Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 12:51 PM EDT

PDB ID	:	6QYC
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 (i) 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 (i)) were used in the production of this report:

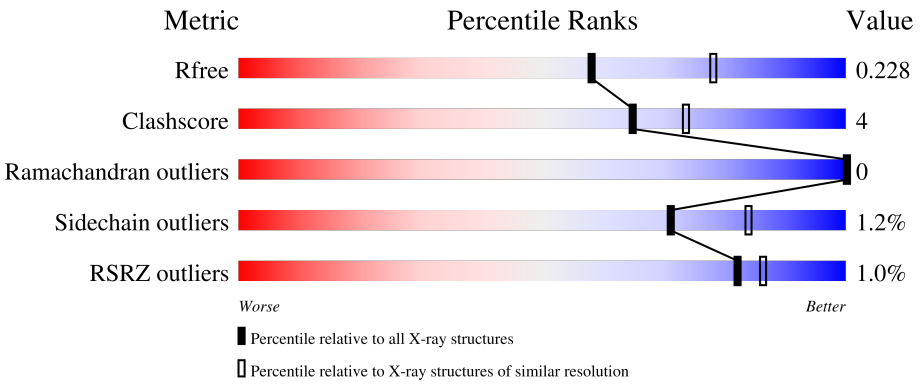
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	3% 87% 12% •

2 Entry composition (i)

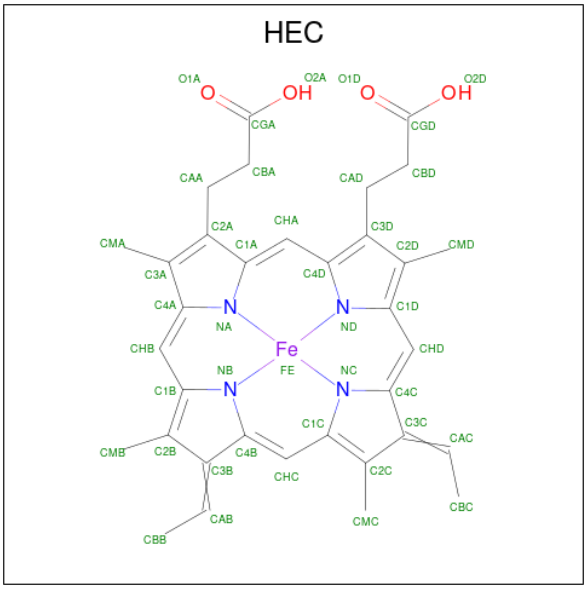
There are 5 unique types of molecules in this entry. The entry contains 15643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	605	4481	2770	782	894	35	0	2	0
1	B	608	4484	2772	781	896	35	0	0	0
1	C	604	4459	2755	777	892	35	0	0	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

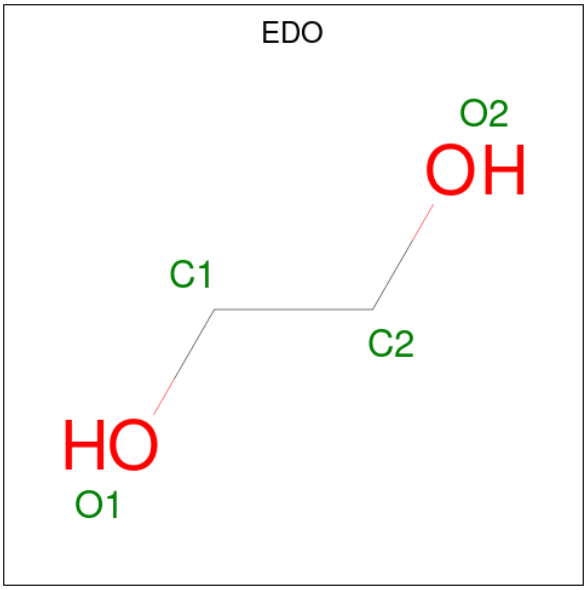
Continued from previous page...

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

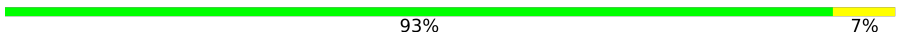
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	333	333	333	0	0
			Total	O		
5	B	335	335	335	0	0
			Total	O		
5	C	245	245	245	0	0

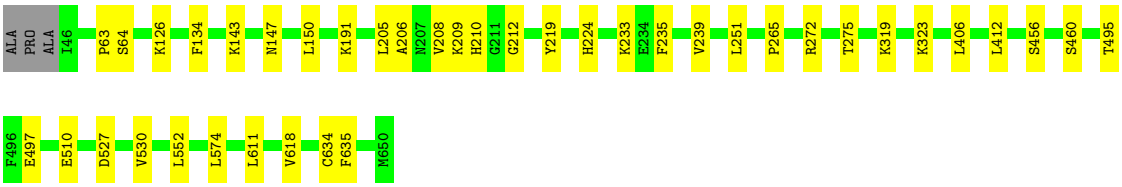
3 Residue-property plots (i)

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

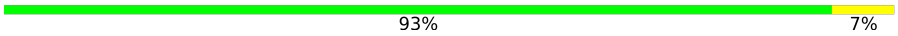
Chain A:

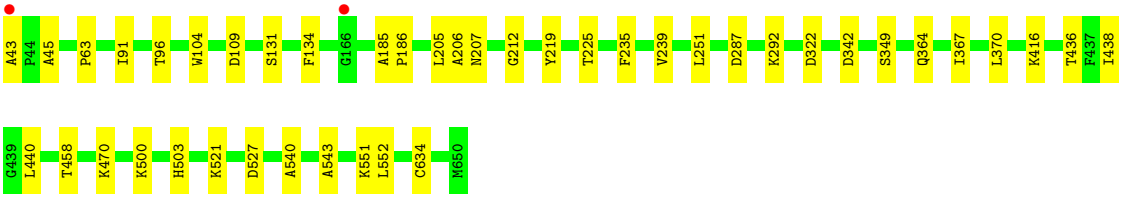




• Molecule 1: Decaheme c-type cytochrome, OmcA/MtrC family

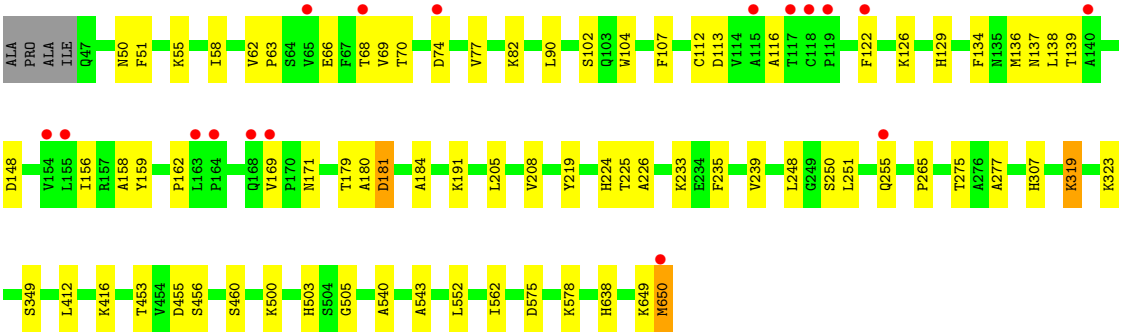
Chain B:





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

Chain C:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.183 , 0.228 0.183 , 0.228	Depositor DCC
R_{free} test set	5313 reflections (5.10%)	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)	0.30 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	0/4577	0.49	0/6225
1	B	0.27	0/4575	0.48	0/6225
1	C	0.27	0/4549	0.48	0/6188
All	All	0.28	0/13701	0.48	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	25	0
1	B	4484	0	4280	25	0
1	C	4459	0	4251	51	0
2	A	430	0	300	12	0
2	B	430	0	300	12	0
2	C	430	0	301	15	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	117	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 (117) 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:C:453:THR:HG22	1:C:455:ASP:H	1.61	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:C:58:ILE:HD12	1:C:62:VAL:C	2.19	0.62
1:A:552:LEU:HD21	2:A:806:HEC:HMB2	1.82	0.60
1:C:248:LEU:HD22	2:C:806:HEC:HMD3	1.86	0.58
1:B:552:LEU:HD11	2:B:806:HEC:HMB2	1.86	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
1:C:55:LYS:NZ	1:C:66:GLU:OE1	2.31	0.58
1:C:552:LEU:HD11	2:C:806:HEC:HMB2	1.86	0.58
1:B:458:THR:O	1:B:500:LYS:NZ	2.31	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:804:HEC:HMD3	1:C:650:MET:SD	2.45	0.57
1:C:70:THR:HG1	1:C:74:ASP:HA	1.70	0.56
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:B:552:LEU:HD12	2:B:808:HEC:HMD2	1.91	0.52
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:C:239:VAL:HG21	2:C:803:HEC:HMD2	1.92	0.51
1:A:510:GLU:H	1:A:510:GLU:CD	2.13	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
2:B:802:HEC:HMC1	2:B:802:HEC:HBC3	1.91	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
2:C:802:HEC:HBC3	2:C:802:HEC:HMC1	1.94	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
2:A:802:HEC:HMC1	2:A:802:HEC:HBC3	1.94	0.49
1:A:143:LYS:NZ	5:A:903:HOH:O	2.27	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:803:HEC:HMB1	2:A:803:HEC:HBB3	1.96	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
1:C:104:TRP:O	1:C:225:THR:HG21	2.15	0.47
1:A:552:LEU:HD22	2:A:808:HEC:HMD2	1.97	0.46
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
2:C:810:HEC:HMB1	2:C:810:HEC:HBB3	1.97	0.46
1:B:239:VAL:HG21	2:B:803:HEC:HMD2	1.97	0.45
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: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: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
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:638:HIS:HE1	2:C:809:HEC:HMA1	1.84	0.42
1:C:58:ILE:HG22	1:C:180:ALA:HA	2.00	0.42
1:C:307:HIS:HE1	2:C:804:HEC:HMA1	1.85	0.42
2:B:810:HEC:HMB1	2:B:810:HEC:HBB3	2.02	0.42
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.90	0.42
1:A:239:VAL:HG21	2:A:803:HEC:HMD2	2.01	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:A:527:ASP:O	1:A:530:VAL:HG22	2.20	0.42
1:C:158:ALA:O	1:C:171:ASN:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:HG23	1:C:184:ALA:O	2.21	0.41
2:A:810:HEC:HMB1	2:A:810:HEC:HBB3	2.02	0.41
1:B:551:LYS:HZ2	2:B:807:HEC:CGD	2.33	0.41
1:C:562:ILE:HD13	2:C:806:HEC:HBC2	2.01	0.41
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 (i)

