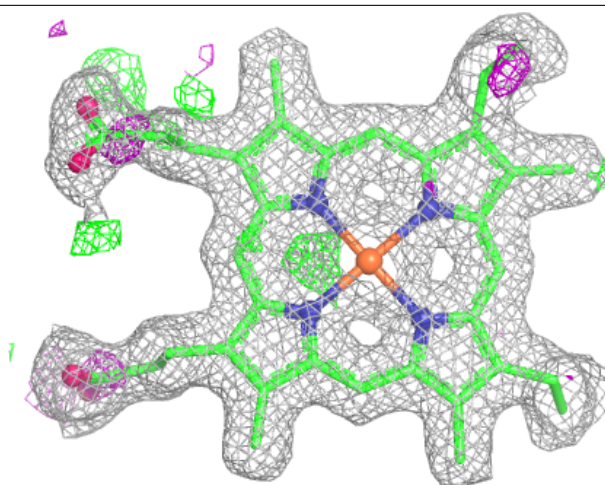
**Electron density around HEC B 605:**

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



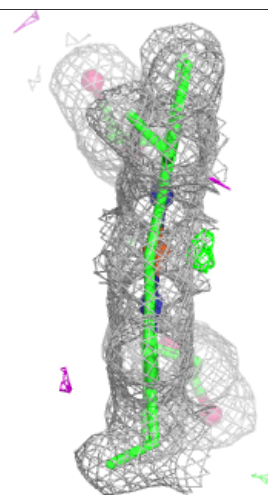
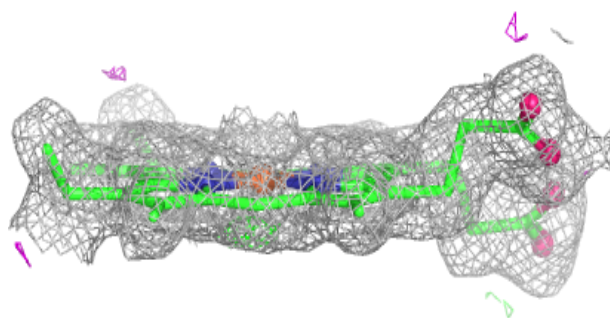
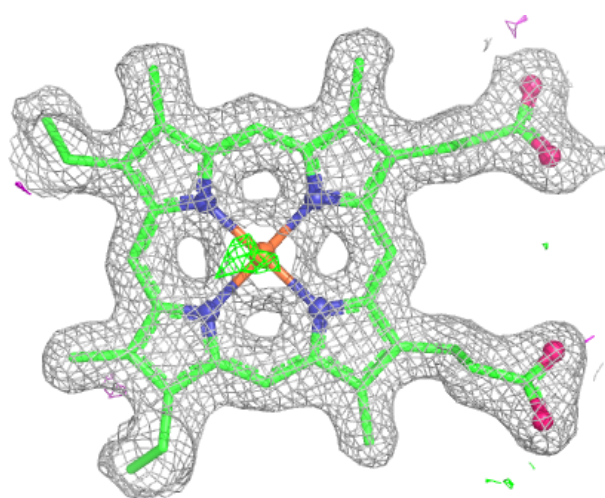
**Electron density around HEC A 607:**

