



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:32 AM UTC

PDB ID : 6QYC / pdb_00006qyc
Title : Crystal structure of MtrC from Shewanella baltica OS185
Authors : Clarke, T.A.; Edwards, M.J.
Deposited on : 2019-03-08
Resolution : 2.29 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

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>.

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

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

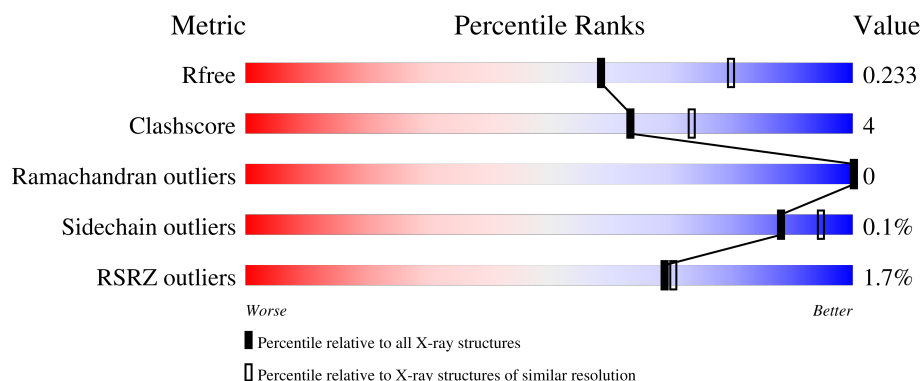
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

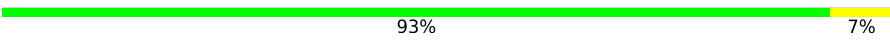
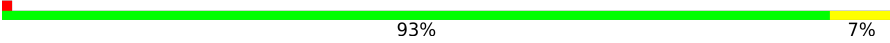
The reported resolution of this entry is 2.29 Å.

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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 ≥ 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	608	 93% 7%
1	B	608	 93% 7%
1	C	608	 4% 88% 11%

2 Entry composition [i](#)

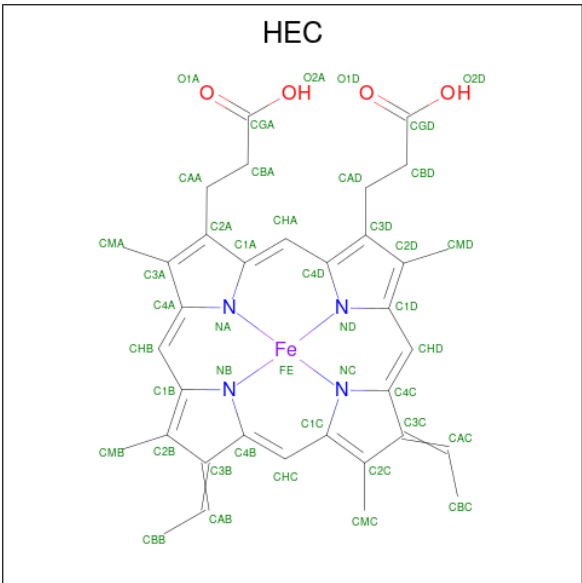
There are 5 unique types of molecules in this entry. The entry contains 15643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Decaheme c-type cytochrome, OmcA/MtrC family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	2	0
			4481	2770	782	894	35			
1	B	608	Total	C	N	O	S	0	0	0
			4484	2772	781	896	35			
1	C	604	Total	C	N	O	S	0	0	0
			4459	2755	777	892	35			

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



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

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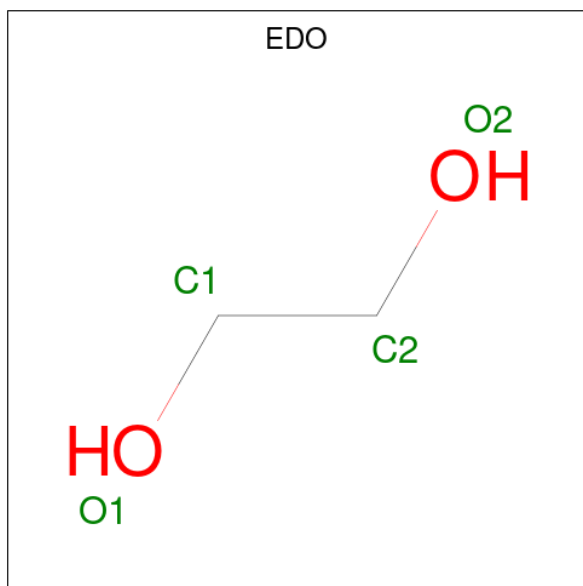
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca		
			2	2	0	0
3	B	3	Total	Ca		
			3	3	0	0
3	C	3	Total	Ca		
			3	3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

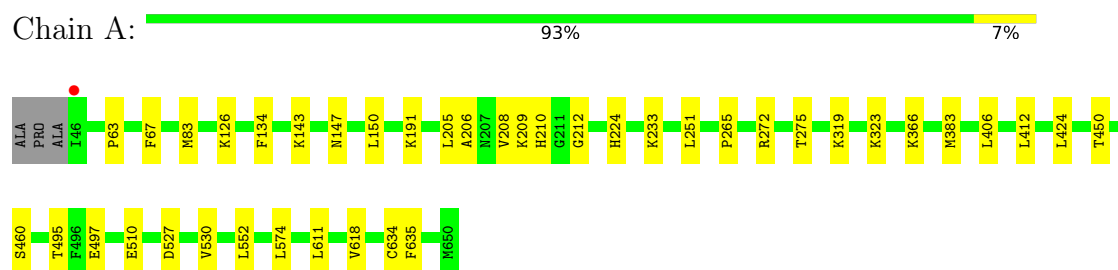
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	333	Total	O	0	0
			333	333		
5	B	335	Total	O	0	0
			335	335		
5	C	245	Total	O	0	0
			245	245		

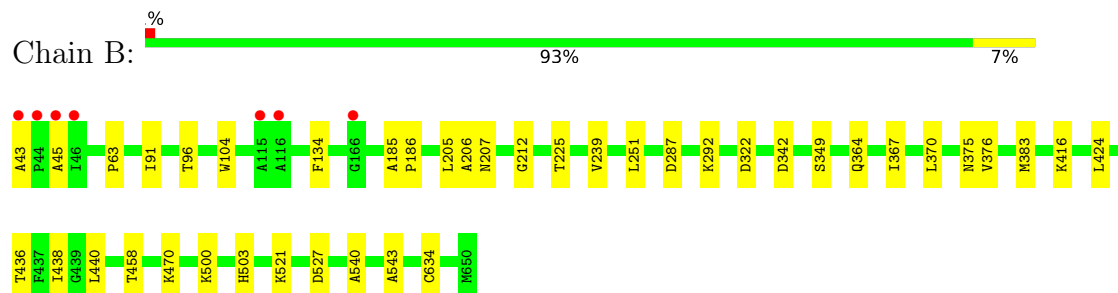
3 Residue-property plots [i](#)

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.

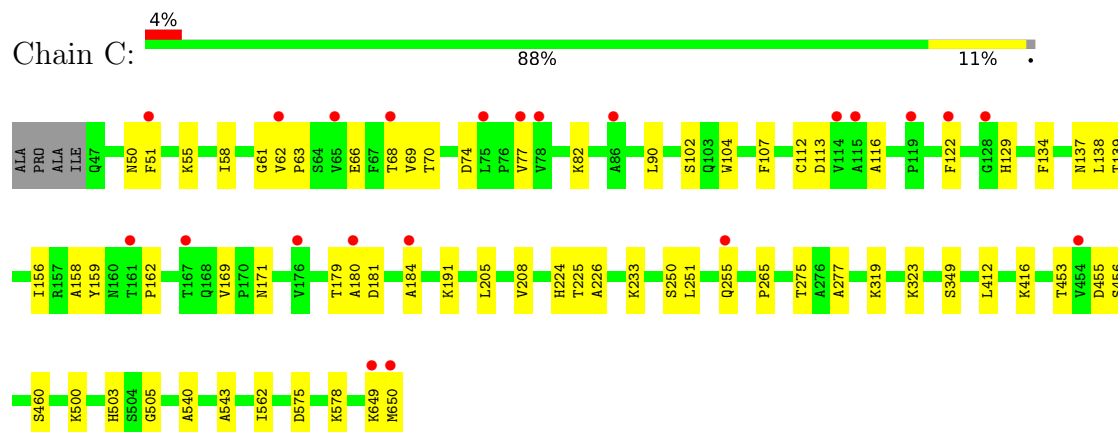
- Molecule 1: Decaheme c-type cytochrome, OmcA/MtrC family



- Molecule 1: Decaheme c-type cytochrome, OmcA/MtrC family



- Molecule 1: Decaheme c-type cytochrome, OmcA/MtrC family



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.52Å 291.50Å 87.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.20 – 2.29 87.20 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.5 (87.20-2.29) 99.5 (87.20-2.29)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.183 , 0.228 0.190 , 0.233	Depositor DCC
R_{free} test set	5313 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15643	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO, CA, 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	0.17	0/4577	0.36	0/6225
1	B	0.16	0/4575	0.35	0/6225
1	C	0.16	0/4549	0.36	0/6188
All	All	0.16	0/13701	0.35	0/18638

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4481	0	4284	27	0
1	B	4484	0	4280	25	0
1	C	4459	0	4251	49	0
2	A	430	0	300	9	0
2	B	430	0	300	8	0
2	C	430	0	301	9	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	8	0	12	0	0
5	A	333	0	0	4	0
5	B	335	0	0	1	1
5	C	245	0	0	1	0
All	All	15643	0	13728	113	1

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 4.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:MET:O	1:C:650:MET:SD	2.33	0.86
1:C:70:THR:OG1	1:C:74:ASP:HA	1.76	0.85
1:C:137:ASN:HD21	1:C:139:THR:HB	1.43	0.84
2:C:803:HEC:HBB3	2:C:804:HEC:HBC2	1.60	0.82
1:C:50:ASN:HB2	1:C:70:THR:HG23	1.62	0.80
1:B:104:TRP:HB2	1:B:225:THR:HG21	1.74	0.70
1:B:375:ASN:HA	1:B:383:MET:HE3	1.75	0.67
1:A:143:LYS:NZ	5:A:903:HOH:O	2.27	0.67
1:C:58:ILE:HD12	1:C:62:VAL:C	2.19	0.67
1:C:453:THR:HG22	1:C:455:ASP:H	1.61	0.65
1:A:552:LEU:HD21	2:A:806:HEC:HMB2	1.79	0.65
1:C:51:PHE:CE2	1:C:156:ILE:HD11	2.33	0.64
1:B:206:ALA:HB1	1:B:212:GLY:HA2	1.79	0.64
2:B:803:HEC:HBB2	2:B:804:HEC:HBC3	1.80	0.63
1:C:63:PRO:HD2	1:C:134:PHE:HB2	1.79	0.63
1:C:255:GLN:NE2	5:C:901:HOH:O	2.30	0.63
1:A:383:MET:HE1	1:A:424:LEU:HD22	1.80	0.62
1:B:383:MET:HE1	1:B:424:LEU:HD22	1.82	0.61
1:B:376:VAL:HG23	1:B:383:MET:HE2	1.85	0.58
1:B:342:ASP:OD1	1:B:470:LYS:NZ	2.35	0.58
2:A:808:HEC:HBB2	2:A:809:HEC:HBC2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:LYS:NZ	1:C:66:GLU:OE1	2.31	0.58
1:B:458:THR:O	1:B:500:LYS:NZ	2.31	0.58
2:A:804:HEC:O1D	5:A:901:HOH:O	2.17	0.57
1:C:191:LYS:HB2	1:C:265:PRO:HD2	1.85	0.57
1:B:251:LEU:HG	2:B:801:HEC:HBC2	1.86	0.57
1:C:70:THR:HG1	1:C:74:ASP:HA	1.71	0.56
1:A:510:GLU:H	1:A:510:GLU:CD	2.13	0.56
1:A:67:PHE:CZ	1:A:83:MET:HE1	2.41	0.55
1:C:69:VAL:HG12	1:C:77:VAL:HG22	1.88	0.55
2:C:808:HEC:HBB2	2:C:809:HEC:HBC2	1.89	0.55
1:A:251:LEU:HG	2:A:801:HEC:HBC2	1.88	0.55
1:B:322:ASP:OD1	5:B:901:HOH:O	2.18	0.54
1:A:147:ASN:HB3	1:A:150:LEU:HG	1.88	0.54
1:C:58:ILE:HD12	1:C:63:PRO:N	2.22	0.54
1:A:272[A]:ARG:NH2	5:A:906:HOH:O	2.37	0.54
1:C:162:PRO:HA	1:C:169:VAL:HG23	1.89	0.53
1:C:575:ASP:OD1	1:C:578:LYS:NZ	2.37	0.53
1:A:323:LYS:HD2	1:A:495:THR:HB	1.91	0.53
1:A:611:LEU:HD13	1:A:618:VAL:HG21	1.92	0.52
1:C:107:PHE:CE2	1:C:138:LEU:HD13	2.44	0.52
1:C:205:LEU:O	1:C:208:VAL:HG22	2.10	0.52
1:B:91:ILE:HG21	1:B:96:THR:HG23	1.92	0.51
1:C:224:HIS:ND1	1:C:233:LYS:O	2.41	0.51
1:B:239:VAL:HG21	2:B:803:HEC:HMD2	1.92	0.51
1:A:205:LEU:O	1:A:208:VAL:HG22	2.09	0.51
1:C:181:ASP:N	1:C:181:ASP:OD1	2.42	0.51
1:C:113:ASP:HB3	1:C:116:ALA:O	2.10	0.51
1:A:126:LYS:N	1:A:126:LYS:HD2	2.25	0.51
1:A:319:LYS:NZ	2:A:804:HEC:HBD1	2.26	0.51
2:A:803:HEC:HBB2	2:A:804:HEC:HBC3	1.92	0.50
1:A:63:PRO:HD2	1:A:134:PHE:HB2	1.93	0.50
1:B:63:PRO:HD2	1:B:134:PHE:HB2	1.93	0.50
1:A:634:CYS:HA	2:A:810:HEC:CHC	2.41	0.49
1:C:453:THR:HB	1:C:456:SER:HB3	1.94	0.49
1:C:275:THR:HG22	1:C:277:ALA:H	1.76	0.49
1:A:275:THR:HG21	5:A:1192:HOH:O	2.12	0.49
1:B:540:ALA:HB1	1:B:543:ALA:HB3	1.95	0.48
1:C:68:THR:HA	1:C:129:HIS:HA	1.95	0.48
1:C:137:ASN:ND2	1:C:139:THR:HB	2.19	0.47
1:C:63:PRO:HB2	1:C:134:PHE:CD1	2.50	0.47
2:B:808:HEC:HBB2	2:B:809:HEC:HBC2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:TRP:O	1:C:225:THR:HG21	2.15	0.47
2:C:806:HEC:HMB3	2:C:806:HEC:HBB3	1.97	0.47
2:A:802:HEC:HBB3	2:A:802:HEC:HMB3	1.97	0.47
1:C:250:SER:HB2	2:C:801:HEC:HBC1	1.98	0.46
1:B:527:ASP:OD1	1:B:527:ASP:N	2.42	0.46
1:B:349:SER:HB2	1:B:416:LYS:HG2	1.98	0.45
2:C:803:HEC:HBB2	2:C:803:HEC:HHC	1.99	0.45
1:B:287:ASP:HB3	1:B:292:LYS:HB3	1.97	0.45
1:C:112:CYS:SG	1:C:122:PHE:HB2	2.57	0.45
1:A:191:LYS:HB2	1:A:265:PRO:HD2	1.98	0.45
1:B:43:ALA:O	1:B:45:ALA:N	2.49	0.45
1:C:649:LYS:HA	1:C:649:LYS:HD2	1.72	0.45
1:B:364:GLN:HA	1:B:367:ILE:HD12	1.98	0.45
1:A:209:LYS:HB3	1:A:210:HIS:CD2	2.52	0.44
1:C:649:LYS:NZ	1:C:650:MET:O	2.50	0.44
1:A:406:LEU:HD11	1:A:412:LEU:CD2	2.48	0.44
1:A:460:SER:HB2	1:A:497:GLU:HG2	1.99	0.44
1:B:634:CYS:HA	2:B:810:HEC:CHC	2.48	0.44
1:A:206:ALA:HB1	1:A:212:GLY:HA2	1.99	0.44
1:A:366:LYS:HG2	1:A:450:THR:C	2.43	0.43
1:B:436:THR:HG22	1:B:438:ILE:HG13	1.99	0.43
1:B:503:HIS:CE1	2:B:807:HEC:HBC2	2.53	0.43
2:B:804:HEC:HBD2	2:B:804:HEC:HMD1	2.00	0.43
1:C:90:LEU:HD11	1:C:102:SER:HB2	2.00	0.43
1:C:225:THR:HG22	1:C:226:ALA:H	1.84	0.43
1:A:574:LEU:HD22	1:A:635:PHE:CZ	2.53	0.43
1:C:251:LEU:HG	2:C:801:HEC:HBC2	1.99	0.43
1:C:460:SER:OG	1:C:505:GLY:HA3	2.19	0.43
1:C:319:LYS:HE3	1:C:323:LYS:HD3	2.00	0.42
1:C:58:ILE:HG22	1:C:180:ALA:HA	2.00	0.42
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.90	0.42
1:B:370:LEU:HG	1:B:440:LEU:HD13	2.01	0.42
1:C:349:SER:HB3	1:C:416:LYS:HG2	2.02	0.42
1:C:575:ASP:CG	1:C:578:LYS:HZ1	2.27	0.42
1:A:527:ASP:O	1:A:530:VAL:HG22	2.20	0.42
2:B:804:HEC:HMD1	1:C:650:MET:SD	2.60	0.41
1:C:58:ILE:HD11	1:C:61:GLY:C	2.46	0.41
1:C:158:ALA:O	1:C:171:ASN:HA	2.20	0.41
1:A:319:LYS:HZ3	2:A:804:HEC:HBD1	1.84	0.41
1:C:179:THR:HG23	1:C:184:ALA:O	2.21	0.41
1:C:562:ILE:HD13	2:C:806:HEC:HBC2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:LYS:HB3	1:C:159:TYR:HB2	2.03	0.41
1:C:503:HIS:CE1	2:C:807:HEC:HBC2	2.56	0.41
1:A:527:ASP:OD1	1:A:527:ASP:N	2.50	0.40
1:B:521:LYS:HD2	1:B:521:LYS:HA	1.92	0.40
1:C:540:ALA:HB1	1:C:543:ALA:HB3	2.03	0.40
2:C:804:HEC:HBA2	2:C:804:HEC:HHA	2.03	0.40
1:A:224:HIS:ND1	1:A:233:LYS:O	2.42	0.40
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.88	0.40
1:C:460:SER:OG	1:C:500:LYS:HD2	2.22	0.40
1:B:185:ALA:HA	1:B:186:PRO:HD3	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:971:HOH:O	5:B:1140:HOH:O[2_555]	2.13	0.07

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	605/608 (100%)	589 (97%)	16 (3%)	0	100	100
1	B	606/608 (100%)	585 (96%)	21 (4%)	0	100	100
1	C	602/608 (99%)	579 (96%)	23 (4%)	0	100	100
All	All	1813/1824 (99%)	1753 (97%)	60 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	484/483 (100%)	484 (100%)	0	100	100
1	B	483/483 (100%)	483 (100%)	0	100	100
1	C	481/483 (100%)	480 (100%)	1 (0%)	87	94
All	All	1448/1449 (100%)	1447 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN
1	A	386	ASN
1	A	559	GLN
1	A	645	HIS
1	A	647	GLN
1	B	168	GLN
1	B	207	ASN
1	B	339	GLN
1	B	386	ASN
1	B	647	GLN
1	C	125	GLN
1	C	137	ASN
1	C	308	ASN
1	C	339	GLN
1	C	407	GLN
1	C	638	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 8 are monoatomic - leaving 32 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$
2	HEC	C	809	1	46,50,50	1.85	6 (13%)	58,82,82	1.81	4 (6%)
2	HEC	A	807	1	46,50,50	1.84	5 (10%)	58,82,82	1.92	4 (6%)
2	HEC	B	805	1	46,50,50	1.87	7 (15%)	58,82,82	1.82	6 (10%)
2	HEC	C	801	1	46,50,50	1.88	7 (15%)	58,82,82	1.83	4 (6%)
4	EDO	A	813	-	3,3,3	0.45	0	2,2,2	0.30	0
2	HEC	A	808	1	46,50,50	1.85	5 (10%)	58,82,82	1.74	4 (6%)
2	HEC	B	809	1	46,50,50	1.85	6 (13%)	58,82,82	1.89	4 (6%)
2	HEC	A	802	1	46,50,50	1.85	4 (8%)	58,82,82	1.78	6 (10%)
2	HEC	C	807	1	46,50,50	1.87	5 (10%)	58,82,82	1.80	4 (6%)
2	HEC	B	807	1	46,50,50	1.84	6 (13%)	58,82,82	1.82	5 (8%)
2	HEC	B	806	1	46,50,50	1.88	7 (15%)	58,82,82	1.76	5 (8%)
2	HEC	B	810	1	46,50,50	1.84	4 (8%)	58,82,82	1.78	4 (6%)
2	HEC	A	806	1	46,50,50	1.86	8 (17%)	58,82,82	1.71	5 (8%)
2	HEC	B	803	1	46,50,50	1.85	5 (10%)	58,82,82	1.86	6 (10%)
4	EDO	A	814	-	3,3,3	0.43	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	B	808	1	46,50,50	1.83	4 (8%)	58,82,82	1.80	4 (6%)
2	HEC	A	804	1	46,50,50	1.88	7 (15%)	58,82,82	1.77	7 (12%)
2	HEC	B	804	1	46,50,50	1.88	9 (19%)	58,82,82	1.78	4 (6%)
2	HEC	A	809	1	46,50,50	1.88	7 (15%)	58,82,82	1.78	4 (6%)
2	HEC	C	804	1	46,50,50	1.88	6 (13%)	58,82,82	1.80	4 (6%)
2	HEC	A	805	1	46,50,50	1.85	4 (8%)	58,82,82	1.89	4 (6%)
2	HEC	C	808	1	46,50,50	1.82	6 (13%)	58,82,82	1.76	5 (8%)
2	HEC	C	802	1	46,50,50	1.86	5 (10%)	58,82,82	1.83	5 (8%)
2	HEC	B	802	1	46,50,50	1.86	6 (13%)	58,82,82	1.82	5 (8%)
2	HEC	C	803	1	46,50,50	1.86	6 (13%)	58,82,82	1.81	7 (12%)
2	HEC	B	801	1	46,50,50	1.86	5 (10%)	58,82,82	1.76	4 (6%)
2	HEC	C	810	1	46,50,50	1.85	5 (10%)	58,82,82	1.75	3 (5%)
2	HEC	A	801	1	46,50,50	1.86	5 (10%)	58,82,82	1.76	5 (8%)
2	HEC	C	806	1	46,50,50	1.85	6 (13%)	58,82,82	1.69	4 (6%)
2	HEC	C	805	1	46,50,50	1.86	5 (10%)	58,82,82	1.79	5 (8%)
2	HEC	A	810	1	46,50,50	1.87	5 (10%)	58,82,82	1.80	4 (6%)
2	HEC	A	803	1	46,50,50	1.85	5 (10%)	58,82,82	1.73	5 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	C	809	1	-	7/14/54/54	-
2	HEC	A	807	1	-	8/14/54/54	-
2	HEC	B	805	1	-	5/14/54/54	-
2	HEC	C	801	1	-	7/14/54/54	-
4	EDO	A	813	-	-	0/1/1/1	-
2	HEC	A	808	1	-	7/14/54/54	-
2	HEC	B	809	1	-	10/14/54/54	-
2	HEC	A	802	1	-	7/14/54/54	-
2	HEC	C	807	1	-	8/14/54/54	-
2	HEC	B	807	1	-	8/14/54/54	-
2	HEC	B	806	1	-	9/14/54/54	-
2	HEC	B	810	1	-	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	806	1	-	7/14/54/54	-
2	HEC	B	803	1	-	6/14/54/54	-
4	EDO	A	814	-	-	0/1/1/1	-
2	HEC	B	808	1	-	7/14/54/54	-
2	HEC	A	804	1	-	8/14/54/54	-
2	HEC	B	804	1	-	10/14/54/54	-
2	HEC	A	809	1	-	9/14/54/54	-
2	HEC	C	804	1	-	9/14/54/54	-
2	HEC	A	805	1	-	5/14/54/54	-
2	HEC	C	808	1	-	6/14/54/54	-
2	HEC	C	802	1	-	8/14/54/54	-
2	HEC	B	802	1	-	9/14/54/54	-
2	HEC	C	803	1	-	8/14/54/54	-
2	HEC	B	801	1	-	9/14/54/54	-
2	HEC	C	810	1	-	5/14/54/54	-
2	HEC	A	801	1	-	10/14/54/54	-
2	HEC	C	806	1	-	9/14/54/54	-
2	HEC	C	805	1	-	2/14/54/54	-
2	HEC	A	810	1	-	5/14/54/54	-
2	HEC	A	803	1	-	4/14/54/54	-

