



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2022 – 11:07 am BST

PDB ID : 7R3V  
Title : Crystal structure of bovine Cytochrome bc1 in complex with inhibitor CK-2-67.  
Authors : Pinthong, N.; Ampornpanai, K.; O'Neill, P.M.; Hasnain, S.S.; Antonyuk, S.  
Deposited on : 2022-02-07  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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                     | : | 4.02b-467  |
| Mogul                          | : | 1.8.4, CSD as541be (2020)  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.29   |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0267   |
| CCP4                           | : | 7.1.010 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.29   |

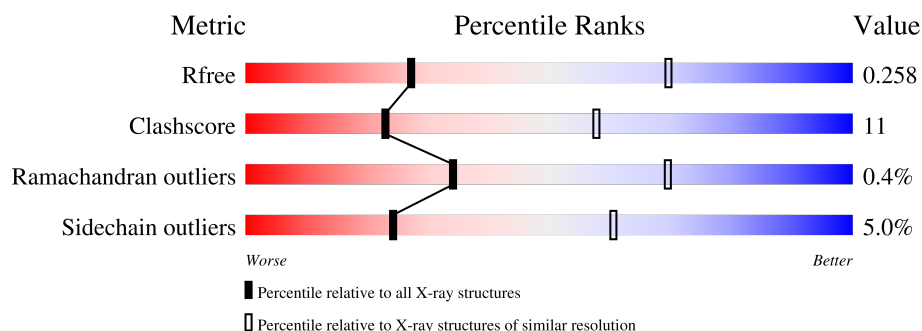
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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






| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1133 (3.20-3.20)                                      |
| Clashscore            | 141614                      | 1253 (3.20-3.20)                                      |
| Ramachandran outliers | 138981                      | 1234 (3.20-3.20)                                      |
| Sidechain outliers    | 138945                      | 1233 (3.20-3.20)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 445    |                  |
| 2   | B     | 418    |                  |
| 3   | C     | 379    |                  |
| 4   | D     | 239    |                  |
| 5   | E     | 196    |                  |
| 6   | F     | 99     |                  |
| 7   | G     | 74     |                  |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 8   | H     | 65     |  <div>68% 31% .</div>   |
| 9   | I     | 46     |  <div>57% 28% 15%</div> |
| 10  | J     | 59     |  <div>78% 22%</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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 16  | PEE  | C     | 406 | X         | -        | -       | -                |
| 16  | PEE  | E     | 204 | X         | -        | -       | -                |

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 16382 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 445      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3449  | 2157 | 608 | 664 | 20 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 226     | GLU      | ASP    | conflict | UNP P31800 |
| A     | 227     | THR      | ALA    | conflict | UNP P31800 |

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 413      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3093  | 1943 | 546 | 597 | 7 |         |         |       |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | C     | 379      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3004  | 2012 | 472 | 501 | 19 |         |         |       |

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 4   | D     | 239      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1884  | 1205 | 321 | 343 | 15 |         |         |       |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | E     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1519  | 957 | 263 | 291 | 8 |         |         |       |

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 99       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 859   | 545 | 156 | 156 | 2 |         |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 56      | ASP      | ASN    | conflict | UNP P00129 |

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 7   | G     | 74       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 620   | 406 | 116 | 97 | 1 |         |         |       |

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 8   | H     | 65       | Total | C   | N  | O   | S | 0       | 0       | 0     |
|     |       |          | 525   | 318 | 95 | 107 | 5 |         |         |       |

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 9   | I     | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 338   | 209 | 64 | 64 | 1 |         |         |       |

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

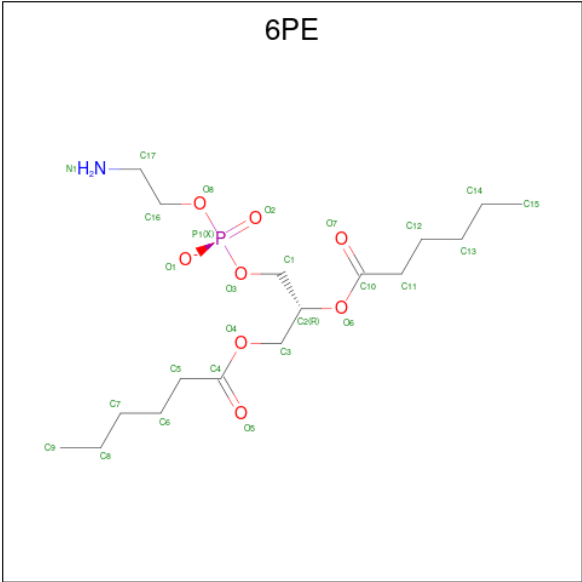
| Mol | Chain | Residues | Atoms |     |    |    |  | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|---------|-------|
| 10  | J     | 59       | Total | C   | N  | O  |  | 0       | 0       | 0     |
|     |       |          | 487   | 320 | 84 | 83 |  |         |         |       |

- Molecule 11 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



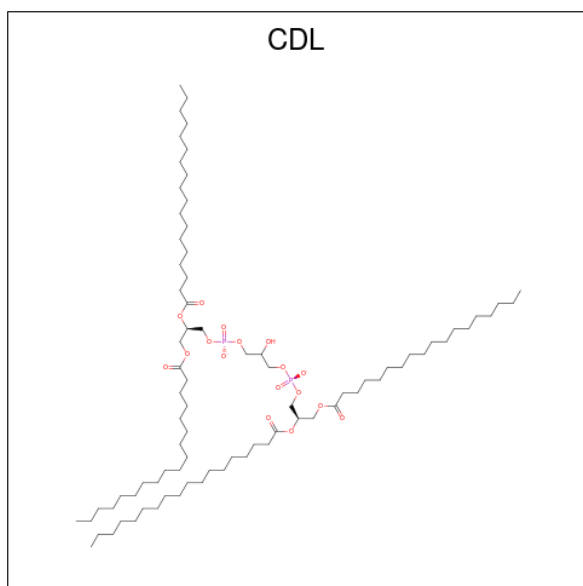
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 11  | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 11  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |
| 11  | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 13    | 8 | 5 |         |         |

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: C<sub>17</sub>H<sub>33</sub>NO<sub>8</sub>P).



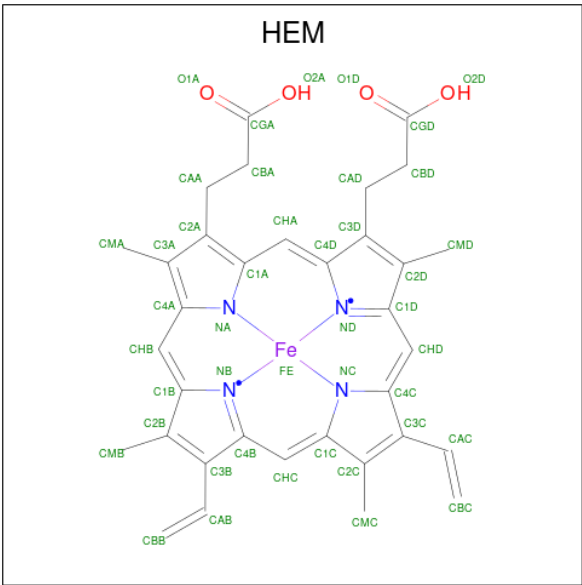
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 12  | A     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 23    | 13 | 1 | 8 | 1 |         |         |

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



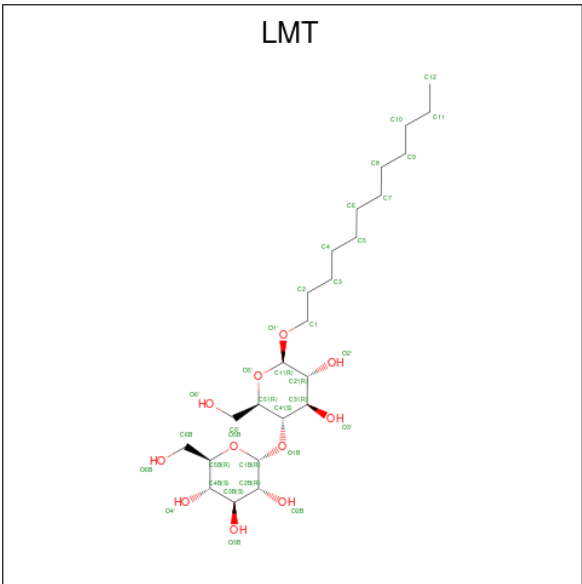
| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 13  | A     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 34    | 17 | 15 | 2 |         |         |
| 13  | D     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 54    | 35 | 17 | 2 |         |         |
| 13  | G     | 1        | Total | C  | O  | P | 0       | 0       |
|     |       |          | 44    | 25 | 17 | 2 |         |         |

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 14  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 14  | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

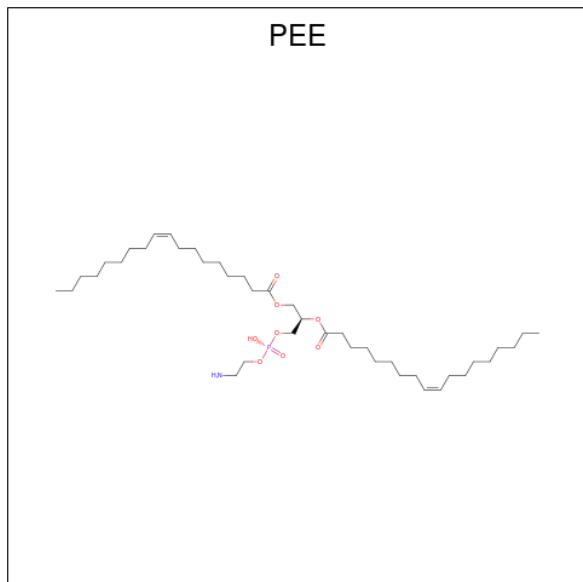
- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---------|---------|
| 15  | C     | 1        | Total | C  | O  | 0       | 0       |
|     |       |          | 35    | 24 | 11 |         |         |

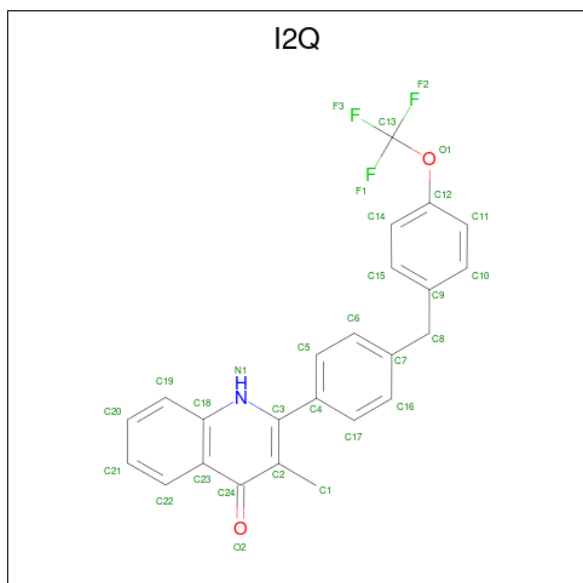


- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



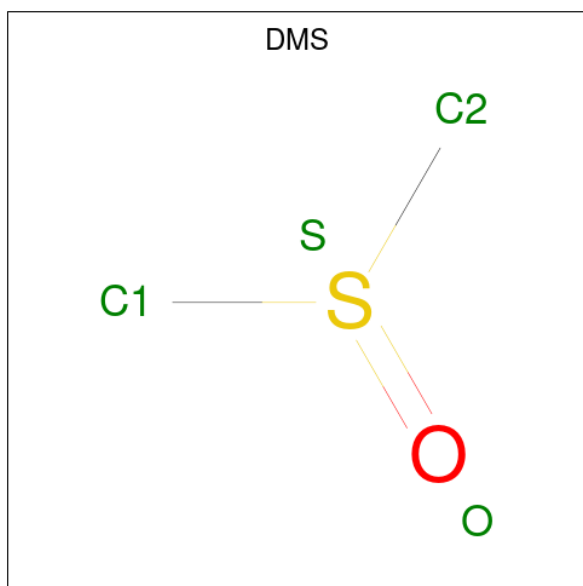
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 16  | C     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |         |
| 16  | E     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |         |

- Molecule 17 is 3-methyl-2-[4-[[4-(trifluoromethoxy)phenyl]methyl]phenyl]-1H-quinolin-4-one (three-letter code: I2Q) (formula: ) (labeled as "Ligand of Interest" by depositor).