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



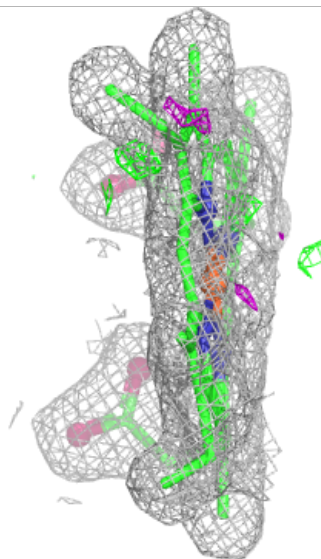
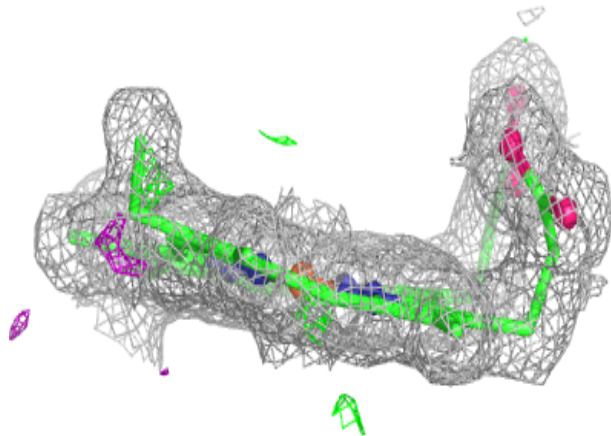
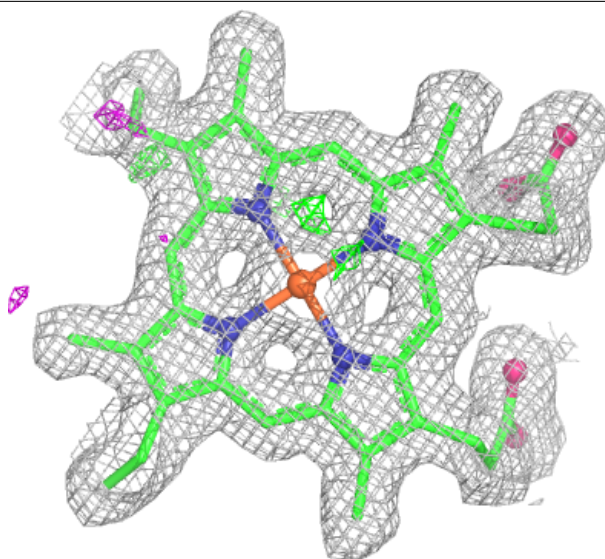
**Electron density around HEC A 608:**

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



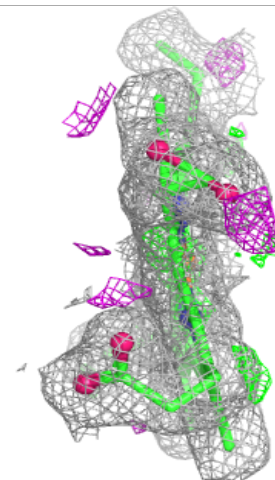
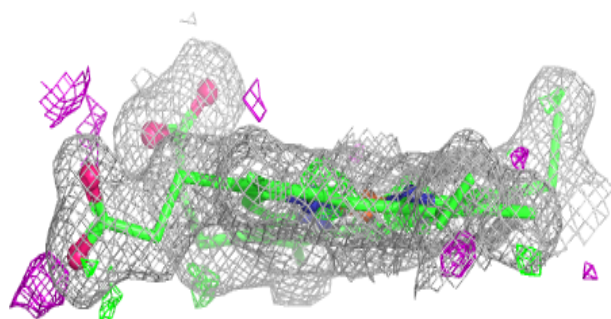
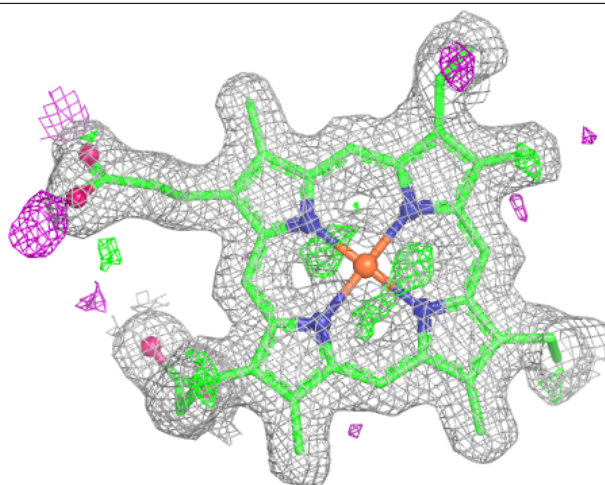
**Electron density around HEC B 601:**

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and green (positive)