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	805	HEC	CAC-C3C	6.53	1.56	1.35
2	A	804	HEC	CAC-C3C	6.52	1.56	1.35
2	A	801	HEC	CAC-C3C	6.51	1.56	1.35
2	C	802	HEC	CAC-C3C	6.49	1.56	1.35
2	C	805	HEC	CAC-C3C	6.49	1.56	1.35
2	C	804	HEC	CAC-C3C	6.48	1.56	1.35
2	C	803	HEC	CAB-C3B	6.47	1.56	1.35
2	B	802	HEC	CAC-C3C	6.45	1.55	1.35
2	B	806	HEC	CAC-C3C	6.45	1.55	1.35
2	C	801	HEC	CAC-C3C	6.45	1.55	1.35
2	B	809	HEC	CAC-C3C	6.44	1.55	1.35
2	A	802	HEC	CAC-C3C	6.43	1.55	1.35
2	A	810	HEC	CAC-C3C	6.43	1.55	1.35
2	B	801	HEC	CAC-C3C	6.41	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	806	HEC	CAC-C3C	6.40	1.55	1.35
2	A	804	HEC	CAB-C3B	6.39	1.55	1.35
2	A	808	HEC	CAB-C3B	6.38	1.55	1.35
2	A	806	HEC	CAC-C3C	6.37	1.55	1.35
2	C	807	HEC	CAB-C3B	6.37	1.55	1.35
2	C	809	HEC	CAC-C3C	6.37	1.55	1.35
2	A	805	HEC	CAC-C3C	6.36	1.55	1.35
2	B	804	HEC	CAC-C3C	6.34	1.55	1.35
2	A	810	HEC	CAB-C3B	6.33	1.55	1.35
2	A	809	HEC	CAC-C3C	6.32	1.55	1.35
2	C	804	HEC	CAB-C3B	6.32	1.55	1.35
2	B	803	HEC	CAC-C3C	6.31	1.55	1.35
2	B	807	HEC	CAC-C3C	6.30	1.55	1.35
2	C	810	HEC	CAC-C3C	6.30	1.55	1.35
2	B	801	HEC	CAB-C3B	6.30	1.55	1.35
2	B	810	HEC	CAB-C3B	6.30	1.55	1.35
2	B	806	HEC	CAB-C3B	6.30	1.55	1.35
2	C	801	HEC	CAB-C3B	6.29	1.55	1.35
2	C	807	HEC	CAC-C3C	6.29	1.55	1.35
2	B	810	HEC	CAC-C3C	6.25	1.55	1.35
2	A	807	HEC	CAB-C3B	6.24	1.55	1.35
2	A	803	HEC	CAC-C3C	6.23	1.55	1.35
2	C	808	HEC	CAB-C3B	6.23	1.55	1.35
2	A	803	HEC	CAB-C3B	6.23	1.55	1.35
2	C	802	HEC	CAB-C3B	6.22	1.55	1.35
2	B	808	HEC	CAB-C3B	6.22	1.55	1.35
2	B	807	HEC	CAB-C3B	6.22	1.55	1.35
2	B	808	HEC	CAC-C3C	6.22	1.55	1.35
2	A	806	HEC	CAB-C3B	6.21	1.55	1.35
2	A	809	HEC	CAB-C3B	6.21	1.55	1.35
2	B	803	HEC	CAB-C3B	6.20	1.55	1.35
2	C	806	HEC	CAB-C3B	6.20	1.55	1.35
2	A	802	HEC	CAB-C3B	6.19	1.55	1.35
2	A	801	HEC	CAB-C3B	6.19	1.55	1.35
2	A	807	HEC	CAC-C3C	6.18	1.55	1.35
2	B	802	HEC	CAB-C3B	6.17	1.55	1.35
2	C	810	HEC	CAB-C3B	6.17	1.55	1.35
2	B	804	HEC	CAB-C3B	6.16	1.55	1.35
2	C	809	HEC	CAB-C3B	6.15	1.55	1.35
2	B	809	HEC	CAB-C3B	6.15	1.55	1.35
2	A	808	HEC	CAC-C3C	6.15	1.55	1.35
2	C	803	HEC	CAC-C3C	6.15	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	805	HEC	CAB-C3B	6.13	1.54	1.35
2	C	808	HEC	CAC-C3C	6.11	1.54	1.35
2	A	805	HEC	CAB-C3B	6.06	1.54	1.35
2	C	805	HEC	CAB-C3B	5.97	1.54	1.35
2	B	804	HEC	C3D-C2D	5.87	1.54	1.38
2	A	809	HEC	C3D-C2D	5.86	1.54	1.38
2	A	805	HEC	C3D-C2D	5.81	1.54	1.38
2	C	804	HEC	C3D-C2D	5.81	1.54	1.38
2	C	806	HEC	C3D-C2D	5.78	1.54	1.38
2	C	805	HEC	C3D-C2D	5.77	1.54	1.38
2	B	805	HEC	C3D-C2D	5.77	1.53	1.38
2	B	803	HEC	C3D-C2D	5.74	1.53	1.38
2	C	801	HEC	C3D-C2D	5.73	1.53	1.38
2	A	801	HEC	C3D-C2D	5.72	1.53	1.38
2	C	803	HEC	C3D-C2D	5.72	1.53	1.38
2	C	807	HEC	C3D-C2D	5.71	1.53	1.38
2	A	808	HEC	C3D-C2D	5.70	1.53	1.38
2	B	810	HEC	C3D-C2D	5.69	1.53	1.38
2	B	802	HEC	C3D-C2D	5.69	1.53	1.38
2	A	810	HEC	C3D-C2D	5.69	1.53	1.38
2	C	810	HEC	C3D-C2D	5.68	1.53	1.38
2	C	802	HEC	C3D-C2D	5.68	1.53	1.38
2	B	806	HEC	C3D-C2D	5.68	1.53	1.38
2	A	803	HEC	C3D-C2D	5.67	1.53	1.38
2	B	808	HEC	C3D-C2D	5.65	1.53	1.38
2	B	801	HEC	C3D-C2D	5.65	1.53	1.38
2	C	809	HEC	C3D-C2D	5.63	1.53	1.38
2	A	807	HEC	C3D-C2D	5.62	1.53	1.38
2	A	806	HEC	C3D-C2D	5.60	1.53	1.38
2	B	809	HEC	C3D-C2D	5.57	1.53	1.38
2	A	802	HEC	C3D-C2D	5.55	1.53	1.38
2	C	808	HEC	C3D-C2D	5.53	1.53	1.38
2	B	807	HEC	C3D-C2D	5.50	1.53	1.38
2	A	804	HEC	C3D-C2D	5.38	1.52	1.38
2	A	806	HEC	CMB-C2B	2.30	1.55	1.50
2	C	803	HEC	C3B-C2B	-2.26	1.33	1.41
2	B	809	HEC	CMC-C2C	2.26	1.55	1.50
2	B	804	HEC	CMC-C2C	2.25	1.55	1.50
2	B	806	HEC	CMB-C2B	2.25	1.55	1.50
2	A	809	HEC	CMD-C2D	2.25	1.55	1.50
2	C	810	HEC	CMB-C2B	2.24	1.55	1.50
2	A	806	HEC	CMC-C2C	2.24	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	807	HEC	CMB-C2B	2.24	1.55	1.50
2	A	809	HEC	CMC-C2C	2.23	1.55	1.50
2	B	801	HEC	CMA-C3A	2.23	1.55	1.50
2	A	803	HEC	CMB-C2B	2.23	1.55	1.50
2	B	804	HEC	CMB-C2B	2.22	1.55	1.50
2	A	804	HEC	CMC-C2C	2.22	1.55	1.50
2	C	807	HEC	CMC-C2C	2.22	1.55	1.50
2	B	806	HEC	CMC-C2C	2.21	1.55	1.50
2	B	801	HEC	CMB-C2B	2.20	1.55	1.50
2	A	804	HEC	CMD-C2D	2.20	1.55	1.50
2	C	801	HEC	CMB-C2B	2.20	1.55	1.50
2	C	809	HEC	CMC-C2C	2.20	1.55	1.50
2	B	805	HEC	C3C-C2C	-2.20	1.33	1.41
2	B	809	HEC	CMB-C2B	2.20	1.55	1.50
2	C	801	HEC	CMA-C3A	2.19	1.55	1.50
2	C	803	HEC	CMC-C2C	2.19	1.55	1.50
2	C	808	HEC	CMC-C2C	2.19	1.55	1.50
2	B	802	HEC	CMB-C2B	2.18	1.55	1.50
2	C	804	HEC	CMC-C2C	2.18	1.55	1.50
2	C	807	HEC	CMB-C2B	2.18	1.55	1.50
2	A	804	HEC	CMB-C2B	2.18	1.55	1.50
2	B	804	HEC	CMD-C2D	2.17	1.55	1.50
2	A	807	HEC	CMC-C2C	2.17	1.55	1.50
2	A	804	HEC	CMA-C3A	2.17	1.55	1.50
2	A	806	HEC	CMA-C3A	2.17	1.55	1.50
2	A	801	HEC	CMC-C2C	2.16	1.55	1.50
2	C	809	HEC	CMA-C3A	2.15	1.55	1.50
2	C	808	HEC	CMA-C3A	2.14	1.55	1.50
2	B	803	HEC	CMC-C2C	2.14	1.55	1.50
2	C	810	HEC	CMC-C2C	2.13	1.55	1.50
2	B	810	HEC	CMB-C2B	2.13	1.55	1.50
2	C	803	HEC	CMA-C3A	2.12	1.55	1.50
2	B	805	HEC	CMB-C2B	2.12	1.55	1.50
2	B	809	HEC	CMA-C3A	2.11	1.55	1.50
2	A	810	HEC	CMB-C2B	2.10	1.55	1.50
2	A	810	HEC	CMA-C3A	2.10	1.55	1.50
2	A	803	HEC	CMD-C2D	2.10	1.55	1.50
2	C	805	HEC	C3B-C2B	-2.10	1.34	1.41
2	B	807	HEC	CMB-C2B	2.10	1.55	1.50
2	C	805	HEC	C3C-C2C	-2.10	1.34	1.41
2	A	809	HEC	CMA-C3A	2.09	1.55	1.50
2	B	802	HEC	CMA-C3A	2.09	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HEC	CMC-C2C	2.08	1.55	1.50
2	C	806	HEC	CMC-C2C	2.08	1.55	1.50
2	C	804	HEC	CMB-C2B	2.07	1.55	1.50
2	B	803	HEC	CMB-C2B	2.07	1.55	1.50
2	A	808	HEC	CMA-C3A	2.06	1.55	1.50
2	A	806	HEC	CMD-C2D	2.06	1.55	1.50
2	B	805	HEC	CMA-C3A	2.06	1.55	1.50
2	B	807	HEC	CMA-C3A	2.06	1.55	1.50
2	C	806	HEC	CMD-C2D	2.06	1.55	1.50
2	A	805	HEC	CMC-C2C	2.06	1.55	1.50
2	C	802	HEC	C3B-C2B	-2.06	1.34	1.41
2	A	802	HEC	CMB-C2B	2.06	1.55	1.50
2	C	801	HEC	CMD-C2D	2.05	1.55	1.50
2	C	804	HEC	CMA-C3A	2.05	1.55	1.50
2	A	806	HEC	C3C-C2C	-2.05	1.34	1.41
2	A	801	HEC	CMA-C3A	2.04	1.55	1.50
2	A	808	HEC	CMC-C2C	2.04	1.55	1.50
2	B	804	HEC	C3B-C2B	-2.04	1.34	1.41
2	B	807	HEC	CMC-C2C	2.04	1.54	1.50
2	B	808	HEC	CMA-C3A	2.03	1.54	1.50
2	C	808	HEC	CMB-C2B	2.03	1.54	1.50
2	A	809	HEC	CMB-C2B	2.03	1.54	1.50
2	B	806	HEC	CMA-C3A	2.03	1.54	1.50
2	B	804	HEC	C3C-C2C	-2.02	1.34	1.41
2	B	802	HEC	C3B-C2B	-2.02	1.34	1.41
2	B	804	HEC	CMA-C3A	2.02	1.54	1.50
2	C	809	HEC	CMD-C2D	2.02	1.54	1.50
2	B	805	HEC	CMC-C2C	2.01	1.54	1.50
2	C	802	HEC	CMA-C3A	2.01	1.54	1.50
2	C	806	HEC	CMA-C3A	2.01	1.54	1.50
2	B	806	HEC	C3B-C2B	-2.01	1.34	1.41

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	805	HEC	CBB-CAB-C3B	-8.93	109.59	127.43
2	A	807	HEC	CBC-CAC-C3C	-8.78	109.89	127.43
2	B	809	HEC	CBB-CAB-C3B	-8.75	109.95	127.43
2	B	805	HEC	CBB-CAB-C3B	-8.73	109.99	127.43
2	B	804	HEC	CBB-CAB-C3B	-8.66	110.12	127.43
2	B	803	HEC	CBB-CAB-C3B	-8.44	110.56	127.43
2	C	802	HEC	CBB-CAB-C3B	-8.43	110.58	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	HEC	CBB-CAB-C3B	-8.28	110.88	127.43
2	A	805	HEC	CBB-CAB-C3B	-8.25	110.95	127.43
2	C	801	HEC	CBB-CAB-C3B	-8.25	110.95	127.43
2	B	802	HEC	CBB-CAB-C3B	-8.16	111.11	127.43
2	A	801	HEC	CBB-CAB-C3B	-8.16	111.12	127.43
2	C	804	HEC	CBB-CAB-C3B	-8.14	111.16	127.43
2	B	806	HEC	CBB-CAB-C3B	-8.09	111.25	127.43
2	A	809	HEC	CBB-CAB-C3B	-7.93	111.58	127.43
2	A	807	HEC	CBB-CAB-C3B	-7.92	111.60	127.43
2	C	810	HEC	CBB-CAB-C3B	-7.90	111.64	127.43
2	A	806	HEC	CBB-CAB-C3B	-7.88	111.69	127.43
2	C	809	HEC	CBB-CAB-C3B	-7.87	111.70	127.43
2	C	803	HEC	CBC-CAC-C3C	-7.82	111.80	127.43
2	A	805	HEC	CBC-CAC-C3C	-7.81	111.82	127.43
2	B	801	HEC	CBB-CAB-C3B	-7.81	111.82	127.43
2	A	804	HEC	CBB-CAB-C3B	-7.80	111.84	127.43
2	B	807	HEC	CBB-CAB-C3B	-7.77	111.91	127.43
2	B	808	HEC	CBC-CAC-C3C	-7.74	111.96	127.43
2	B	807	HEC	CBC-CAC-C3C	-7.72	112.01	127.43
2	B	810	HEC	CBC-CAC-C3C	-7.69	112.06	127.43
2	C	807	HEC	CBB-CAB-C3B	-7.68	112.08	127.43
2	A	810	HEC	CBC-CAC-C3C	-7.67	112.11	127.43
2	C	807	HEC	CBC-CAC-C3C	-7.58	112.28	127.43
2	A	810	HEC	CBB-CAB-C3B	-7.51	112.43	127.43
2	C	808	HEC	CBC-CAC-C3C	-7.42	112.60	127.43
2	B	808	HEC	CBB-CAB-C3B	-7.42	112.61	127.43
2	A	808	HEC	CBC-CAC-C3C	-7.34	112.76	127.43
2	C	808	HEC	CBB-CAB-C3B	-7.33	112.78	127.43
2	C	806	HEC	CBB-CAB-C3B	-7.32	112.80	127.43
2	B	803	HEC	CBC-CAC-C3C	-7.18	113.08	127.43
2	A	808	HEC	CBB-CAB-C3B	-7.18	113.08	127.43
2	B	810	HEC	CBB-CAB-C3B	-7.13	113.18	127.43
2	A	803	HEC	CBB-CAB-C3B	-7.11	113.22	127.43
2	C	810	HEC	CBC-CAC-C3C	-7.06	113.32	127.43
2	B	809	HEC	CBC-CAC-C3C	-6.99	113.46	127.43
2	C	809	HEC	CBC-CAC-C3C	-6.99	113.47	127.43
2	A	809	HEC	CBC-CAC-C3C	-6.98	113.48	127.43
2	A	803	HEC	CBC-CAC-C3C	-6.94	113.57	127.43
2	C	801	HEC	CBC-CAC-C3C	-6.86	113.73	127.43
2	C	804	HEC	CBC-CAC-C3C	-6.79	113.86	127.43
2	C	802	HEC	CBC-CAC-C3C	-6.41	114.62	127.43
2	B	801	HEC	CBC-CAC-C3C	-6.21	115.01	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEC	CBC-CAC-C3C	-6.03	115.38	127.43
2	C	803	HEC	CBB-CAB-C3B	-5.93	115.58	127.43
2	A	802	HEC	CBC-CAC-C3C	-5.91	115.63	127.43
2	B	802	HEC	CBC-CAC-C3C	-5.83	115.78	127.43
2	B	804	HEC	CBC-CAC-C3C	-5.79	115.86	127.43
2	B	806	HEC	CBC-CAC-C3C	-5.74	115.96	127.43
2	A	804	HEC	CBC-CAC-C3C	-5.73	115.98	127.43
2	A	806	HEC	CBC-CAC-C3C	-5.73	115.99	127.43
2	B	805	HEC	CBC-CAC-C3C	-5.68	116.09	127.43
2	C	806	HEC	CBC-CAC-C3C	-5.59	116.27	127.43
2	C	805	HEC	CBC-CAC-C3C	-5.22	117.00	127.43
2	A	805	HEC	C4D-ND-C1D	3.90	112.17	105.82
2	B	802	HEC	C4D-ND-C1D	3.85	112.09	105.82
2	B	806	HEC	C4D-ND-C1D	3.84	112.09	105.82
2	C	806	HEC	C4D-ND-C1D	3.83	112.06	105.82
2	A	801	HEC	C4D-ND-C1D	3.82	112.05	105.82
2	B	805	HEC	C4D-ND-C1D	3.82	112.04	105.82
2	C	801	HEC	C4D-ND-C1D	3.81	112.03	105.82
2	B	804	HEC	C4D-ND-C1D	3.74	111.91	105.82
2	A	804	HEC	C4D-ND-C1D	3.73	111.91	105.82
2	A	808	HEC	C4D-ND-C1D	3.70	111.85	105.82
2	B	803	HEC	C4D-ND-C1D	3.69	111.84	105.82
2	C	807	HEC	C4D-ND-C1D	3.69	111.84	105.82
2	C	803	HEC	C4D-ND-C1D	3.69	111.83	105.82
2	B	808	HEC	C4D-ND-C1D	3.66	111.79	105.82
2	C	804	HEC	C4D-ND-C1D	3.65	111.77	105.82
2	C	805	HEC	C4D-ND-C1D	3.64	111.75	105.82
2	B	809	HEC	C4D-ND-C1D	3.63	111.74	105.82
2	B	801	HEC	C4D-ND-C1D	3.62	111.73	105.82
2	B	810	HEC	C4D-ND-C1D	3.62	111.73	105.82
2	C	809	HEC	C4D-ND-C1D	3.60	111.70	105.82
2	C	802	HEC	C4D-ND-C1D	3.60	111.69	105.82
2	A	807	HEC	C4D-ND-C1D	3.55	111.61	105.82
2	A	806	HEC	C4D-ND-C1D	3.55	111.60	105.82
2	A	810	HEC	C4D-ND-C1D	3.52	111.56	105.82
2	C	810	HEC	C4D-ND-C1D	3.46	111.46	105.82
2	C	808	HEC	C4D-ND-C1D	3.45	111.45	105.82
2	A	809	HEC	C4D-ND-C1D	3.44	111.43	105.82
2	A	803	HEC	C4D-ND-C1D	3.44	111.42	105.82
2	A	804	HEC	CBD-CAD-C3D	-3.40	103.13	112.53
2	A	802	HEC	C4D-ND-C1D	3.40	111.36	105.82
2	B	807	HEC	C4D-ND-C1D	3.26	111.13	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	HEC	C2A-C1A-NA	-3.01	107.42	110.32
2	B	806	HEC	C2A-C1A-NA	-2.89	107.53	110.32
2	A	805	HEC	C2A-C1A-NA	-2.81	107.61	110.32
2	C	806	HEC	C2A-C1A-NA	-2.79	107.63	110.32
2	B	804	HEC	C2A-C1A-NA	-2.75	107.67	110.32
2	C	804	HEC	C2A-C1A-NA	-2.72	107.69	110.32
2	C	803	HEC	CAD-CBD-CGD	-2.67	106.59	113.67
2	B	810	HEC	C2A-C1A-NA	-2.62	107.79	110.32
2	A	802	HEC	C2A-C1A-NA	-2.62	107.80	110.32
2	B	809	HEC	C2A-C1A-NA	-2.60	107.81	110.32
2	C	803	HEC	CHD-C4C-NC	2.57	127.25	124.45
2	C	802	HEC	C2A-C1A-NA	-2.57	107.84	110.32
2	C	803	HEC	CHC-C4B-C3B	2.49	129.40	125.21
2	A	809	HEC	C2A-C1A-NA	-2.46	107.95	110.32
2	B	805	HEC	C2A-C1A-NA	-2.45	107.96	110.32
2	C	805	HEC	C2A-C1A-NA	-2.44	107.97	110.32
2	C	807	HEC	C2A-C1A-NA	-2.41	107.99	110.32
2	C	805	HEC	CHD-C4C-C3C	2.39	129.24	125.21
2	A	804	HEC	CMD-C2D-C1D	2.37	129.03	125.42
2	C	801	HEC	C2A-C1A-NA	-2.35	108.05	110.32
2	C	802	HEC	CMC-C2C-C1C	-2.35	121.84	125.42
2	C	809	HEC	C2A-C1A-NA	-2.35	108.06	110.32
2	B	802	HEC	CMC-C2C-C1C	-2.34	121.86	125.42
2	A	806	HEC	CAA-CBA-CGA	-2.32	107.52	113.67
2	B	803	HEC	CAD-CBD-CGD	-2.31	107.53	113.67
2	A	807	HEC	C2A-C1A-NA	-2.31	108.09	110.32
2	C	808	HEC	CAD-CBD-CGD	-2.31	107.54	113.67
2	A	804	HEC	C2A-C1A-NA	-2.31	108.10	110.32
2	B	801	HEC	C2A-C1A-NA	-2.29	108.11	110.32
2	B	805	HEC	CHD-C4C-C3C	2.27	129.04	125.21
2	A	808	HEC	C2A-C1A-NA	-2.26	108.14	110.32
2	B	805	HEC	CAD-CBD-CGD	-2.26	107.68	113.67
2	B	807	HEC	C2A-C1A-NA	-2.21	108.19	110.32
2	A	810	HEC	C2A-C1A-NA	-2.21	108.19	110.32
2	A	803	HEC	CAD-CBD-CGD	-2.20	107.83	113.67
2	C	803	HEC	CAA-CBA-CGA	-2.19	107.85	113.67
2	A	803	HEC	C2A-C1A-NA	-2.17	108.23	110.32
2	A	801	HEC	CAD-C3D-C4D	2.16	129.16	124.94
2	B	808	HEC	CAD-CBD-CGD	-2.13	108.03	113.67
2	B	806	HEC	CHA-C1A-C2A	2.07	128.14	124.86
2	C	808	HEC	C2A-C1A-NA	-2.07	108.32	110.32
2	B	803	HEC	C2A-C1A-NA	-2.07	108.33	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	804	HEC	C3D-C4D-ND	-2.07	107.86	110.15
2	B	803	HEC	CAA-CBA-CGA	-2.06	108.20	113.67
2	A	802	HEC	CBD-CAD-C3D	-2.06	106.84	112.53
2	A	801	HEC	CAD-CBD-CGD	-2.06	108.21	113.67
2	A	806	HEC	CBD-CAD-C3D	-2.05	106.87	112.53
2	A	802	HEC	CAA-CBA-CGA	-2.04	108.25	113.67
2	B	807	HEC	CHA-C1A-NA	2.00	126.63	124.45

There are no chirality outliers.

All (221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEC	C2B-C3B-CAB-CBB
2	A	801	HEC	C4B-C3B-CAB-CBB
2	A	801	HEC	C2C-C3C-CAC-CBC
2	A	801	HEC	C4C-C3C-CAC-CBC
2	A	802	HEC	C2B-C3B-CAB-CBB
2	A	802	HEC	C4B-C3B-CAB-CBB
2	A	802	HEC	C2C-C3C-CAC-CBC
2	A	802	HEC	C4C-C3C-CAC-CBC
2	A	802	HEC	C3D-CAD-CBD-CGD
2	A	803	HEC	C2B-C3B-CAB-CBB
2	A	803	HEC	C4B-C3B-CAB-CBB
2	A	803	HEC	C2C-C3C-CAC-CBC
2	A	803	HEC	C4C-C3C-CAC-CBC
2	A	804	HEC	C2B-C3B-CAB-CBB
2	A	804	HEC	C4B-C3B-CAB-CBB
2	A	804	HEC	C2C-C3C-CAC-CBC
2	A	804	HEC	C4C-C3C-CAC-CBC
2	A	805	HEC	C2B-C3B-CAB-CBB
2	A	805	HEC	C4B-C3B-CAB-CBB
2	A	805	HEC	C2C-C3C-CAC-CBC
2	A	805	HEC	C4C-C3C-CAC-CBC
2	A	806	HEC	C2B-C3B-CAB-CBB
2	A	806	HEC	C4B-C3B-CAB-CBB
2	A	806	HEC	C2C-C3C-CAC-CBC
2	A	806	HEC	C4C-C3C-CAC-CBC
2	A	807	HEC	C2B-C3B-CAB-CBB
2	A	807	HEC	C4B-C3B-CAB-CBB
2	A	807	HEC	C2C-C3C-CAC-CBC
2	A	807	HEC	C4C-C3C-CAC-CBC
2	A	808	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	A	808	HEC	C4B-C3B-CAB-CBB
2	A	808	HEC	C2C-C3C-CAC-CBC
2	A	808	HEC	C4C-C3C-CAC-CBC
2	A	809	HEC	C2B-C3B-CAB-CBB
2	A	809	HEC	C4B-C3B-CAB-CBB
2	A	809	HEC	C2C-C3C-CAC-CBC
2	A	809	HEC	C4C-C3C-CAC-CBC
2	A	810	HEC	C2B-C3B-CAB-CBB
2	A	810	HEC	C4B-C3B-CAB-CBB
2	A	810	HEC	C2C-C3C-CAC-CBC
2	A	810	HEC	C4C-C3C-CAC-CBC
2	B	801	HEC	C2B-C3B-CAB-CBB
2	B	801	HEC	C4B-C3B-CAB-CBB
2	B	801	HEC	C2C-C3C-CAC-CBC
2	B	801	HEC	C4C-C3C-CAC-CBC
2	B	802	HEC	C2B-C3B-CAB-CBB
2	B	802	HEC	C4B-C3B-CAB-CBB
2	B	802	HEC	C2C-C3C-CAC-CBC
2	B	802	HEC	C4C-C3C-CAC-CBC
2	B	803	HEC	C2B-C3B-CAB-CBB
2	B	803	HEC	C4B-C3B-CAB-CBB
2	B	803	HEC	C2C-C3C-CAC-CBC
2	B	803	HEC	C4C-C3C-CAC-CBC
2	B	804	HEC	C2B-C3B-CAB-CBB
2	B	804	HEC	C2C-C3C-CAC-CBC
2	B	804	HEC	C4C-C3C-CAC-CBC
2	B	805	HEC	C2B-C3B-CAB-CBB
2	B	805	HEC	C4B-C3B-CAB-CBB
2	B	806	HEC	C2B-C3B-CAB-CBB
2	B	806	HEC	C4B-C3B-CAB-CBB
2	B	806	HEC	C2C-C3C-CAC-CBC
2	B	806	HEC	C4C-C3C-CAC-CBC
2	B	807	HEC	C2B-C3B-CAB-CBB
2	B	807	HEC	C4B-C3B-CAB-CBB
2	B	807	HEC	C2C-C3C-CAC-CBC
2	B	807	HEC	C4C-C3C-CAC-CBC
2	B	808	HEC	C2B-C3B-CAB-CBB
2	B	808	HEC	C4B-C3B-CAB-CBB
2	B	808	HEC	C2C-C3C-CAC-CBC
2	B	808	HEC	C4C-C3C-CAC-CBC
2	B	809	HEC	C2B-C3B-CAB-CBB
2	B	809	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	B	809	HEC	C2C-C3C-CAC-CBC
2	B	809	HEC	C4C-C3C-CAC-CBC
2	B	810	HEC	C2B-C3B-CAB-CBB
2	B	810	HEC	C4B-C3B-CAB-CBB
2	B	810	HEC	C2C-C3C-CAC-CBC
2	B	810	HEC	C4C-C3C-CAC-CBC
2	C	801	HEC	C2B-C3B-CAB-CBB
2	C	801	HEC	C4B-C3B-CAB-CBB
2	C	801	HEC	C2C-C3C-CAC-CBC
2	C	801	HEC	C4C-C3C-CAC-CBC
2	C	802	HEC	C2B-C3B-CAB-CBB
2	C	802	HEC	C4B-C3B-CAB-CBB
2	C	802	HEC	C2C-C3C-CAC-CBC
2	C	802	HEC	C4C-C3C-CAC-CBC
2	C	803	HEC	C4B-C3B-CAB-CBB
2	C	803	HEC	C2C-C3C-CAC-CBC
2	C	803	HEC	C4C-C3C-CAC-CBC
2	C	804	HEC	C2B-C3B-CAB-CBB
2	C	804	HEC	C4B-C3B-CAB-CBB
2	C	804	HEC	C2C-C3C-CAC-CBC
2	C	804	HEC	C4C-C3C-CAC-CBC
2	C	805	HEC	C2C-C3C-CAC-CBC
2	C	806	HEC	C2B-C3B-CAB-CBB
2	C	806	HEC	C4B-C3B-CAB-CBB
2	C	806	HEC	C2C-C3C-CAC-CBC
2	C	806	HEC	C4C-C3C-CAC-CBC
2	C	807	HEC	C2B-C3B-CAB-CBB
2	C	807	HEC	C4B-C3B-CAB-CBB
2	C	807	HEC	C2C-C3C-CAC-CBC
2	C	807	HEC	C4C-C3C-CAC-CBC
2	C	808	HEC	C2B-C3B-CAB-CBB
2	C	808	HEC	C4B-C3B-CAB-CBB
2	C	808	HEC	C2C-C3C-CAC-CBC
2	C	808	HEC	C4C-C3C-CAC-CBC
2	C	809	HEC	C2B-C3B-CAB-CBB
2	C	809	HEC	C4B-C3B-CAB-CBB
2	C	809	HEC	C2C-C3C-CAC-CBC
2	C	809	HEC	C4C-C3C-CAC-CBC
2	C	810	HEC	C2B-C3B-CAB-CBB
2	C	810	HEC	C4B-C3B-CAB-CBB
2	C	810	HEC	C2C-C3C-CAC-CBC
2	C	810	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
2	B	810	HEC	C2A-CAA-CBA-CGA
2	C	801	HEC	C2A-CAA-CBA-CGA
2	A	806	HEC	C1A-C2A-CAA-CBA
2	B	801	HEC	C1A-C2A-CAA-CBA
2	B	802	HEC	C3D-CAD-CBD-CGD
2	C	804	HEC	C3D-CAD-CBD-CGD
2	B	801	HEC	C3A-C2A-CAA-CBA
2	A	801	HEC	C4D-C3D-CAD-CBD
2	A	804	HEC	C1A-C2A-CAA-CBA
2	A	806	HEC	C3A-C2A-CAA-CBA
2	A	804	HEC	C3A-C2A-CAA-CBA
2	A	810	HEC	C3D-CAD-CBD-CGD
2	A	801	HEC	C2D-C3D-CAD-CBD
2	C	810	HEC	C3D-CAD-CBD-CGD
2	C	804	HEC	C1A-C2A-CAA-CBA
2	B	804	HEC	C4B-C3B-CAB-CBB
2	C	805	HEC	C4B-C3B-CAB-CBB
2	C	803	HEC	C2B-C3B-CAB-CBB
2	B	804	HEC	C2A-CAA-CBA-CGA
2	A	801	HEC	CAD-CBD-CGD-O2D
2	B	806	HEC	CAD-CBD-CGD-O1D
2	A	804	HEC	CAD-CBD-CGD-O1D
2	C	804	HEC	CAD-CBD-CGD-O1D
2	C	804	HEC	CAD-CBD-CGD-O2D
2	C	807	HEC	CAA-CBA-CGA-O1A
2	A	807	HEC	CAA-CBA-CGA-O2A
2	B	806	HEC	CAD-CBD-CGD-O2D
2	B	807	HEC	CAA-CBA-CGA-O2A
2	C	806	HEC	CAD-CBD-CGD-O1D
2	A	804	HEC	CAD-CBD-CGD-O2D
2	B	805	HEC	CAA-CBA-CGA-O1A
2	B	804	HEC	CAA-CBA-CGA-O1A
2	B	809	HEC	CAD-CBD-CGD-O1D
2	B	802	HEC	CAA-CBA-CGA-O1A
2	C	807	HEC	CAA-CBA-CGA-O2A
2	A	809	HEC	CAD-CBD-CGD-O2D
2	B	806	HEC	CAA-CBA-CGA-O1A
2	C	804	HEC	C3A-C2A-CAA-CBA
2	A	807	HEC	CAA-CBA-CGA-O1A
2	B	807	HEC	CAA-CBA-CGA-O1A
2	C	807	HEC	CAD-CBD-CGD-O2D
2	A	807	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
2	A	801	HEC	CAD-CBD-CGD-O1D
2	B	804	HEC	CAA-CBA-CGA-O2A
2	B	805	HEC	CAA-CBA-CGA-O2A
2	C	806	HEC	CAA-CBA-CGA-O1A
2	C	806	HEC	CAD-CBD-CGD-O2D
2	B	809	HEC	CAD-CBD-CGD-O2D
2	B	809	HEC	C3D-CAD-CBD-CGD
2	B	802	HEC	CAA-CBA-CGA-O2A
2	B	806	HEC	CAA-CBA-CGA-O2A
2	B	810	HEC	CAA-CBA-CGA-O2A
2	A	802	HEC	CAD-CBD-CGD-O2D
2	B	804	HEC	CAD-CBD-CGD-O2D
2	B	807	HEC	CAD-CBD-CGD-O2D
2	C	802	HEC	CAD-CBD-CGD-O2D
2	B	809	HEC	C1A-C2A-CAA-CBA
2	B	804	HEC	CAD-CBD-CGD-O1D
2	C	801	HEC	CAA-CBA-CGA-O2A
2	A	809	HEC	CAD-CBD-CGD-O1D
2	B	810	HEC	CAD-CBD-CGD-O2D
2	C	807	HEC	CAD-CBD-CGD-O1D
2	A	809	HEC	CAA-CBA-CGA-O2A
2	B	801	HEC	CAD-CBD-CGD-O1D
2	B	810	HEC	CAD-CBD-CGD-O1D
2	C	801	HEC	CAA-CBA-CGA-O1A
2	C	806	HEC	C1A-C2A-CAA-CBA
2	B	801	HEC	CAD-CBD-CGD-O2D
2	A	807	HEC	CAD-CBD-CGD-O1D
2	B	807	HEC	CAD-CBD-CGD-O1D
2	B	810	HEC	CAA-CBA-CGA-O1A
2	C	802	HEC	CAD-CBD-CGD-O1D
2	B	804	HEC	C2D-C3D-CAD-CBD
2	C	802	HEC	CAA-CBA-CGA-O2A
2	A	802	HEC	CAD-CBD-CGD-O1D
2	C	802	HEC	CAA-CBA-CGA-O1A
2	C	806	HEC	CAA-CBA-CGA-O2A
2	A	809	HEC	CAA-CBA-CGA-O1A
2	B	802	HEC	CAD-CBD-CGD-O1D
2	A	809	HEC	C2A-CAA-CBA-CGA
2	B	808	HEC	CAA-CBA-CGA-O2A
2	C	809	HEC	CAD-CBD-CGD-O2D
2	A	808	HEC	CAA-CBA-CGA-O2A
2	A	801	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	803	HEC	CAA-CBA-CGA-O2A
2	B	803	HEC	CAA-CBA-CGA-O2A
2	C	803	HEC	CAD-CBD-CGD-O2D
2	B	806	HEC	C1A-C2A-CAA-CBA
2	A	801	HEC	CAA-CBA-CGA-O2A
2	A	806	HEC	CAA-CBA-CGA-O2A
2	B	802	HEC	CAD-CBD-CGD-O2D
2	B	805	HEC	C4C-C3C-CAC-CBC
2	A	808	HEC	CAA-CBA-CGA-O1A
2	B	808	HEC	CAA-CBA-CGA-O1A
2	B	808	HEC	CAD-CBD-CGD-O2D
2	C	809	HEC	CAD-CBD-CGD-O1D
2	A	805	HEC	CAD-CBD-CGD-O2D
2	C	803	HEC	CAA-CBA-CGA-O1A
2	C	803	HEC	CAD-CBD-CGD-O1D
2	C	809	HEC	CAA-CBA-CGA-O2A
2	B	809	HEC	CAA-CBA-CGA-O2A
2	C	808	HEC	CAD-CBD-CGD-O2D
2	A	808	HEC	CAD-CBD-CGD-O2D
2	B	801	HEC	CAA-CBA-CGA-O1A
2	C	808	HEC	CAD-CBD-CGD-O1D
2	B	809	HEC	CAA-CBA-CGA-O1A
2	B	803	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