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%)	480 (99%)	4 (1%)	81	91
1	B	483/483 (100%)	479 (99%)	4 (1%)	81	91
1	C	481/483 (100%)	472 (98%)	9 (2%)	57	73
All	All	1448/1449 (100%)	1431 (99%)	17 (1%)	71	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	SER
1	A	219	TYR
1	A	235	PHE
1	A	456	SER
1	B	109	ASP
1	B	131	SER
1	B	219	TYR
1	B	235	PHE
1	C	126	LYS
1	C	136	MET
1	C	148	ASP
1	C	181	ASP
1	C	219	TYR
1	C	235	PHE
1	C	319	LYS
1	C	412	LEU
1	C	650	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	GLN
1	B	207	ASN
1	C	125	GLN
1	C	137	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	803	1	32,50,50	2.22	5 (15%)	24,82,82	1.42	5 (20%)
2	HEC	C	810	1	32,50,50	2.11	3 (9%)	24,82,82	1.66	6 (25%)
2	HEC	C	802	1	32,50,50	2.11	3 (9%)	24,82,82	1.83	5 (20%)
2	HEC	C	808	1	32,50,50	2.09	3 (9%)	24,82,82	1.62	6 (25%)
2	HEC	A	804	1	32,50,50	2.13	3 (9%)	24,82,82	1.78	4 (16%)
2	HEC	A	809	1	32,50,50	2.18	4 (12%)	24,82,82	1.53	4 (16%)
2	HEC	A	803	1	32,50,50	2.11	4 (12%)	24,82,82	1.54	5 (20%)
2	HEC	B	803	1	32,50,50	2.11	3 (9%)	24,82,82	1.53	4 (16%)
2	HEC	A	801	1	32,50,50	2.07	4 (12%)	24,82,82	1.58	3 (12%)
2	HEC	B	806	1	32,50,50	2.15	3 (9%)	24,82,82	1.49	3 (12%)
2	HEC	A	805	1	32,50,50	2.14	4 (12%)	24,82,82	1.63	4 (16%)
2	HEC	A	802	1	32,50,50	2.07	3 (9%)	24,82,82	1.74	6 (25%)
2	HEC	A	806	1	32,50,50	2.13	3 (9%)	24,82,82	1.73	6 (25%)
2	HEC	A	810	1	32,50,50	2.10	4 (12%)	24,82,82	1.55	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEC	A	808	1	32,50,50	2.09	3 (9%)	24,82,82	1.43	2 (8%)
2	HEC	B	808	1	32,50,50	2.08	4 (12%)	24,82,82	1.63	5 (20%)
2	HEC	C	805	1	32,50,50	2.22	4 (12%)	24,82,82	1.55	4 (16%)
2	HEC	B	802	1	32,50,50	2.11	3 (9%)	24,82,82	1.78	4 (16%)
2	HEC	B	810	1	32,50,50	2.09	4 (12%)	24,82,82	1.57	4 (16%)
2	HEC	B	807	1	32,50,50	2.10	4 (12%)	24,82,82	1.39	2 (8%)
4	EDO	A	814	-	3,3,3	0.46	0	2,2,2	0.33	0
2	HEC	B	804	1	32,50,50	2.21	4 (12%)	24,82,82	1.42	3 (12%)
4	EDO	A	813	-	3,3,3	0.49	0	2,2,2	0.25	0
2	HEC	A	807	1	32,50,50	2.11	4 (12%)	24,82,82	1.54	3 (12%)
2	HEC	B	805	1	32,50,50	2.24	5 (15%)	24,82,82	1.42	2 (8%)
2	HEC	C	806	1	32,50,50	2.07	3 (9%)	24,82,82	1.56	4 (16%)
2	HEC	B	809	1	32,50,50	2.08	3 (9%)	24,82,82	1.60	3 (12%)
2	HEC	B	801	1	32,50,50	2.08	3 (9%)	24,82,82	1.61	4 (16%)
2	HEC	C	809	1	32,50,50	2.13	4 (12%)	24,82,82	1.56	5 (20%)
2	HEC	C	807	1	32,50,50	2.13	4 (12%)	24,82,82	1.32	2 (8%)
2	HEC	C	801	1	32,50,50	2.10	3 (9%)	24,82,82	1.56	5 (20%)
2	HEC	C	804	1	32,50,50	2.13	4 (12%)	24,82,82	1.45	2 (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	803	1	-	4/10/54/54	-
2	HEC	C	810	1	-	2/10/54/54	-
2	HEC	C	802	1	-	4/10/54/54	-
2	HEC	C	808	1	-	2/10/54/54	-
2	HEC	A	804	1	-	4/10/54/54	-
2	HEC	A	809	1	-	4/10/54/54	-
2	HEC	A	803	1	-	0/10/54/54	-
2	HEC	B	803	1	-	2/10/54/54	-
2	HEC	A	801	1	-	6/10/54/54	-
2	HEC	B	806	1	-	4/10/54/54	-
2	HEC	A	805	1	-	1/10/54/54	-
2	HEC	A	802	1	-	3/10/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	806	1	-	4/10/54/54	-
2	HEC	A	810	1	-	1/10/54/54	-
2	HEC	A	808	1	-	4/10/54/54	-
2	HEC	B	808	1	-	3/10/54/54	-
2	HEC	C	805	1	-	0/10/54/54	-
2	HEC	B	802	1	-	6/10/54/54	-
2	HEC	B	810	1	-	5/10/54/54	-
2	HEC	B	807	1	-	4/10/54/54	-
4	EDO	A	814	-	-	0/1/1/1	-
2	HEC	B	804	1	-	7/10/54/54	-
4	EDO	A	813	-	-	0/1/1/1	-
2	HEC	A	807	1	-	4/10/54/54	-
2	HEC	B	805	1	-	2/10/54/54	-
2	HEC	C	806	1	-	4/10/54/54	-
2	HEC	B	809	1	-	4/10/54/54	-
2	HEC	B	801	1	-	6/10/54/54	-
2	HEC	C	809	1	-	3/10/54/54	-
2	HEC	C	807	1	-	4/10/54/54	-
2	HEC	C	801	1	-	3/10/54/54	-
2	HEC	C	804	1	-	5/10/54/54	-