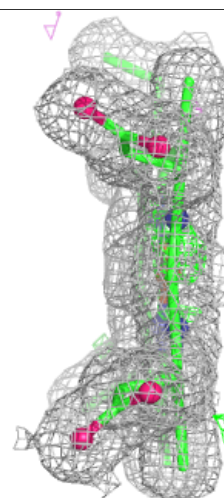
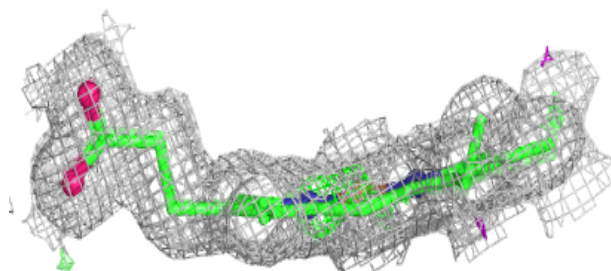
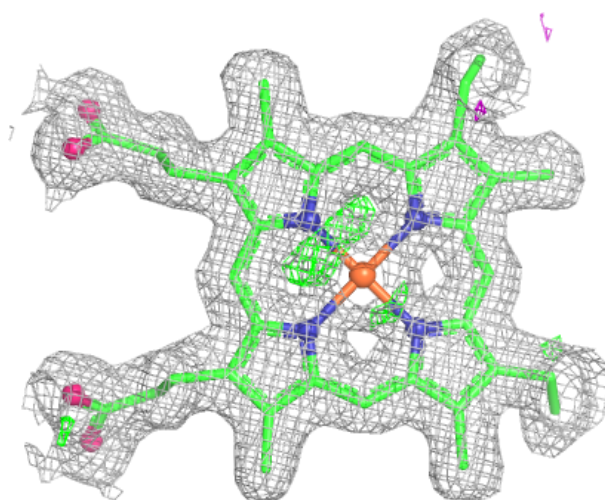
**Electron density around HEC B 602:**

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



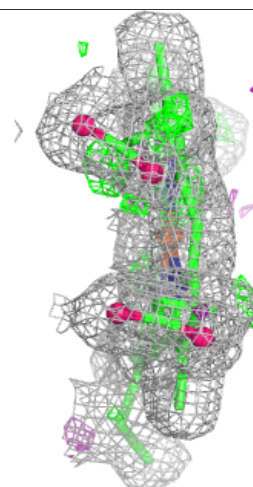
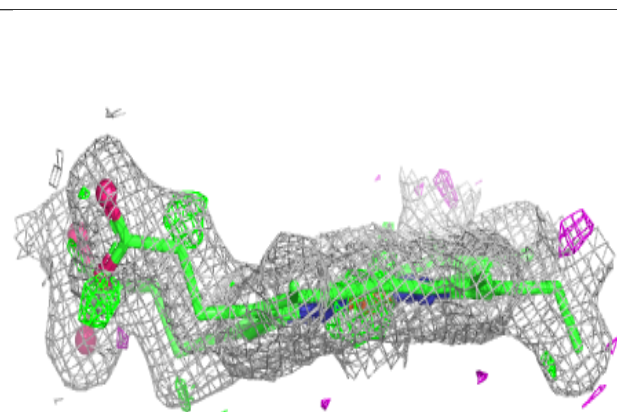
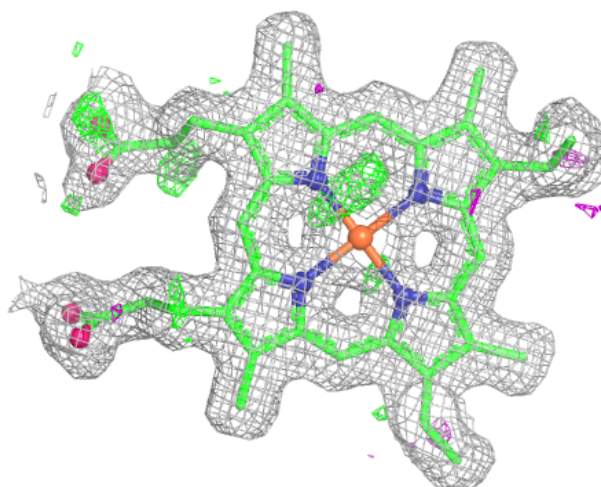
**Electron density around HEC B 603:**