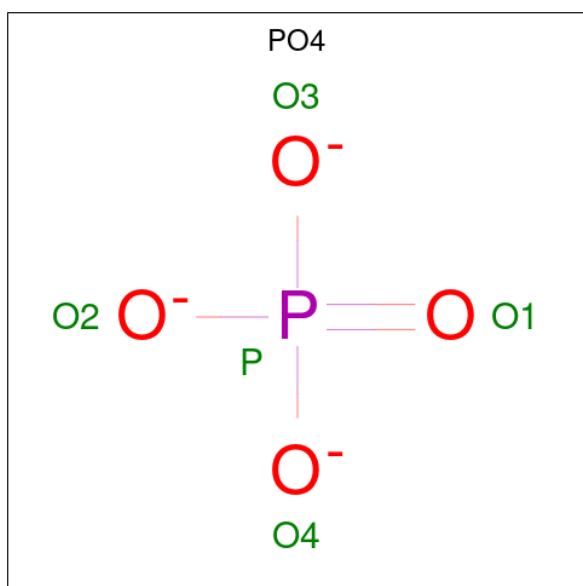
| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 17  | C     | 1        | Total | C  | F | N | O | 0       | 0       |
|     |       |          | 30    | 24 | 3 | 1 | 2 |         |         |

- Molecule 18 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $\text{C}_2\text{H}_6\text{OS}$ ).



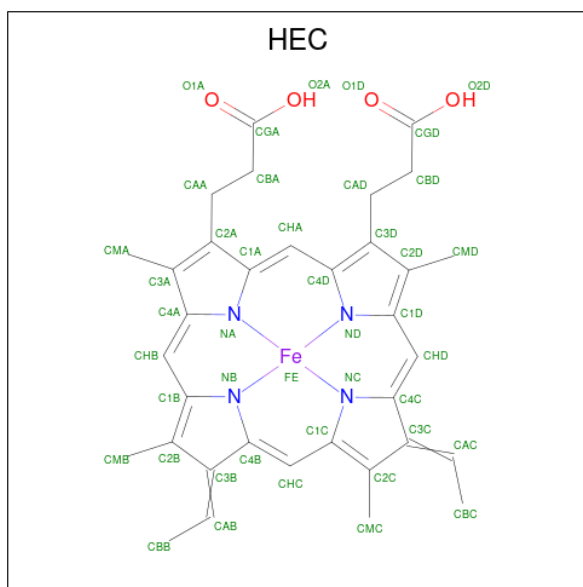
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 18  | C     | 1        | Total | C | O | S | 0       | 0       |
|     |       |          | 4     | 2 | 1 | 1 |         |         |

- Molecule 19 is PHOSPHATE ION (three-letter code: PO4) (formula:  $\text{O}_4\text{P}$ ).



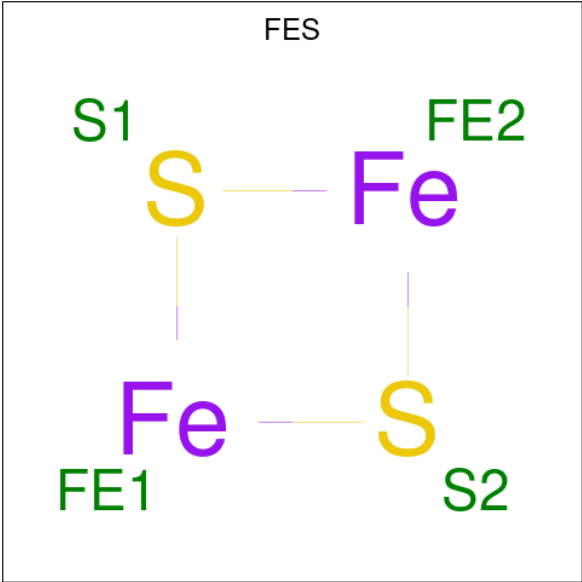
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 19  | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | D     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | E     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | F     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 19  | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 20 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



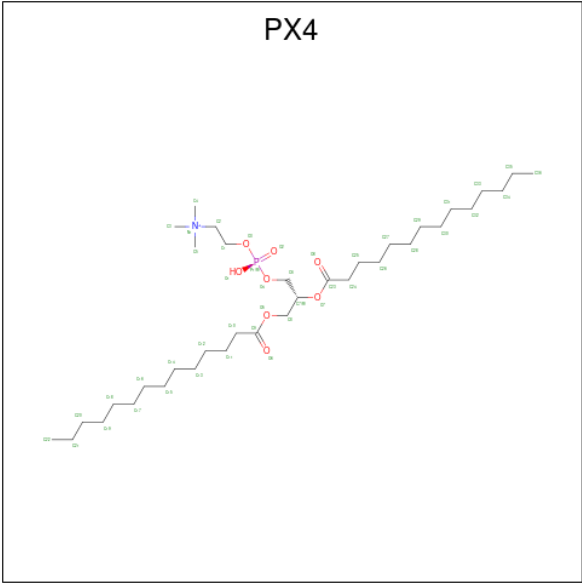
| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 20  | D     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 21  | E     | 1        | Total | Fe | S | 0       | 0       |
|     |       |          | 4     | 2  | 2 |         |         |

- Molecule 22 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C<sub>36</sub>H<sub>73</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 22  | E     | 1        | Total | C  | N | O | P | 0       | 0       |
|     |       |          | 37    | 27 | 1 | 8 | 1 |         |         |

- Molecule 23 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 23  | A     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 23  | B     | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 23  | C     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 23  | D     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 23  | E     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 23  | F     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 23  | G     | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 23  | J     | 1        | Total<br>1  | O<br>1  | 0       | 0       |

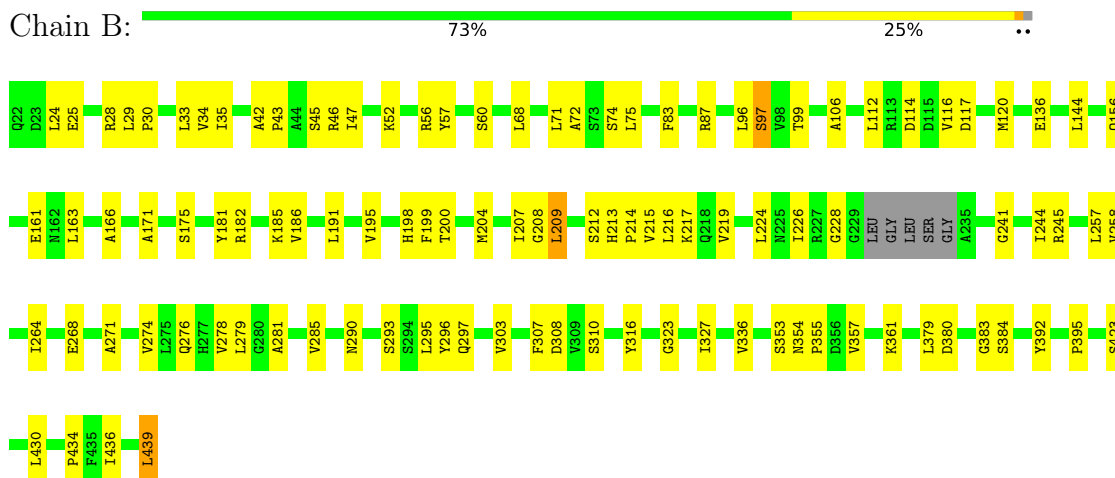
### 3 Residue-property plots

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

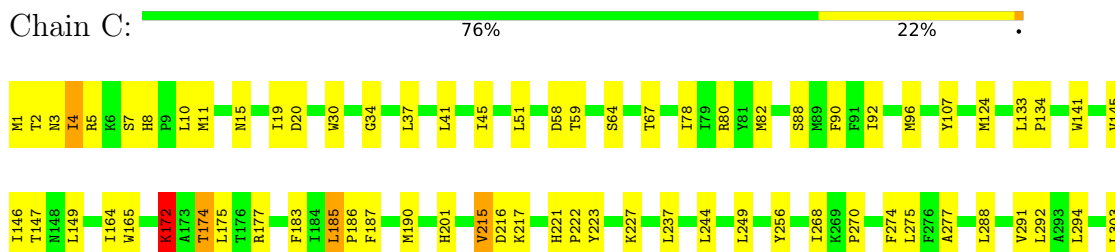
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 3: Cytochrome b





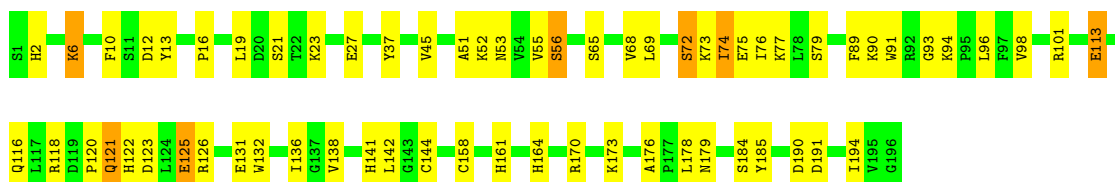
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 79% 20% .



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 67% 29% .



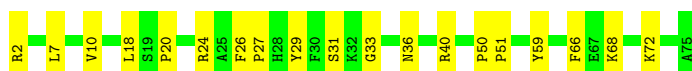
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F: 82% 17% .



- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain G: 74% 26% .



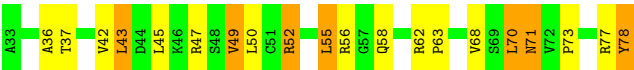
- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain H: 68% 31% .

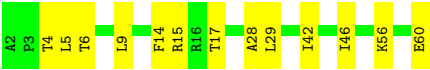
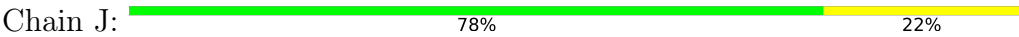


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I: 57% 28% 15% .



- Molecule 10: Cytochrome b-c1 complex subunit 9





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 65 2 2  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 209.59Å 209.59Å 342.43Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)  | 49.86 – 3.20<br>49.81 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.1 (49.86-3.20)<br>95.1 (49.81-3.20)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.62 (at 3.19Å)   | Xtrriage         |
| Refinement program  | REFMAC 5.8.0267   | Depositor        |
| R, $R_{free}$   | 0.205 , 0.256<br>0.207 , 0.258                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3441 reflections (4.92%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 85.7  | Xtrriage         |
| Anisotropy  | 0.158   | Xtrriage         |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | (Not available) , (Not available)                           | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtrriage         |
| Estimated twinning fraction   | No twinning to report.                                      | Xtrriage         |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 16382   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 87.0  | wwPDB-VP         |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PX4, PG4, FES, HEM, 6PE, LMT, DMS, I2Q, PEE, CDL, HEC, PO4