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	803	HEC	C2B-C3B	-6.91	1.33	1.40
2	B	805	HEC	C3C-C2C	-6.71	1.33	1.40
2	C	805	HEC	C2B-C3B	-6.39	1.34	1.40
2	C	805	HEC	C3C-C2C	-6.38	1.34	1.40
2	C	802	HEC	C2B-C3B	-6.25	1.34	1.40
2	A	806	HEC	C3C-C2C	-6.22	1.34	1.40
2	B	804	HEC	C2B-C3B	-6.20	1.34	1.40
2	B	804	HEC	C3C-C2C	-6.15	1.34	1.40
2	B	802	HEC	C2B-C3B	-6.15	1.34	1.40
2	B	806	HEC	C2B-C3B	-6.09	1.34	1.40
2	A	809	HEC	C2B-C3B	-6.07	1.34	1.40
2	A	804	HEC	C3C-C2C	-6.03	1.34	1.40
2	B	805	HEC	C2B-C3B	-6.02	1.34	1.40
2	C	804	HEC	C2B-C3B	-6.00	1.34	1.40
2	A	805	HEC	C2B-C3B	-5.99	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	807	HEC	C2B-C3B	-5.96	1.34	1.40
2	B	808	HEC	C2B-C3B	-5.95	1.34	1.40
2	A	802	HEC	C2B-C3B	-5.94	1.34	1.40
2	B	809	HEC	C2B-C3B	-5.94	1.34	1.40
2	C	807	HEC	C2B-C3B	-5.90	1.34	1.40
2	B	810	HEC	C3C-C2C	-5.90	1.34	1.40
2	C	809	HEC	C2B-C3B	-5.89	1.34	1.40
2	A	804	HEC	C2B-C3B	-5.89	1.34	1.40
2	A	810	HEC	C3C-C2C	-5.85	1.34	1.40
2	C	808	HEC	C2B-C3B	-5.85	1.34	1.40
2	A	805	HEC	C3C-C2C	-5.84	1.34	1.40
2	B	807	HEC	C2B-C3B	-5.83	1.34	1.40
2	A	803	HEC	C3C-C2C	-5.83	1.34	1.40
2	C	801	HEC	C2B-C3B	-5.79	1.34	1.40
2	C	810	HEC	C3C-C2C	-5.78	1.34	1.40
2	C	809	HEC	C3C-C2C	-5.77	1.34	1.40
2	A	809	HEC	C3C-C2C	-5.76	1.34	1.40
2	B	810	HEC	C2B-C3B	-5.75	1.34	1.40
2	C	807	HEC	C3C-C2C	-5.75	1.34	1.40
2	C	808	HEC	C3C-C2C	-5.74	1.34	1.40
2	A	806	HEC	C2B-C3B	-5.73	1.34	1.40
2	B	803	HEC	C2B-C3B	-5.70	1.34	1.40
2	B	803	HEC	C3C-C2C	-5.69	1.34	1.40
2	A	808	HEC	C2B-C3B	-5.69	1.34	1.40
2	B	801	HEC	C3C-C2C	-5.69	1.34	1.40
2	B	806	HEC	C3C-C2C	-5.69	1.34	1.40
2	C	810	HEC	C2B-C3B	-5.68	1.34	1.40
2	A	801	HEC	C2B-C3B	-5.68	1.34	1.40
2	C	803	HEC	C3C-C2C	-5.66	1.34	1.40
2	A	808	HEC	C3C-C2C	-5.64	1.34	1.40
2	A	803	HEC	C2B-C3B	-5.63	1.34	1.40
2	B	807	HEC	C3C-C2C	-5.59	1.34	1.40
2	B	801	HEC	C2B-C3B	-5.59	1.34	1.40
2	B	804	HEC	C3D-C2D	5.58	1.54	1.37
2	A	809	HEC	C3D-C2D	5.57	1.54	1.37
2	A	810	HEC	C2B-C3B	-5.54	1.35	1.40
2	A	805	HEC	C3D-C2D	5.53	1.54	1.37
2	A	807	HEC	C3C-C2C	-5.53	1.35	1.40
2	C	804	HEC	C3D-C2D	5.52	1.54	1.37
2	C	806	HEC	C3C-C2C	-5.51	1.35	1.40
2	C	806	HEC	C3D-C2D	5.51	1.54	1.37
2	C	805	HEC	C3D-C2D	5.49	1.54	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	805	HEC	C3D-C2D	5.49	1.53	1.37
2	B	803	HEC	C3D-C2D	5.46	1.53	1.37
2	C	804	HEC	C3C-C2C	-5.46	1.35	1.40
2	B	802	HEC	C3C-C2C	-5.46	1.35	1.40
2	B	808	HEC	C3C-C2C	-5.46	1.35	1.40
2	C	801	HEC	C3D-C2D	5.45	1.53	1.37
2	A	801	HEC	C3D-C2D	5.45	1.53	1.37
2	C	803	HEC	C3D-C2D	5.45	1.53	1.37
2	C	807	HEC	C3D-C2D	5.44	1.53	1.37
2	A	808	HEC	C3D-C2D	5.43	1.53	1.37
2	C	806	HEC	C2B-C3B	-5.43	1.35	1.40
2	B	810	HEC	C3D-C2D	5.42	1.53	1.37
2	B	802	HEC	C3D-C2D	5.42	1.53	1.37
2	A	810	HEC	C3D-C2D	5.42	1.53	1.37
2	C	810	HEC	C3D-C2D	5.42	1.53	1.37
2	C	802	HEC	C3D-C2D	5.42	1.53	1.37
2	A	802	HEC	C3C-C2C	-5.41	1.35	1.40
2	B	806	HEC	C3D-C2D	5.41	1.53	1.37
2	A	803	HEC	C3D-C2D	5.40	1.53	1.37
2	B	808	HEC	C3D-C2D	5.39	1.53	1.37
2	C	801	HEC	C3C-C2C	-5.39	1.35	1.40
2	B	801	HEC	C3D-C2D	5.39	1.53	1.37
2	C	809	HEC	C3D-C2D	5.37	1.53	1.37
2	A	807	HEC	C3D-C2D	5.36	1.53	1.37
2	C	802	HEC	C3C-C2C	-5.35	1.35	1.40
2	A	806	HEC	C3D-C2D	5.34	1.53	1.37
2	B	809	HEC	C3D-C2D	5.32	1.53	1.37
2	B	809	HEC	C3C-C2C	-5.30	1.35	1.40
2	A	802	HEC	C3D-C2D	5.30	1.53	1.37
2	A	801	HEC	C3C-C2C	-5.29	1.35	1.40
2	C	808	HEC	C3D-C2D	5.29	1.53	1.37
2	B	807	HEC	C3D-C2D	5.26	1.53	1.37
2	A	804	HEC	C3D-C2D	5.15	1.52	1.37
2	B	805	HEC	C3C-C4C	2.37	1.47	1.43
2	A	801	HEC	CAD-C3D	2.32	1.55	1.52
2	C	805	HEC	C3C-C4C	2.31	1.47	1.43
2	B	804	HEC	CAD-C3D	2.25	1.55	1.52
2	C	804	HEC	CAD-C3D	2.18	1.55	1.52
2	C	803	HEC	C4B-C3B	2.16	1.47	1.43
2	A	807	HEC	CAD-C3D	2.15	1.55	1.52
2	B	805	HEC	CAD-C3D	2.15	1.55	1.52
2	C	803	HEC	CAD-C3D	2.13	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	809	HEC	CAD-C3D	2.12	1.55	1.52
2	A	809	HEC	CAD-C3D	2.11	1.55	1.52
2	B	808	HEC	CAD-C3D	2.09	1.55	1.52
2	B	810	HEC	CAD-C3D	2.07	1.55	1.52
2	B	807	HEC	CAD-C3D	2.04	1.55	1.52
2	A	803	HEC	CAD-C3D	2.02	1.55	1.52
2	A	810	HEC	CAD-C3D	2.02	1.55	1.52
2	C	807	HEC	CAD-C3D	2.01	1.55	1.52
2	A	805	HEC	CAD-C3D	2.00	1.55	1.52