22 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	809	HEC	1	0
2	C	801	HEC	2	0
2	A	808	HEC	1	0
2	B	809	HEC	1	0
2	A	802	HEC	1	0
2	C	807	HEC	1	0
2	B	807	HEC	1	0
2	B	810	HEC	1	0
2	A	806	HEC	1	0
2	B	803	HEC	2	0
2	B	808	HEC	1	0
2	A	804	HEC	4	0
2	B	804	HEC	3	0
2	A	809	HEC	1	0

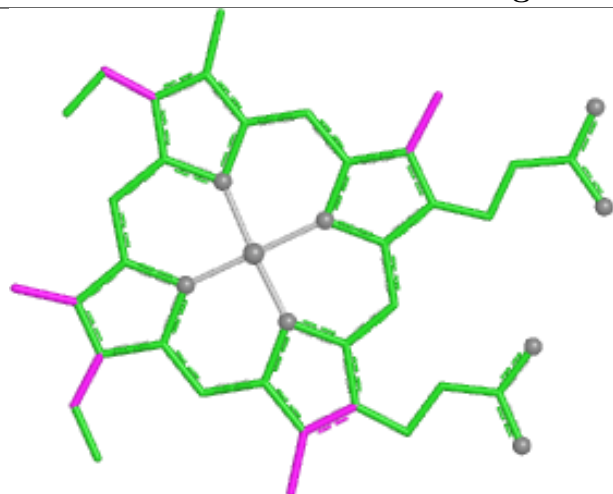
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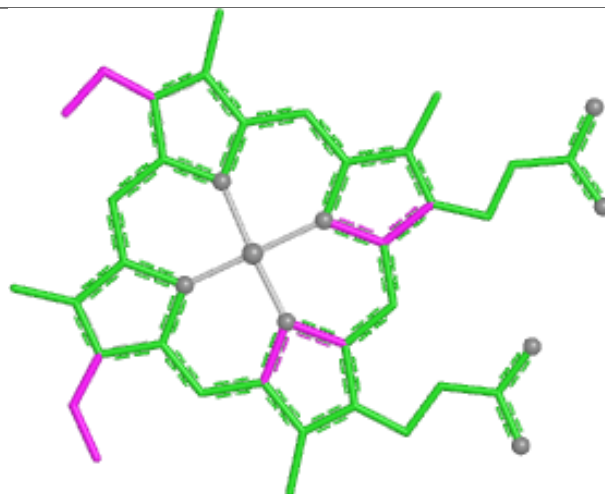
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	804	HEC	2	0
2	C	808	HEC	1	0
2	C	803	HEC	2	0
2	B	801	HEC	1	0
2	A	801	HEC	1	0
2	C	806	HEC	2	0
2	A	810	HEC	1	0
2	A	803	HEC	1	0

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.

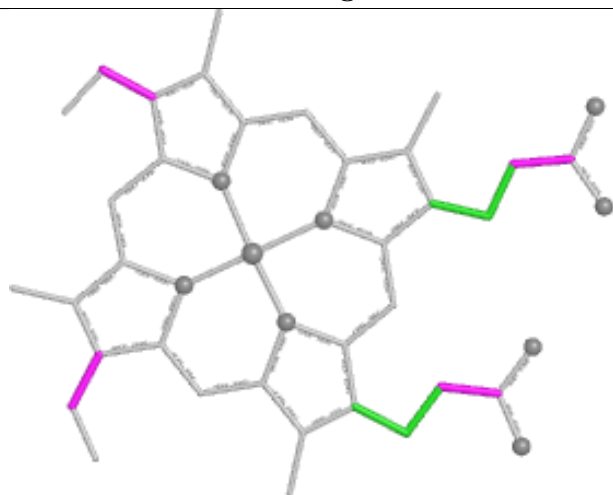
Ligand HEC C 809



Bond lengths



Bond angles

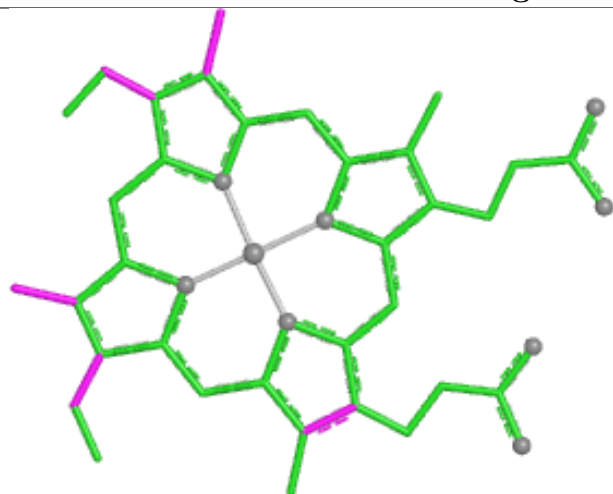


Torsions

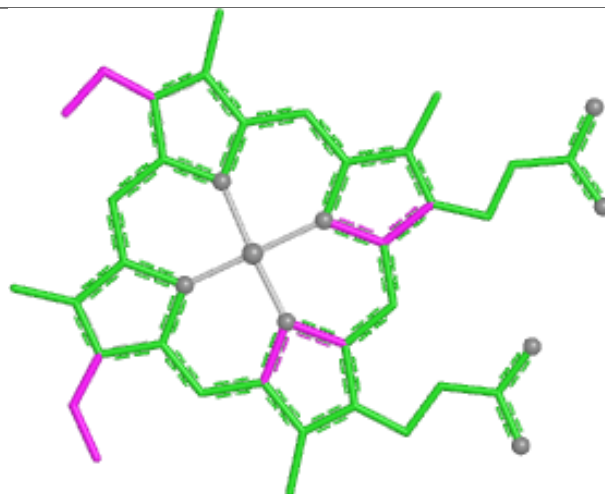


Rings

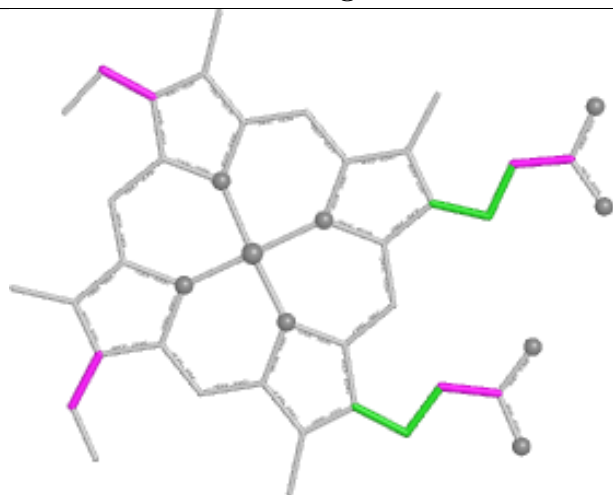
Ligand HEC A 807



Bond lengths



Bond angles

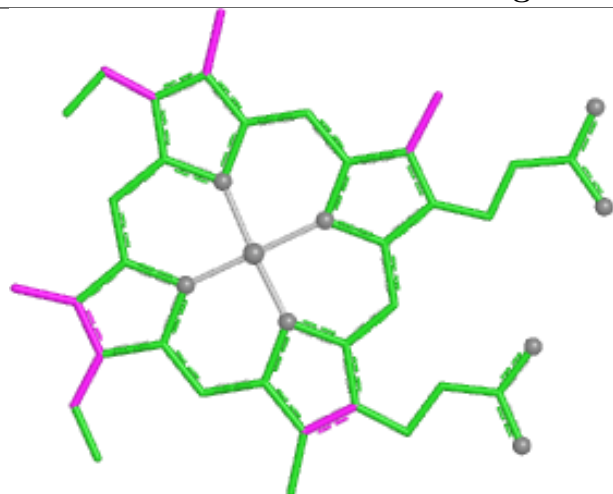


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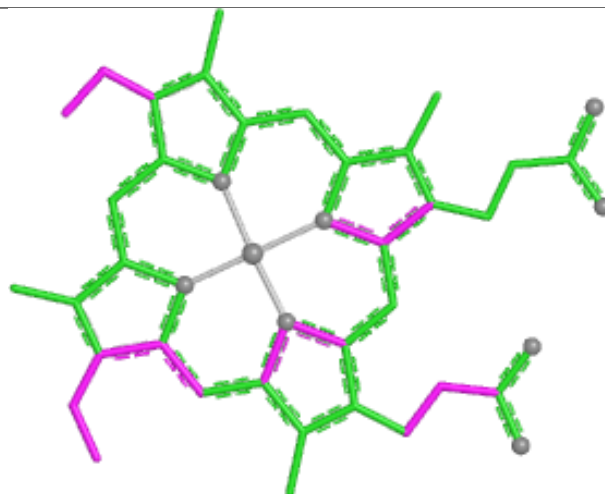


Rings

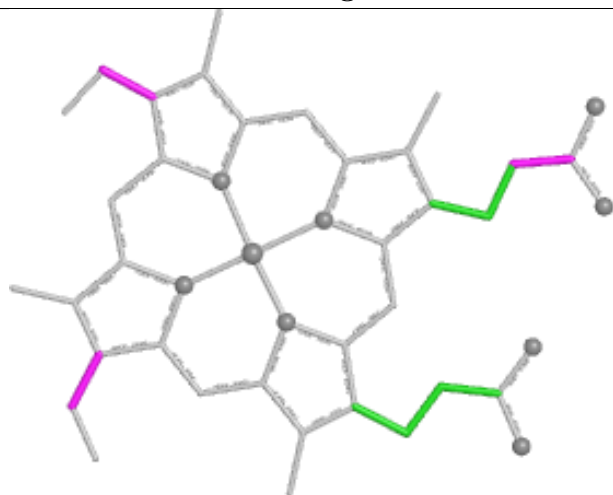
Ligand HEC B 805



Bond lengths



Bond angles

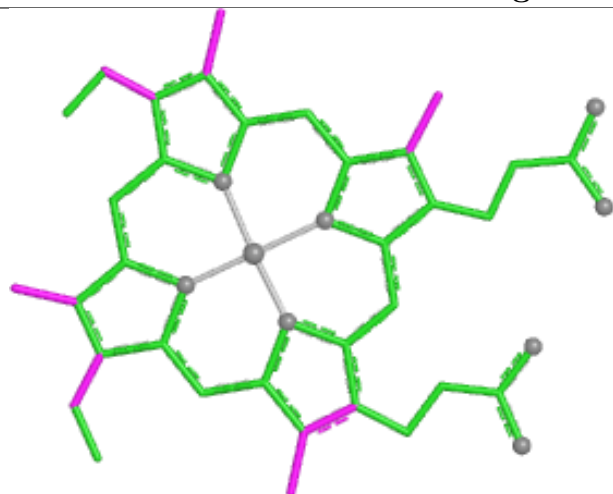


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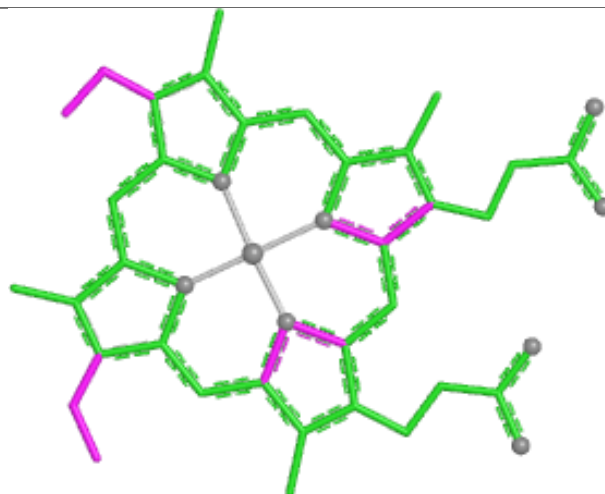


Rings

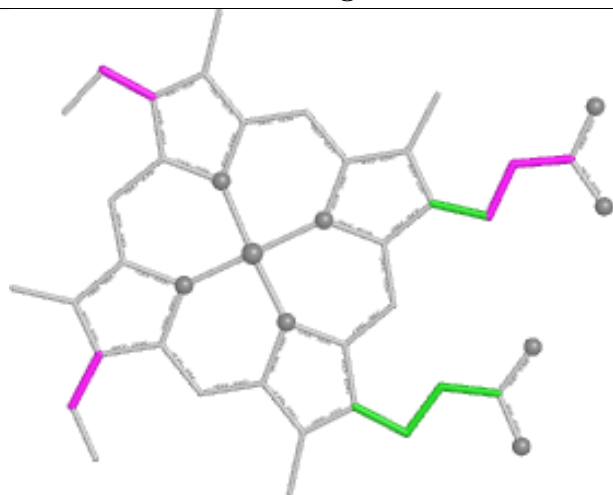
Ligand HEC C 801



Bond lengths



Bond angles

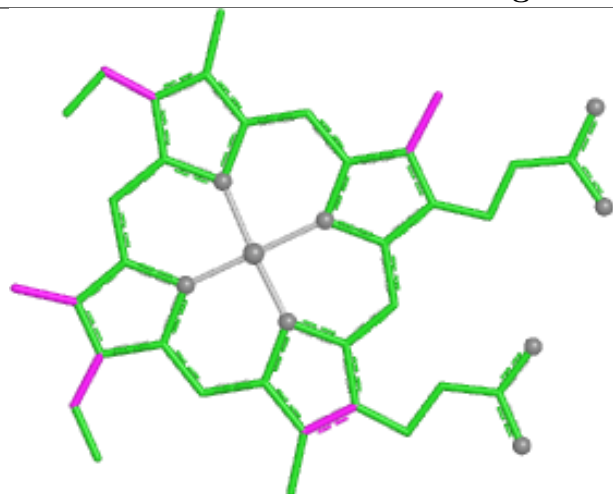


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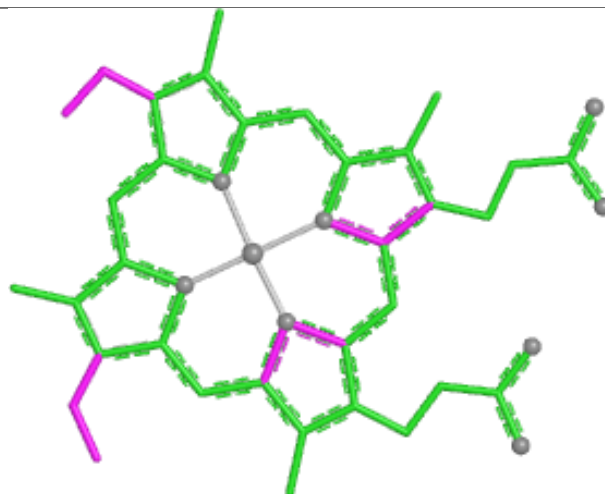


Rings

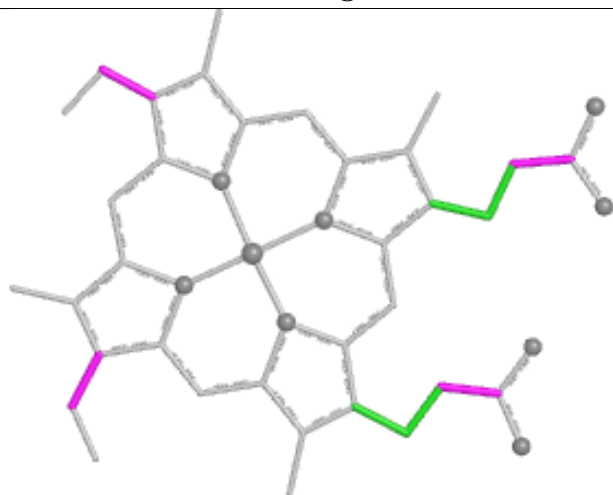
Ligand HEC A 808



Bond lengths



Bond angles

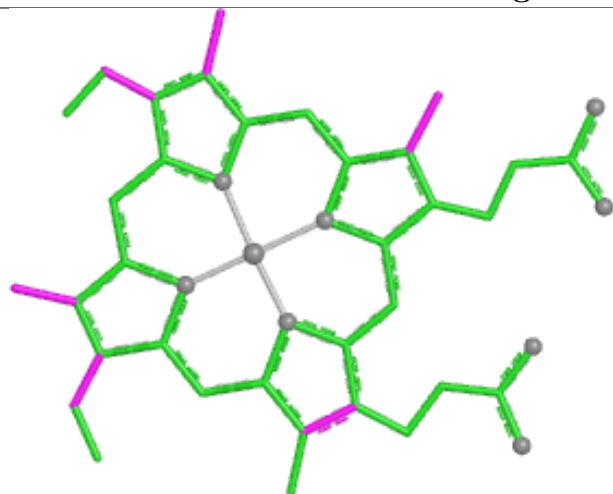


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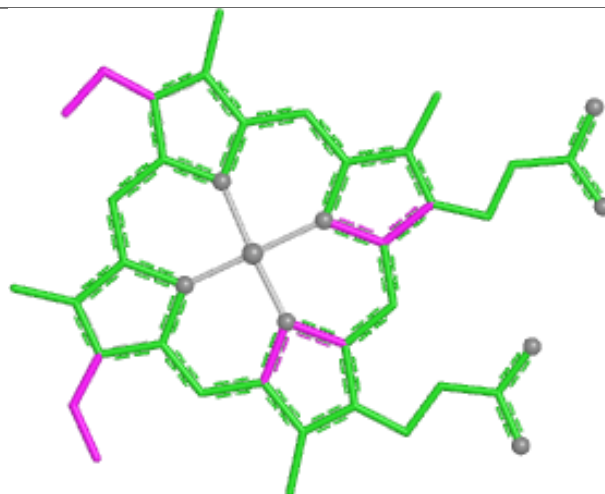


Rings

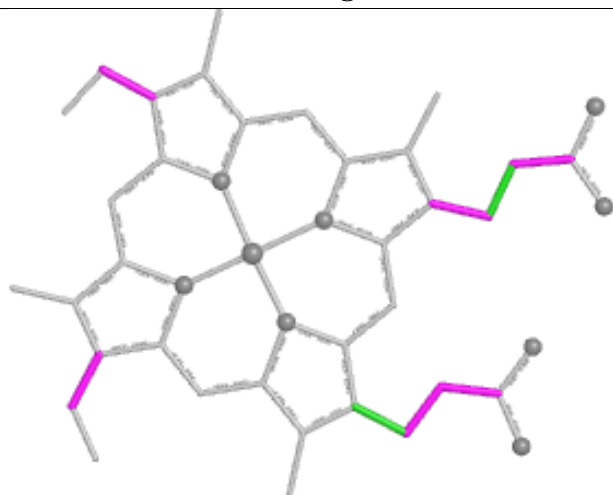
Ligand HEC B 809



Bond lengths



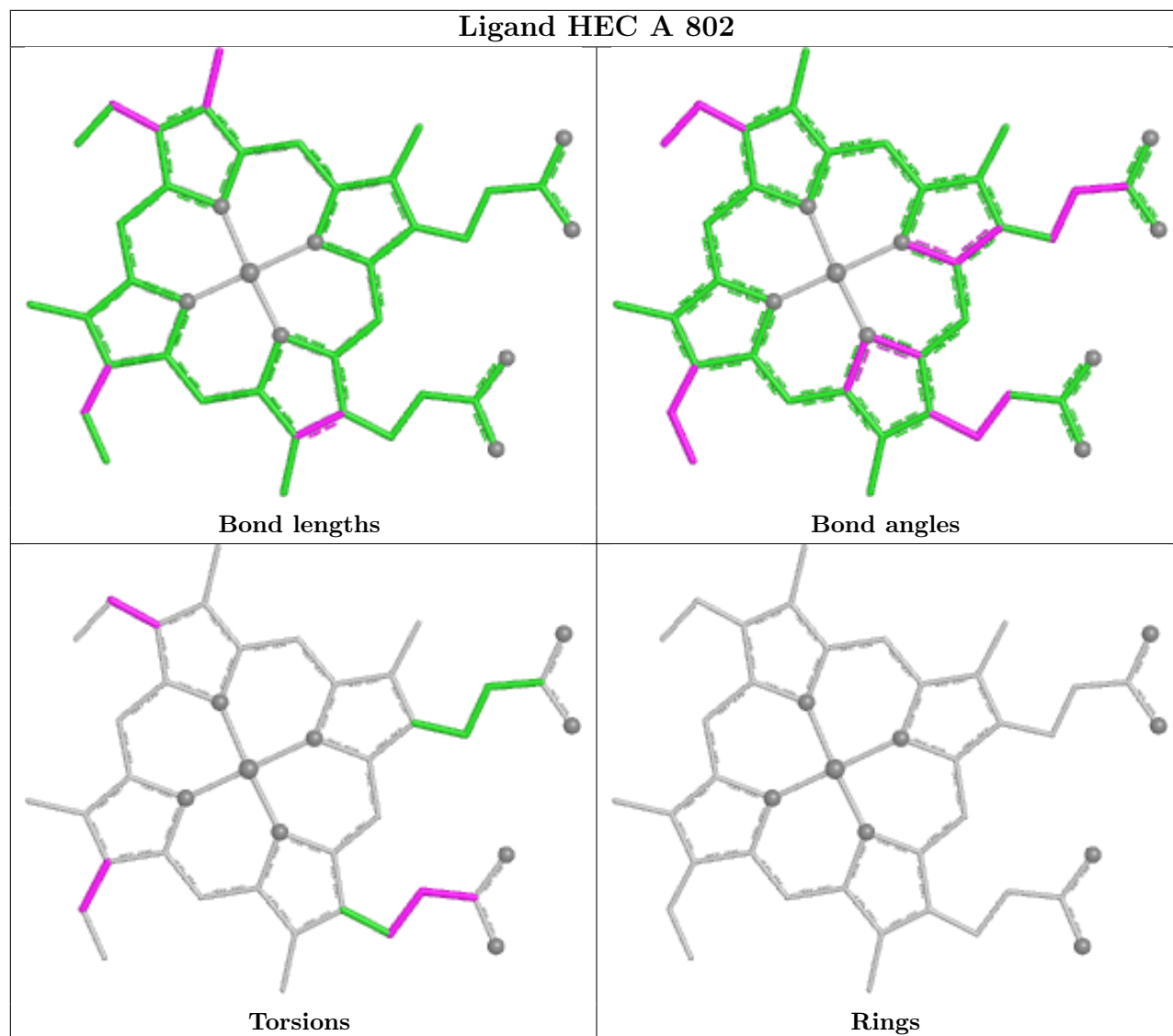
Bond angles



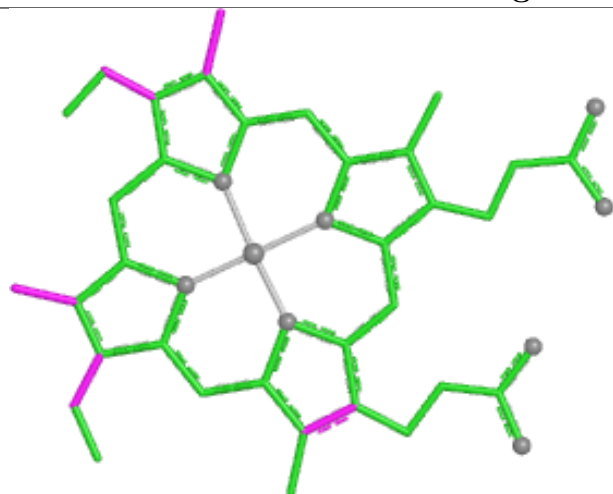
Torsions



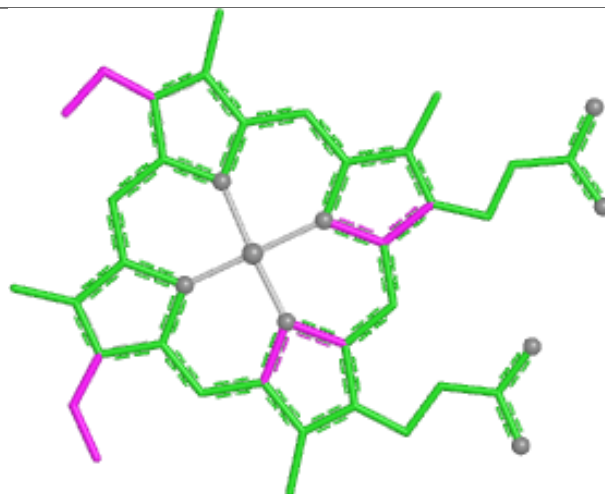
Rings



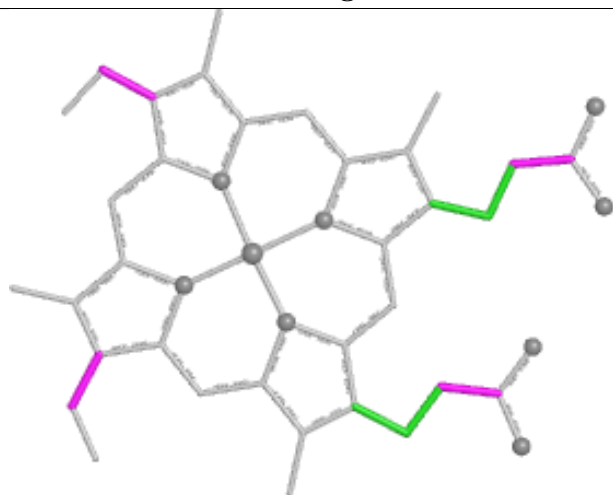
Ligand HEC C 807



Bond lengths



Bond angles

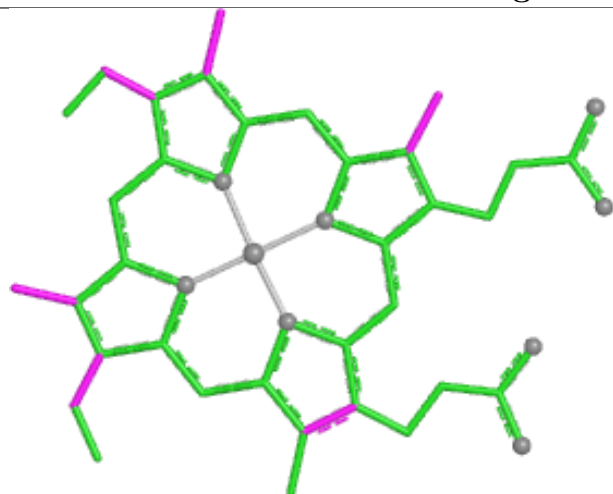


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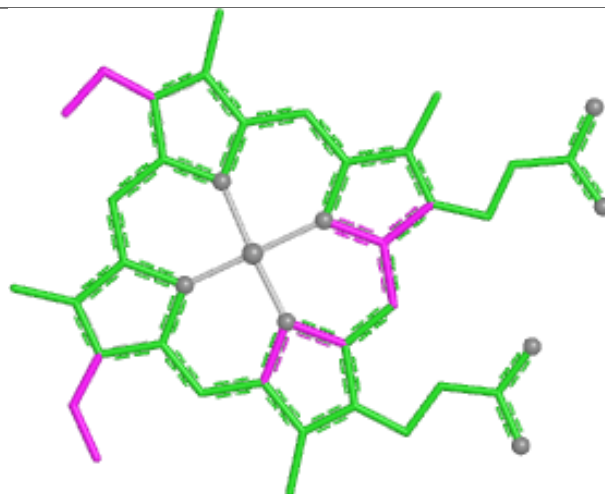