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     | 0.43         | 0/3522  | 0.89        | 0/4781  |
| 2   | B     | 0.41         | 0/3148  | 0.85        | 0/4270  |
| 3   | C     | 0.39         | 0/3100  | 0.78        | 0/4241  |
| 4   | D     | 0.40         | 0/1943  | 0.81        | 0/2642  |
| 5   | E     | 0.42         | 0/1553  | 0.84        | 0/2100  |
| 6   | F     | 0.42         | 0/878   | 0.91        | 0/1181  |
| 7   | G     | 0.43         | 0/641   | 0.93        | 0/868   |
| 8   | H     | 0.38         | 0/530   | 0.83        | 0/714   |
| 9   | I     | 0.46         | 0/342   | 1.11        | 0/464   |
| 10  | J     | 0.39         | 0/500   | 0.81        | 0/675   |
| All | All   | 0.41         | 0/16157 | 0.85        | 0/21936 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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     | 3449  | 0        | 3346     | 81      | 0            |
| 2   | B     | 3093  | 0        | 3064     | 75      | 0            |
| 3   | C     | 3004  | 0        | 3070     | 67      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | D     | 1884  | 0        | 1814     | 56      | 0            |
| 5   | E     | 1519  | 0        | 1503     | 45      | 0            |
| 6   | F     | 859   | 0        | 836      | 14      | 0            |
| 7   | G     | 620   | 0        | 624      | 17      | 0            |
| 8   | H     | 525   | 0        | 500      | 23      | 0            |
| 9   | I     | 338   | 0        | 356      | 25      | 0            |
| 10  | J     | 487   | 0        | 487      | 8       | 0            |
| 11  | A     | 13    | 0        | 18       | 0       | 0            |
| 11  | C     | 26    | 0        | 36       | 1       | 0            |
| 12  | A     | 23    | 0        | 19       | 4       | 0            |
| 13  | A     | 34    | 0        | 24       | 3       | 0            |
| 13  | D     | 54    | 0        | 52       | 1       | 0            |
| 13  | G     | 44    | 0        | 32       | 1       | 0            |
| 14  | C     | 86    | 0        | 60       | 12      | 0            |
| 15  | C     | 35    | 0        | 46       | 2       | 0            |
| 16  | C     | 40    | 0        | 54       | 1       | 0            |
| 16  | E     | 41    | 0        | 59       | 3       | 0            |
| 17  | C     | 30    | 0        | 0        | 1       | 0            |
| 18  | C     | 4     | 0        | 6        | 0       | 0            |
| 19  | C     | 10    | 0        | 0        | 0       | 0            |
| 19  | D     | 5     | 0        | 0        | 0       | 0            |
| 19  | E     | 5     | 0        | 0        | 0       | 0            |
| 19  | F     | 10    | 0        | 0        | 0       | 0            |
| 19  | G     | 15    | 0        | 0        | 0       | 0            |
| 20  | D     | 43    | 0        | 32       | 15      | 0            |
| 21  | E     | 4     | 0        | 0        | 0       | 0            |
| 22  | E     | 37    | 0        | 51       | 4       | 0            |
| 23  | A     | 10    | 0        | 0        | 0       | 0            |
| 23  | B     | 9     | 0        | 0        | 0       | 0            |
| 23  | C     | 10    | 0        | 0        | 0       | 0            |
| 23  | D     | 4     | 0        | 0        | 0       | 0            |
| 23  | E     | 4     | 0        | 0        | 1       | 0            |
| 23  | F     | 5     | 0        | 0        | 0       | 0            |
| 23  | G     | 2     | 0        | 0        | 0       | 0            |
| 23  | J     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 16382 | 0        | 16089    | 369     | 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 11.

The worst 5 of 369 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:C:402:HEM:HBC2 | 14:C:402:HEM:HMC2 | 1.41                     | 1.00              |
| 7:G:50:PRO:HB2    | 7:G:51:PRO:HD3    | 1.47                     | 0.97              |
| 5:E:16:PRO:HA     | 5:E:19:LEU:HD12   | 1.51                     | 0.93              |
| 1:A:86:LEU:HB3    | 2:B:285:VAL:HG22  | 1.54                     | 0.89              |
| 1:A:4:TYR:HB3     | 2:B:114:ASP:OD2   | 1.75                     | 0.87              |

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     | 443/445 (100%)  | 417 (94%)  | 25 (6%) | 1 (0%)   | 47          | 79  |
| 2   | B     | 409/418 (98%)   | 395 (97%)  | 14 (3%) | 0        | 100         | 100 |
| 3   | C     | 377/379 (100%)  | 354 (94%)  | 22 (6%) | 1 (0%)   | 41          | 74  |
| 4   | D     | 237/239 (99%)   | 224 (94%)  | 10 (4%) | 3 (1%)   | 12          | 47  |
| 5   | E     | 194/196 (99%)   | 187 (96%)  | 5 (3%)  | 2 (1%)   | 15          | 54  |
| 6   | F     | 97/99 (98%)     | 95 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 7   | G     | 72/74 (97%)     | 69 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 8   | H     | 63/65 (97%)     | 56 (89%)   | 7 (11%) | 0        | 100         | 100 |
| 9   | I     | 44/46 (96%)     | 42 (96%)   | 2 (4%)  | 0        | 100         | 100 |
| 10  | J     | 57/59 (97%)     | 54 (95%)   | 3 (5%)  | 0        | 100         | 100 |
| All | All   | 1993/2020 (99%) | 1893 (95%) | 93 (5%) | 7 (0%)   | 34          | 69  |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 227 | THR  |
| 5   | E     | 120 | PRO  |
| 3   | C     | 172 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 121 | GLN  |
| 4   | D     | 162 | PRO  |

### 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     | 369/370 (100%)  | 356 (96%)  | 13 (4%)  | 36          | 69 |
| 2   | B     | 322/327 (98%)   | 311 (97%)  | 11 (3%)  | 37          | 70 |
| 3   | C     | 326/327 (100%)  | 311 (95%)  | 15 (5%)  | 27          | 63 |
| 4   | D     | 200/204 (98%)   | 192 (96%)  | 8 (4%)   | 31          | 66 |
| 5   | E     | 168/168 (100%)  | 153 (91%)  | 15 (9%)  | 9           | 35 |
| 6   | F     | 88/91 (97%)     | 82 (93%)   | 6 (7%)   | 16          | 49 |
| 7   | G     | 65/66 (98%)     | 62 (95%)   | 3 (5%)   | 27          | 63 |
| 8   | H     | 61/62 (98%)     | 59 (97%)   | 2 (3%)   | 38          | 71 |
| 9   | I     | 38/38 (100%)    | 28 (74%)   | 10 (26%) | 0           | 2  |
| 10  | J     | 49/49 (100%)    | 47 (96%)   | 2 (4%)   | 30          | 66 |
| All | All   | 1686/1702 (99%) | 1601 (95%) | 85 (5%)  | 24          | 60 |

5 of 85 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 118 | ARG  |
| 8   | H     | 29  | LYS  |
| 5   | E     | 170 | ARG  |
| 6   | F     | 17  | ARG  |
| 9   | I     | 47  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | E     | 161 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 49  | GLN  |
| 8   | H     | 23  | GLN  |
| 1   | A     | 311 | ASN  |
| 4   | D     | 225 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 11  | PG4  | A     | 501 | -    | 12,12,12     | 0.24 | 0           | 11,11,11    | 0.16 | 0           |
| 13  | CDL  | A     | 503 | -    | 33,33,99     | 0.51 | 0           | 37,43,111   | 0.86 | 0           |
| 17  | I2Q  | C     | 407 | -    | 33,33,33     | 0.78 | 1 (3%)      | 46,48,48    | 0.70 | 0           |
| 16  | PEE  | E     | 204 | -    | 40,40,50     | 0.79 | 1 (2%)      | 43,45,55    | 0.88 | 1 (2%)      |
| 13  | CDL  | G     | 101 | -    | 43,43,99     | 0.66 | 1 (2%)      | 49,55,111   | 1.03 | 6 (12%)     |
| 19  | PO4  | F     | 501 | -    | 4,4,4        | 1.21 | 1 (25%)     | 6,6,6       | 0.49 | 0           |
| 19  | PO4  | G     | 103 | -    | 4,4,4        | 0.93 | 0           | 6,6,6       | 0.45 | 0           |
| 20  | HEC  | D     | 501 | 4    | 32,50,50     | 2.38 | 10 (31%)    | 24,82,82    | 2.26 | 6 (25%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | PO4  | G     | 104 | -    | 4,4,4        | 1.35 | 1 (25%)  | 6,6,6       | 0.52 | 0        |
| 19  | PO4  | D     | 502 | -    | 4,4,4        | 0.69 | 0        | 6,6,6       | 0.54 | 0        |
| 19  | PO4  | F     | 502 | -    | 4,4,4        | 0.65 | 0        | 6,6,6       | 0.46 | 0        |
| 19  | PO4  | G     | 102 | -    | 4,4,4        | 1.11 | 0        | 6,6,6       | 0.38 | 0        |
| 15  | LMT  | C     | 403 | -    | 36,36,36     | 0.88 | 1 (2%)   | 47,47,47    | 1.65 | 13 (27%) |
| 19  | PO4  | C     | 409 | -    | 4,4,4        | 0.50 | 0        | 6,6,6       | 0.65 | 0        |
| 19  | PO4  | E     | 203 | -    | 4,4,4        | 0.91 | 0        | 6,6,6       | 0.39 | 0        |
| 19  | PO4  | C     | 410 | -    | 4,4,4        | 0.87 | 0        | 6,6,6       | 0.35 | 0        |
| 11  | PG4  | C     | 404 | -    | 12,12,12     | 0.42 | 0        | 11,11,11    | 0.37 | 0        |
| 14  | HEM  | C     | 402 | 3    | 41,50,50     | 1.44 | 5 (12%)  | 45,82,82    | 1.88 | 10 (22%) |
| 13  | CDL  | D     | 503 | -    | 53,53,99     | 0.62 | 1 (1%)   | 59,65,111   | 0.82 | 1 (1%)   |
| 11  | PG4  | C     | 405 | -    | 12,12,12     | 0.30 | 0        | 11,11,11    | 0.30 | 0        |
| 16  | PEE  | C     | 406 | -    | 39,39,50     | 0.80 | 1 (2%)   | 42,44,55    | 0.73 | 0        |
| 18  | DMS  | C     | 408 | -    | 3,3,3        | 0.35 | 0        | 3,3,3       | 0.26 | 0        |
| 22  | PX4  | E     | 202 | -    | 36,36,45     | 0.62 | 0        | 42,44,53    | 0.92 | 2 (4%)   |
| 12  | 6PE  | A     | 502 | -    | 22,22,26     | 0.50 | 0        | 25,27,31    | 0.89 | 1 (4%)   |
| 21  | FES  | E     | 201 | 5    | 0,4,4        | -    | -        | -           | -    | -        |
| 14  | HEM  | C     | 401 | 3    | 41,50,50     | 1.53 | 7 (17%)  | 45,82,82    | 2.09 | 16 (35%) |

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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 15  | LMT  | C     | 403 | -    | -       | 14/21/61/61  | 0/2/2/2 |
| 20  | HEC  | D     | 501 | 4    | -       | 0/10/54/54   | -       |
| 22  | PX4  | E     | 202 | -    | -       | 17/40/40/49  | -       |
| 14  | HEM  | C     | 402 | 3    | -       | 3/12/54/54   | -       |
| 11  | PG4  | A     | 501 | -    | -       | 7/10/10/10   | -       |
| 13  | CDL  | A     | 503 | -    | -       | 15/41/41/110 | -       |
| 17  | I2Q  | C     | 407 | -    | -       | 2/13/13/13   | 0/4/4/4 |
| 12  | 6PE  | A     | 502 | -    | -       | 12/26/26/30  | -       |
| 16  | PEE  | E     | 204 | -    | 1/1/4/8 | 26/44/44/54  | -       |
| 11  | PG4  | C     | 404 | -    | -       | 8/10/10/10   | -       |
| 13  | CDL  | G     | 101 | -    | -       | 17/52/52/110 | -       |
| 13  | CDL  | D     | 503 | -    | -       | 28/63/63/110 | -       |
| 21  | FES  | E     | 201 | 5    | -       | -            | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings |
|-----|------|-------|-----|------|---------|-------------|-------|
| 14  | HEM  | C     | 401 | 3    | -       | 4/12/54/54  | -     |
| 11  | PG4  | C     | 405 | -    | -       | 5/10/10/10  | -     |
| 16  | PEE  | C     | 406 | -    | 1/1/4/8 | 19/43/43/54 | -     |

The worst 5 of 30 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 20  | D     | 501 | HEC  | C2B-C3B | 6.53  | 1.47        | 1.40     |
| 20  | D     | 501 | HEC  | C3C-C2C | 6.32  | 1.47        | 1.40     |
| 20  | D     | 501 | HEC  | C3C-C4C | 4.47  | 1.51        | 1.43     |
| 14  | C     | 402 | HEM  | C1B-NB  | -4.24 | 1.33        | 1.40     |
| 16  | C     | 406 | PEE  | C18-C19 | 3.91  | 1.54        | 1.31     |