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



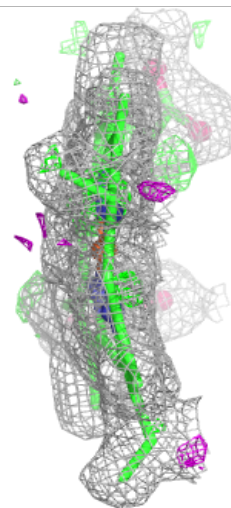
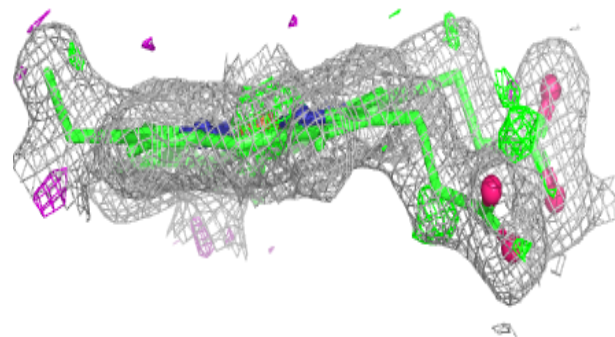
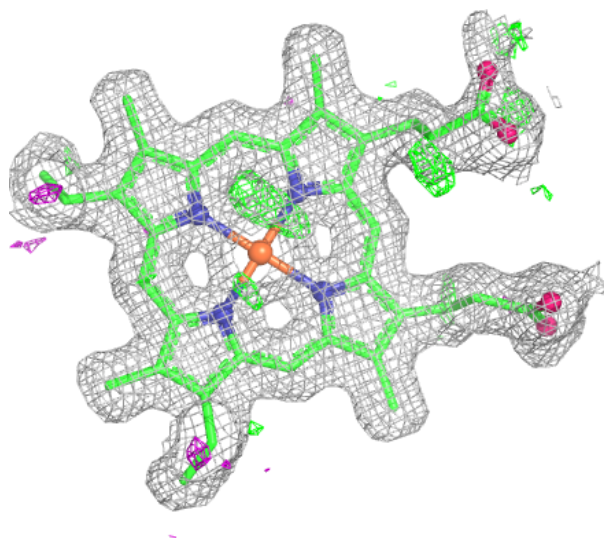
**Electron density around HEC B 604 (A):**

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



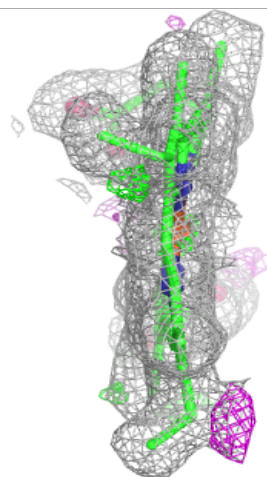
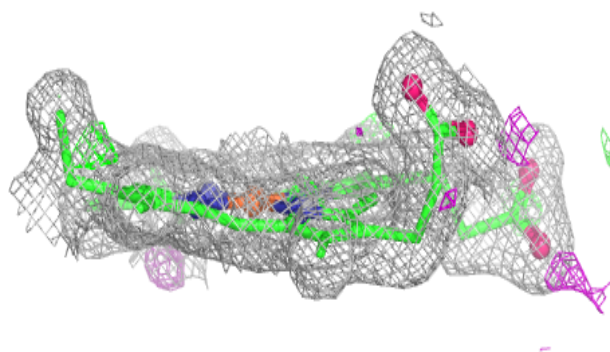
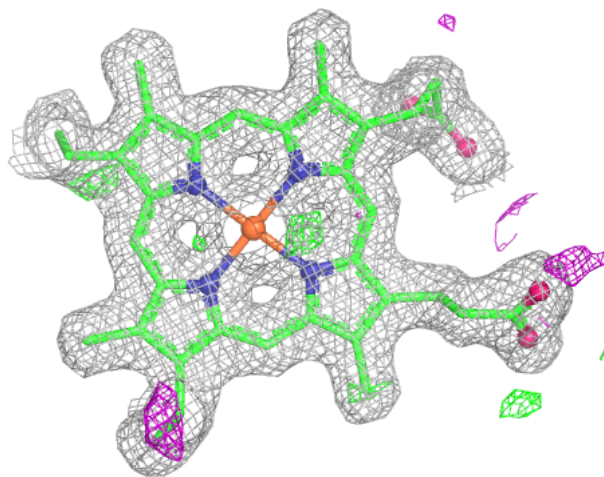
**Electron density around HEC B 604 (B):**