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	804	HEC	CBD-CAD-C3D	-5.56	103.13	112.62
2	C	802	HEC	CMC-C2C-C1C	-4.31	121.84	128.46
2	B	802	HEC	CMC-C2C-C1C	-4.30	121.86	128.46
2	B	808	HEC	CMC-C2C-C1C	-3.87	122.51	128.46
2	A	801	HEC	CMC-C2C-C1C	-3.83	122.58	128.46
2	A	807	HEC	CMC-C2C-C1C	-3.80	122.62	128.46
2	A	802	HEC	CMC-C2C-C1C	-3.62	122.89	128.46
2	C	804	HEC	CMC-C2C-C1C	-3.59	122.94	128.46
2	C	808	HEC	CMC-C2C-C1C	-3.53	123.05	128.46
2	C	801	HEC	CMC-C2C-C1C	-3.50	123.08	128.46
2	C	810	HEC	CMB-C2B-C1B	-3.42	123.20	128.46
2	A	809	HEC	CMC-C2C-C1C	-3.42	123.22	128.46
2	C	802	HEC	CMB-C2B-C1B	-3.39	123.25	128.46
2	A	802	HEC	CBD-CAD-C3D	-3.39	106.84	112.62
2	A	806	HEC	CBD-CAD-C3D	-3.37	106.87	112.62
2	A	810	HEC	CMB-C2B-C1B	-3.32	123.35	128.46
2	C	806	HEC	CMC-C2C-C1C	-3.31	123.37	128.46
2	A	808	HEC	CMC-C2C-C1C	-3.31	123.37	128.46
2	C	805	HEC	CMC-C2C-C1C	-3.30	123.39	128.46
2	C	809	HEC	CMB-C2B-C1B	-3.28	123.42	128.46
2	B	810	HEC	CBA-CAA-C2A	-3.27	107.10	112.60
2	C	802	HEC	CMC-C2C-C3C	3.26	129.65	125.82
2	C	801	HEC	CBD-CAD-C3D	-3.24	107.08	112.62
2	A	805	HEC	CMC-C2C-C1C	-3.22	123.52	128.46
2	A	804	HEC	CMC-C2C-C1C	-3.21	123.52	128.46
2	B	804	HEC	CMC-C2C-C1C	-3.21	123.54	128.46
2	A	802	HEC	CMB-C2B-C1B	-3.18	123.58	128.46
2	C	810	HEC	CBA-CAA-C2A	-3.14	107.31	112.60
2	B	801	HEC	CMB-C2B-C1B	-3.13	123.66	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	806	HEC	CMC-C2C-C1C	-3.12	123.67	128.46
2	A	803	HEC	CMB-C2B-C1B	-3.09	123.71	128.46
2	C	808	HEC	CMB-C2B-C1B	-3.09	123.72	128.46
2	B	809	HEC	CBD-CAD-C3D	-3.04	107.43	112.62
2	B	808	HEC	CMB-C2B-C1B	-3.01	123.83	128.46
2	B	801	HEC	CMC-C2C-C1C	-3.01	123.84	128.46
2	B	802	HEC	CMB-C2B-C1B	-2.99	123.87	128.46
2	B	803	HEC	CMC-C2C-C1C	-2.97	123.90	128.46
2	A	804	HEC	C1D-C2D-C3D	-2.97	104.93	107.00
2	A	801	HEC	CMB-C2B-C1B	-2.96	123.92	128.46
2	A	806	HEC	C1D-C2D-C3D	-2.94	104.95	107.00
2	C	806	HEC	CMB-C2B-C1B	-2.90	124.00	128.46
2	B	810	HEC	CMB-C2B-C1B	-2.88	124.04	128.46
2	B	806	HEC	CMB-C2B-C1B	-2.87	124.05	128.46
2	A	806	HEC	CMB-C2B-C1B	-2.87	124.06	128.46
2	B	802	HEC	CMC-C2C-C3C	2.86	129.19	125.82
2	B	802	HEC	CBA-CAA-C2A	-2.83	107.83	112.60
2	C	810	HEC	CMC-C2C-C1C	-2.82	124.12	128.46
2	C	803	HEC	CMC-C2C-C1C	-2.81	124.14	128.46
2	A	805	HEC	CMB-C2B-C1B	-2.81	124.15	128.46
2	A	808	HEC	CMB-C2B-C1B	-2.78	124.19	128.46
2	C	807	HEC	CMC-C2C-C1C	-2.78	124.20	128.46
2	B	809	HEC	CMC-C2C-C1C	-2.76	124.22	128.46
2	B	807	HEC	CMC-C2C-C1C	-2.75	124.24	128.46
2	A	806	HEC	CMC-C2C-C1C	-2.73	124.27	128.46
2	C	809	HEC	CMC-C2C-C1C	-2.73	124.27	128.46
2	A	805	HEC	CBA-CAA-C2A	-2.72	108.03	112.60
2	B	809	HEC	CMB-C2B-C1B	-2.69	124.33	128.46
2	C	805	HEC	CBA-CAA-C2A	-2.67	108.11	112.60
2	A	810	HEC	CMC-C2C-C1C	-2.64	124.40	128.46
2	B	803	HEC	CMB-C2B-C1B	-2.63	124.43	128.46
2	B	805	HEC	CMB-C2B-C1B	-2.62	124.44	128.46
2	A	805	HEC	CBD-CAD-C3D	-2.62	108.15	112.62
2	A	803	HEC	CMC-C2C-C1C	-2.62	124.44	128.46
2	A	809	HEC	CMB-C2B-C1B	-2.61	124.46	128.46
2	C	810	HEC	CMB-C2B-C3B	2.59	128.86	125.82
2	B	807	HEC	CBA-CAA-C2A	-2.58	108.25	112.60
2	A	807	HEC	CMB-C2B-C1B	-2.56	124.53	128.46
2	A	802	HEC	CMC-C2C-C3C	2.56	128.83	125.82
2	C	803	HEC	CAD-CBD-CGD	-2.56	106.59	113.76
2	A	810	HEC	CBD-CAD-C3D	-2.50	108.35	112.62
2	C	810	HEC	CBD-CAD-C3D	-2.48	108.38	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	802	HEC	CBA-CAA-C2A	-2.47	108.45	112.60
2	C	801	HEC	CBA-CAA-C2A	2.46	116.75	112.60
2	C	804	HEC	CMB-C2B-C1B	-2.43	124.72	128.46
2	B	810	HEC	CMC-C2C-C1C	-2.43	124.73	128.46
2	C	806	HEC	C1D-C2D-C3D	-2.35	105.36	107.00
2	A	810	HEC	CMB-C2B-C3B	2.35	128.58	125.82
2	B	801	HEC	C1D-C2D-C3D	-2.34	105.36	107.00
2	C	802	HEC	CMB-C2B-C3B	2.30	128.53	125.82
2	C	809	HEC	CMB-C2B-C3B	2.29	128.51	125.82
2	B	806	HEC	C1D-C2D-C3D	-2.29	105.41	107.00
2	A	801	HEC	CMC-C2C-C3C	2.28	128.50	125.82
2	A	809	HEC	C1D-C2D-C3D	-2.27	105.42	107.00
2	C	808	HEC	C1D-C2D-C3D	-2.26	105.42	107.00
2	C	801	HEC	C1D-C2D-C3D	-2.25	105.43	107.00
2	A	803	HEC	C1D-C2D-C3D	-2.24	105.44	107.00
2	A	807	HEC	CBA-CAA-C2A	-2.24	108.84	112.60
2	A	806	HEC	CAA-CBA-CGA	-2.22	107.52	113.76
2	B	803	HEC	CAD-CBD-CGD	-2.22	107.53	113.76
2	C	808	HEC	CAD-CBD-CGD	-2.22	107.54	113.76
2	A	803	HEC	CMB-C2B-C3B	2.21	128.42	125.82
2	C	809	HEC	C1D-C2D-C3D	-2.19	105.47	107.00
2	C	808	HEC	CMB-C2B-C3B	2.19	128.40	125.82
2	B	810	HEC	CBD-CAD-C3D	-2.18	108.89	112.62
2	B	805	HEC	CAD-CBD-CGD	-2.17	107.68	113.76
2	C	809	HEC	CBD-CAD-C3D	-2.17	108.92	112.62
2	C	801	HEC	CMB-C2B-C1B	-2.15	125.15	128.46
2	A	802	HEC	CBA-CAA-C2A	-2.15	108.99	112.60
2	B	804	HEC	C1D-C2D-C3D	-2.13	105.51	107.00
2	C	810	HEC	C1D-C2D-C3D	-2.12	105.52	107.00
2	A	803	HEC	CAD-CBD-CGD	-2.12	107.83	113.76
2	B	808	HEC	C1D-C2D-C3D	-2.11	105.53	107.00
2	C	803	HEC	CAA-CBA-CGA	-2.11	107.85	113.76
2	A	806	HEC	CMA-C3A-C2A	2.11	128.91	124.94
2	C	807	HEC	CMB-C2B-C1B	-2.10	125.23	128.46
2	A	810	HEC	C1D-C2D-C3D	-2.10	105.53	107.00
2	B	801	HEC	CMA-C3A-C2A	2.09	128.89	124.94
2	A	804	HEC	CMB-C2B-C1B	-2.09	125.25	128.46
2	A	809	HEC	CMC-C2C-C3C	2.08	128.26	125.82
2	C	803	HEC	C4C-C3C-C2C	2.07	108.58	106.35
2	C	805	HEC	C3C-C4C-NC	-2.06	107.06	110.94
2	C	803	HEC	C3C-C4C-NC	-2.06	107.06	110.94
2	C	808	HEC	CBA-CAA-C2A	-2.05	109.15	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	808	HEC	CAD-CBD-CGD	-2.04	108.03	113.76
2	C	806	HEC	CMB-C2B-C3B	2.04	128.22	125.82
2	C	805	HEC	CBD-CAD-C3D	-2.03	109.16	112.62
2	A	802	HEC	CMB-C2B-C3B	2.03	128.20	125.82
2	B	808	HEC	CMC-C2C-C3C	2.03	128.20	125.82
2	B	803	HEC	CMC-C2C-C3C	2.02	128.20	125.82
2	B	804	HEC	CMB-C2B-C1B	-2.01	125.37	128.46

There are no chirality outliers.

All (105) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	807	HEC	CAD-CBD-CGD-O1D
2	B	807	HEC	CAD-CBD-CGD-O1D
2	A	802	HEC	CAD-CBD-CGD-O1D
2	A	801	HEC	CAA-CBA-CGA-O2A
2	B	802	HEC	CAD-CBD-CGD-O2D
2	B	808	HEC	CAA-CBA-CGA-O2A
2	C	803	HEC	CAA-CBA-CGA-O2A
2	C	809	HEC	CAD-CBD-CGD-O2D
2	A	808	HEC	CAA-CBA-CGA-O2A
2	B	803	HEC	CAA-CBA-CGA-O2A
2	C	803	HEC	CAD-CBD-CGD-O2D
2	B	802	HEC	C2A-CAA-CBA-CGA
2	B	804	HEC	C2A-CAA-CBA-CGA
2	B	808	HEC	CAD-CBD-CGD-O2D
2	A	808	HEC	CAA-CBA-CGA-O1A
2	B	809	HEC	CAA-CBA-CGA-O2A
2	C	808	HEC	CAD-CBD-CGD-O2D
2	A	805	HEC	CAD-CBD-CGD-O2D
2	A	806	HEC	CAA-CBA-CGA-O2A
2	B	808	HEC	CAA-CBA-CGA-O1A
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	C	803	HEC	CAA-CBA-CGA-O1A
2	C	803	HEC	CAD-CBD-CGD-O1D
2	C	809	HEC	CAA-CBA-CGA-O2A
2	C	809	HEC	CAD-CBD-CGD-O1D
2	A	808	HEC	CAD-CBD-CGD-O2D
2	B	801	HEC	CAA-CBA-CGA-O2A
2	A	806	HEC	CAA-CBA-CGA-O1A
2	A	808	HEC	CAD-CBD-CGD-O1D
2	B	803	HEC	CAA-CBA-CGA-O1A
2	C	810	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