The worst 5 of 56 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 20  | D     | 501 | HEC  | C1D-C2D-C3D | -5.95 | 102.86      | 107.00   |
| 14  | C     | 401 | HEM  | CBA-CAA-C2A | -5.56 | 103.13      | 112.62   |
| 14  | C     | 402 | HEM  | CHC-C4B-NB  | 5.41  | 130.31      | 124.43   |
| 20  | D     | 501 | HEC  | CMB-C2B-C3B | 4.82  | 131.49      | 125.82   |
| 14  | C     | 402 | HEM  | CMD-C2D-C1D | 4.38  | 131.71      | 125.04   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 16  | C     | 406 | PEE  | C2   |
| 16  | E     | 204 | PEE  | C2   |

5 of 177 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 12  | A     | 502 | 6PE  | C1-O3-P1-O1   |
| 12  | A     | 502 | 6PE  | C1-O3-P1-O2   |
| 12  | A     | 502 | 6PE  | C1-O3-P1-O8   |
| 12  | A     | 502 | 6PE  | C11-C10-O6-C2 |
| 12  | A     | 502 | 6PE  | O8-C16-C17-N1 |

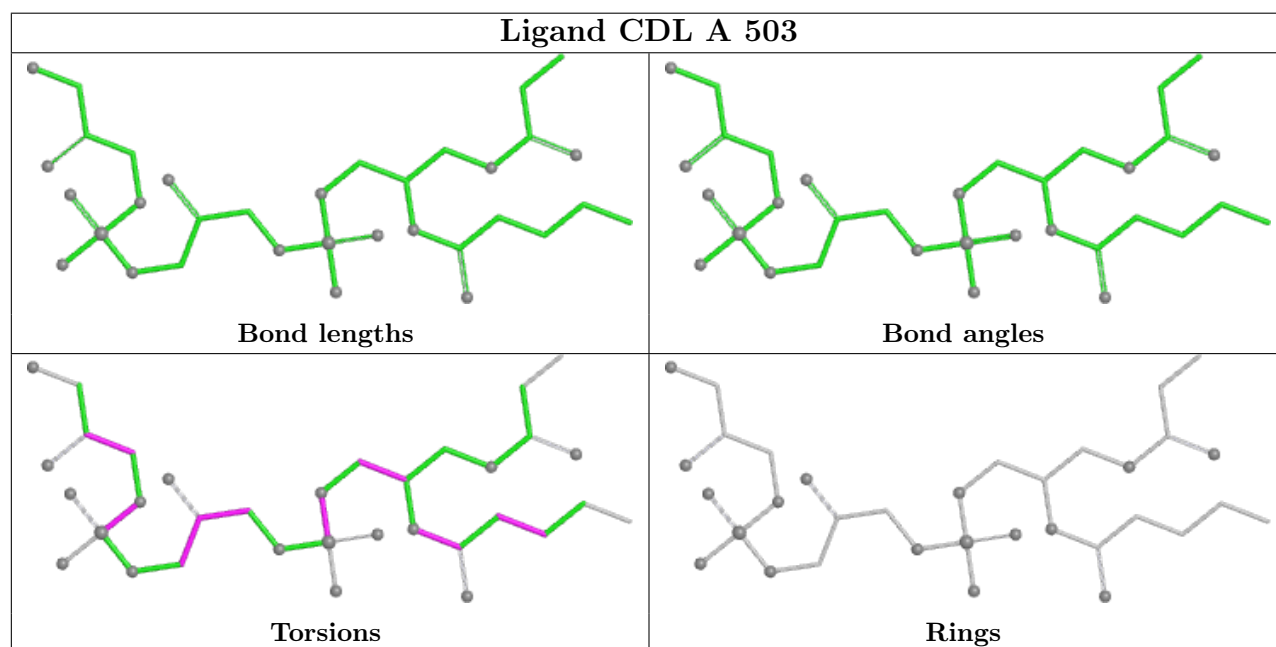
There are no ring outliers.

13 monomers are involved in 45 short contacts:

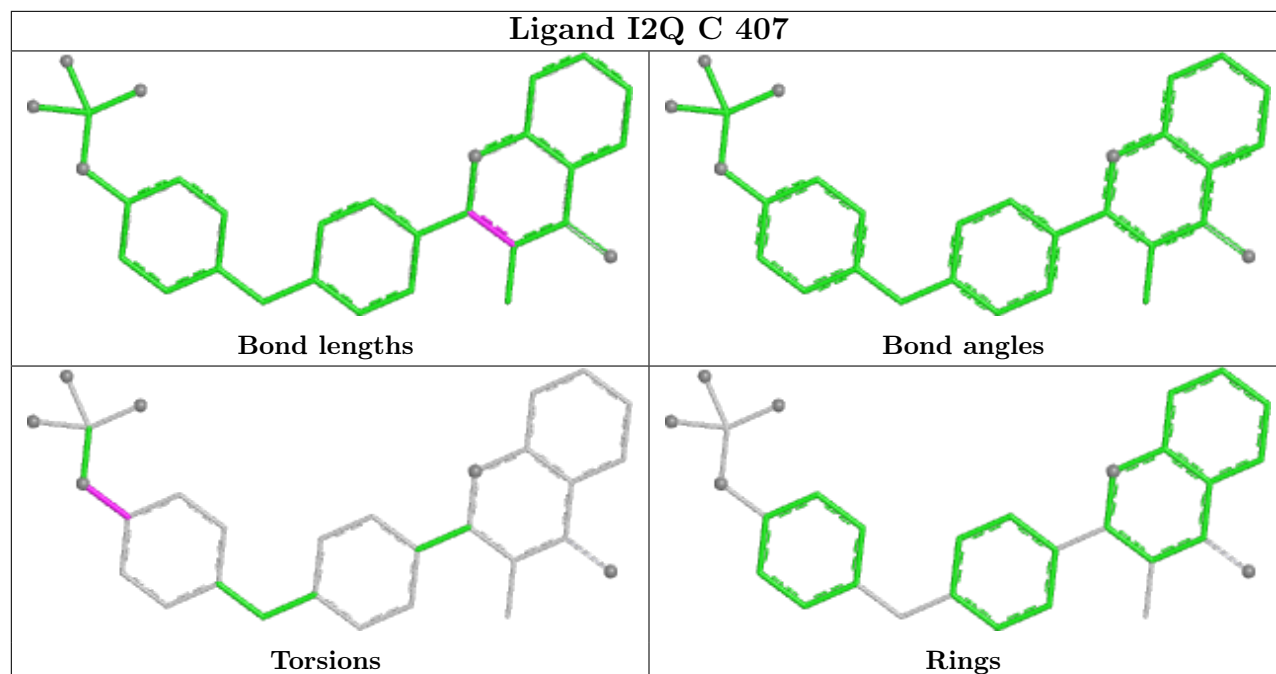


| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 13  | A     | 503 | CDL  | 3       | 0            |
| 17  | C     | 407 | I2Q  | 1       | 0            |
| 16  | E     | 204 | PEE  | 3       | 0            |
| 13  | G     | 101 | CDL  | 1       | 0            |
| 20  | D     | 501 | HEC  | 15      | 0            |
| 15  | C     | 403 | LMT  | 2       | 0            |
| 14  | C     | 402 | HEM  | 7       | 0            |
| 13  | D     | 503 | CDL  | 1       | 0            |
| 11  | C     | 405 | PG4  | 1       | 0            |
| 16  | C     | 406 | PEE  | 1       | 0            |
| 22  | E     | 202 | PX4  | 4       | 0            |
| 12  | A     | 502 | 6PE  | 4       | 0            |
| 14  | C     | 401 | HEM  | 5       | 0            |

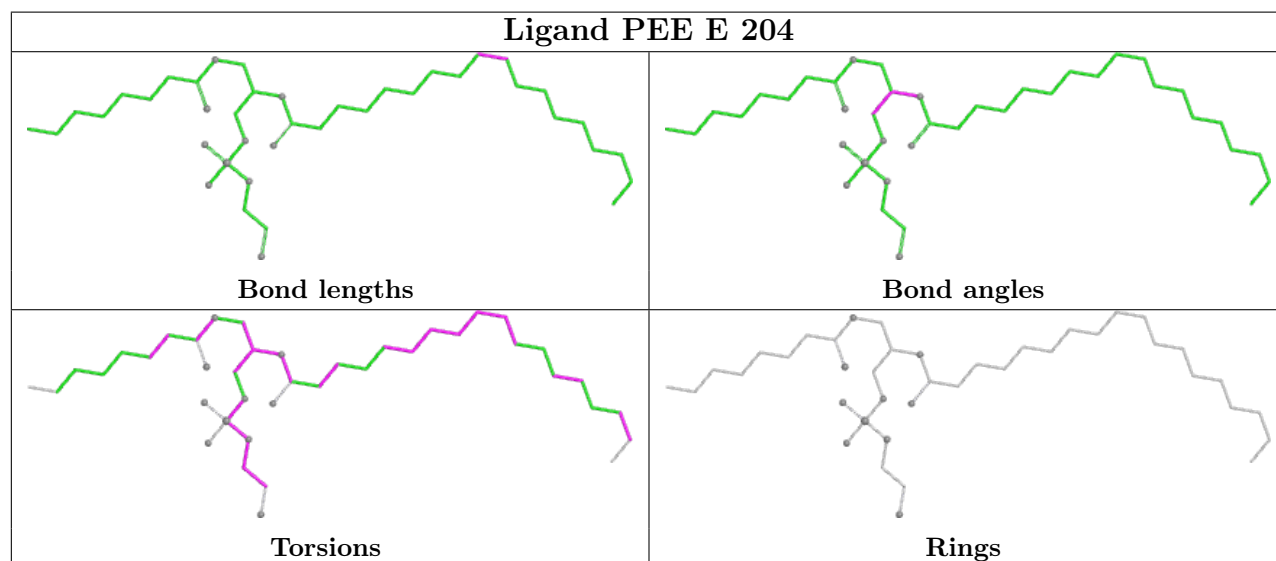
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