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and green (positive)



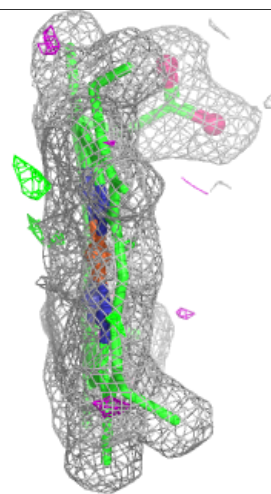
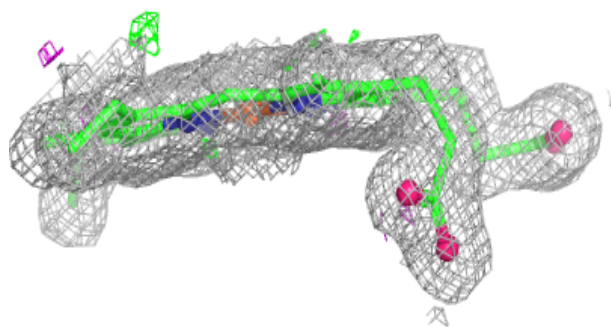
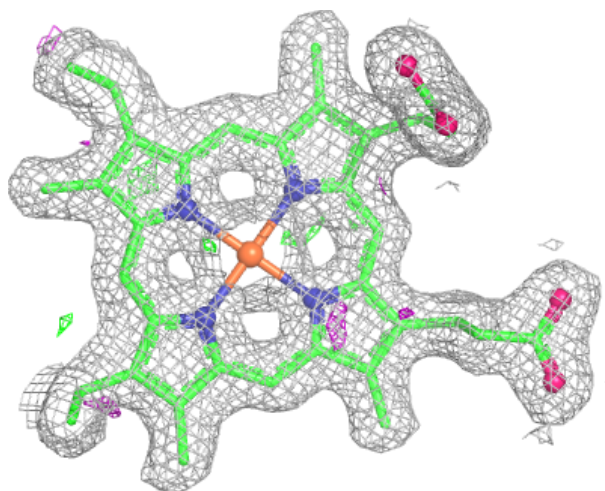
**Electron density around HEC A 602:**

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



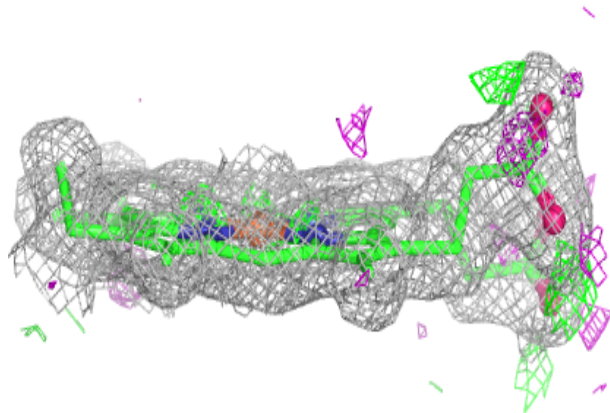
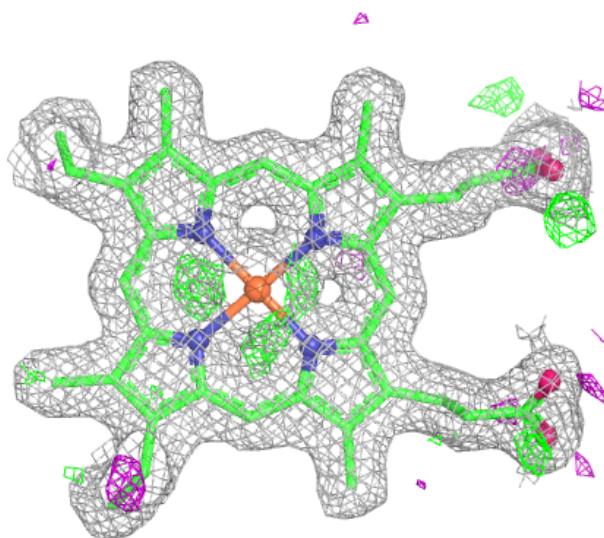
**Electron density around HEC B 606:**