26 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	803	HEC	3	0
2	C	810	HEC	1	0
2	C	802	HEC	1	0
2	C	808	HEC	1	0

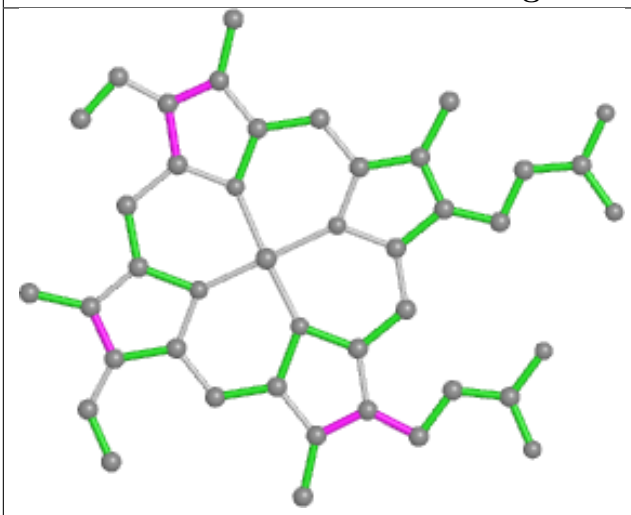
Continued on next page...

Continued from previous page...

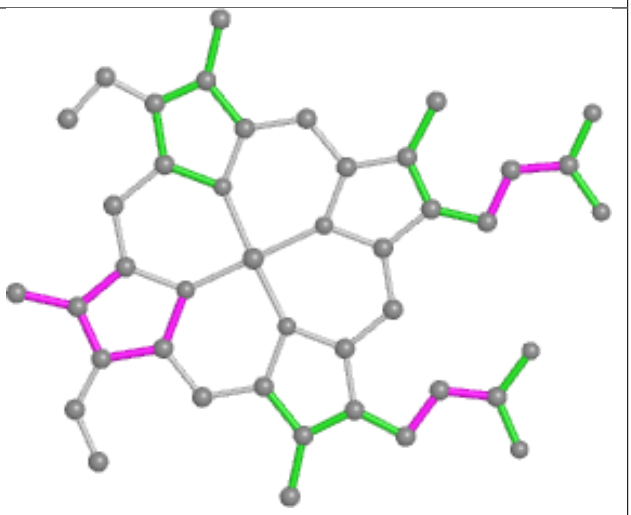
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	HEC	3	0
2	A	809	HEC	1	0
2	A	803	HEC	3	0
2	B	803	HEC	2	0
2	A	801	HEC	1	0
2	B	806	HEC	1	0
2	A	802	HEC	1	0
2	A	806	HEC	1	0
2	A	810	HEC	2	0
2	A	808	HEC	2	0
2	B	808	HEC	2	0
2	B	802	HEC	1	0
2	B	810	HEC	2	0
2	B	807	HEC	2	0
2	B	804	HEC	2	0
2	C	806	HEC	3	0
2	B	809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