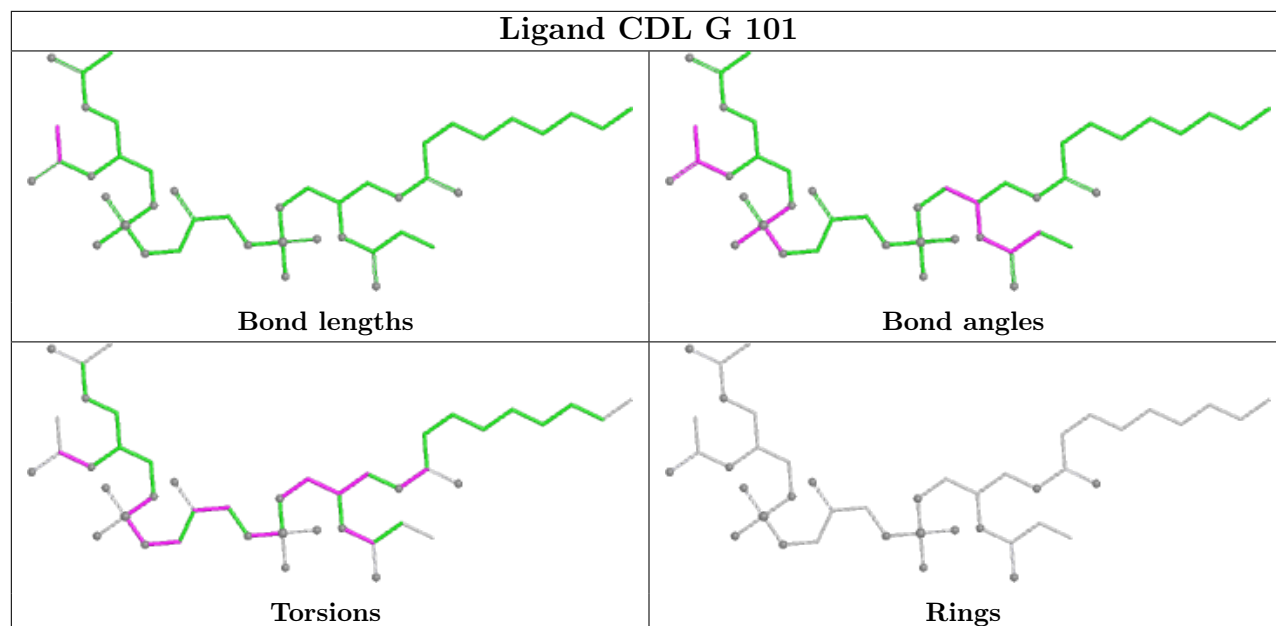
## Ligand I2Q C 407



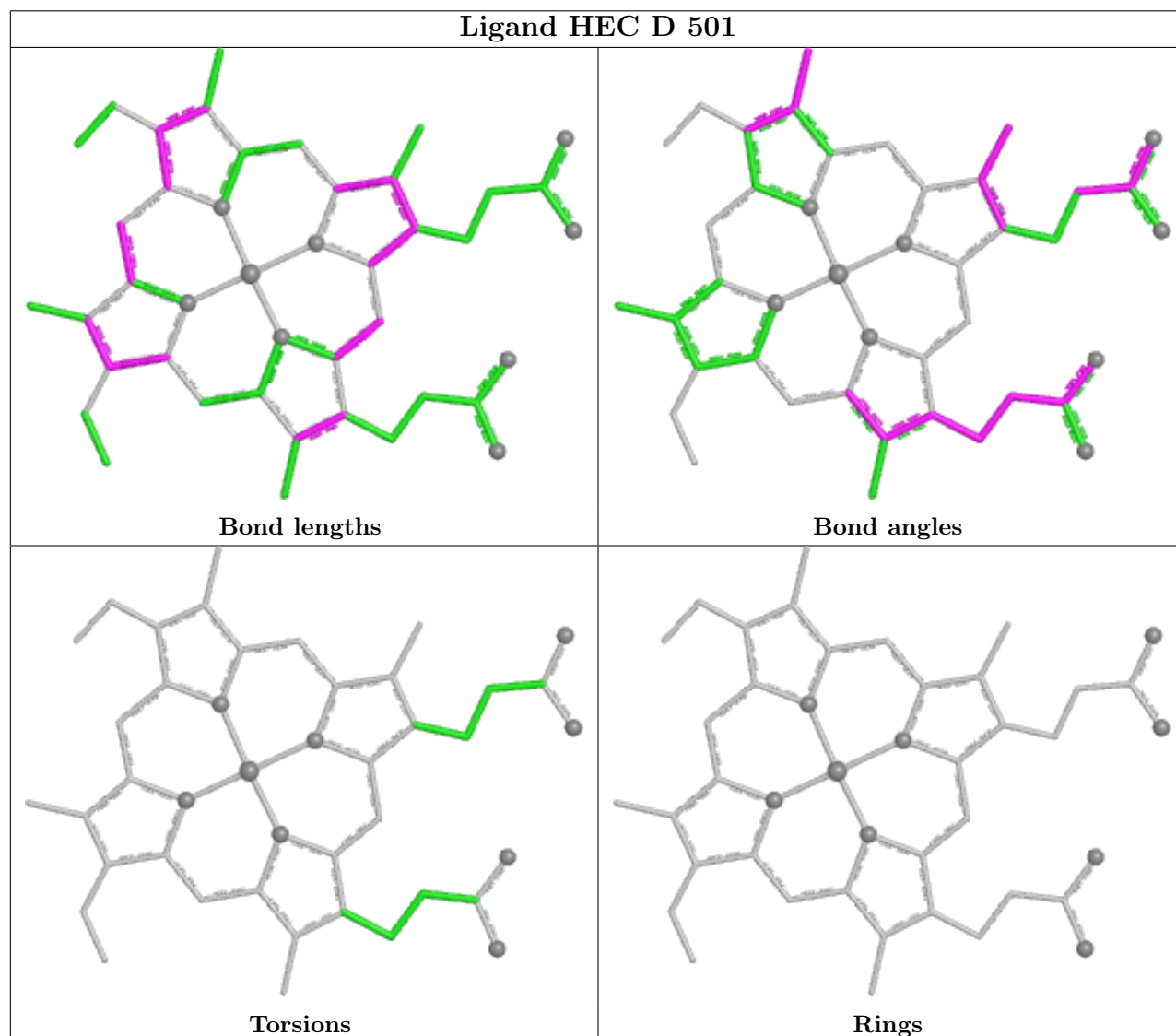
## Ligand PEE E 204

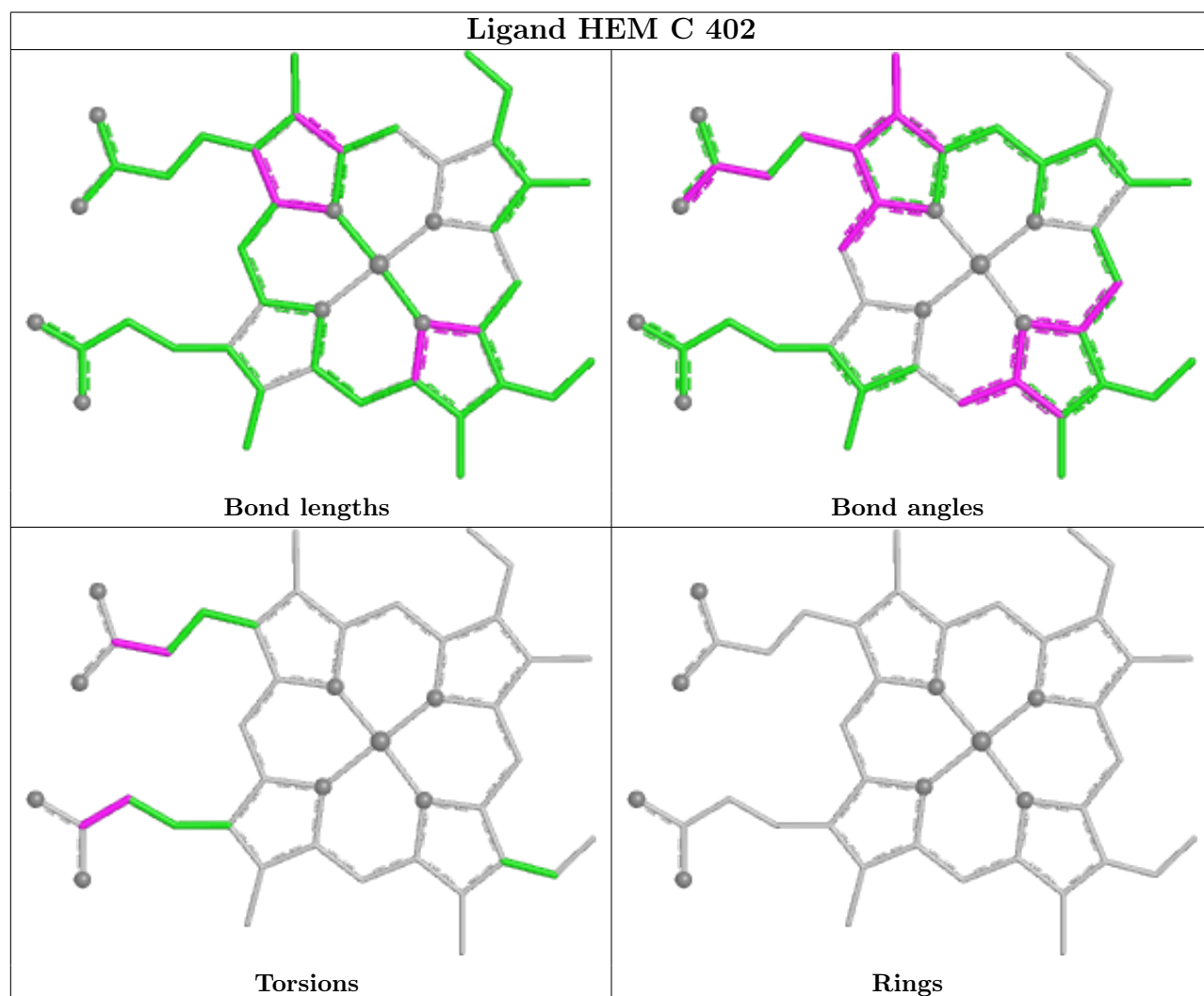
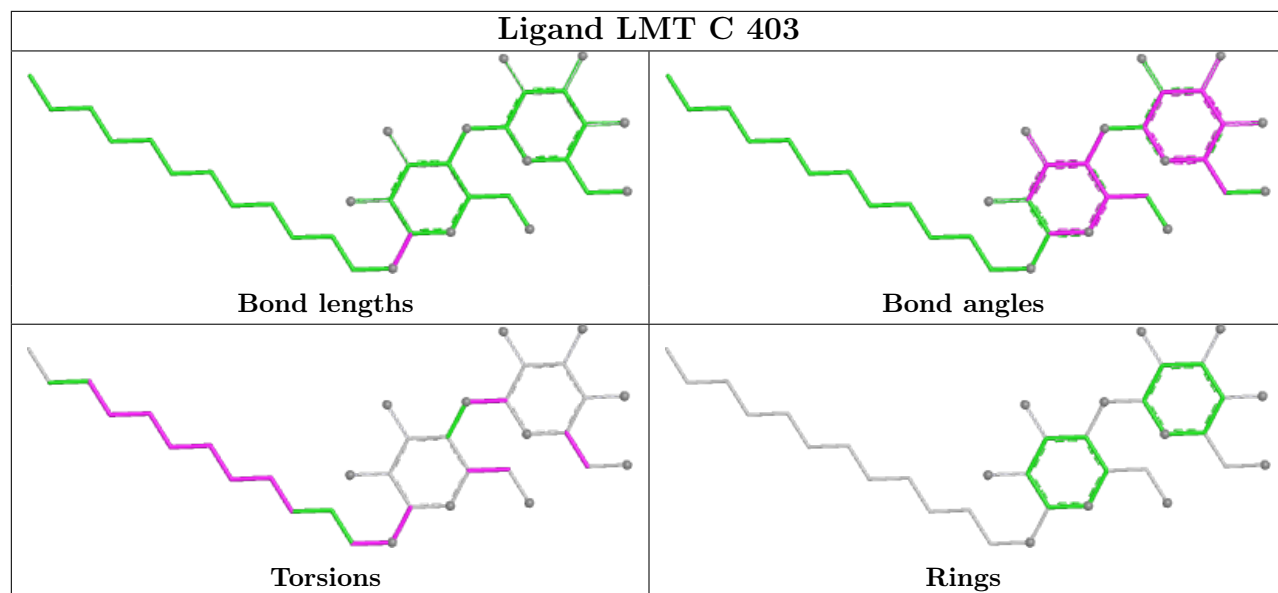