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and green (positive)



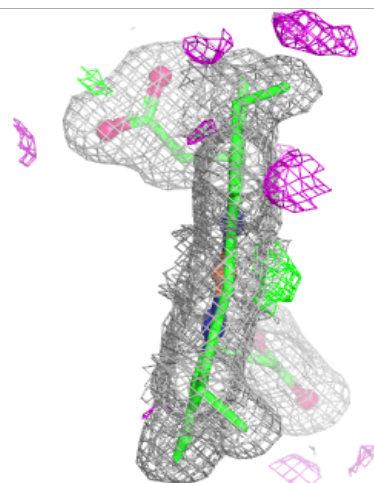
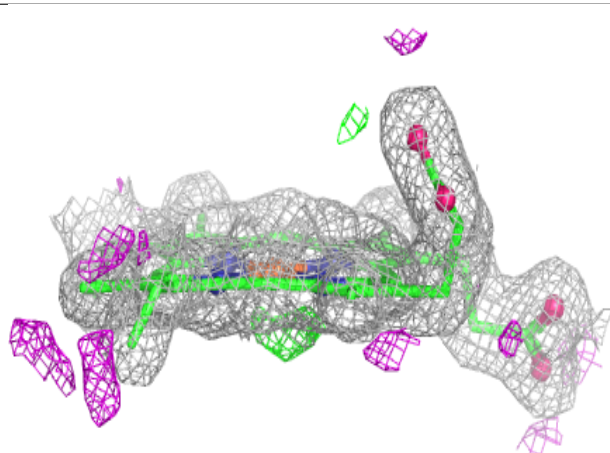
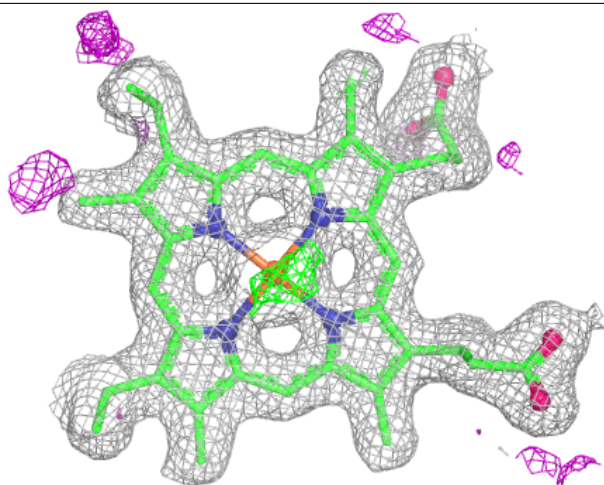
**Electron density around HEC B 607:**

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and green (positive)