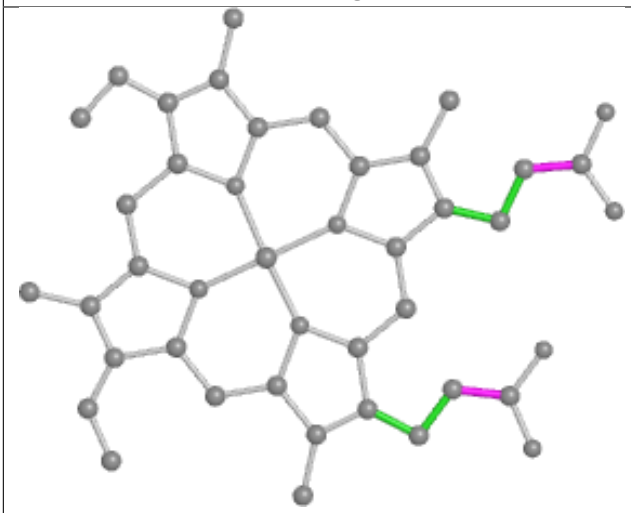
Ligand HEC C 803



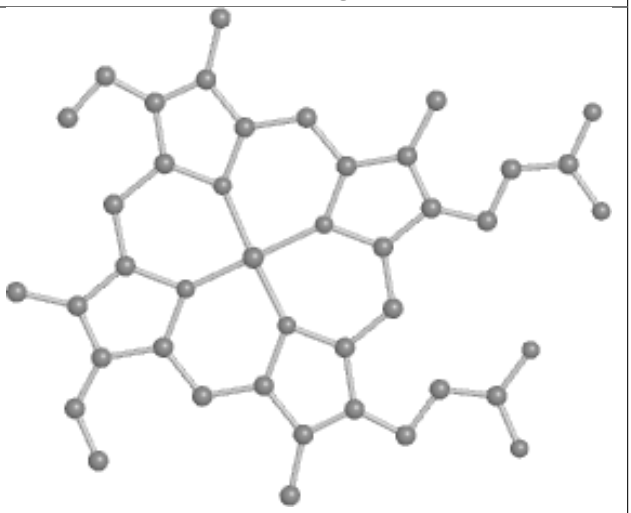
Bond lengths



Bond angles

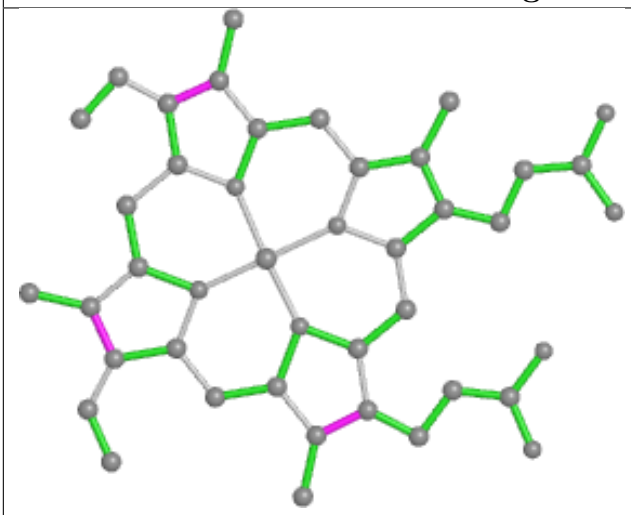


Torsions

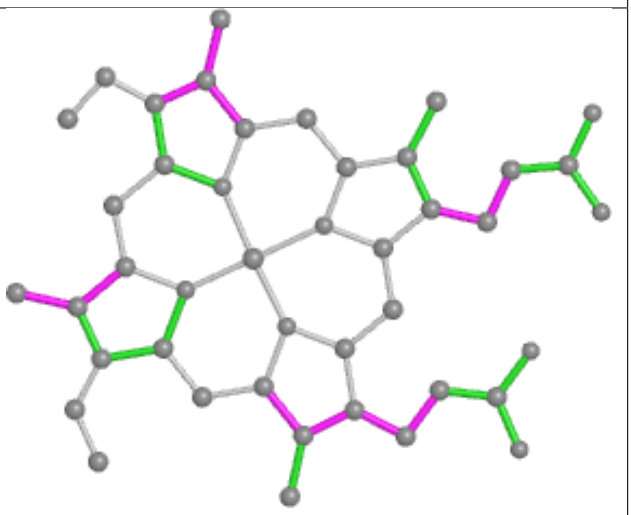


Rings

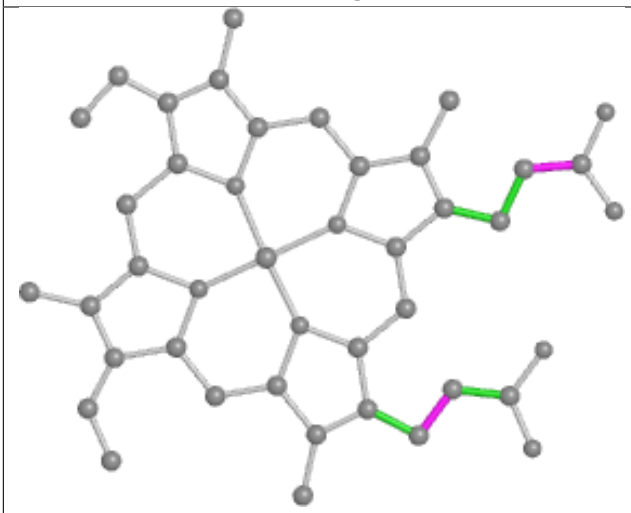
Ligand HEC C 810



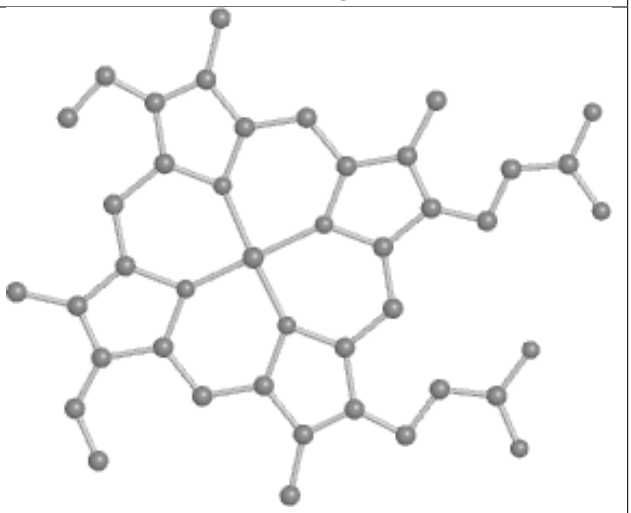
Bond lengths



Bond angles

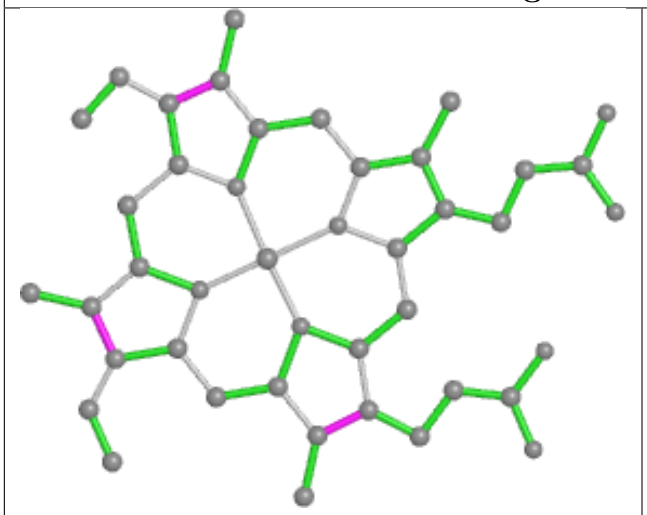


Torsions

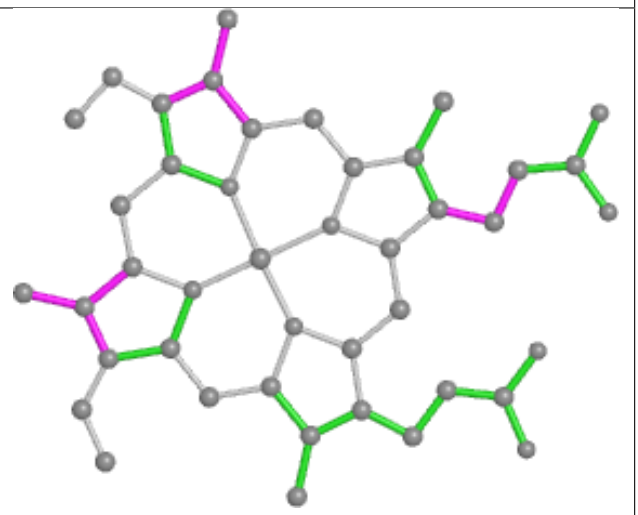


Rings

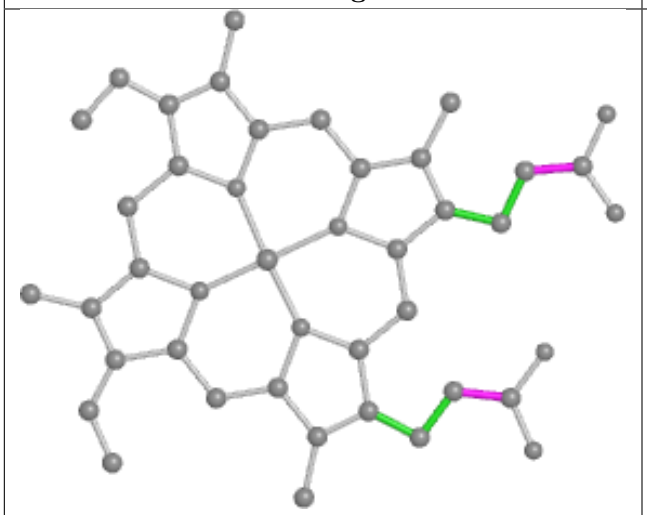
Ligand HEC C 802



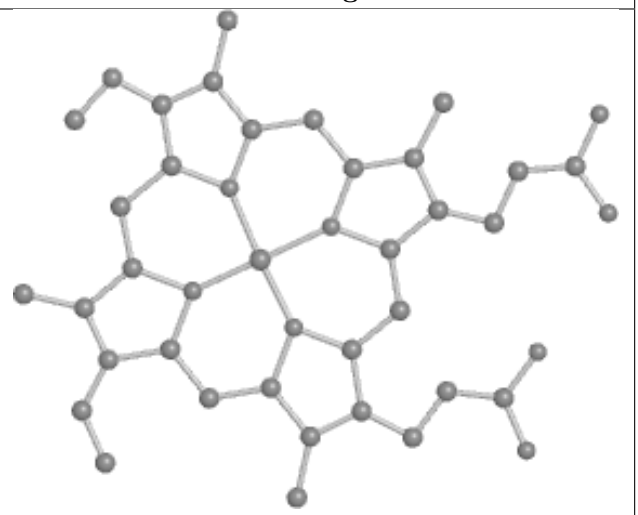
Bond lengths