Rings

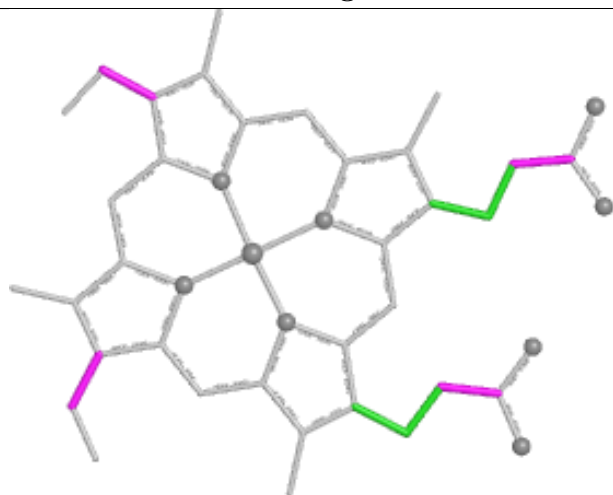
Ligand HEC B 807



Bond lengths



Bond angles

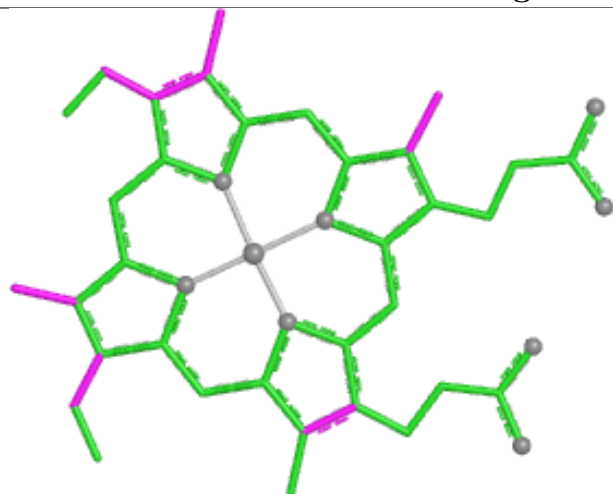


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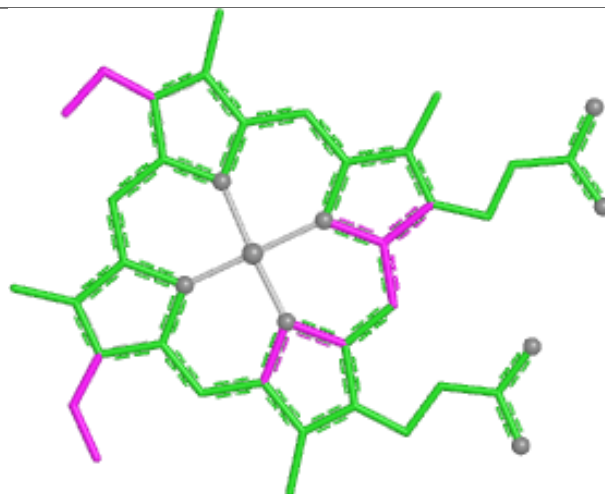


Rings

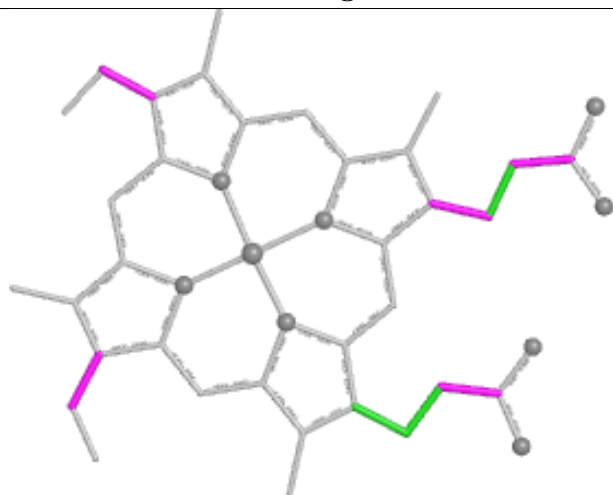
Ligand HEC B 806



Bond lengths



Bond angles

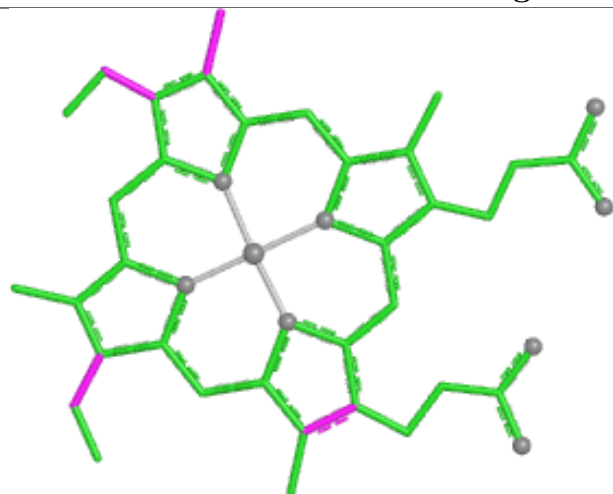


Torsions

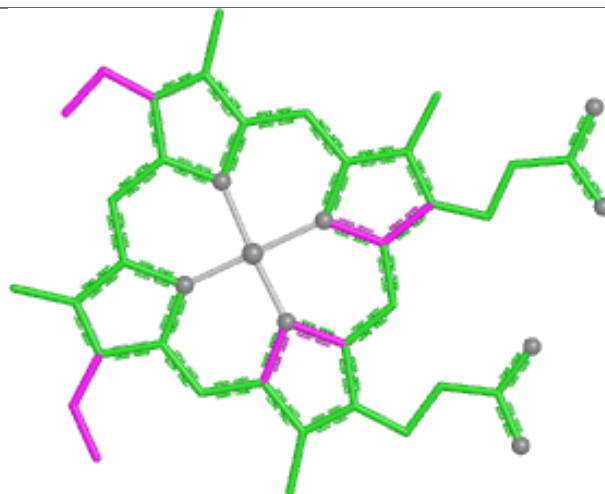


Rings

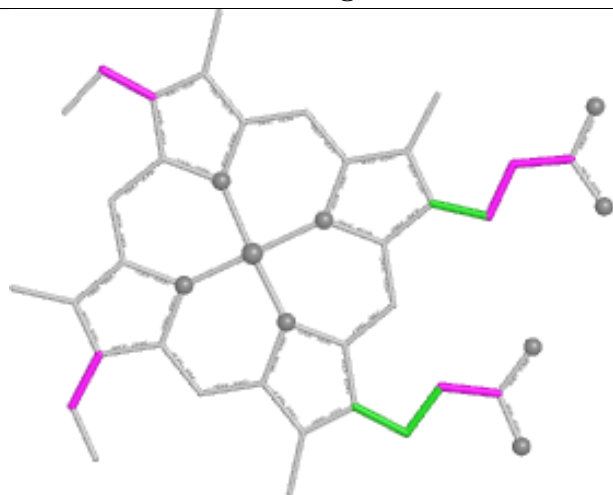
Ligand HEC B 810



Bond lengths



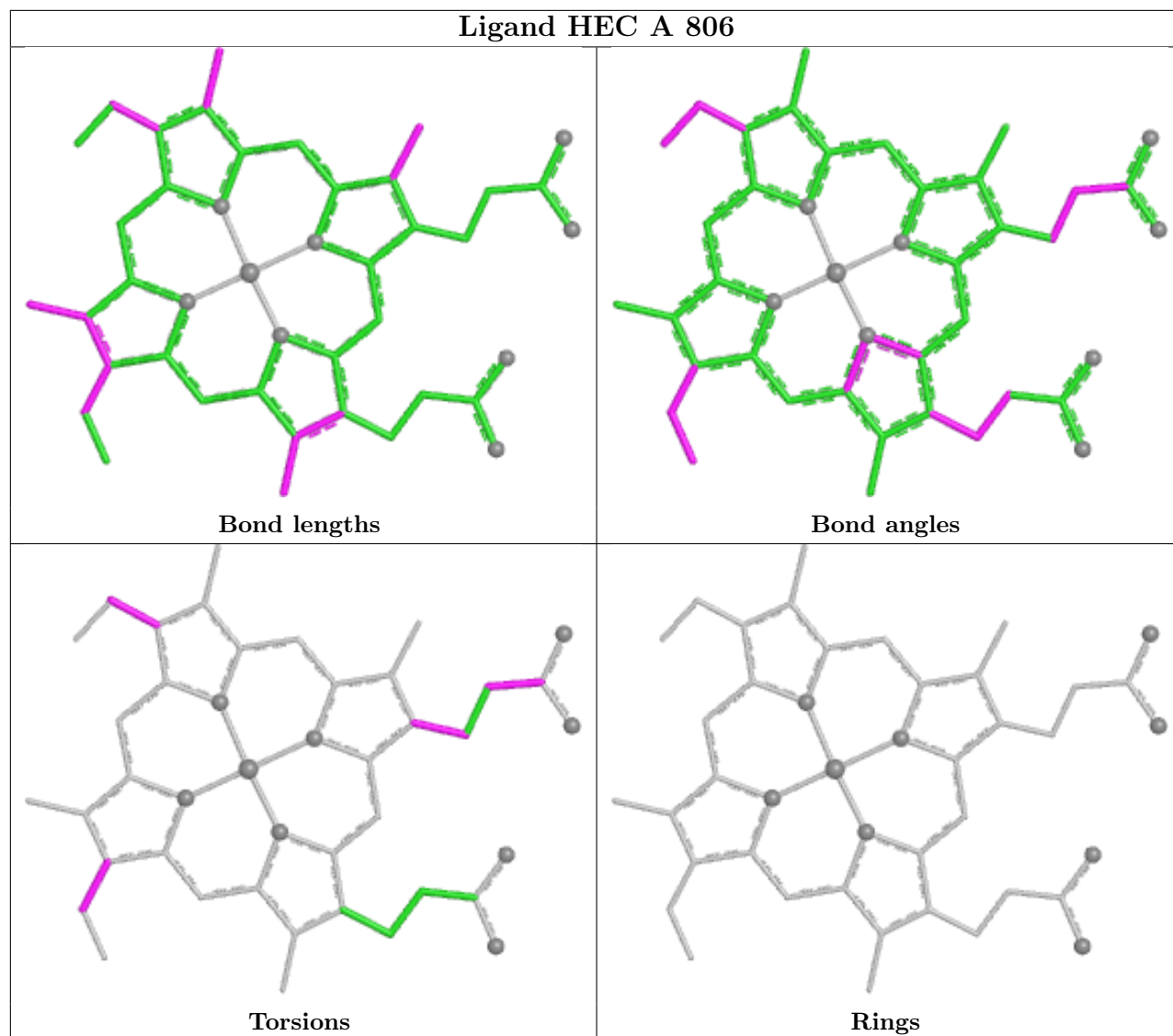
Bond angles



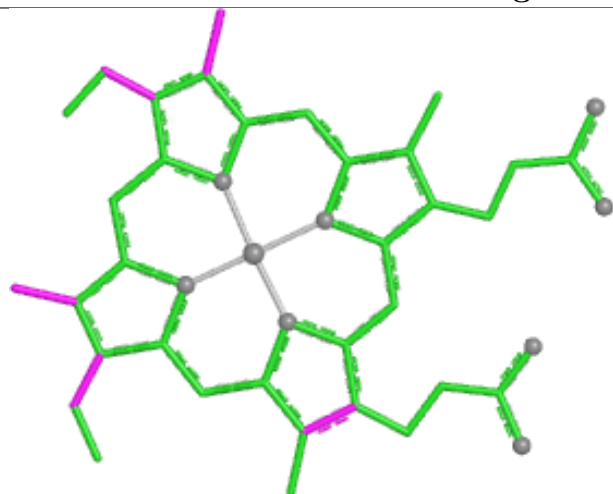
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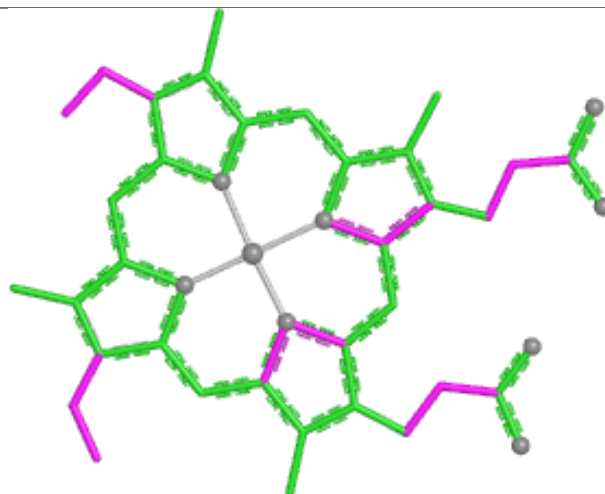
Rings



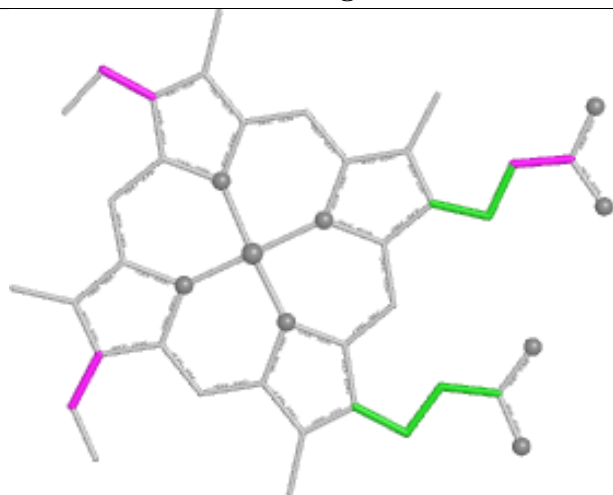
Ligand HEC B 803



Bond lengths



Bond angles

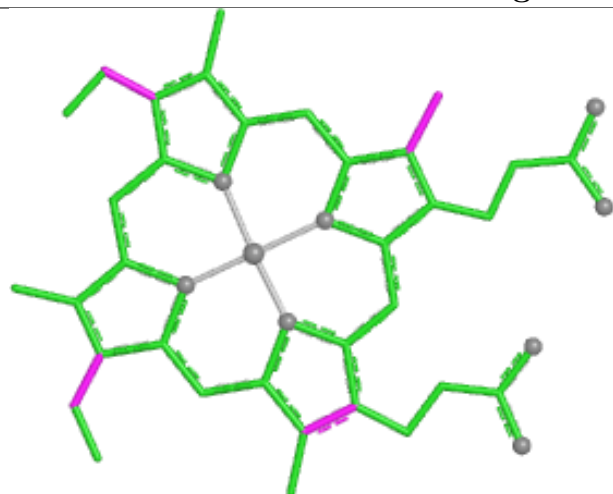


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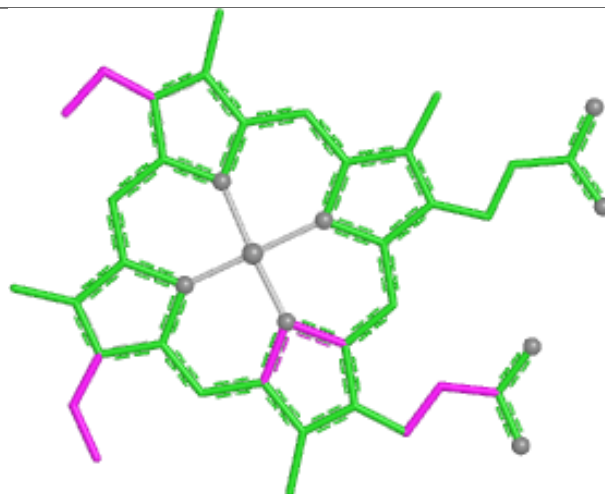


Rings

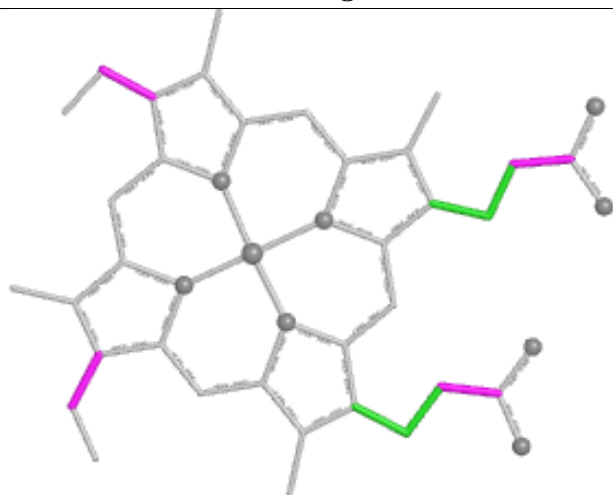
Ligand HEC B 808



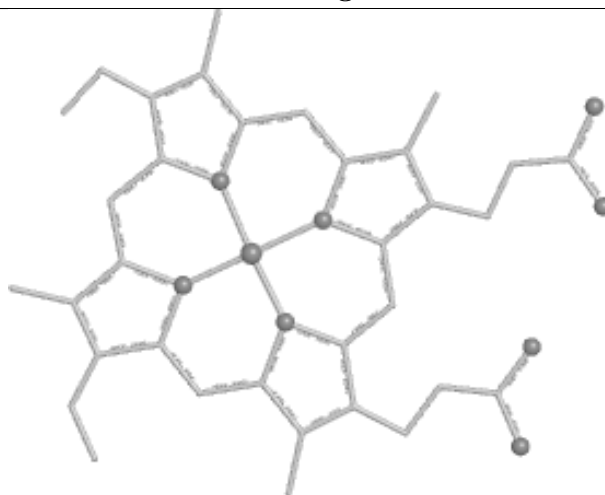
Bond lengths



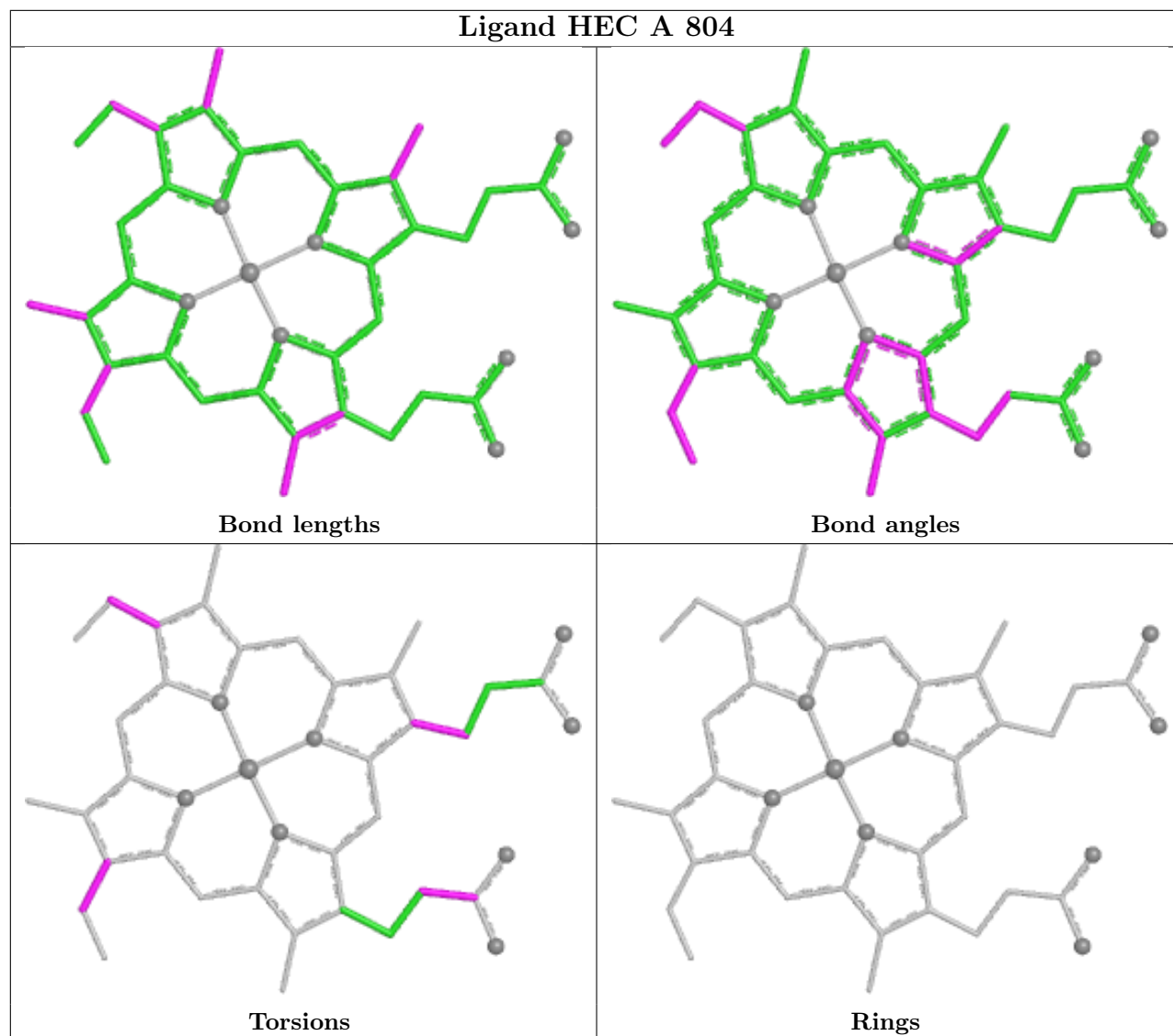
Bond angles



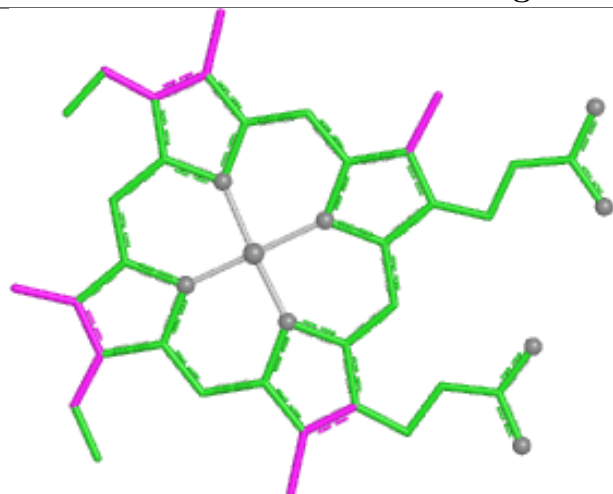
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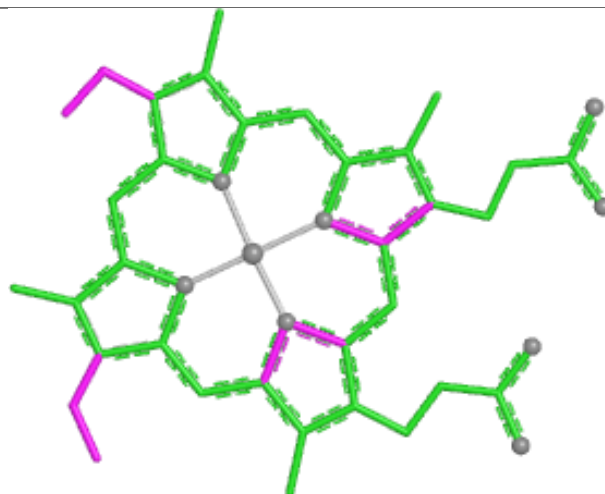
Rings