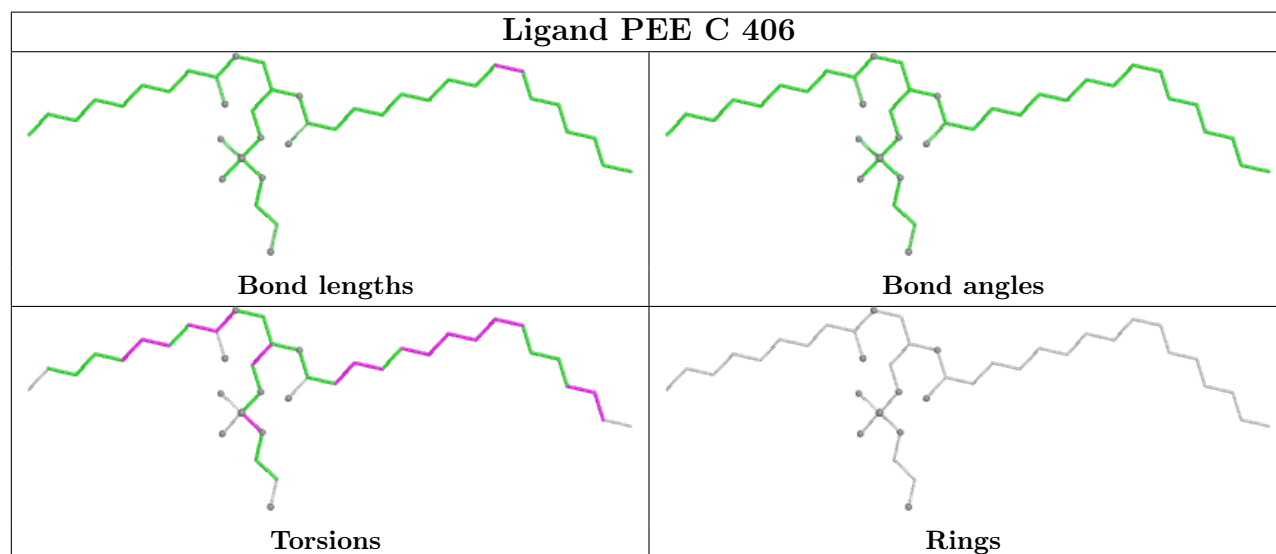
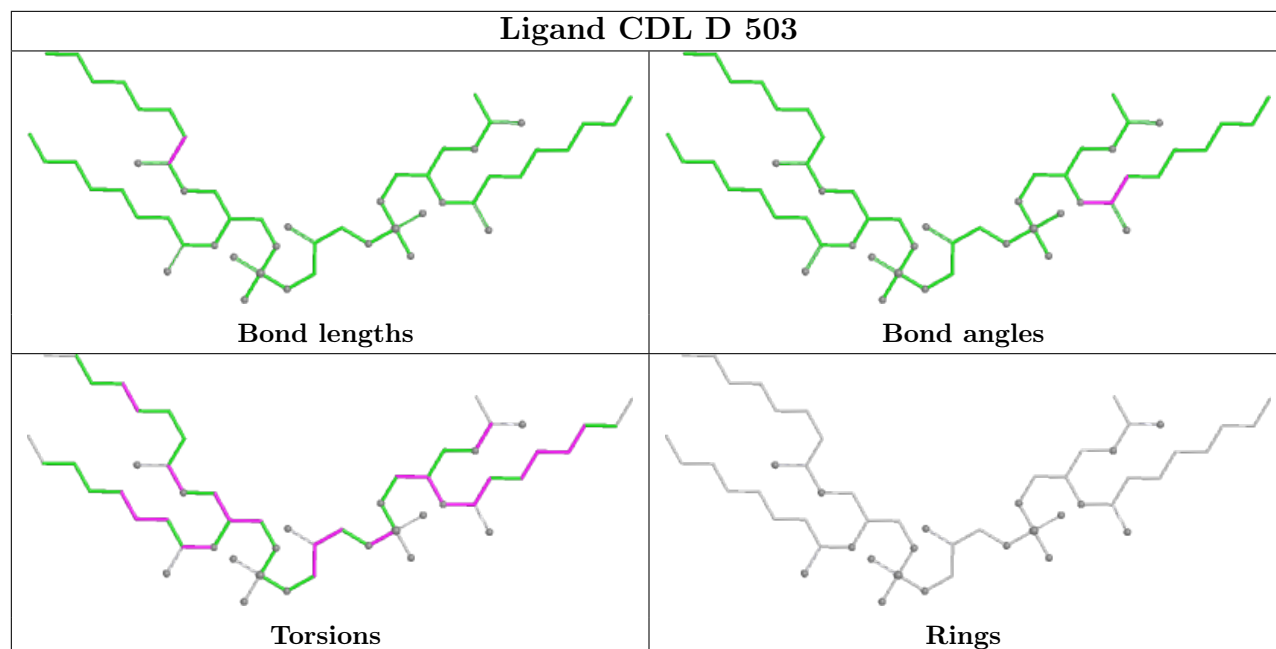
## Ligand CDL G 101