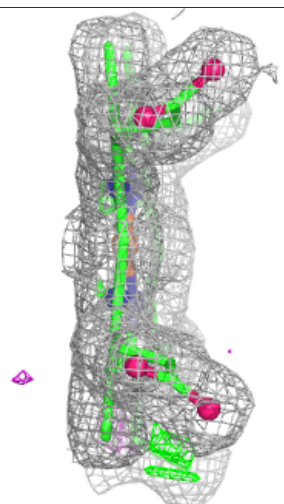
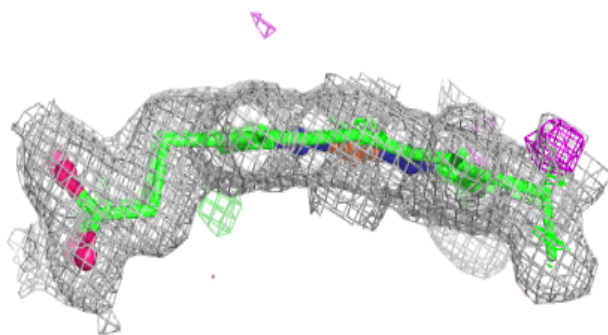
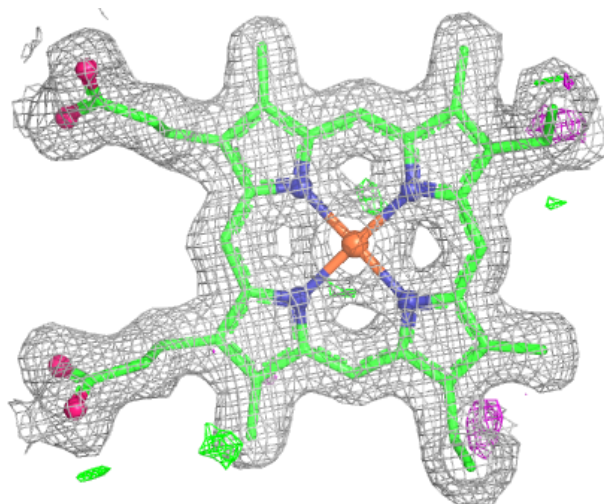
**Electron density around HEC B 608:**

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and green (positive)



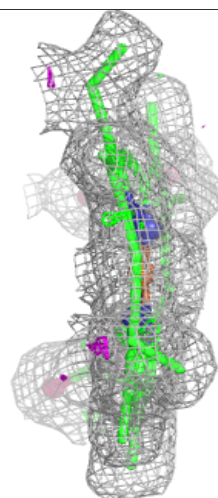
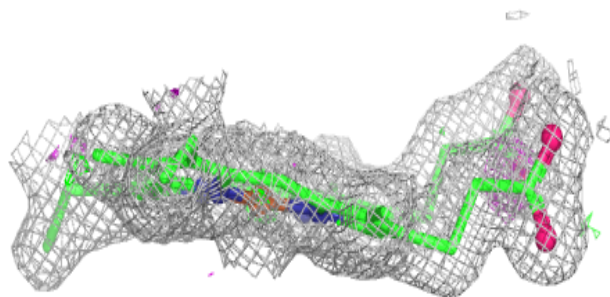
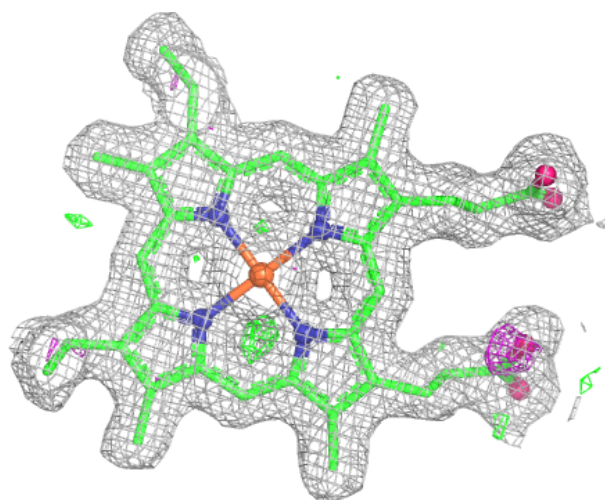
**Electron density around HEC A 603:**

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and green (positive)