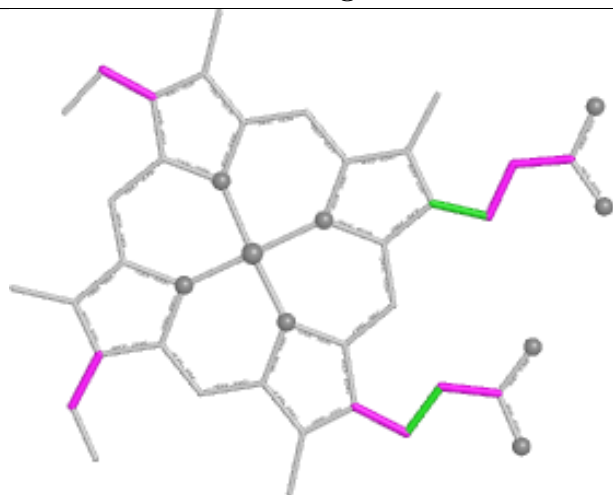
Ligand HEC B 804



Bond lengths



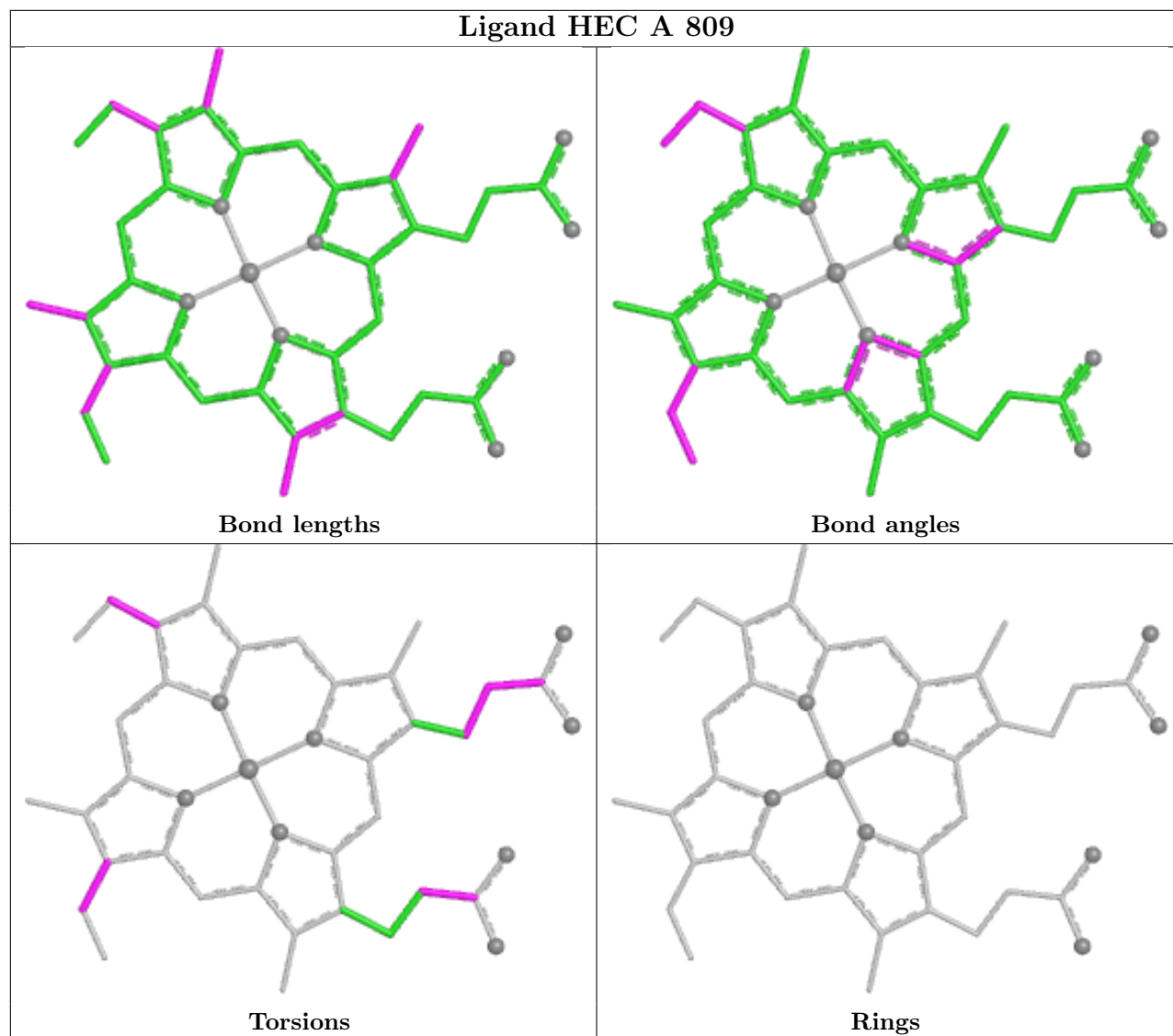
Bond angles



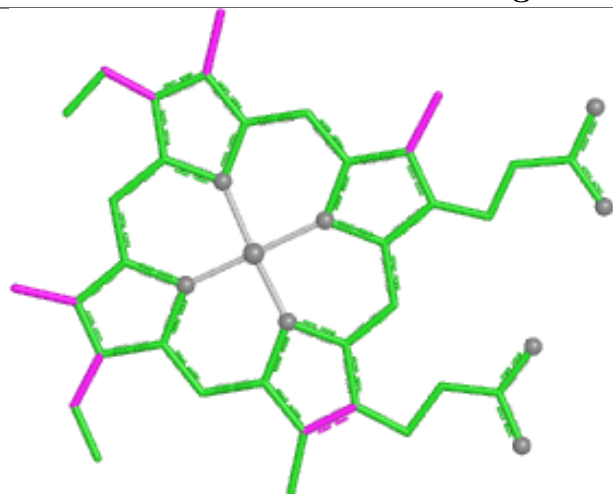
Torsions



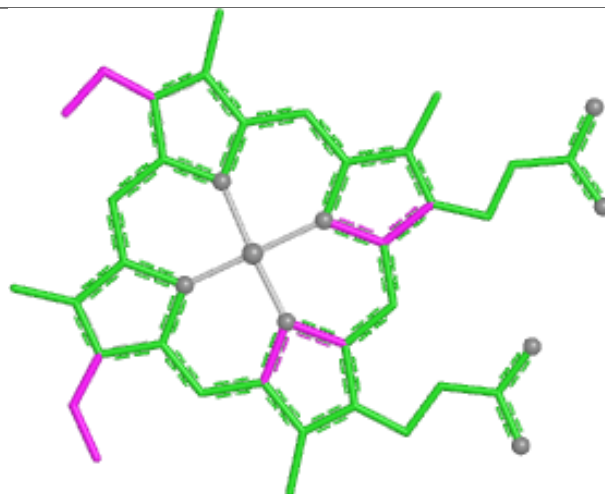
Rings



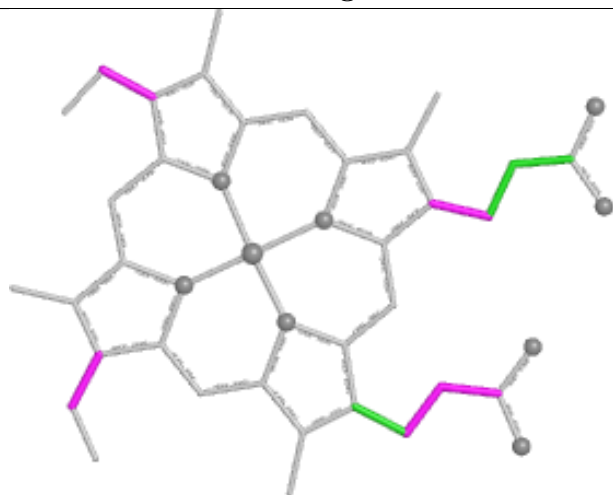
Ligand HEC C 804



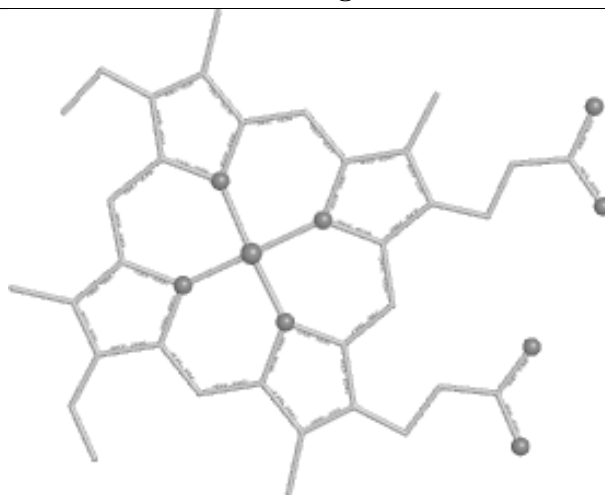
Bond lengths



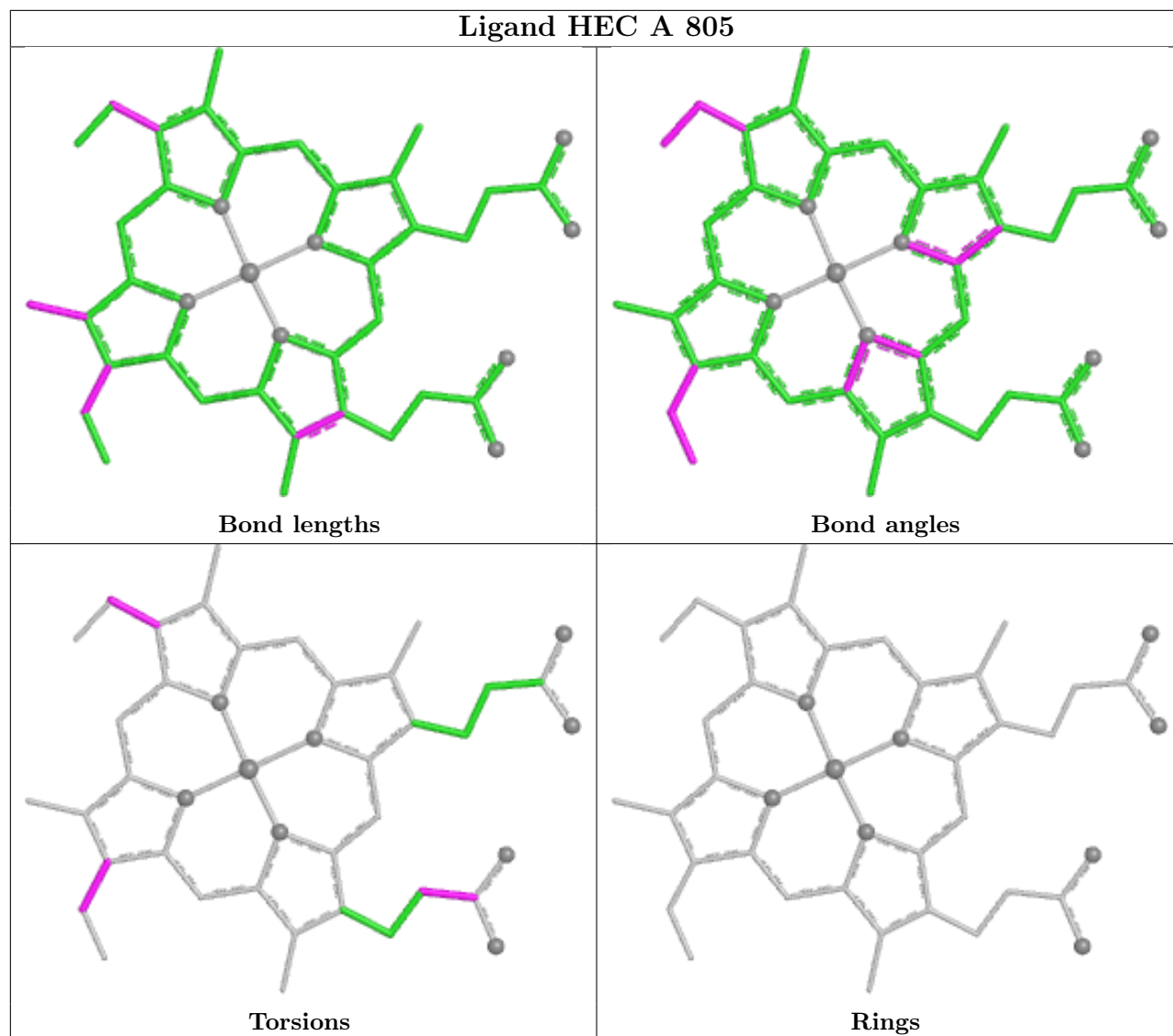
Bond angles



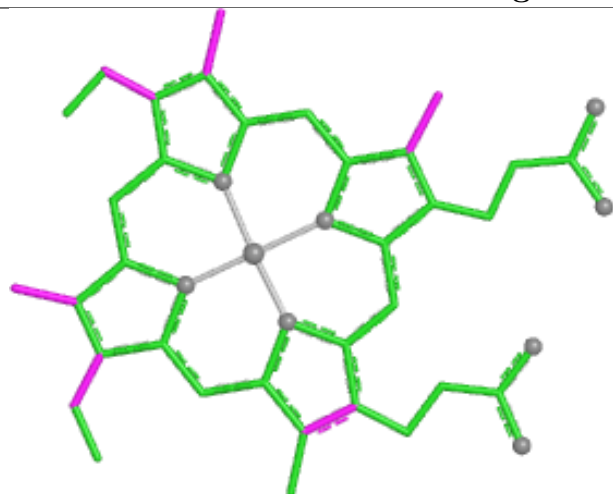
Torsions



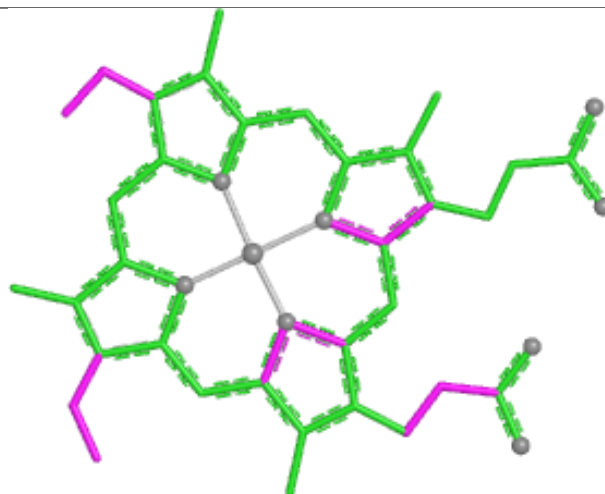
Rings



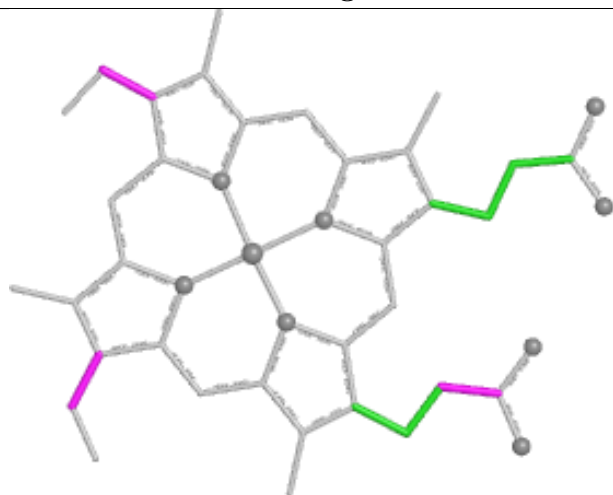
Ligand HEC C 808



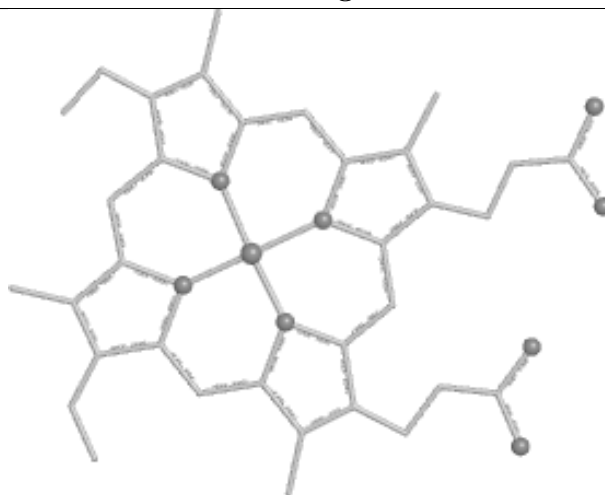
Bond lengths



Bond angles

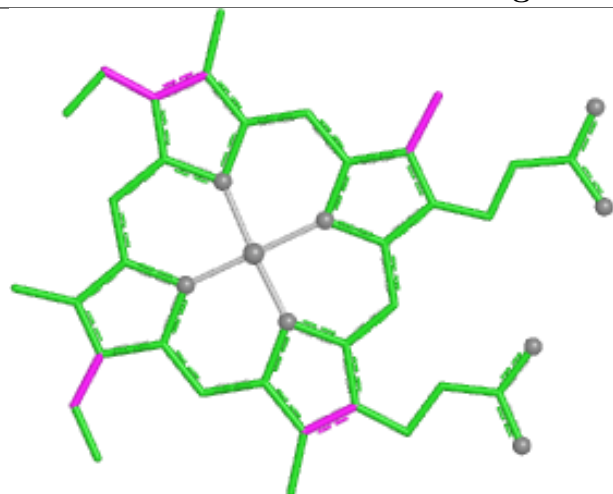


Torsions

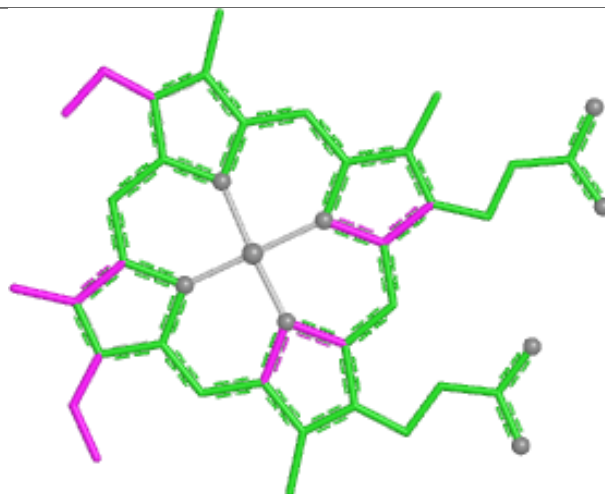


Rings

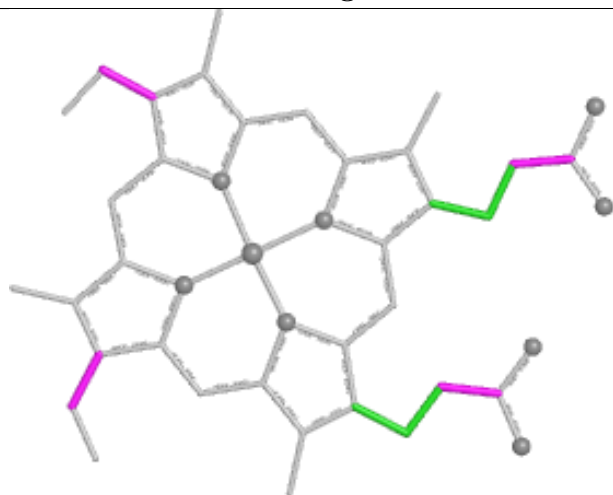
Ligand HEC C 802



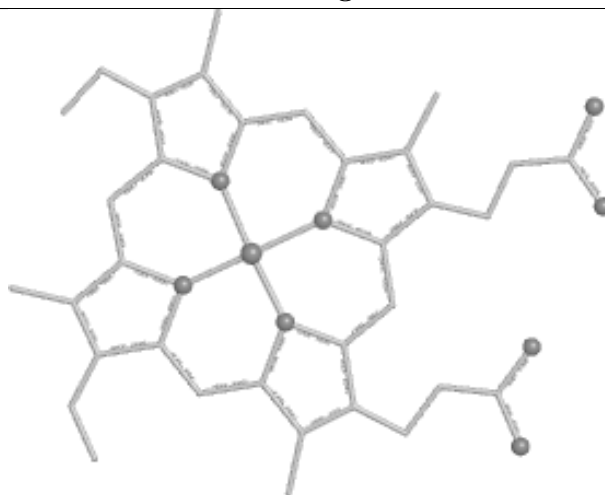
Bond lengths



Bond angles

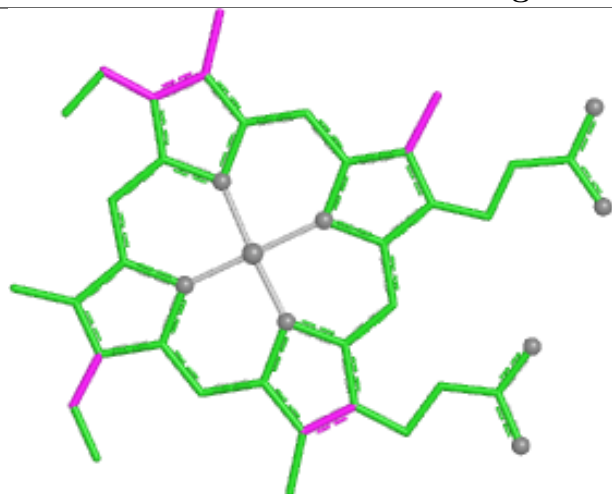


Torsions

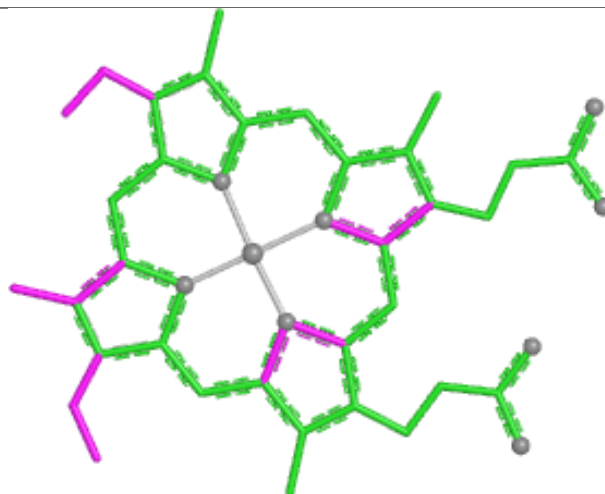


Rings

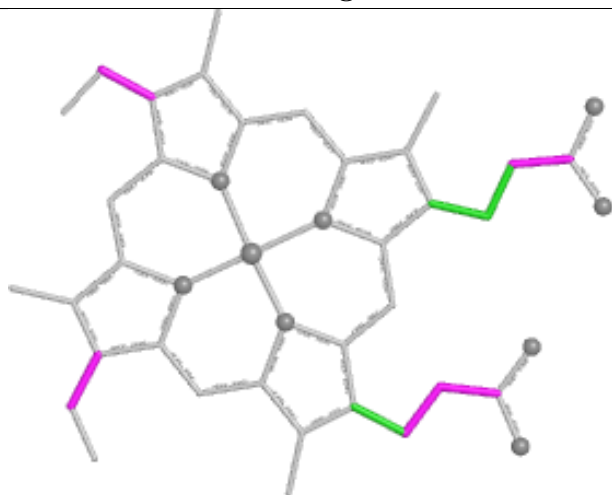
Ligand HEC B 802



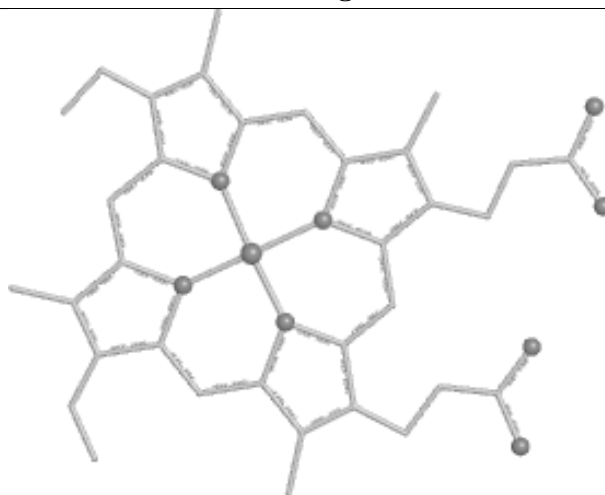
Bond lengths



Bond angles

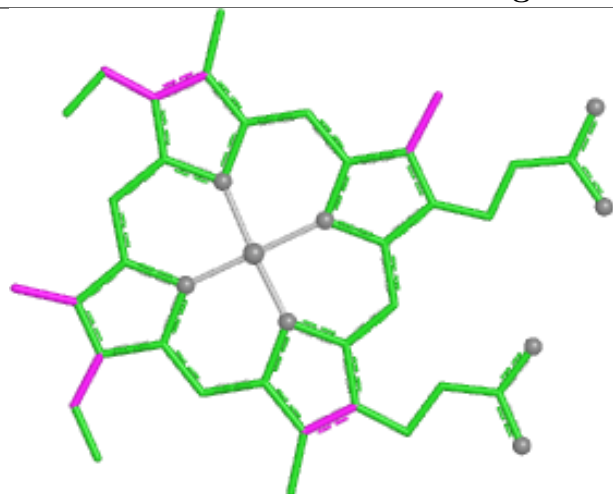


Torsions

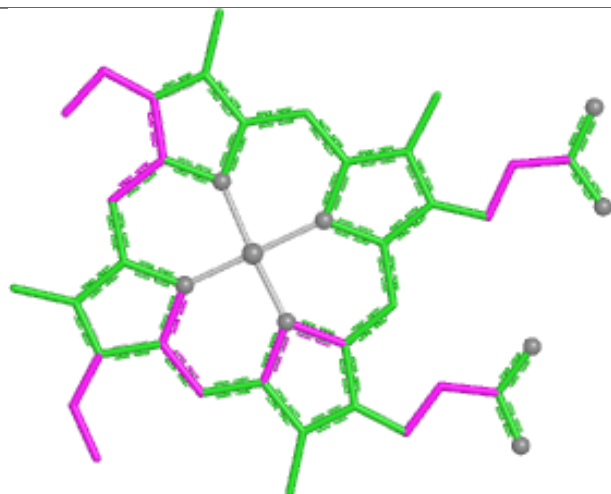


Rings

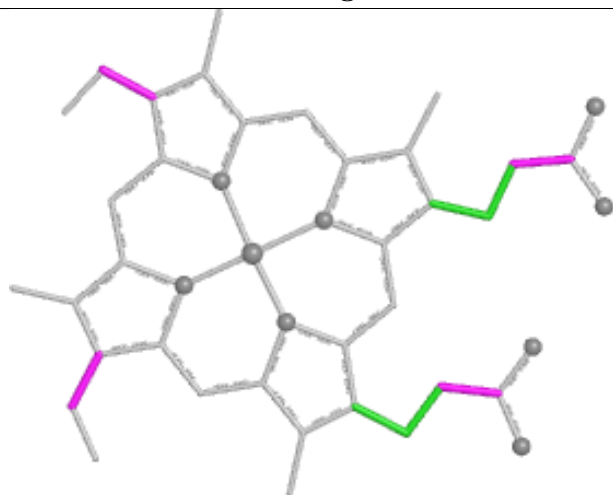
Ligand HEC C 803



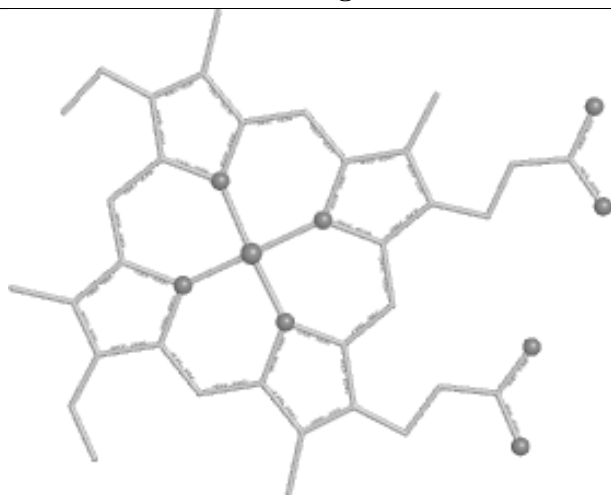
Bond lengths



Bond angles

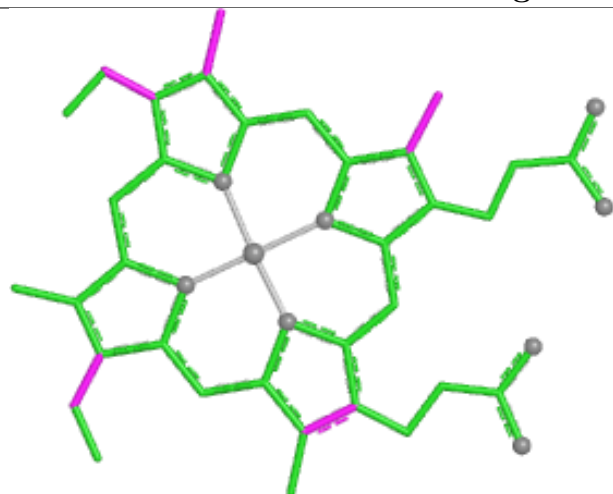


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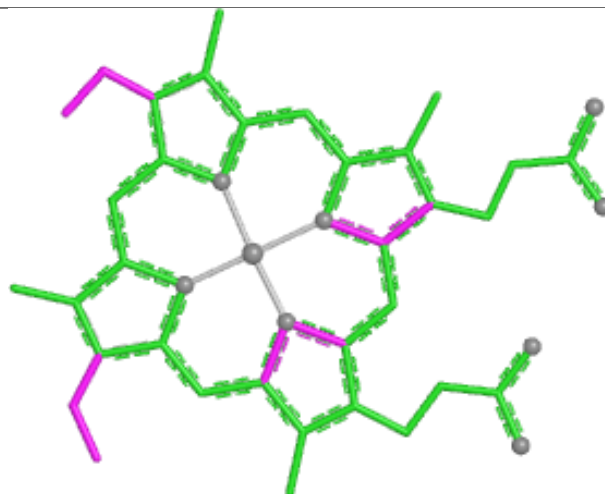


Rings

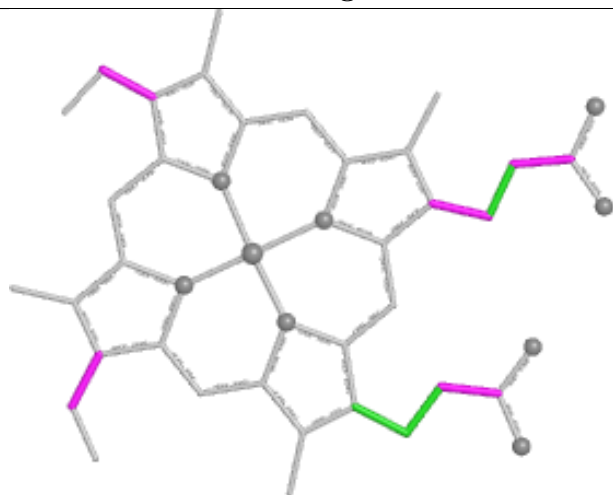
Ligand HEC B 801



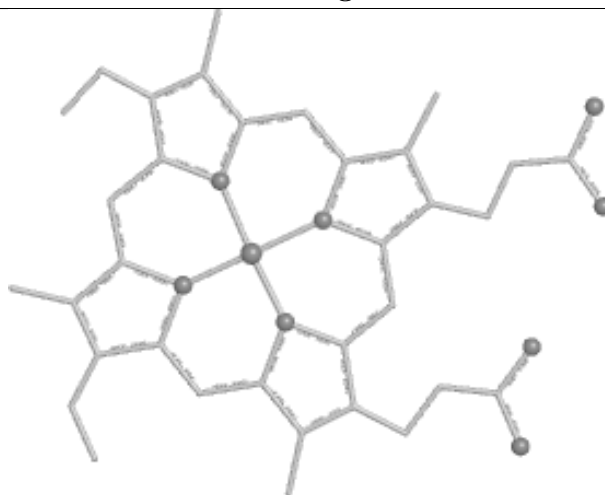
Bond lengths



Bond angles

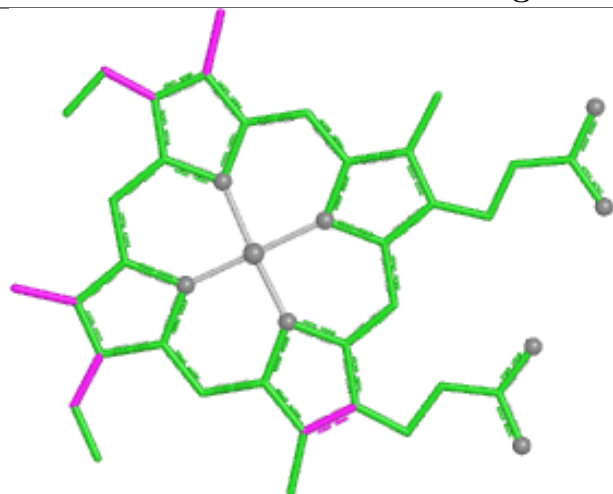


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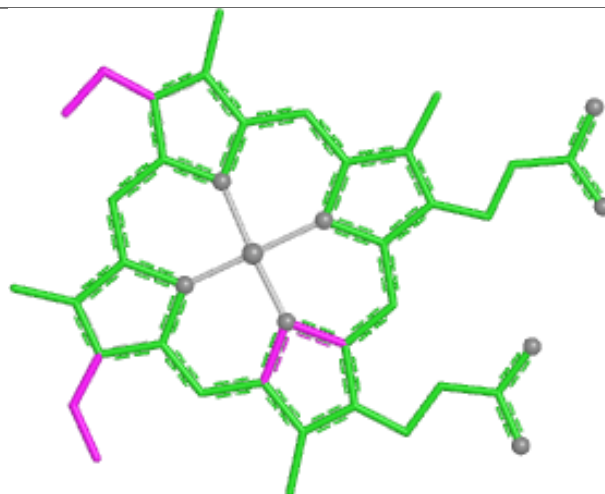


Rings

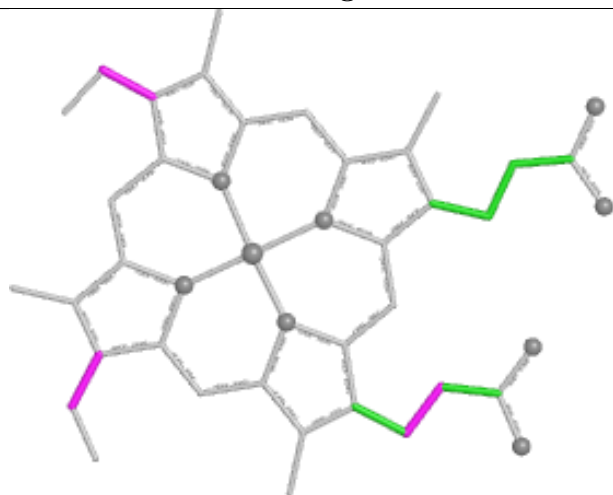
Ligand HEC C 810



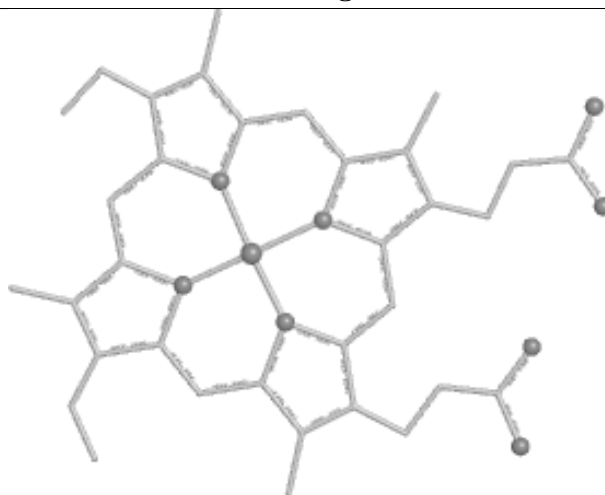
Bond lengths



Bond angles

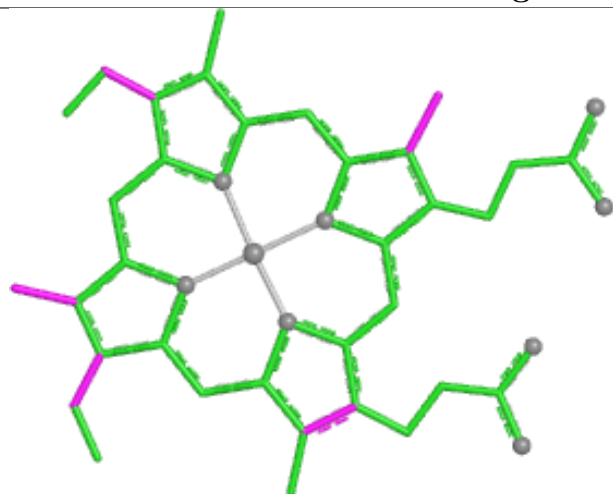


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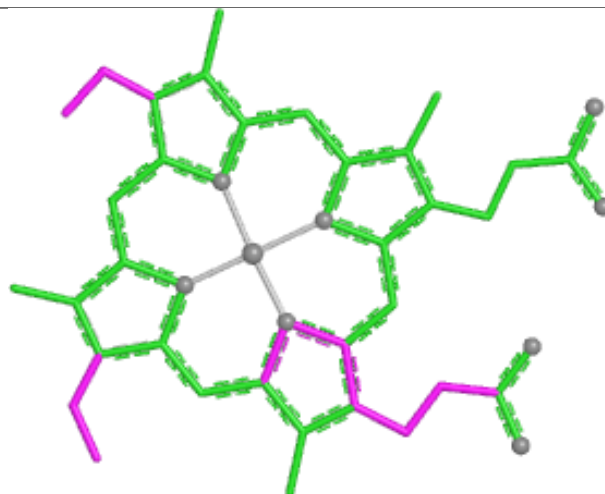