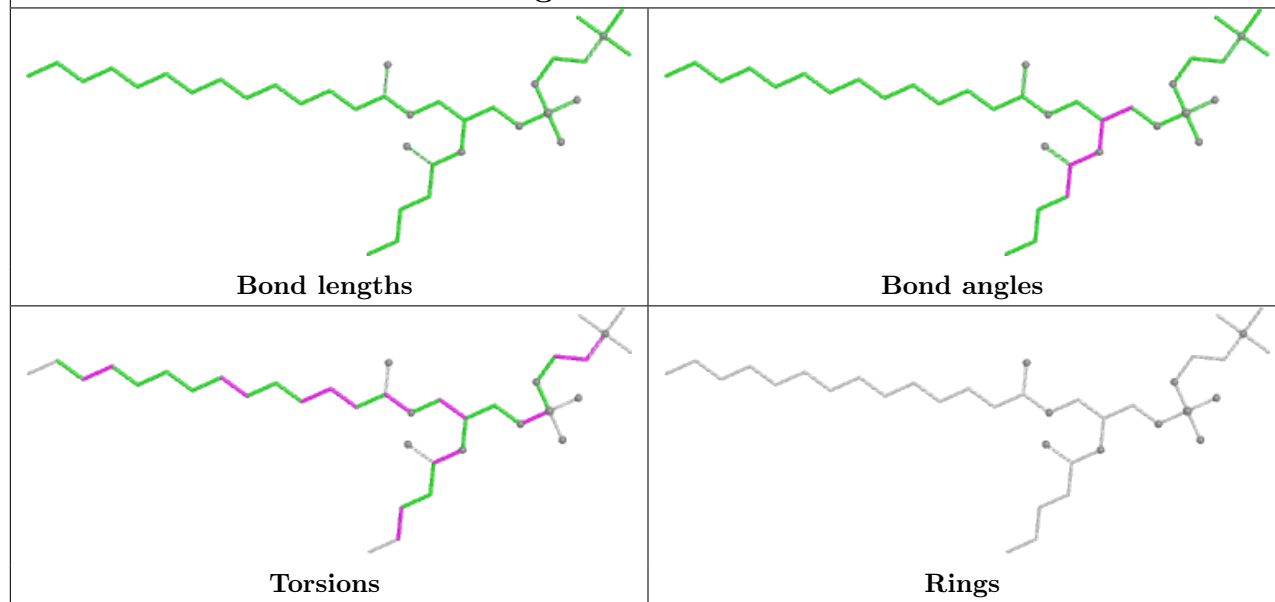
## Ligand HEC D 501



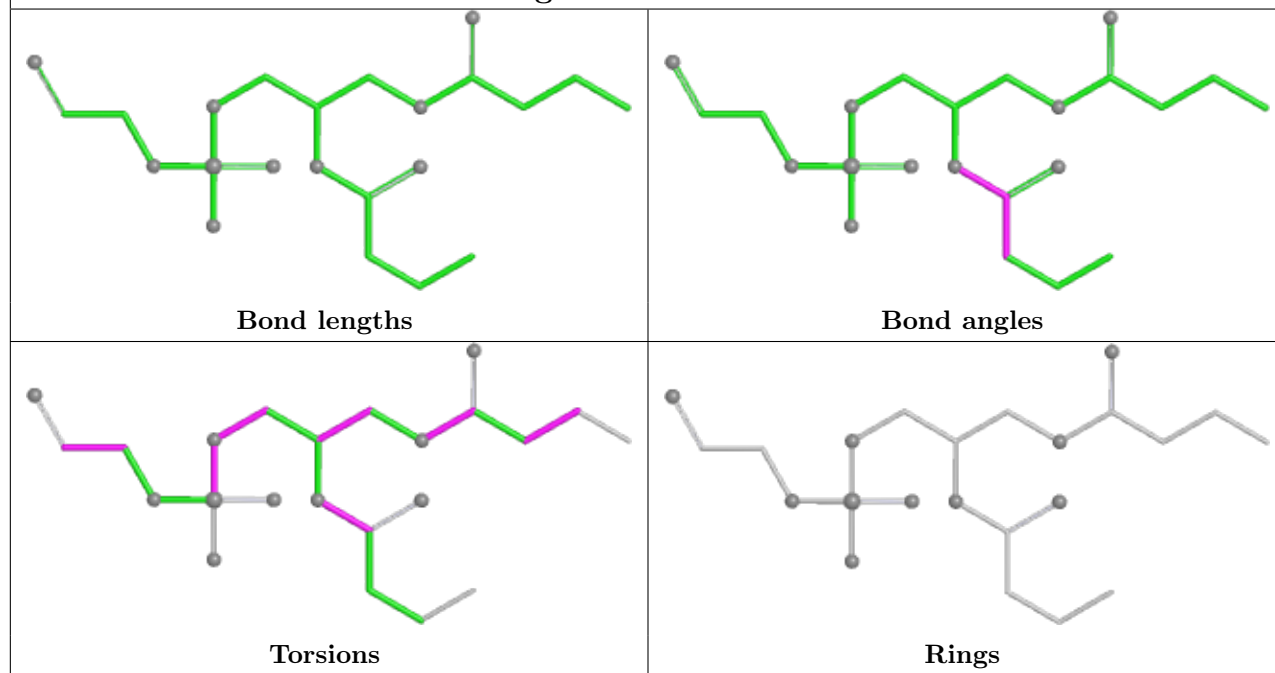


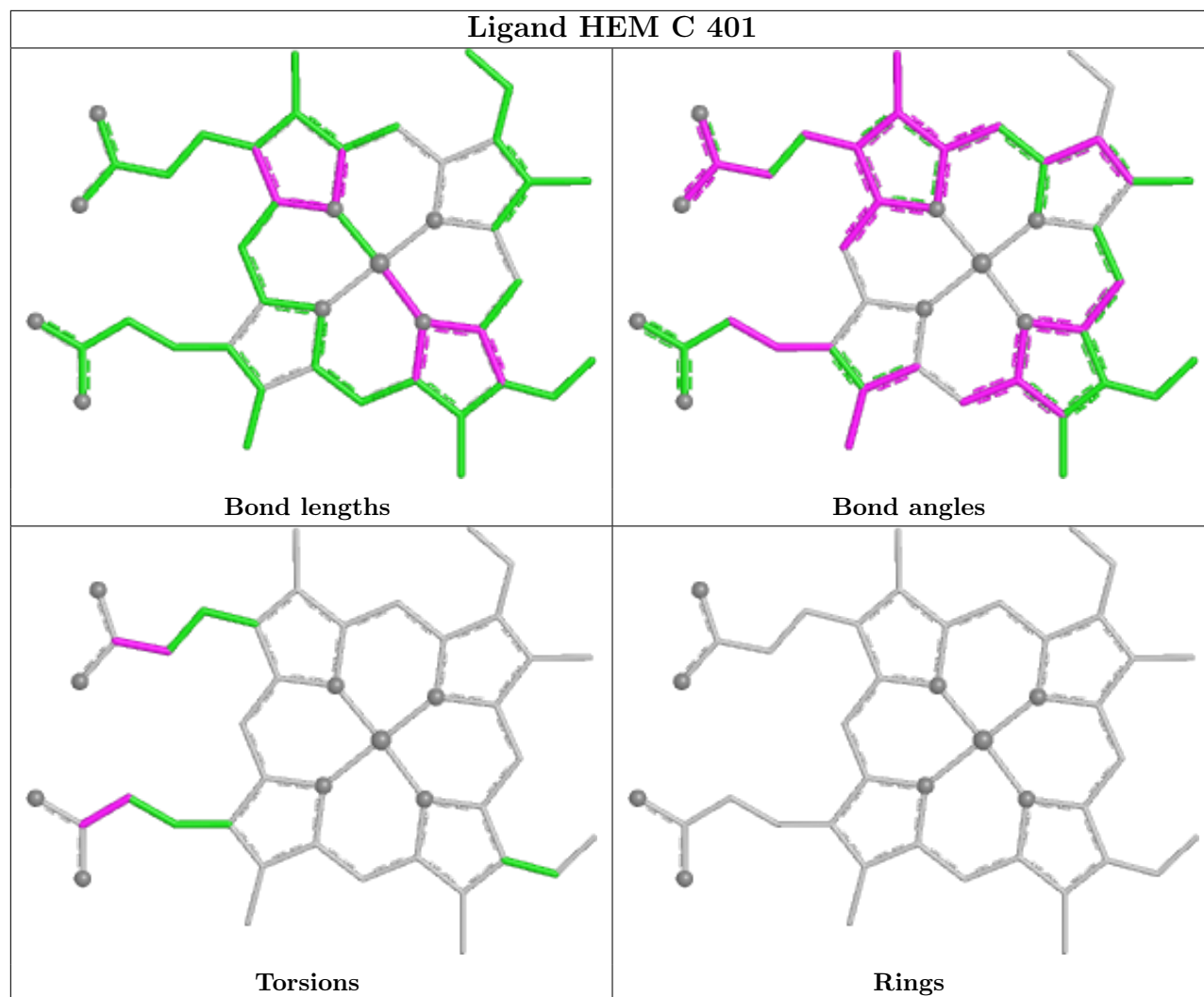


## Ligand PX4 E 202



## Ligand 6PE A 502





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

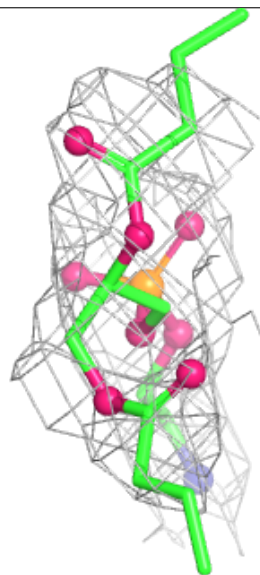
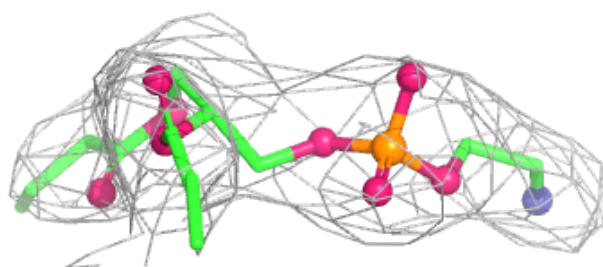
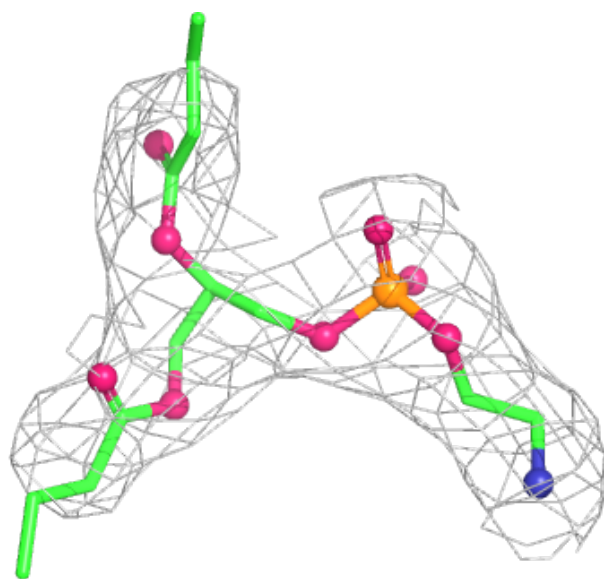
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



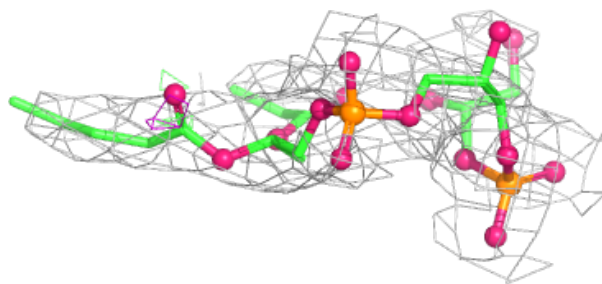
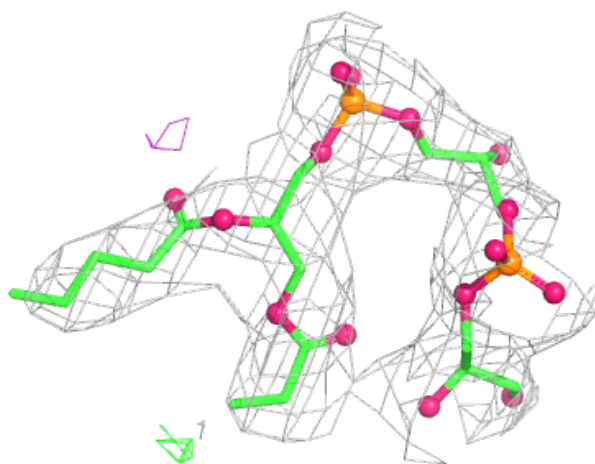
**Electron density around 6PE A 502:**

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



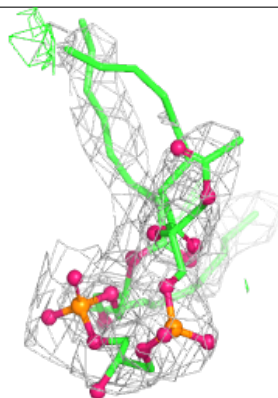
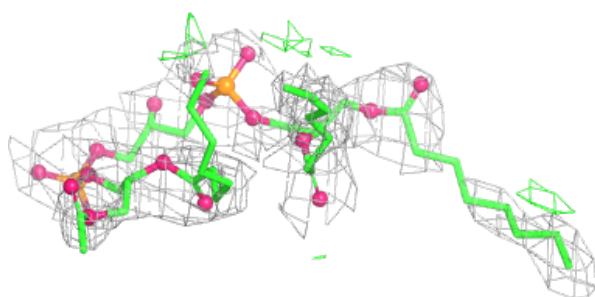
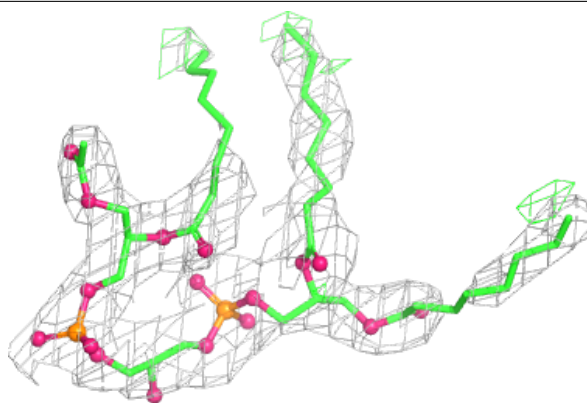
**Electron density around CDL A 503:**

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



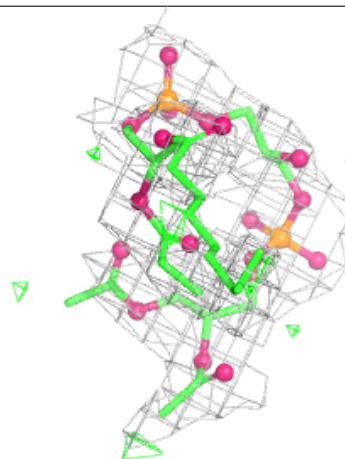
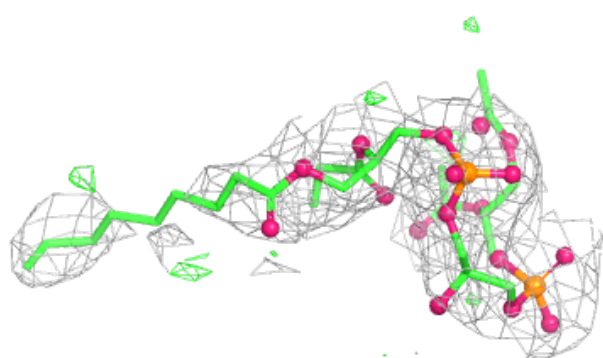
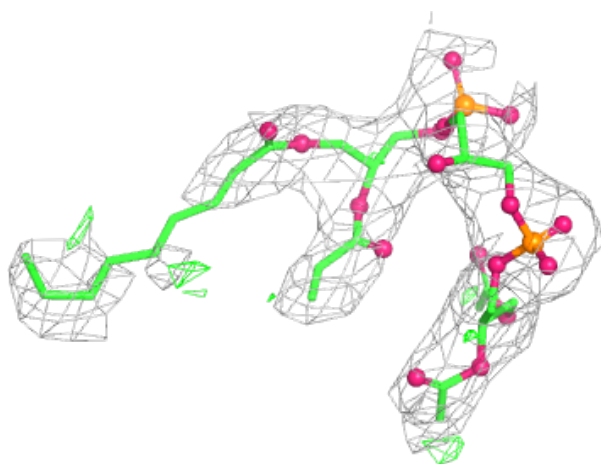
**Electron density around CDL D 503:**

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



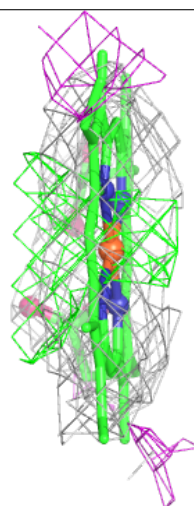
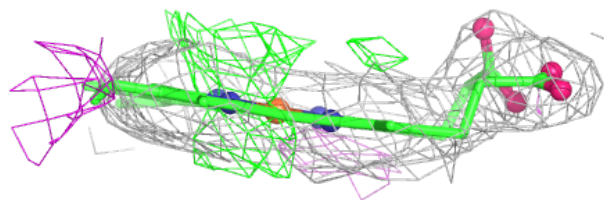
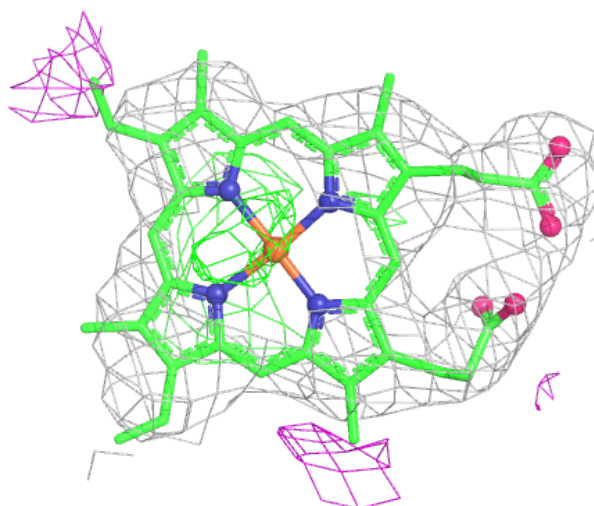
**Electron density around CDL G 101:**

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



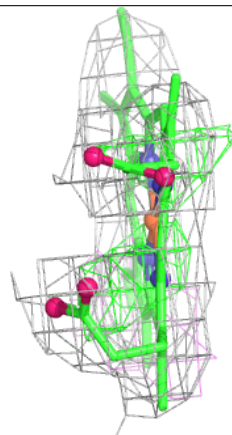
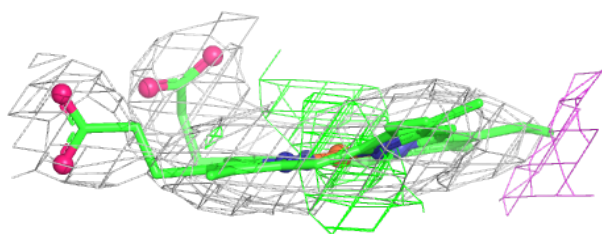
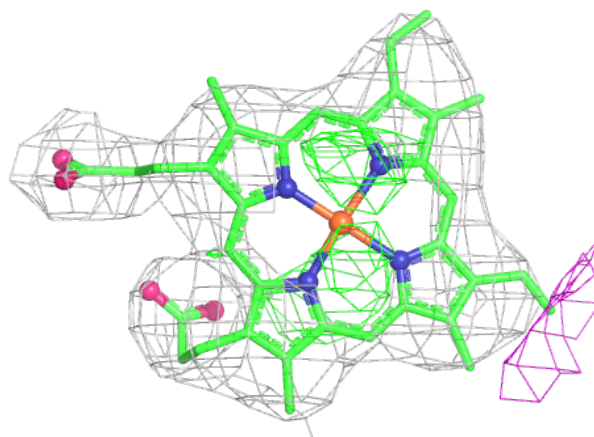
**Electron density around HEM C 401:**