Bond angles

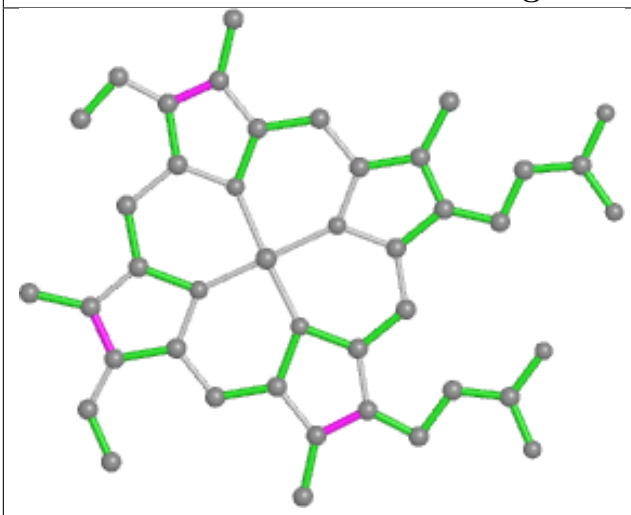


Torsions

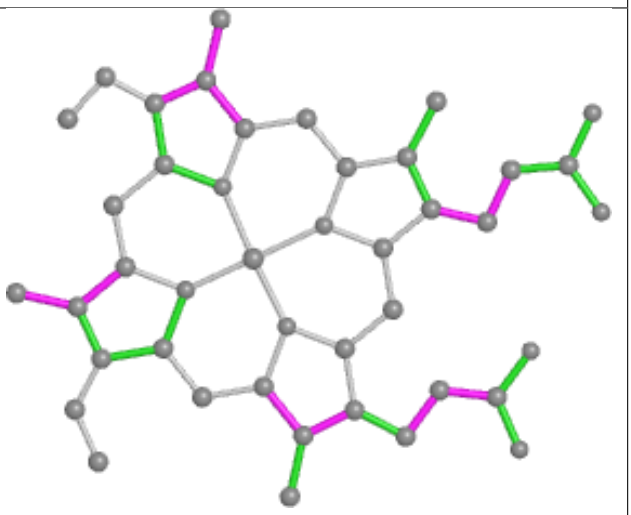


Rings

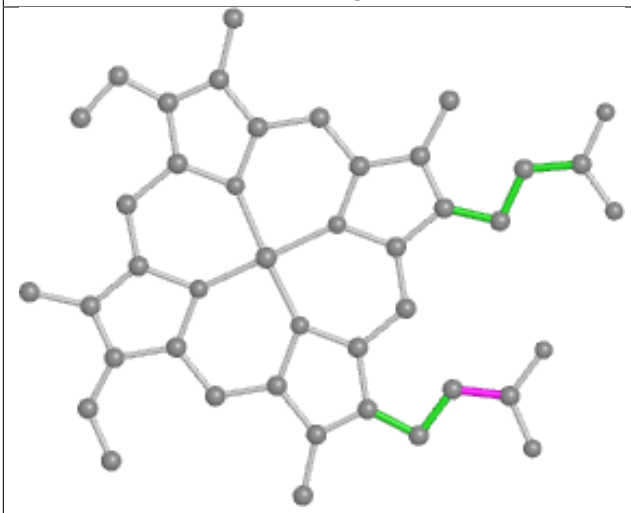
Ligand HEC C 808



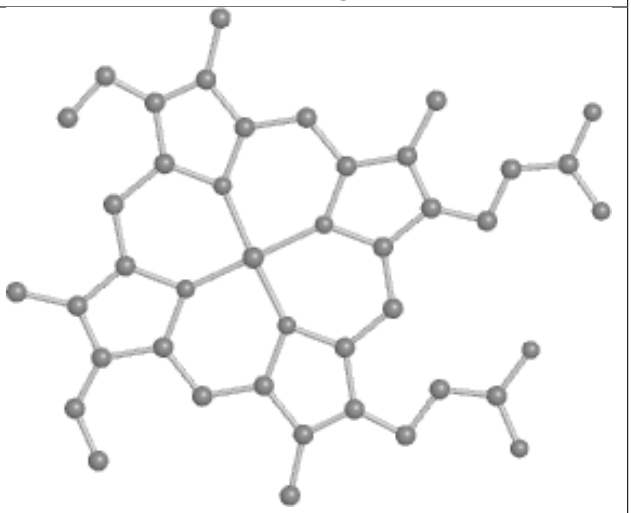
Bond lengths



Bond angles

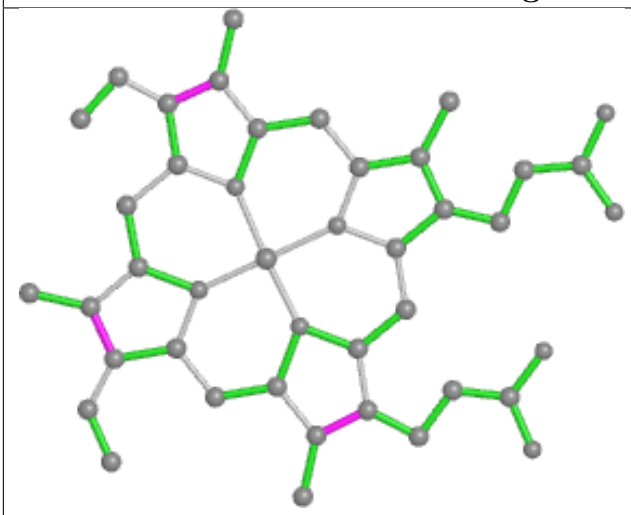


Torsions

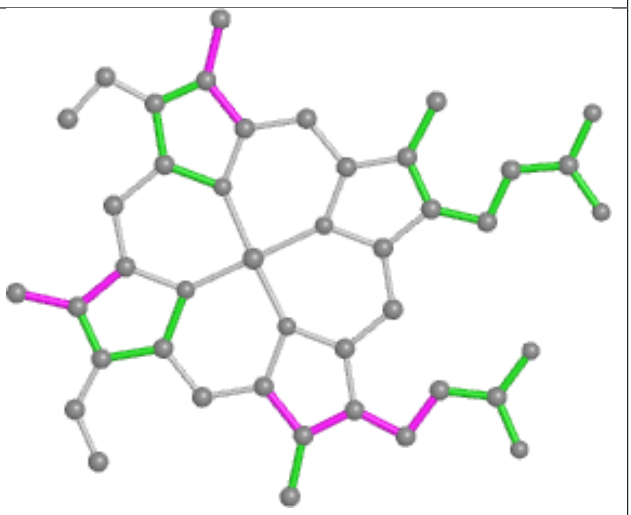


Rings

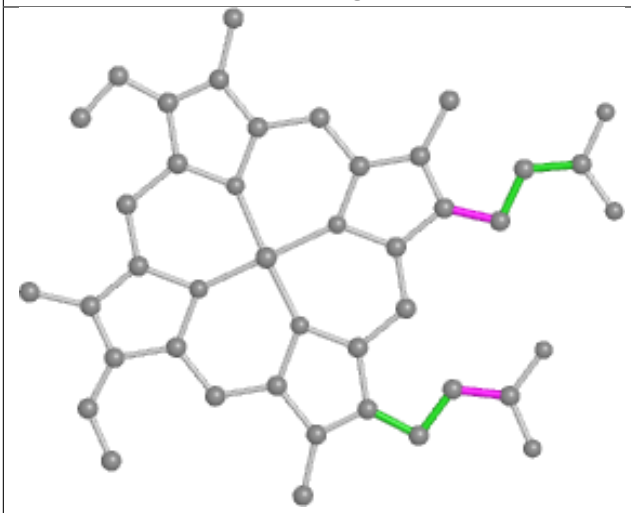
Ligand HEC A 804



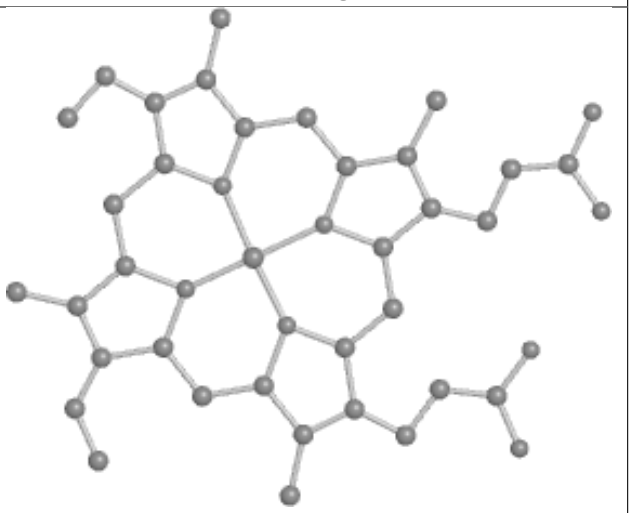
Bond lengths



Bond angles

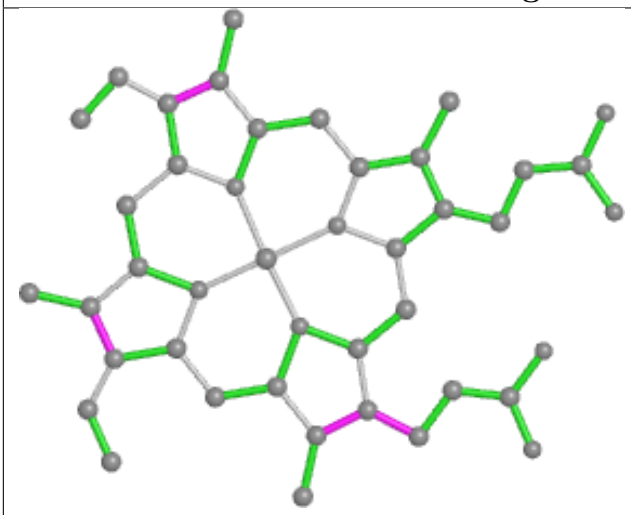


Torsions

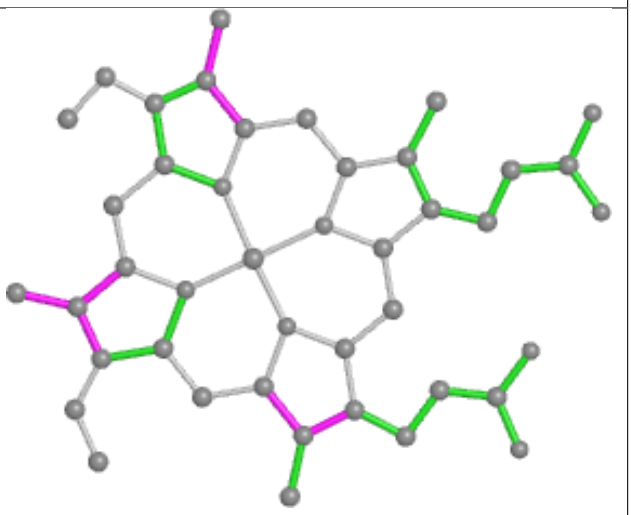


Rings