Rings

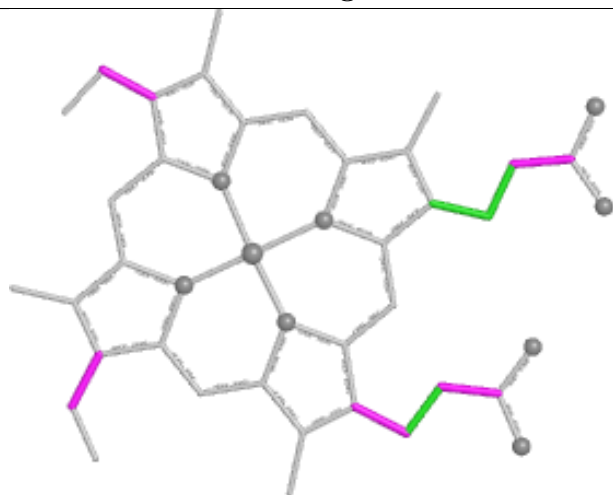
Ligand HEC A 801



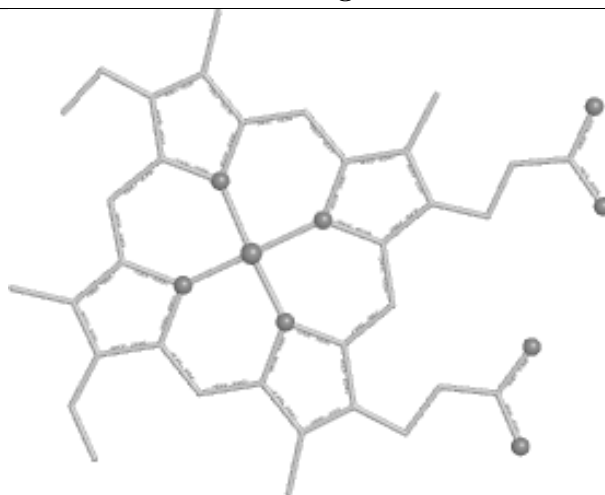
Bond lengths



Bond angles

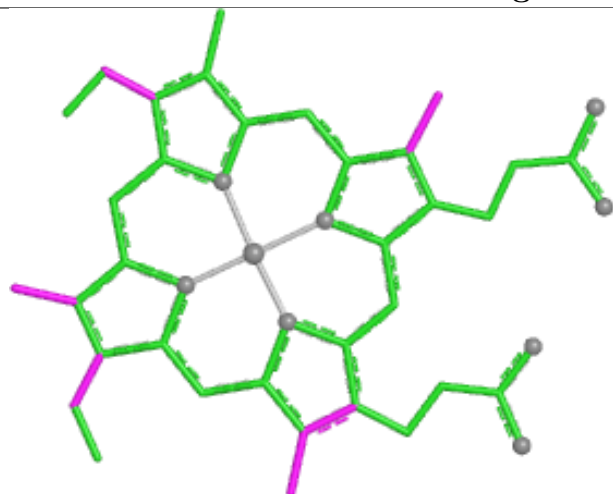


Torsions

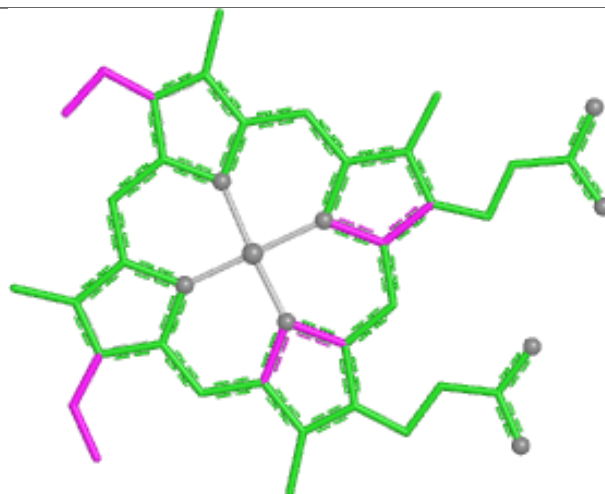


Rings

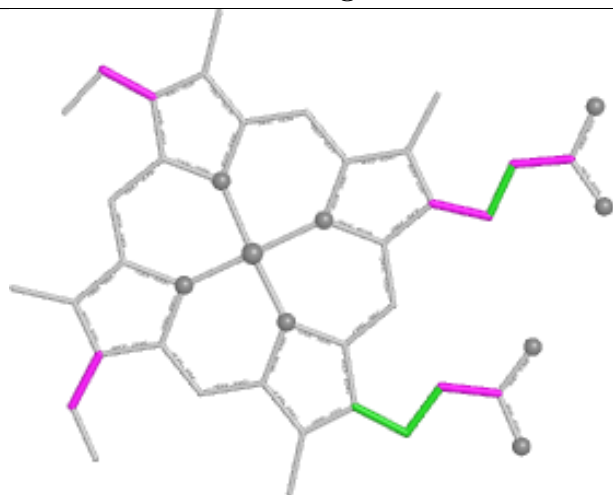
Ligand HEC C 806



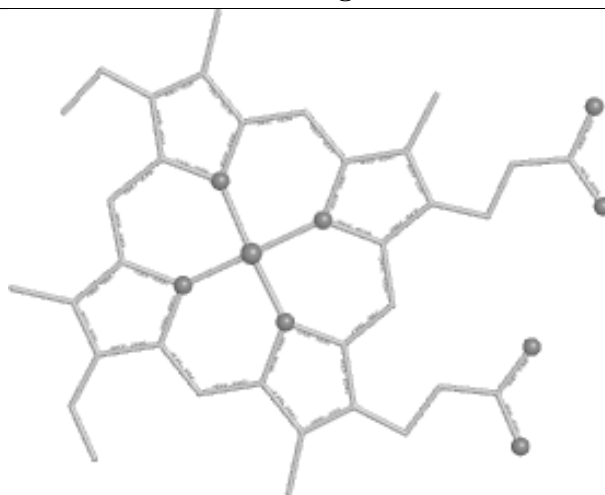
Bond lengths



Bond angles

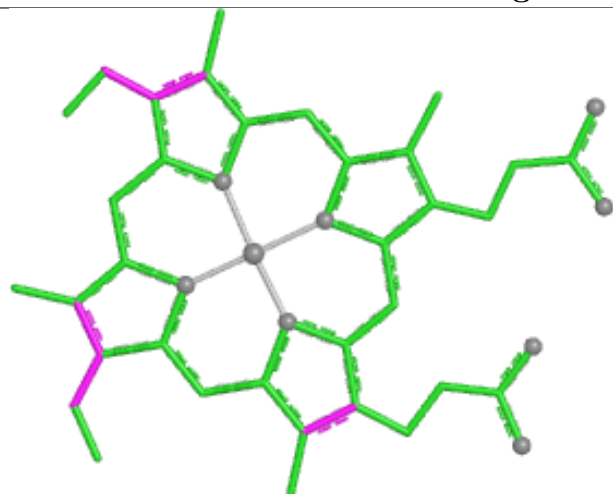


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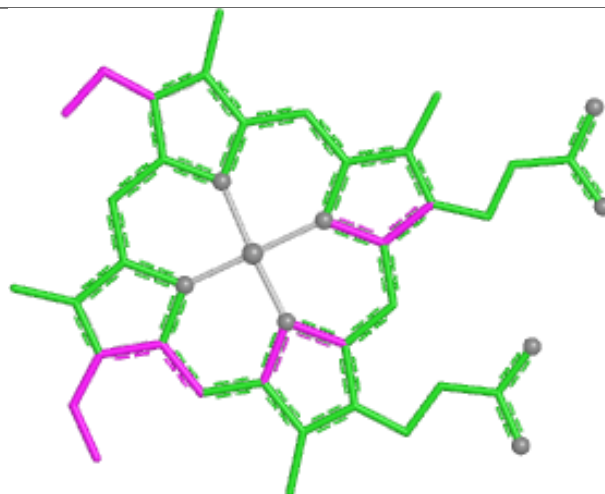


Rings

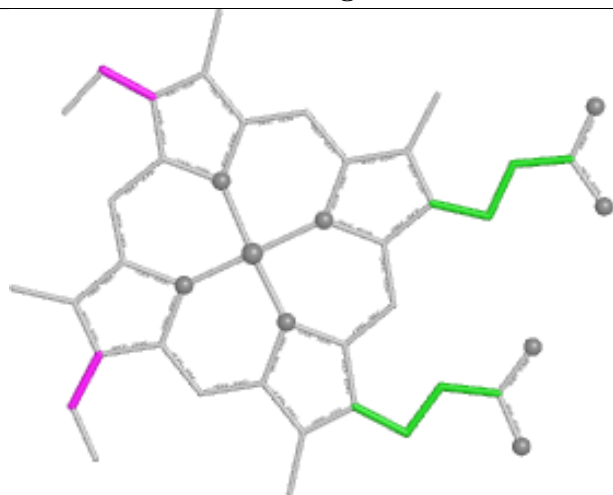
Ligand HEC C 805



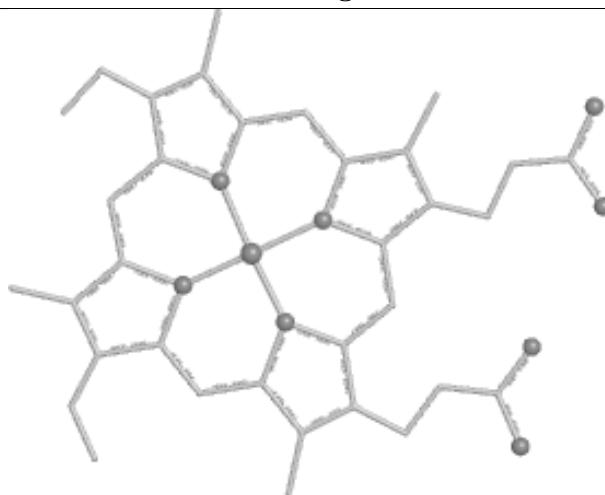
Bond lengths



Bond angles

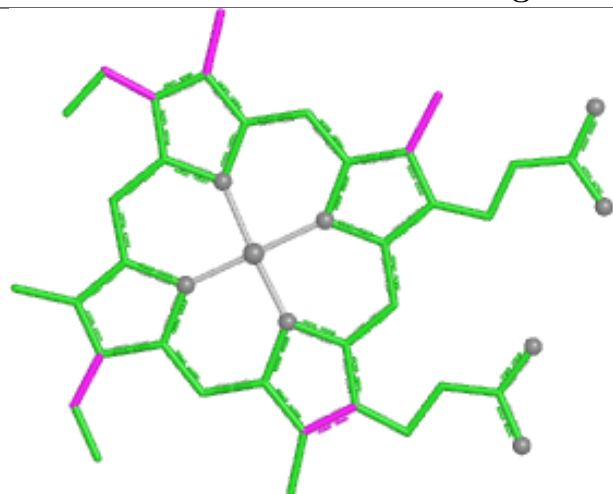


Torsions

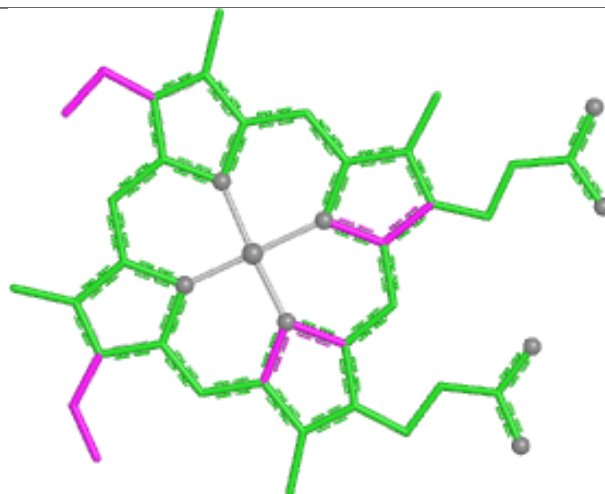


Rings

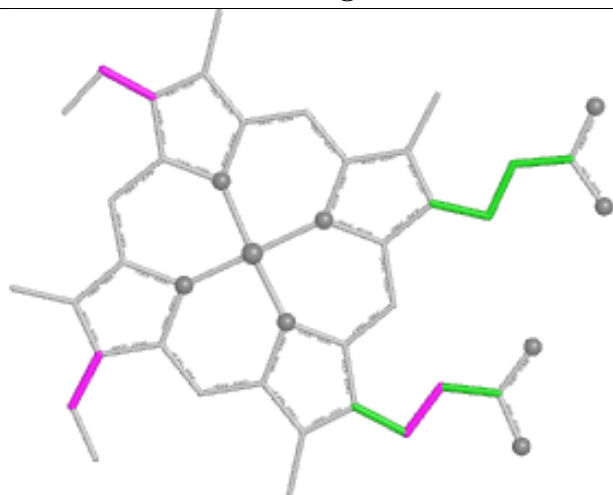
Ligand HEC A 810



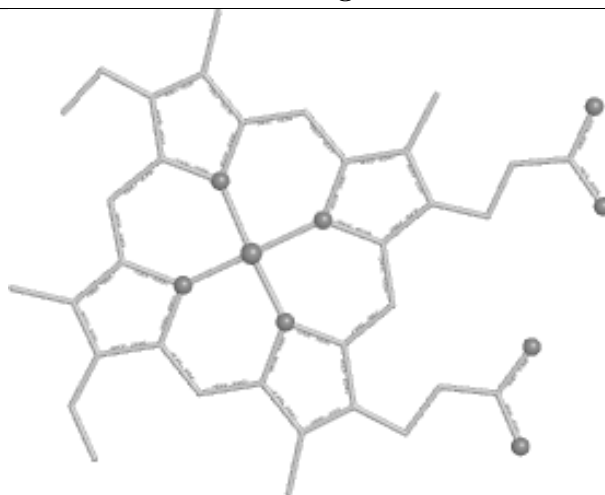
Bond lengths



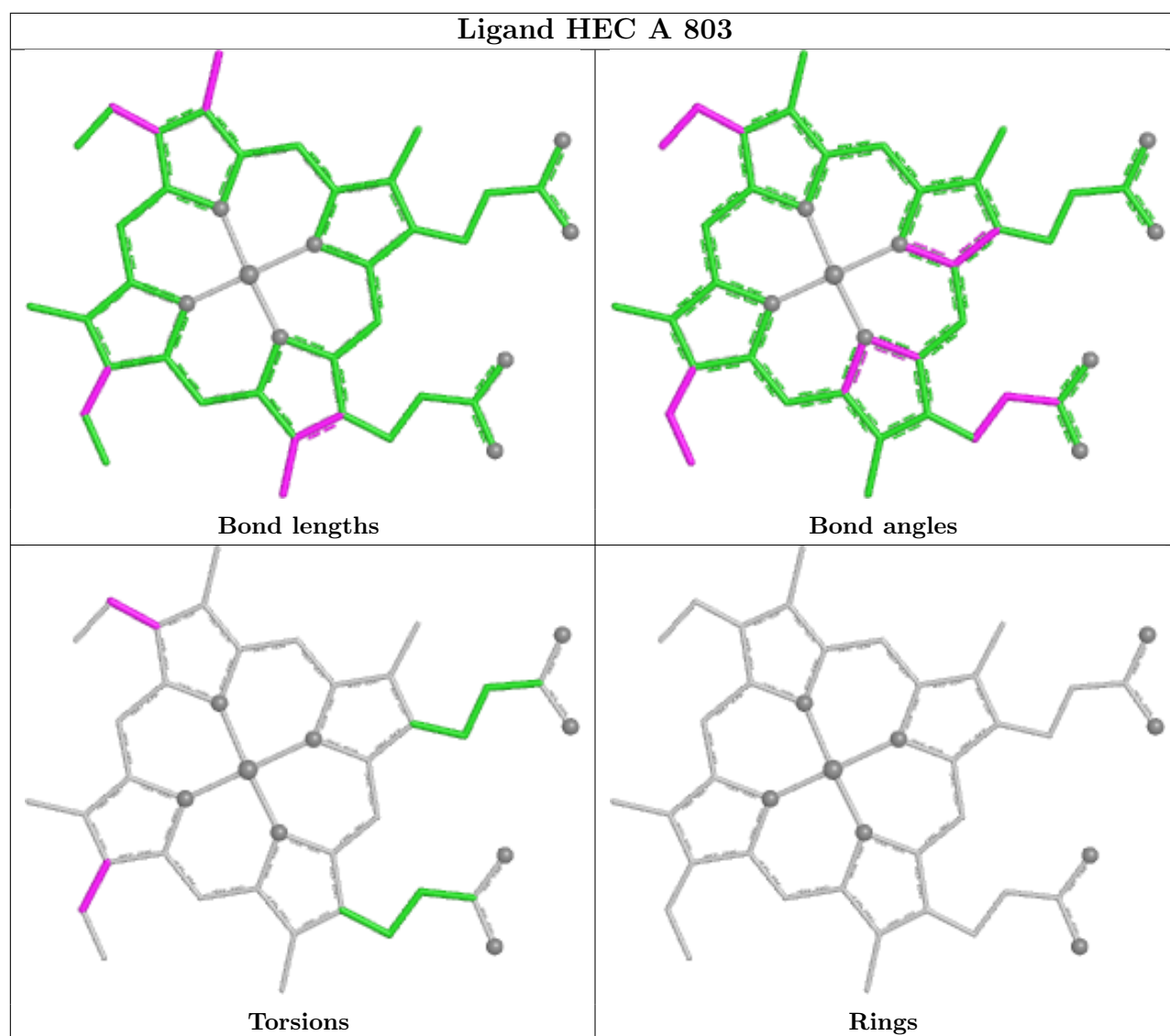
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	605/608 (99%)	-0.13	1 (0%) 91 91	26, 48, 63, 89	2 (0%)
1	B	608/608 (100%)	-0.06	7 (1%) 76 77	38, 49, 65, 113	0
1	C	604/608 (99%)	0.23	22 (3%) 46 48	38, 54, 93, 112	0
All	All	1817/1824 (99%)	0.01	30 (1%) 69 70	26, 50, 78, 113	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	650	MET	6.7
1	B	43	ALA	5.7
1	A	46	ILE	4.4
1	C	115	ALA	4.2
1	B	44	PRO	3.5
1	C	119	PRO	2.8
1	C	167	THR	2.8
1	C	77	VAL	2.8
1	C	128	GLY	2.7
1	C	78	VAL	2.6
1	C	122	PHE	2.5
1	C	62	VAL	2.5
1	C	180	ALA	2.5
1	B	45	ALA	2.4
1	C	649	LYS	2.4
1	C	65	VAL	2.4
1	B	46	ILE	2.3
1	C	176	VAL	2.3
1	C	51	PHE	2.2
1	C	255	GLN	2.2
1	C	75	LEU	2.2
1	C	161	THR	2.2
1	C	454	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	116	ALA	2.2
1	B	166	GLY	2.1
1	B	115	ALA	2.1
1	C	114	VAL	2.1
1	C	68	THR	2.0
1	C	86	ALA	2.0
1	C	184	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	C	812	1/1	0.81	0.39	83,83,83,83	0
4	EDO	A	814	4/4	0.84	0.15	58,58,64,64	0
3	CA	B	812	1/1	0.86	0.38	77,77,77,77	0
4	EDO	A	813	4/4	0.94	0.12	51,52,53,56	0
2	HEC	C	802	43/43	0.94	0.11	50,56,70,78	0
2	HEC	A	802	43/43	0.95	0.11	41,46,66,80	0
2	HEC	C	804	43/43	0.95	0.10	45,52,70,80	0
2	HEC	C	805	43/43	0.95	0.10	51,60,66,73	0
2	HEC	A	806	43/43	0.95	0.10	36,41,53,59	0
3	CA	B	813	1/1	0.95	0.06	81,81,81,81	0
2	HEC	B	802	43/43	0.95	0.10	41,48,66,73	0
3	CA	C	813	1/1	0.95	0.05	80,80,80,80	0
2	HEC	B	805	43/43	0.95	0.09	38,44,53,62	0
2	HEC	C	801	43/43	0.95	0.10	38,49,60,66	0
2	HEC	B	804	43/43	0.96	0.10	36,42,70,78	0
2	HEC	C	806	43/43	0.96	0.09	31,42,49,53	0

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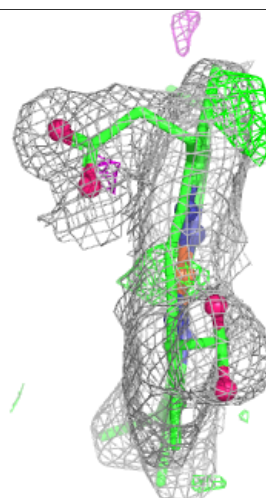
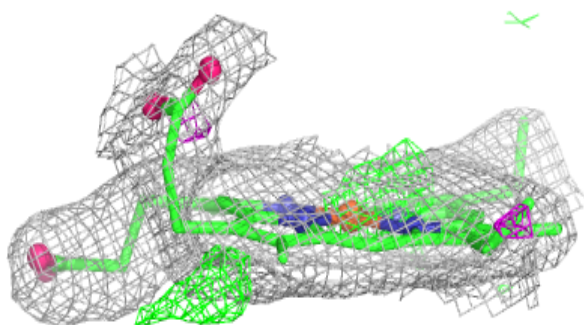
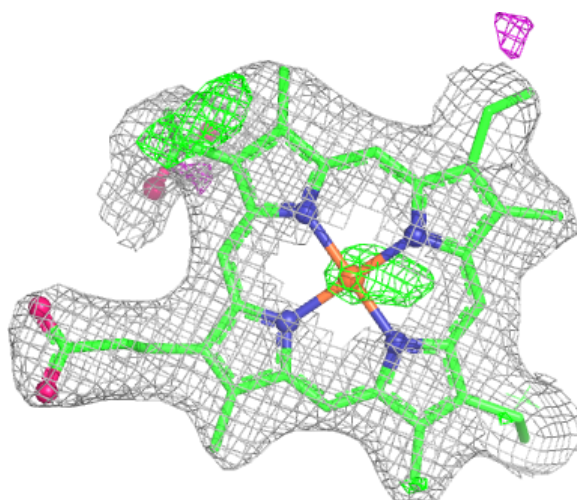
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	812	1/1	0.96	0.11	77,77,77,77	0
2	HEC	A	805	43/43	0.96	0.09	41,51,63,66	0
2	HEC	B	806	43/43	0.96	0.09	37,43,52,54	0
2	HEC	A	801	43/43	0.96	0.09	36,44,63,69	0
2	HEC	A	809	43/43	0.96	0.08	37,44,59,65	0
2	HEC	C	803	43/43	0.96	0.08	44,48,56,58	0
2	HEC	A	804	43/43	0.96	0.09	34,48,67,72	0
2	HEC	B	808	43/43	0.97	0.07	35,40,43,46	0
2	HEC	C	807	43/43	0.97	0.07	35,41,45,46	0
2	HEC	C	808	43/43	0.97	0.07	35,41,44,47	0
2	HEC	C	809	43/43	0.97	0.08	31,39,54,61	0
2	HEC	C	810	43/43	0.97	0.08	33,39,52,62	0
2	HEC	B	809	43/43	0.97	0.09	34,42,58,71	0
2	HEC	B	810	43/43	0.97	0.09	37,43,58,64	0
2	HEC	A	807	43/43	0.97	0.07	32,40,45,50	0
2	HEC	A	803	43/43	0.97	0.07	35,42,44,47	0
2	HEC	A	810	43/43	0.97	0.07	37,45,52,57	0
2	HEC	B	801	43/43	0.97	0.08	35,41,55,63	0
2	HEC	B	807	43/43	0.97	0.07	34,41,45,49	0
2	HEC	B	803	43/43	0.98	0.07	35,41,46,50	0
3	CA	C	811	1/1	0.98	0.09	47,47,47,47	0
2	HEC	A	808	43/43	0.98	0.06	34,39,45,46	0
3	CA	A	811	1/1	0.99	0.05	47,47,47,47	0
3	CA	B	811	1/1	1.00	0.10	45,45,45,45	0

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

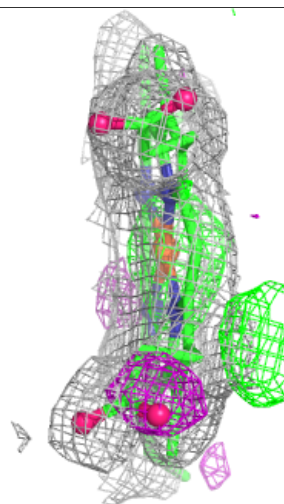
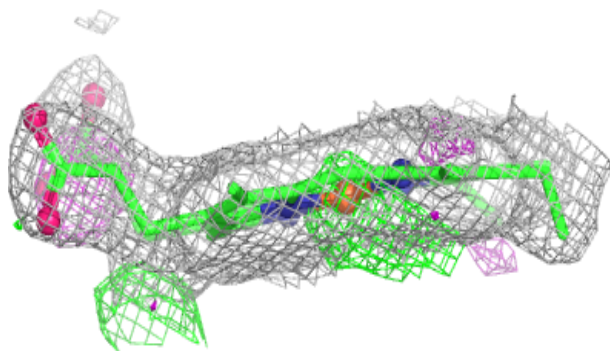
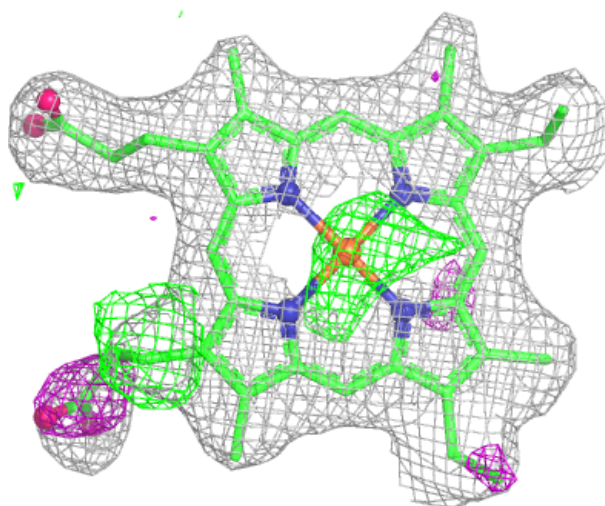
Electron density around HEC C 802:

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



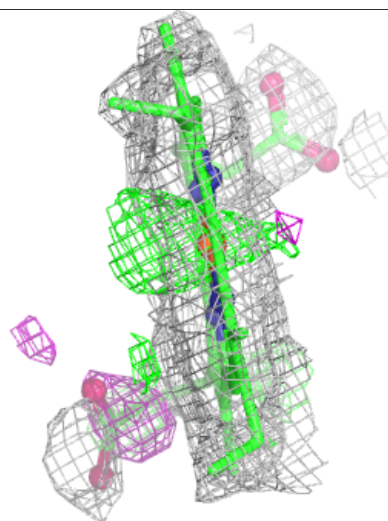
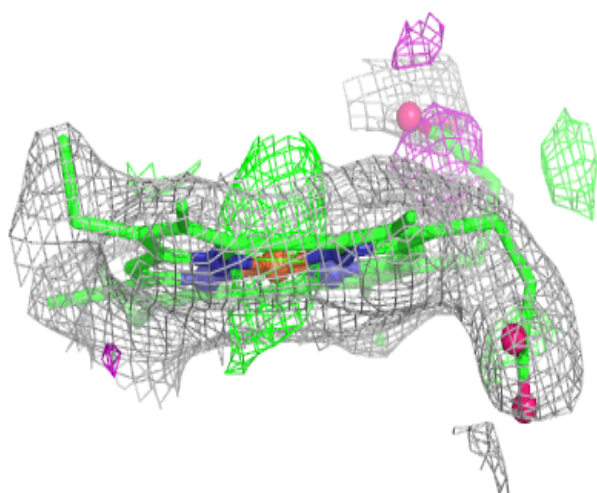
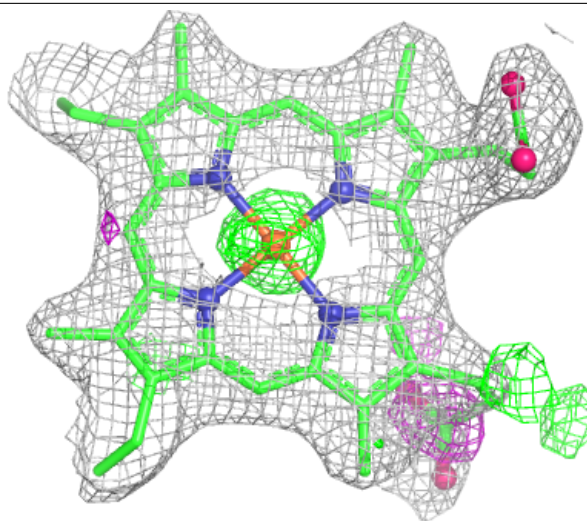
Electron density around HEC A 802:

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



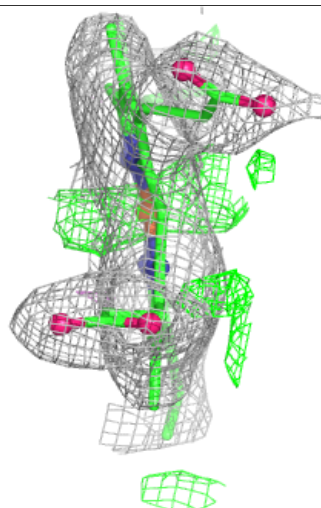
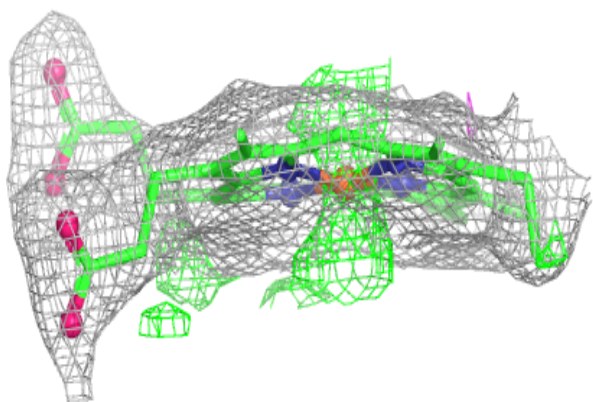
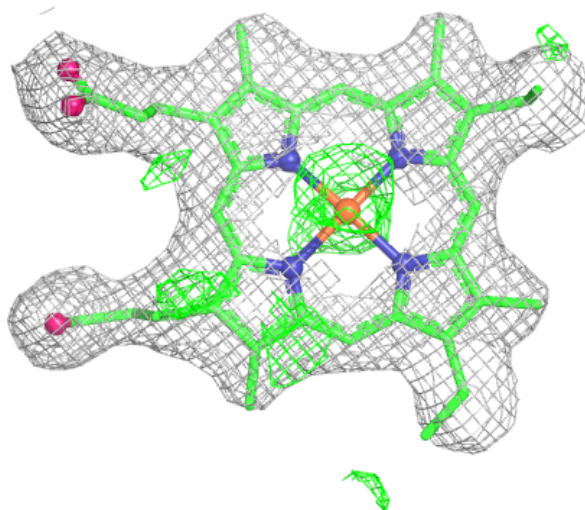
Electron density around HEC C 804:

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



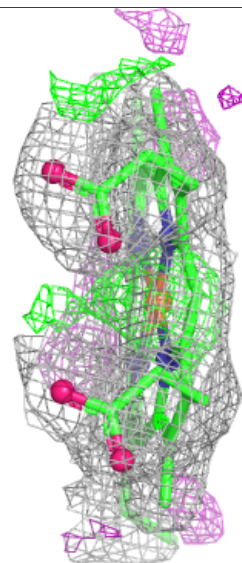
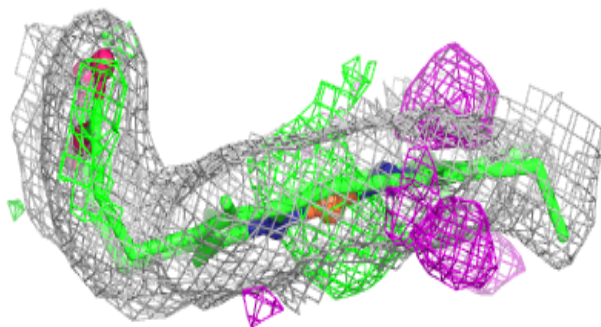
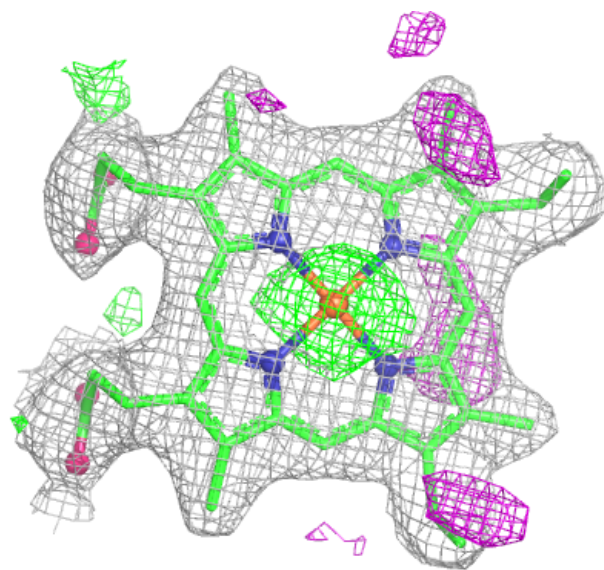
Electron density around HEC C 805:

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



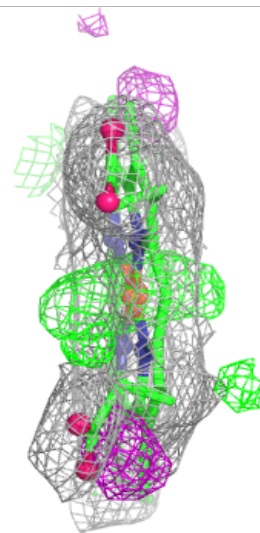
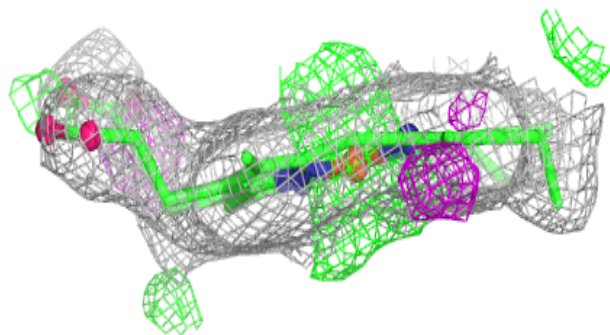
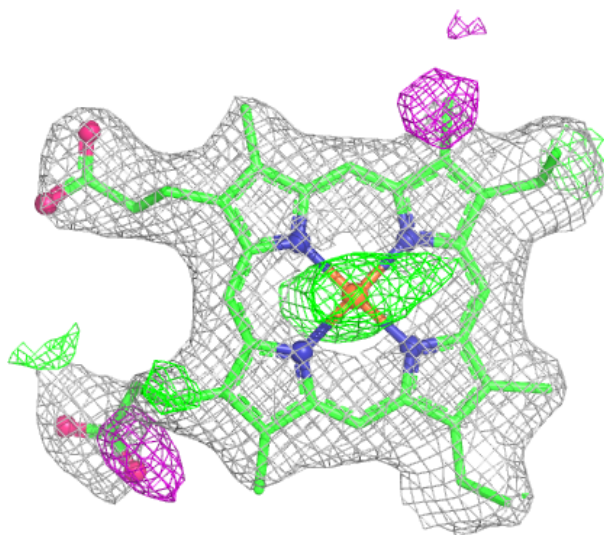
Electron density around HEC A 806:

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



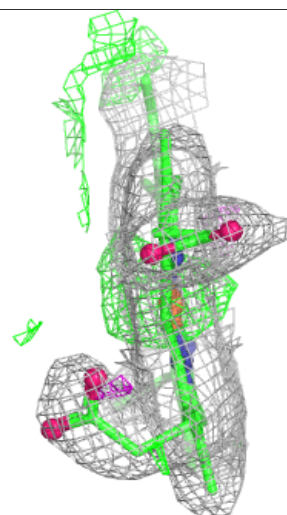
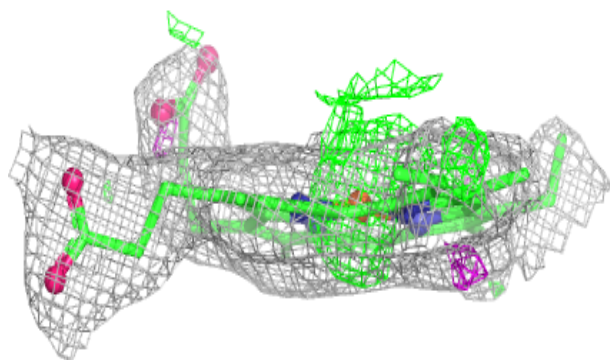
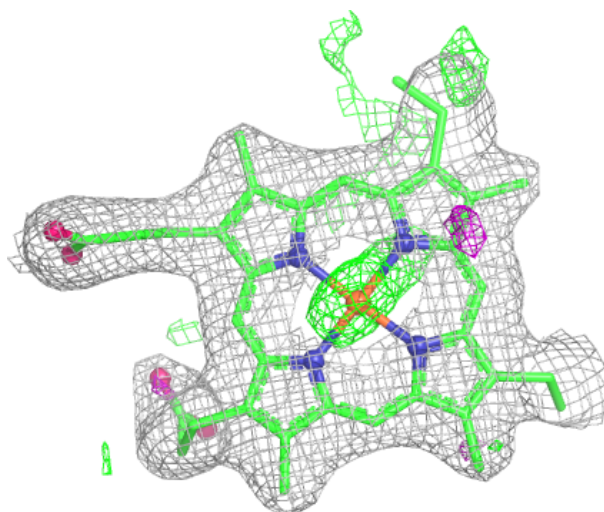
Electron density around HEC B 802:

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



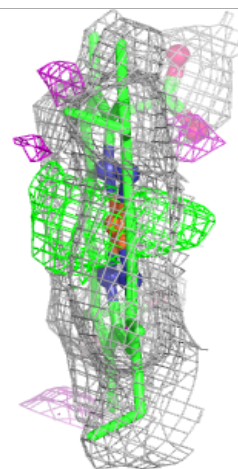
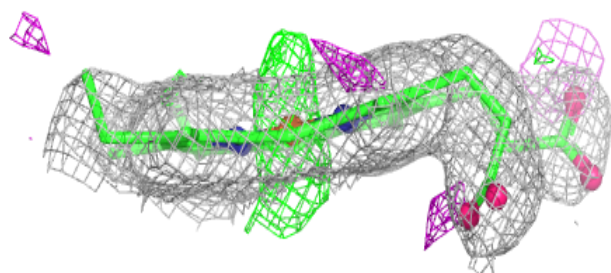
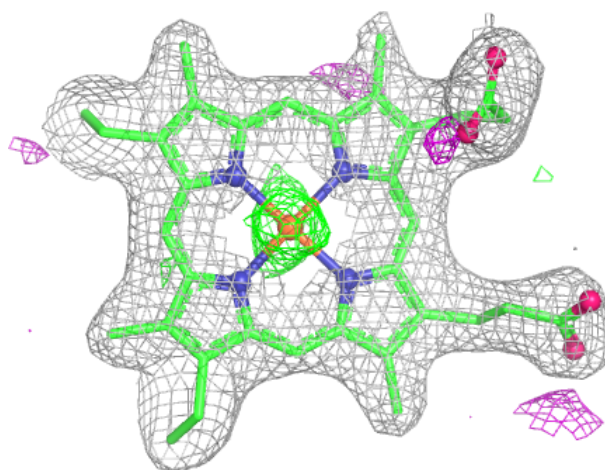
Electron density around HEC B 805:

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



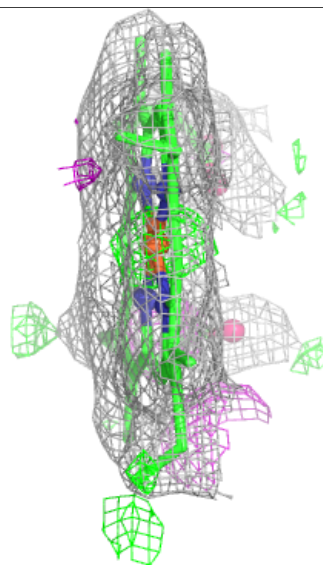
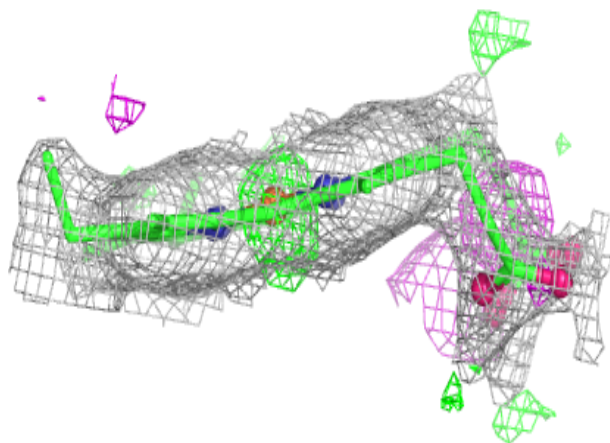
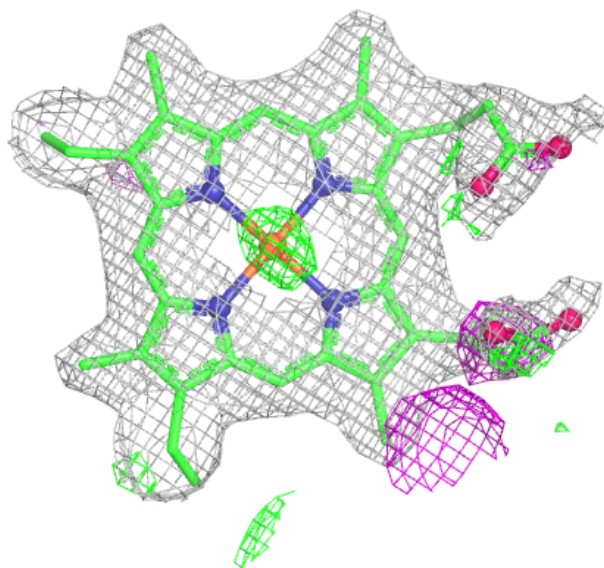
Electron density around HEC C 801:

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



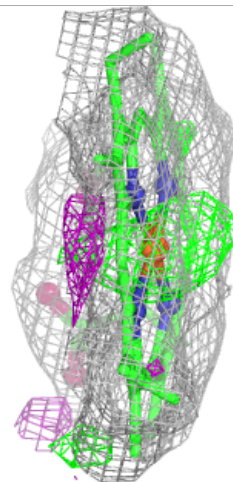
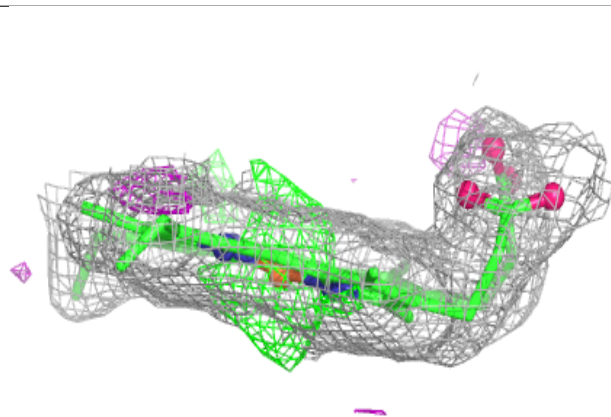
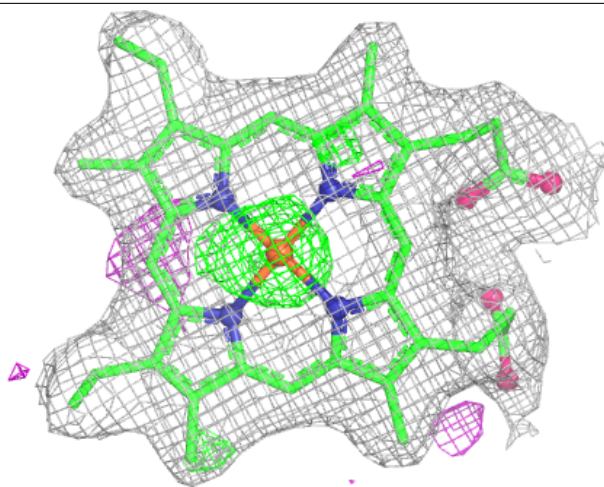
Electron density around HEC B 804:

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



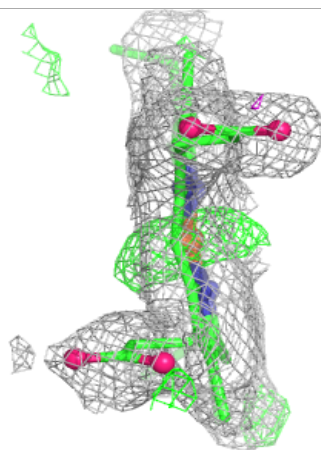
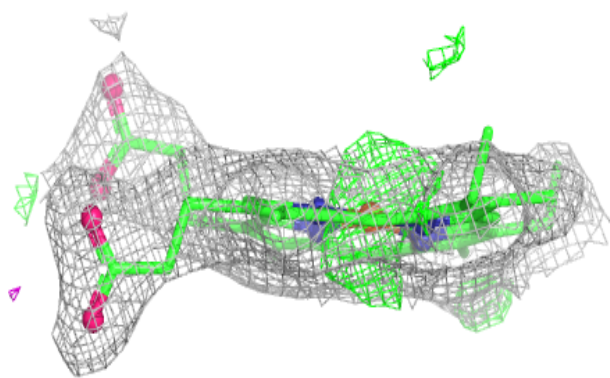
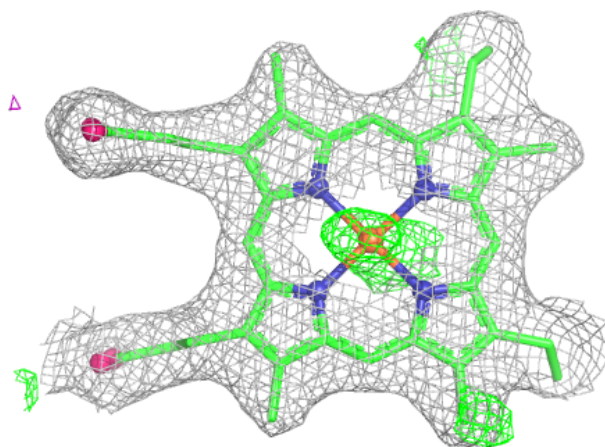
Electron density around HEC C 806:

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



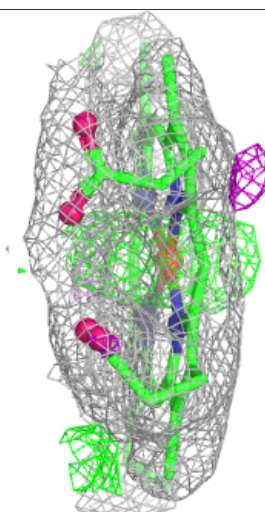
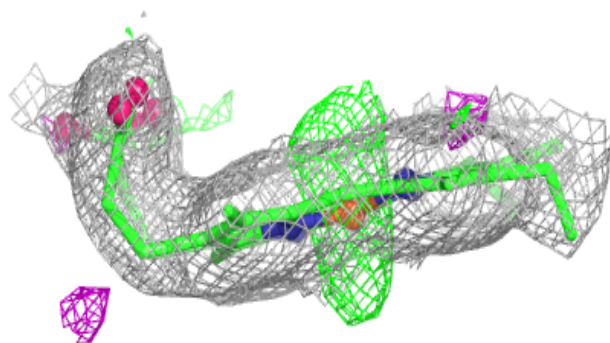
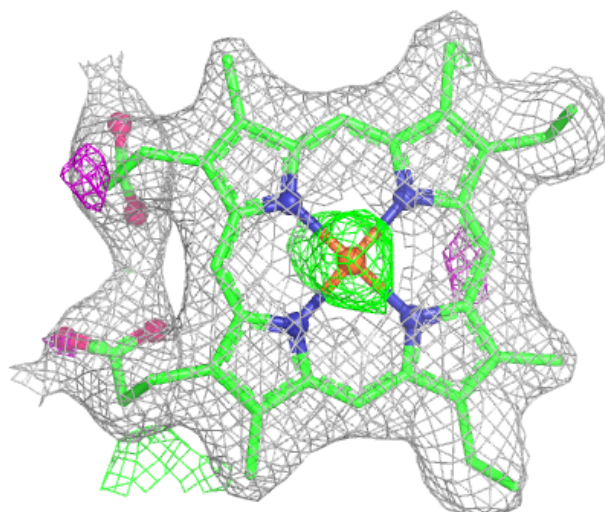
Electron density around HEC A 805:

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



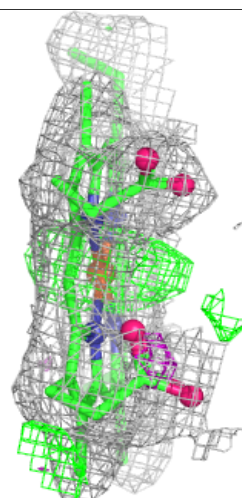
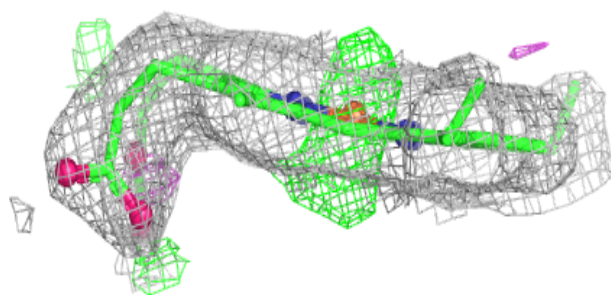
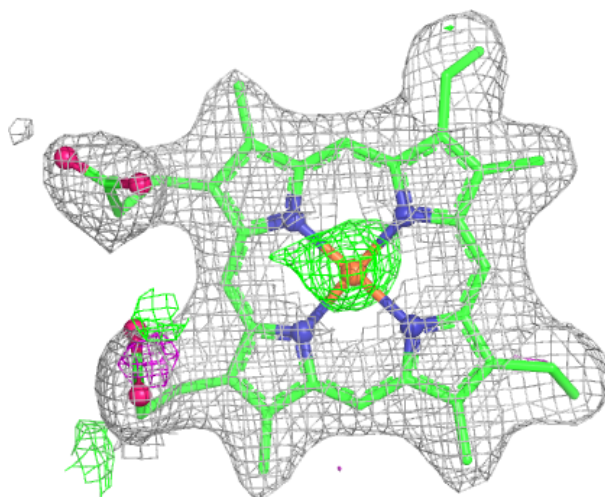
Electron density around HEC B 806:

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



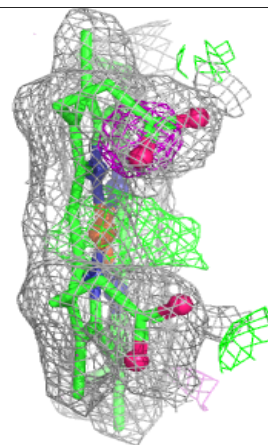
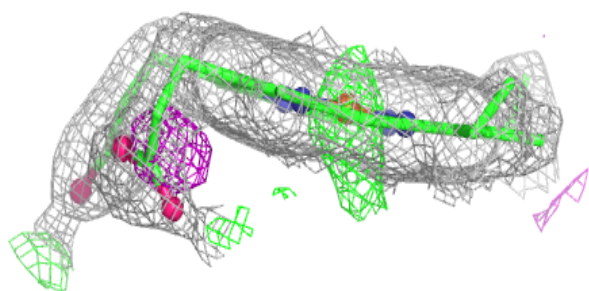
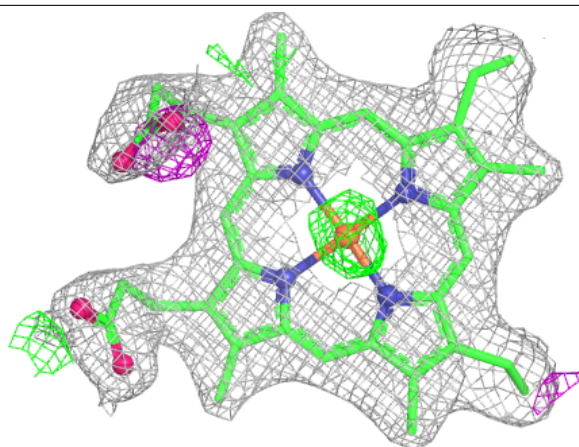
Electron density around HEC A 801:

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

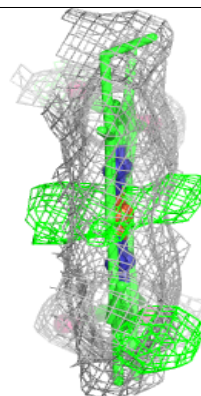
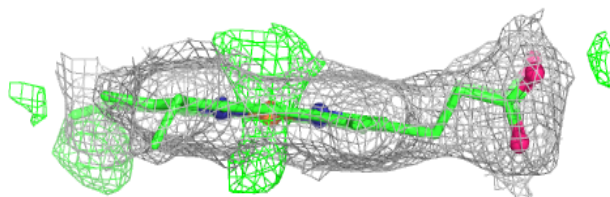
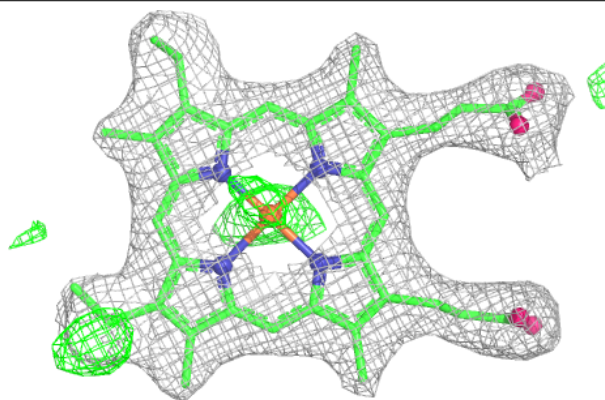


Electron density around HEC A 809:

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

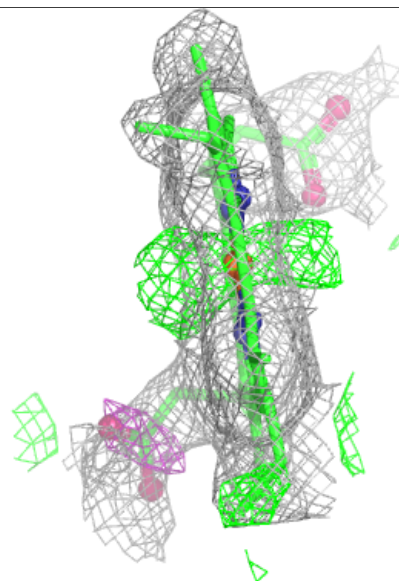
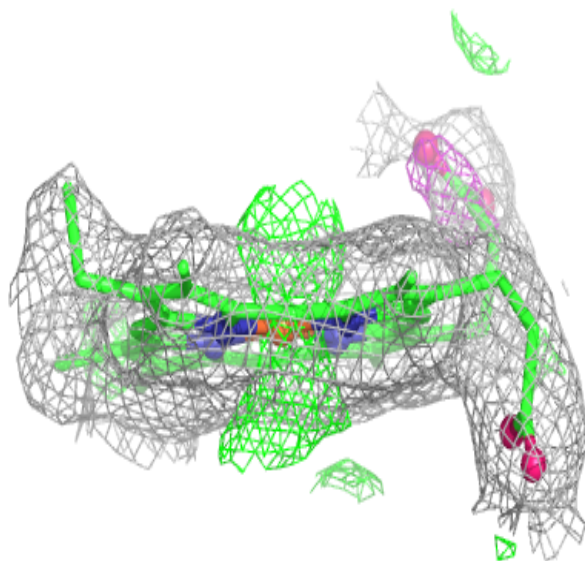
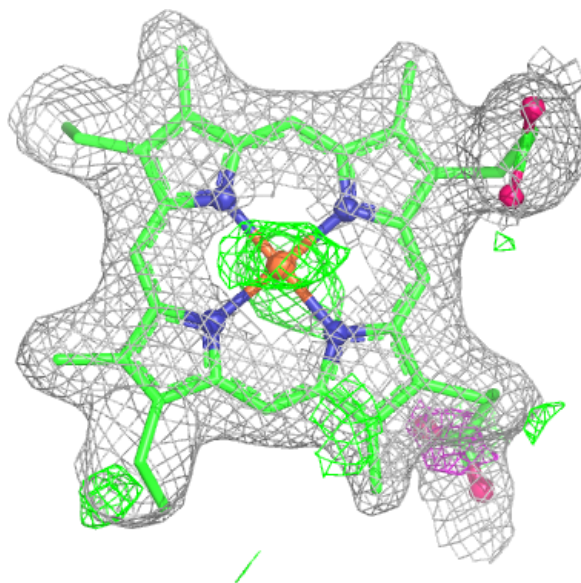
**Electron density around HEC C 803:**