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

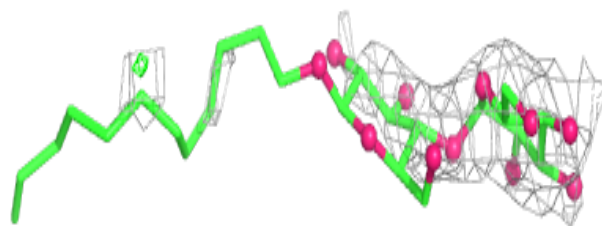
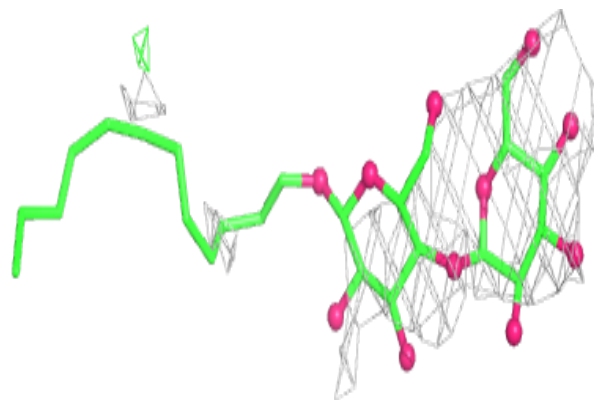


**Electron density around HEM C 402:**

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

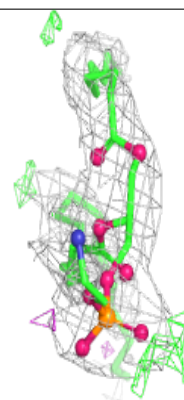
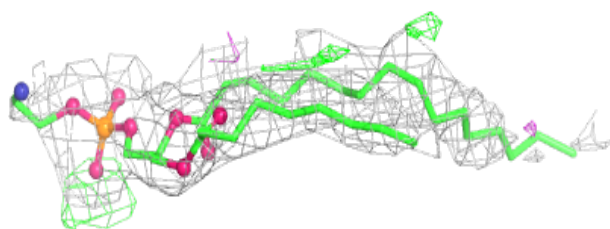
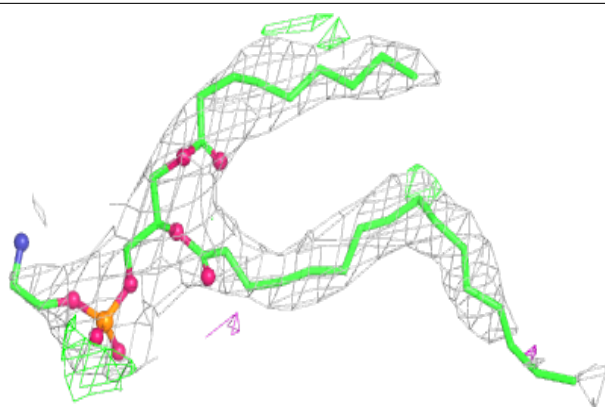
**Electron density around LMT C 403:**

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

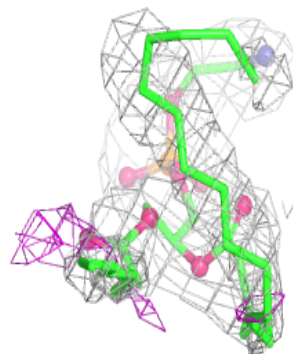
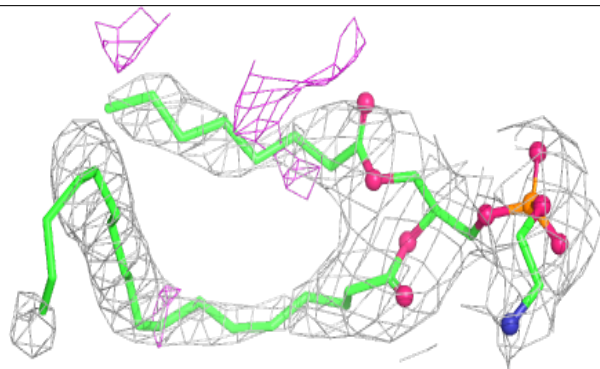
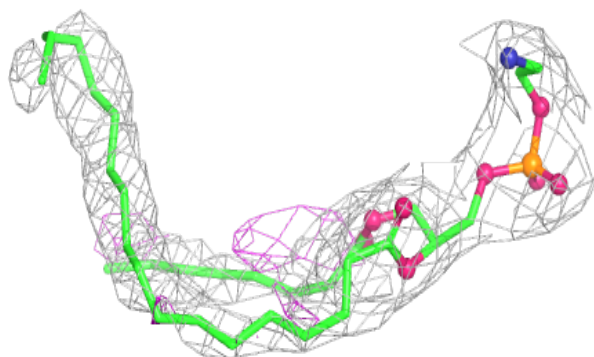


**Electron density around PEE C 406:**

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

**Electron density around PEE E 204:**

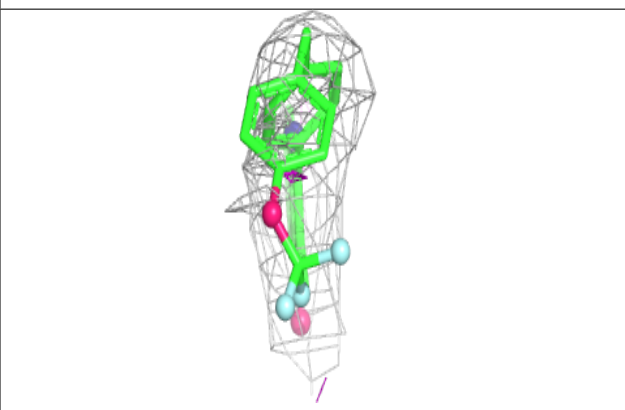
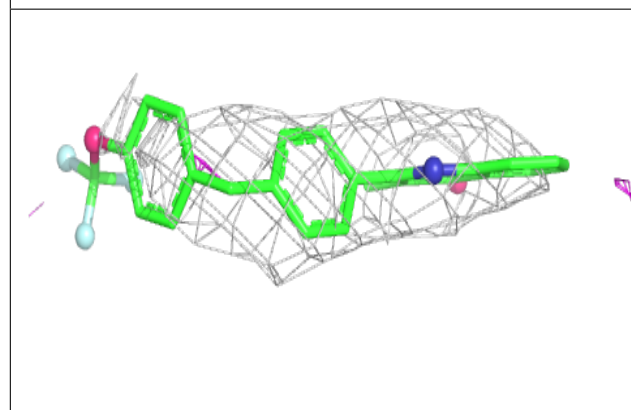
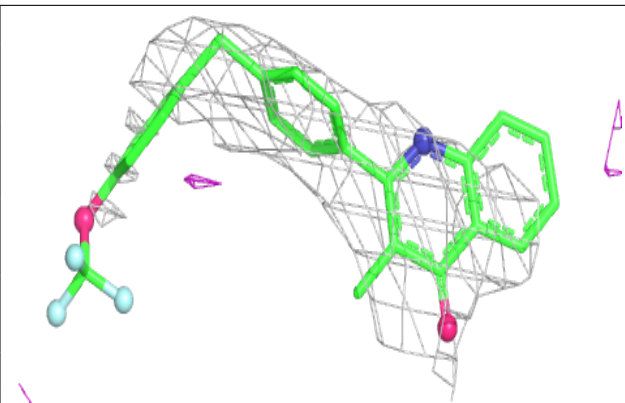
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around I2Q C 407:**

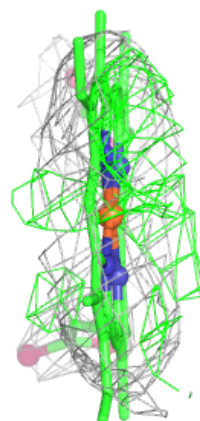
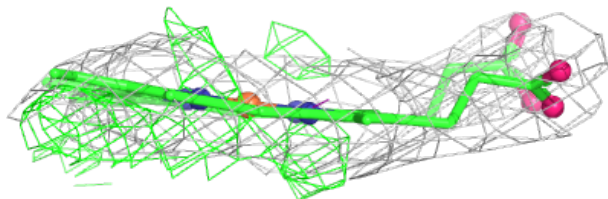
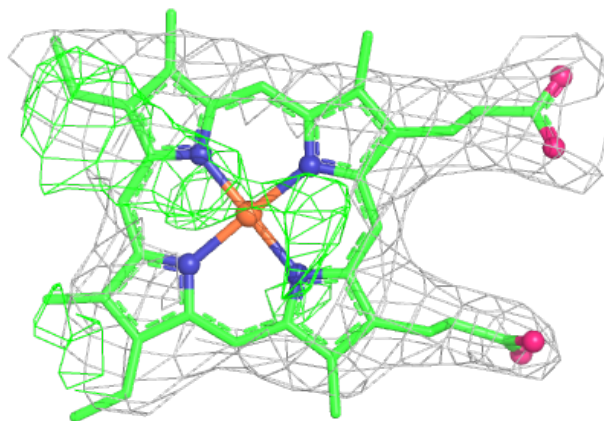
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

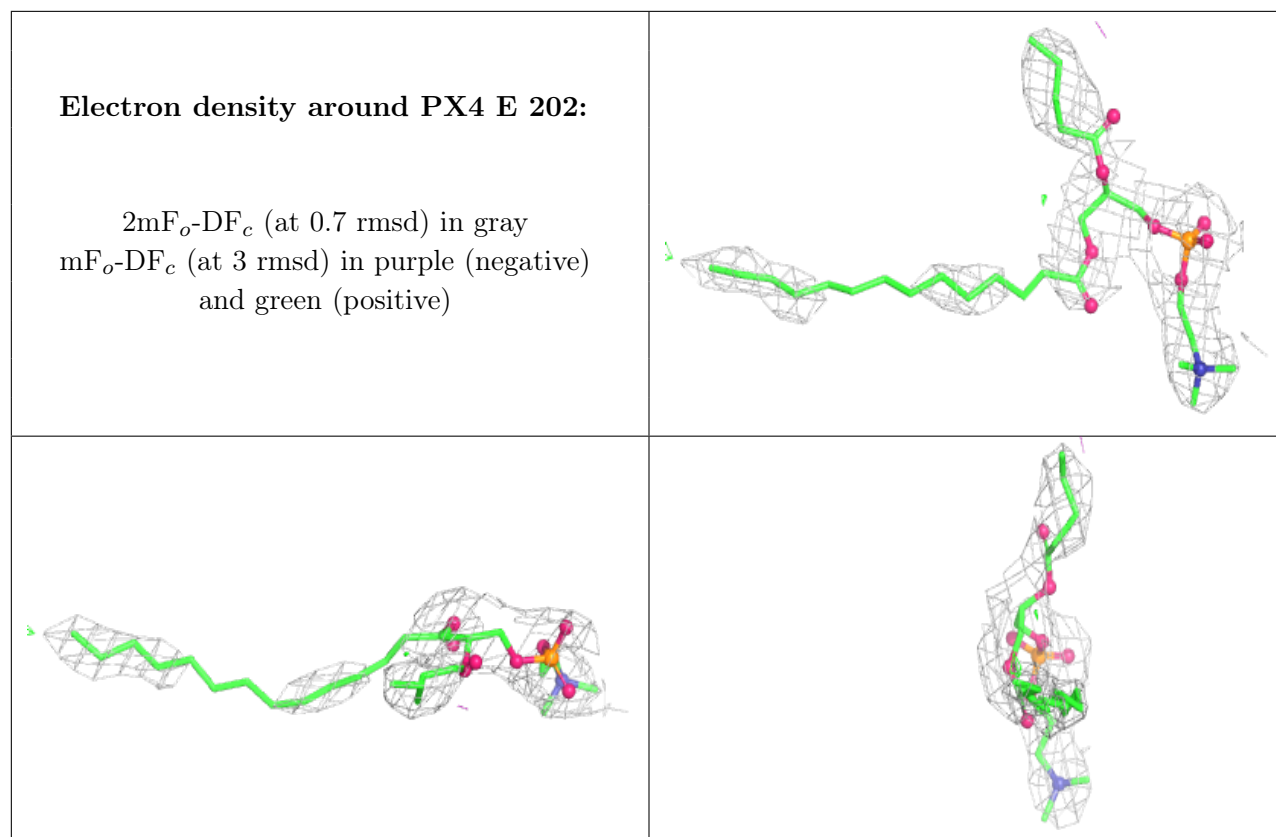




**Electron density around HEC D 501:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.