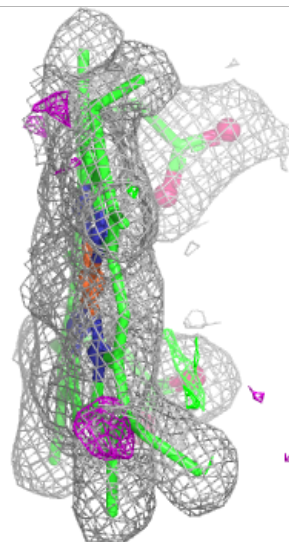
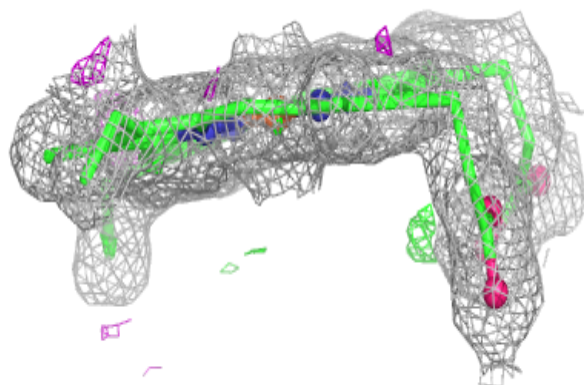
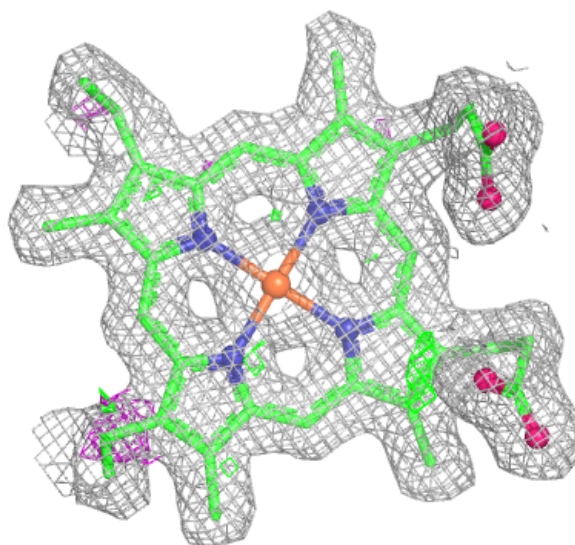
**Electron density around HEC A 604:**

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



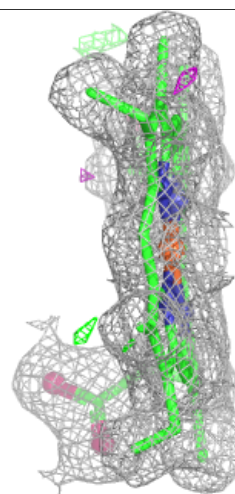
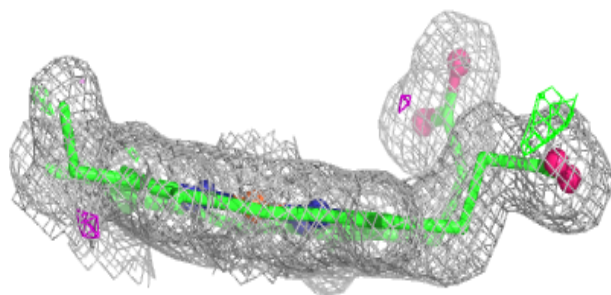
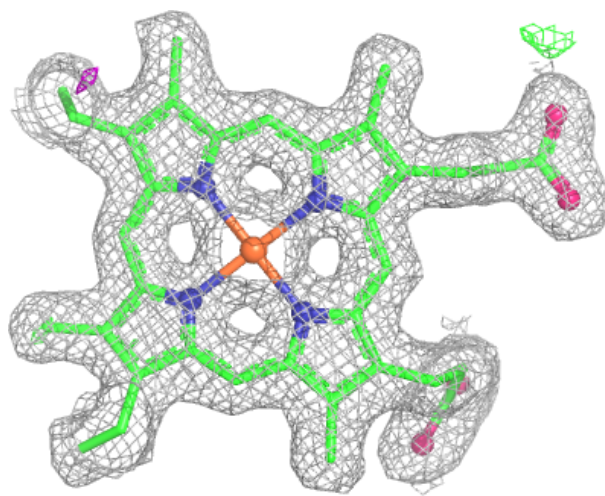
**Electron density around HEC A 601:**

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



**Electron density around HEC A 606:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.