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



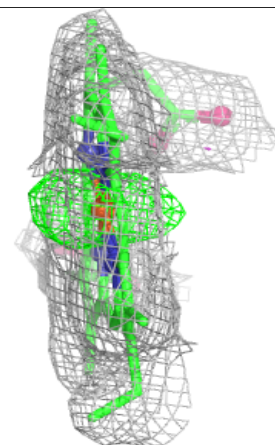
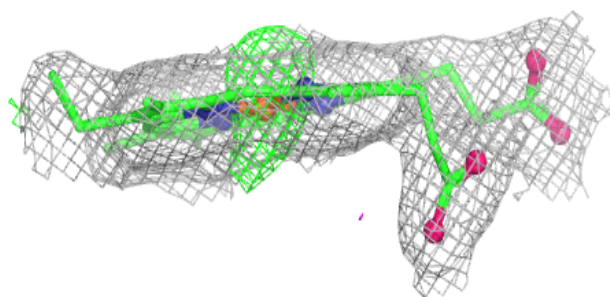
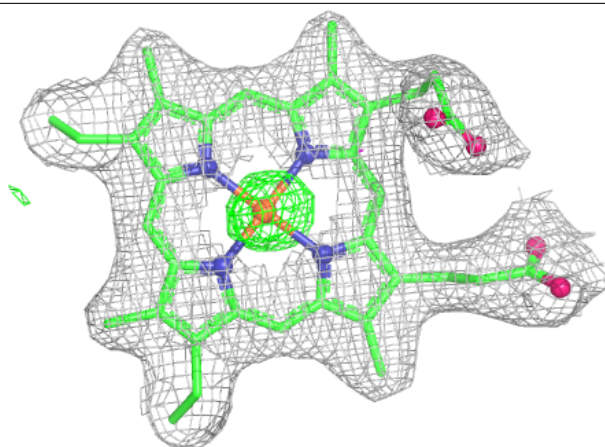
Electron density around HEC A 804:

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



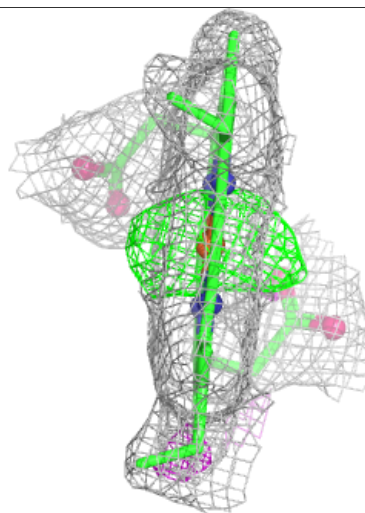
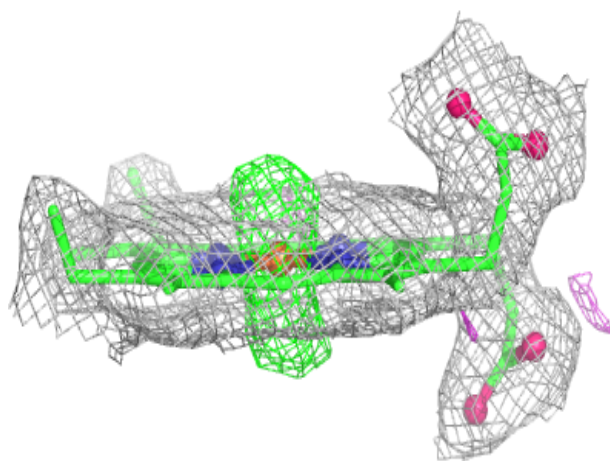
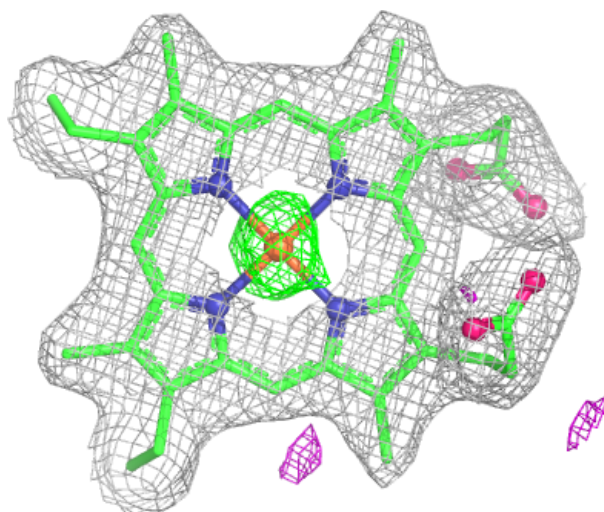
Electron density around HEC B 808:

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



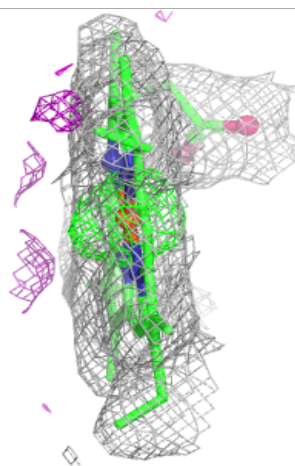
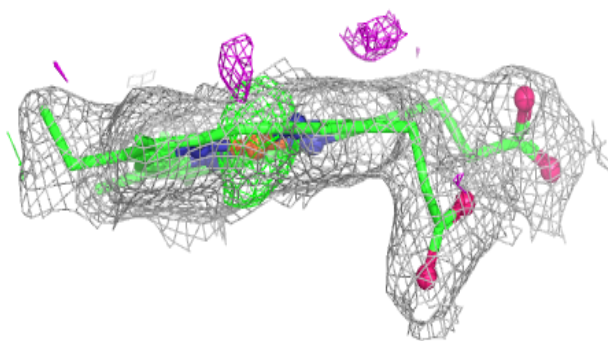
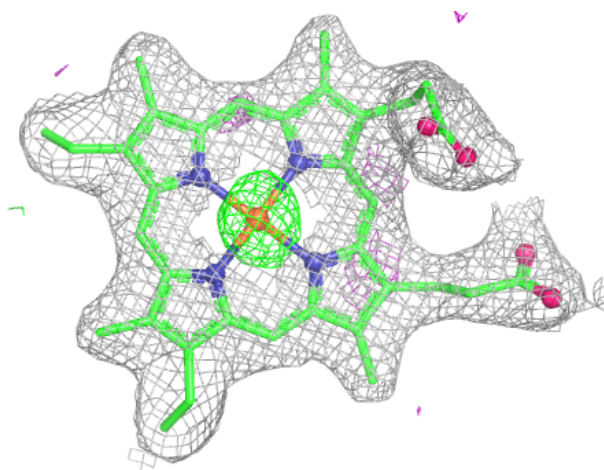
Electron density around HEC C 807:

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



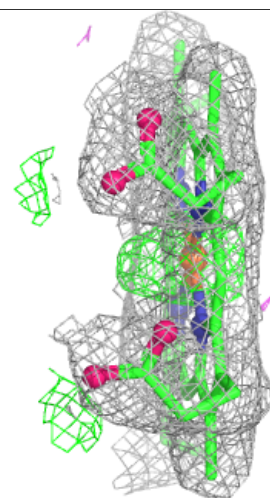
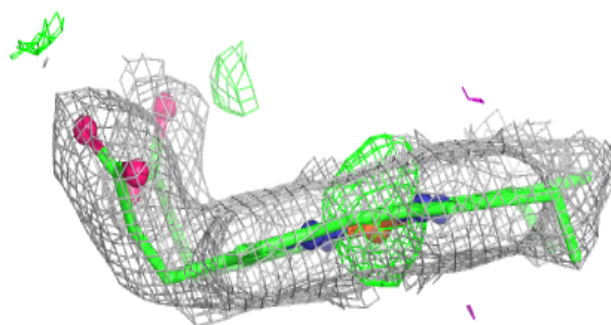
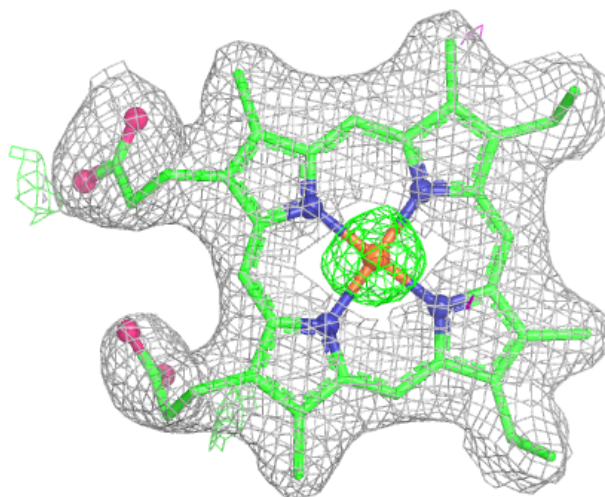
Electron density around HEC C 808:

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



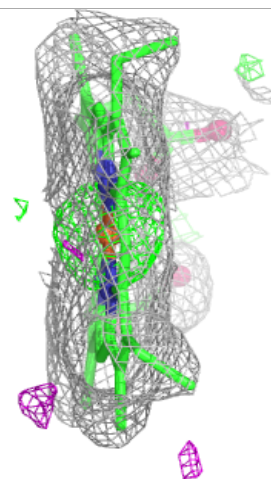
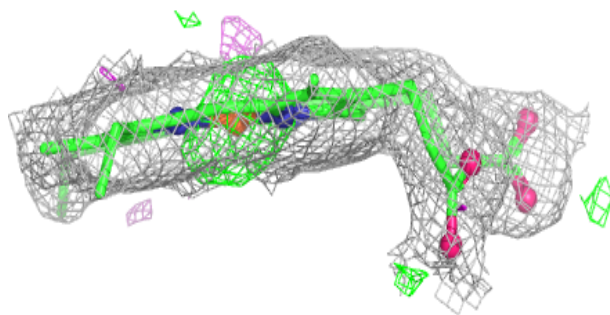
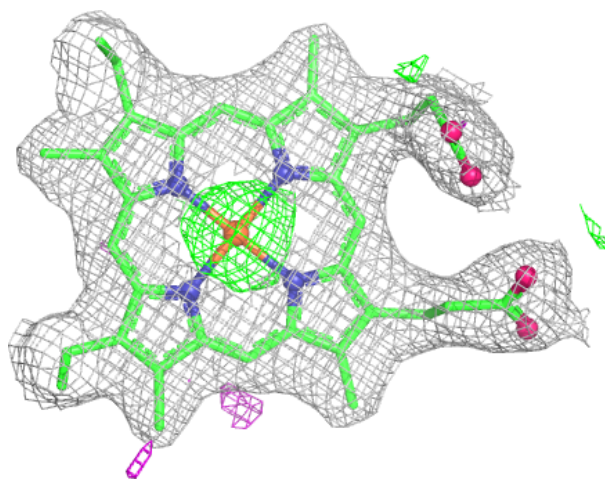
Electron density around HEC C 809:

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



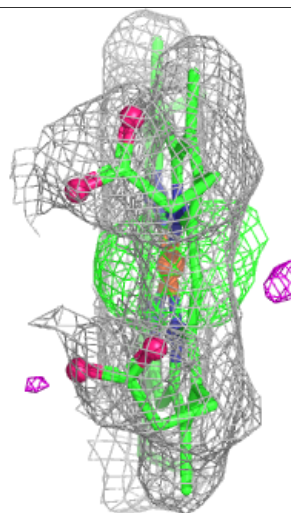
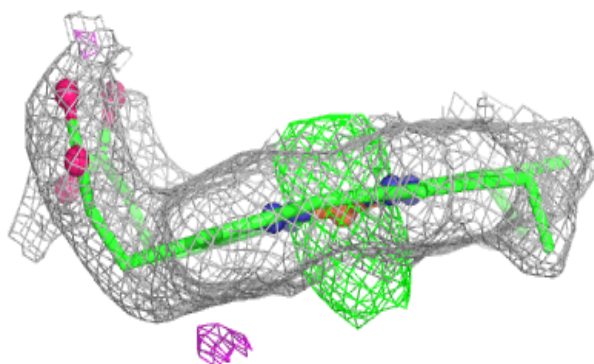
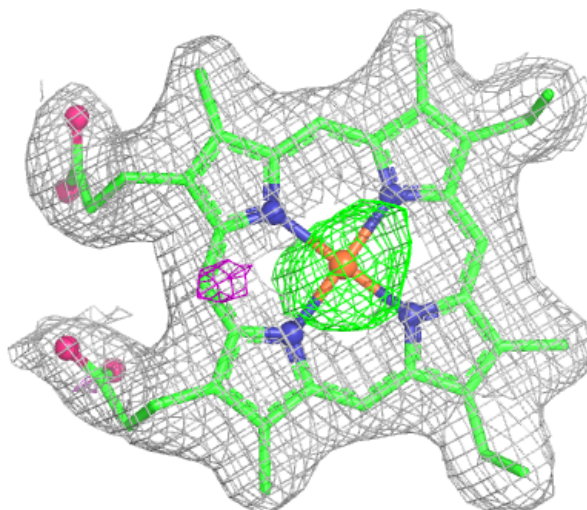
Electron density around HEC C 810:

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



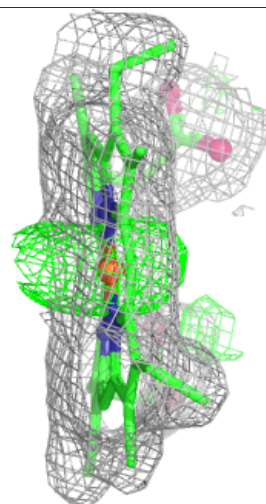
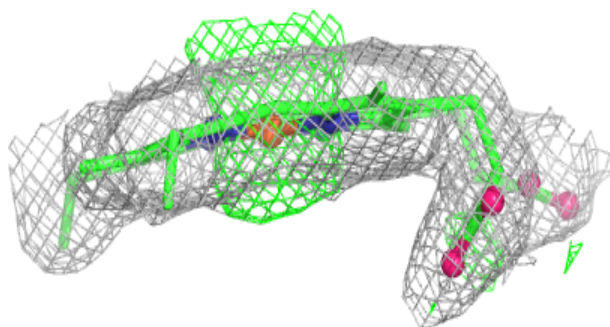
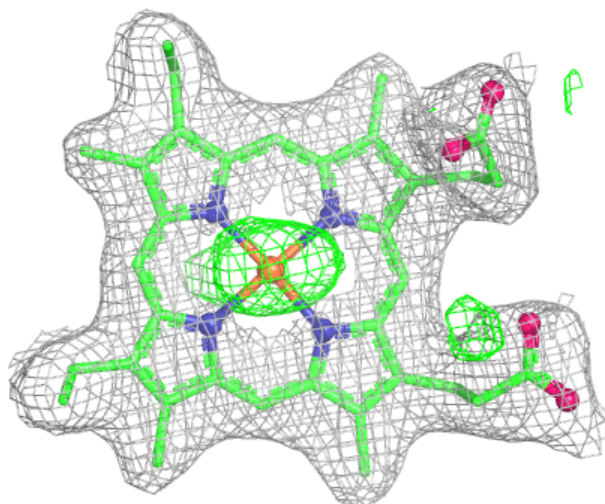
Electron density around HEC B 809:

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



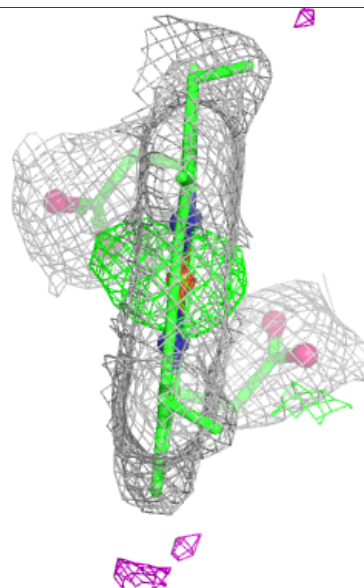
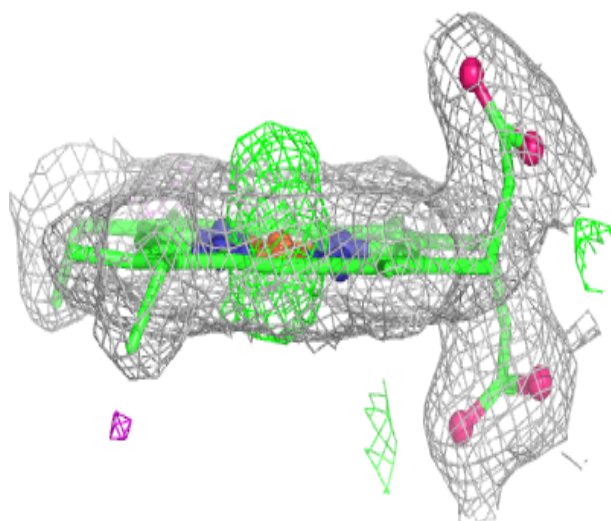
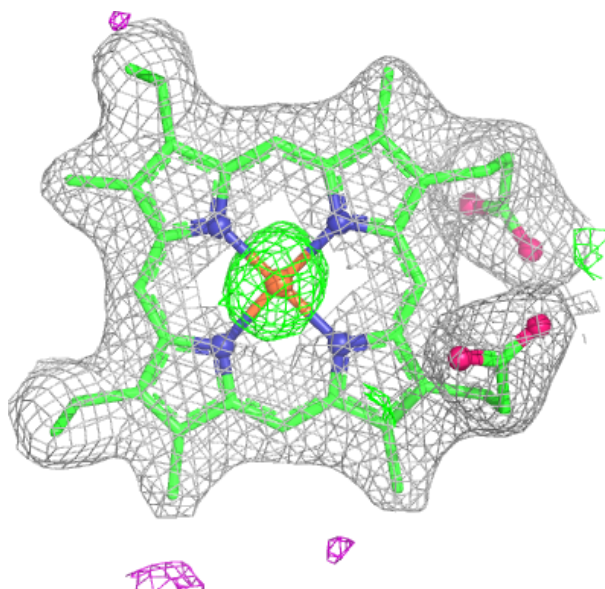
Electron density around HEC B 810:

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



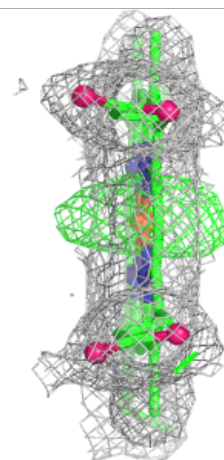
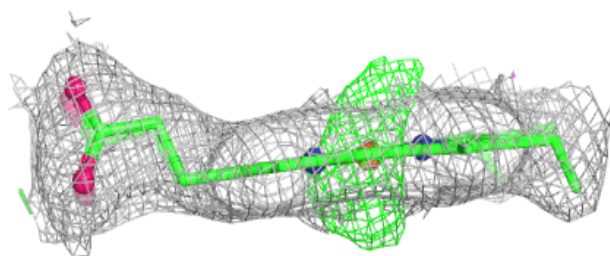
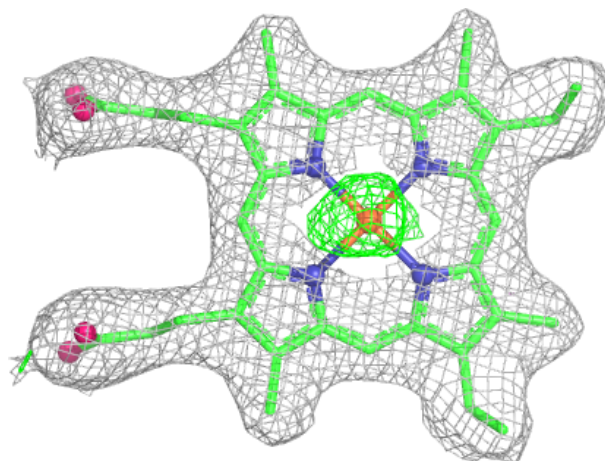
Electron density around HEC A 807:

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



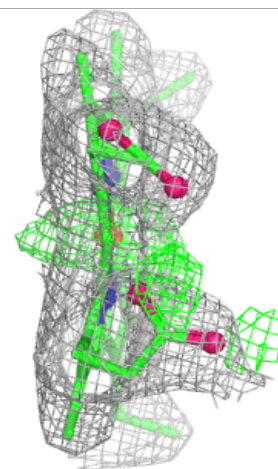
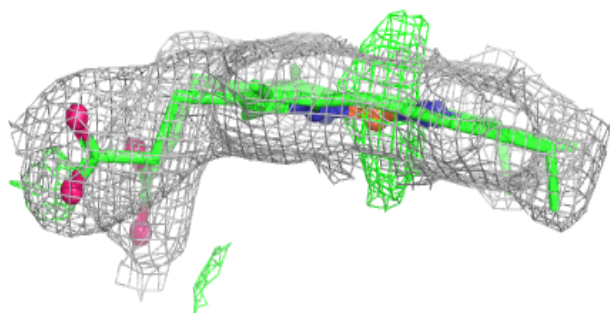
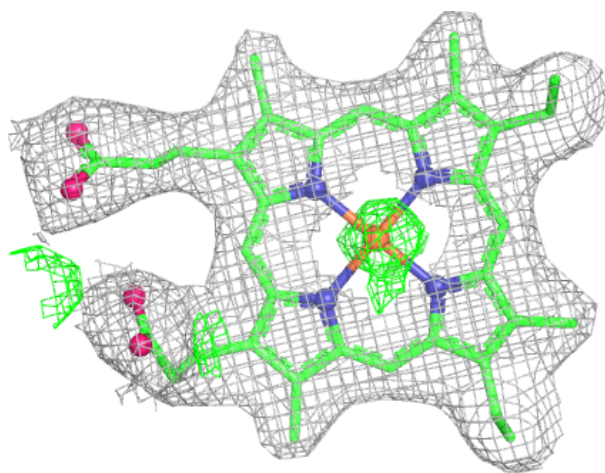
Electron density around HEC A 803:

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



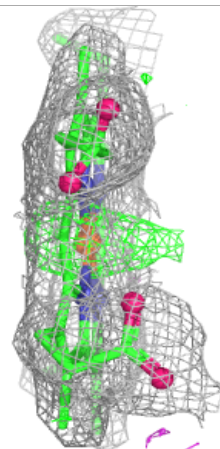
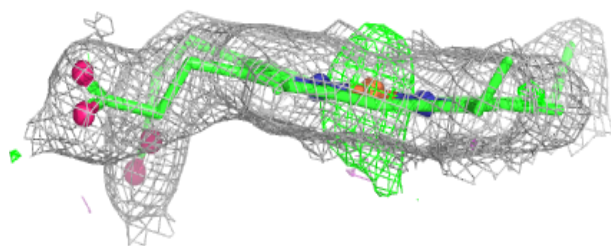
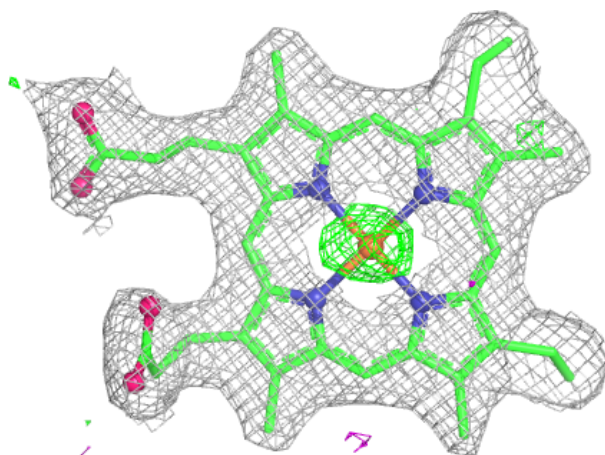
Electron density around HEC A 810:

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



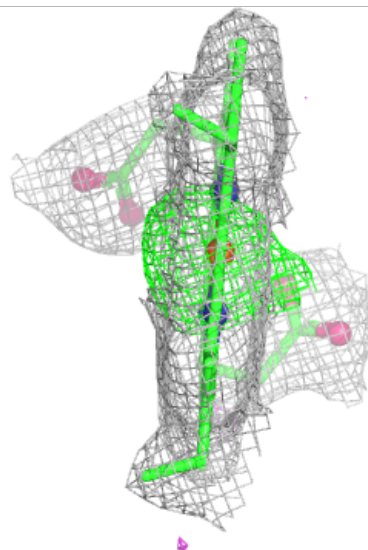
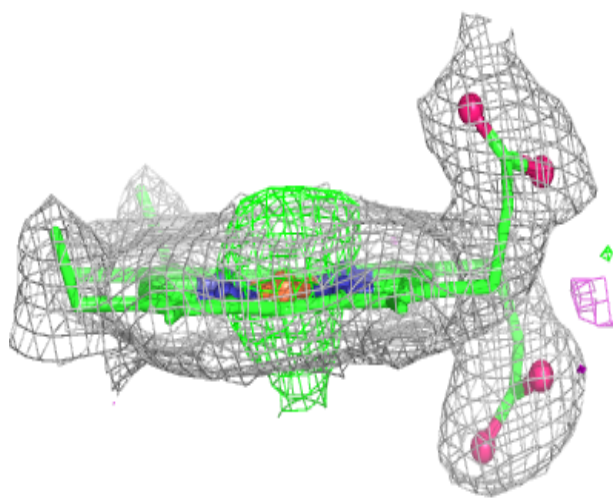
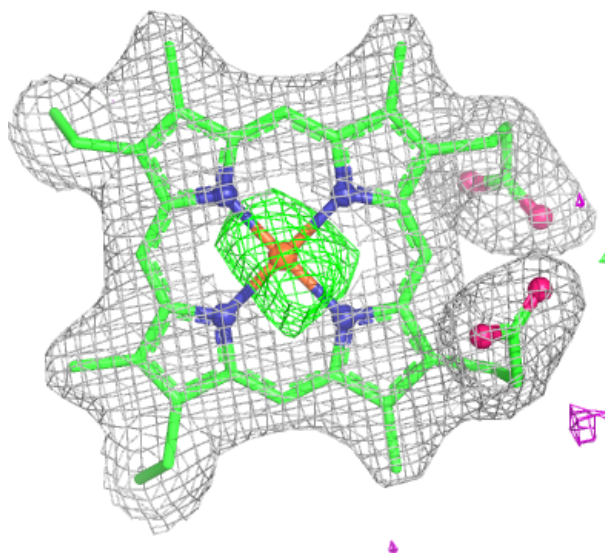
Electron density around HEC B 801:

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



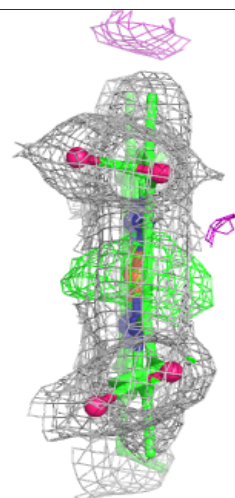
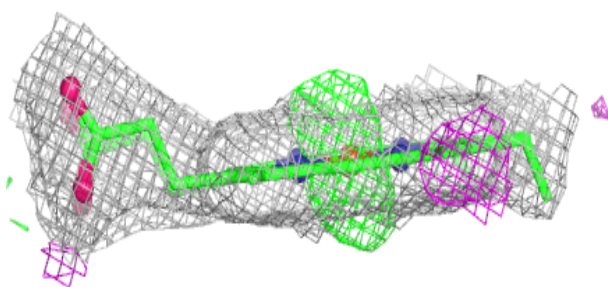
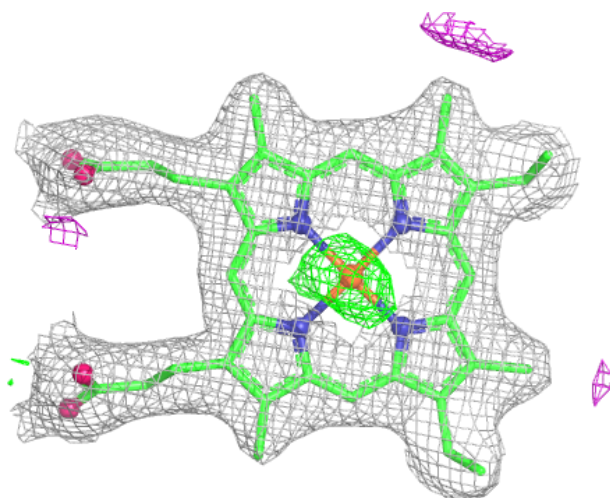
Electron density around HEC B 807:

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



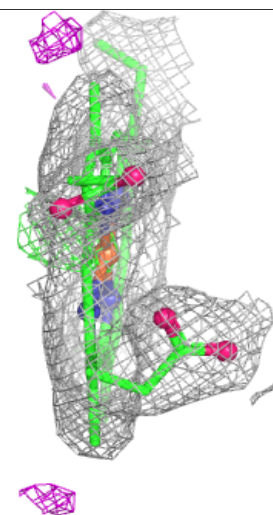
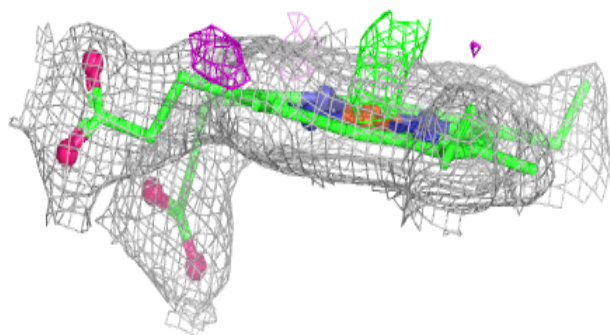
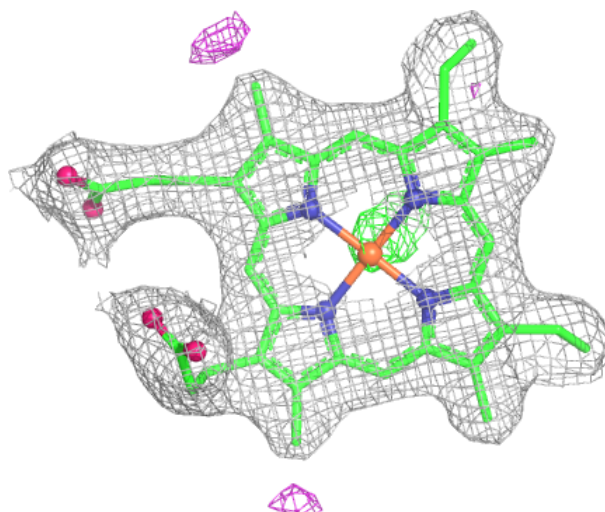
Electron density around HEC B 803:

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



Electron density around HEC A 808:

$2mF_o-DF_c$ (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.