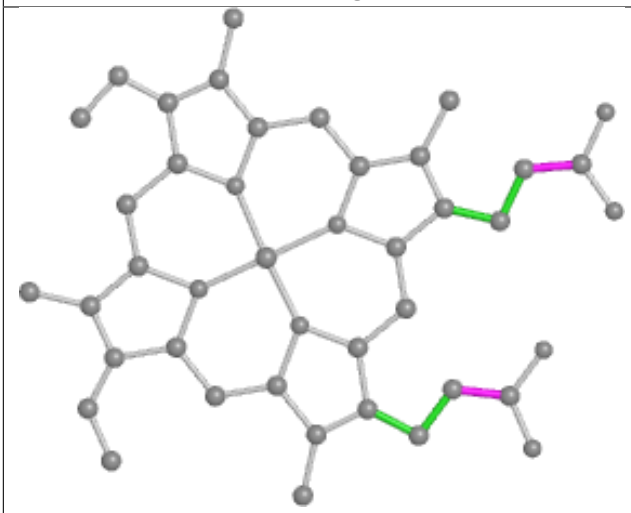
Ligand HEC A 809



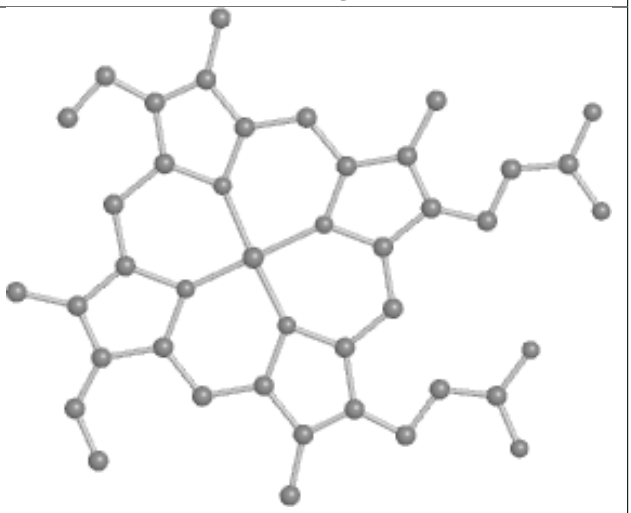
Bond lengths



Bond angles

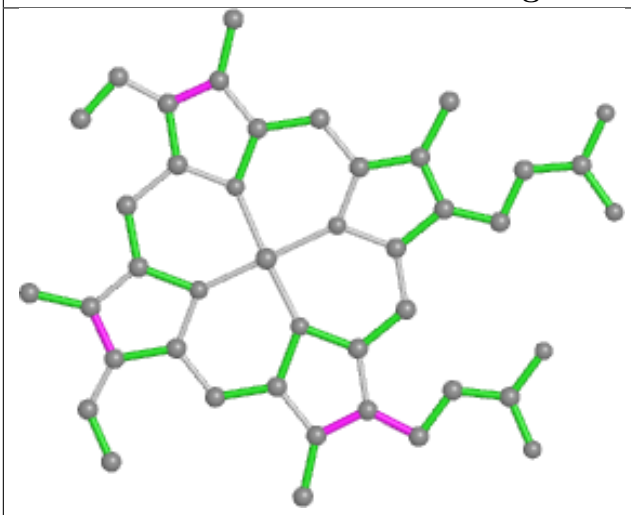


Torsions

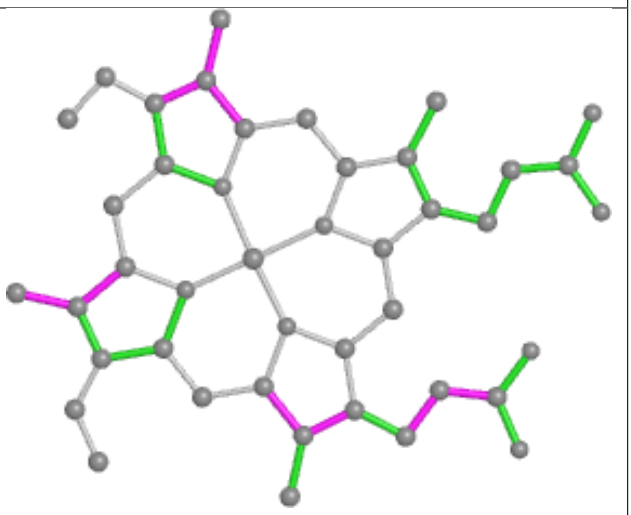


Rings

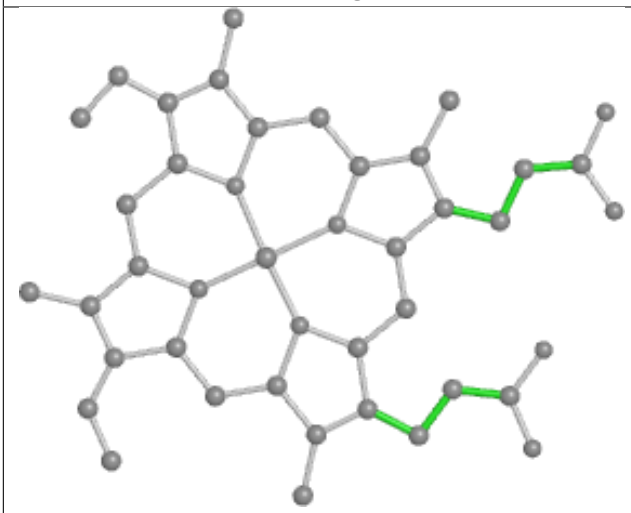
Ligand HEC A 803



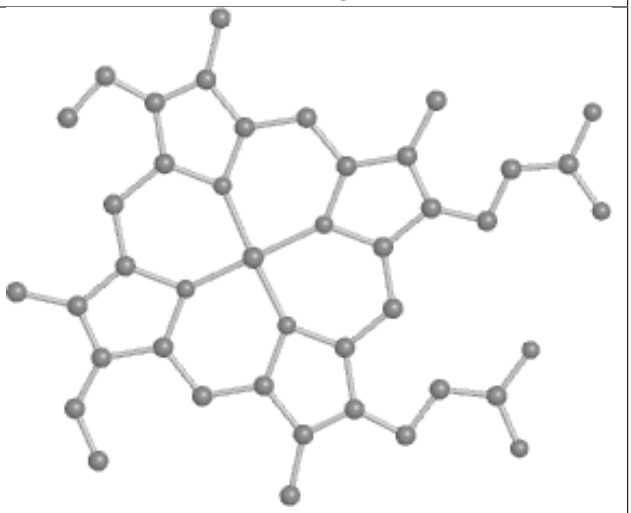
Bond lengths



Bond angles

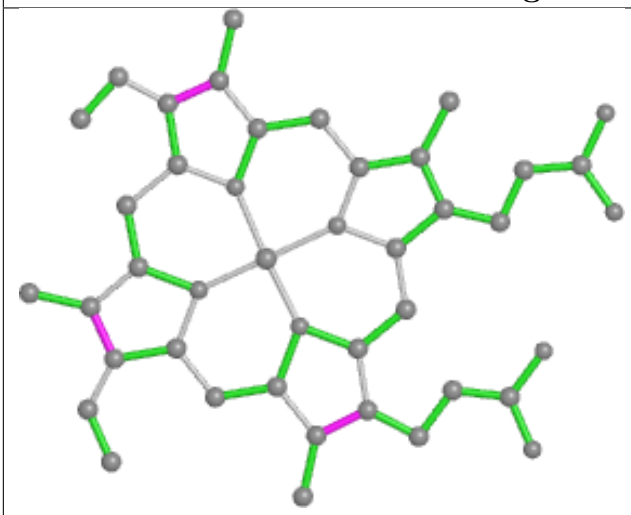


Torsions

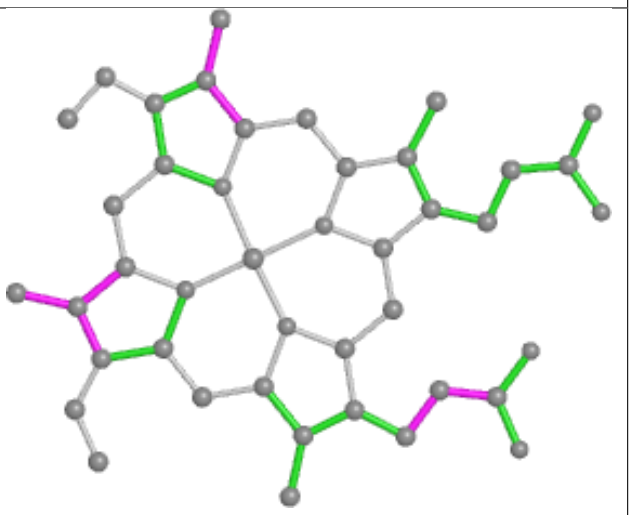


Rings

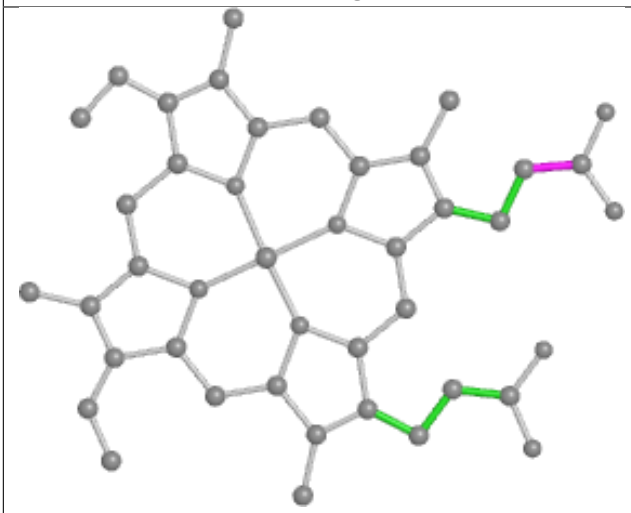
Ligand HEC B 803



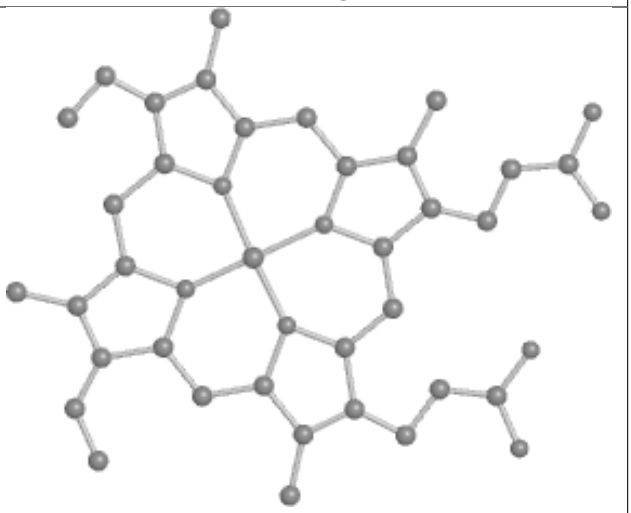
Bond lengths



Bond angles

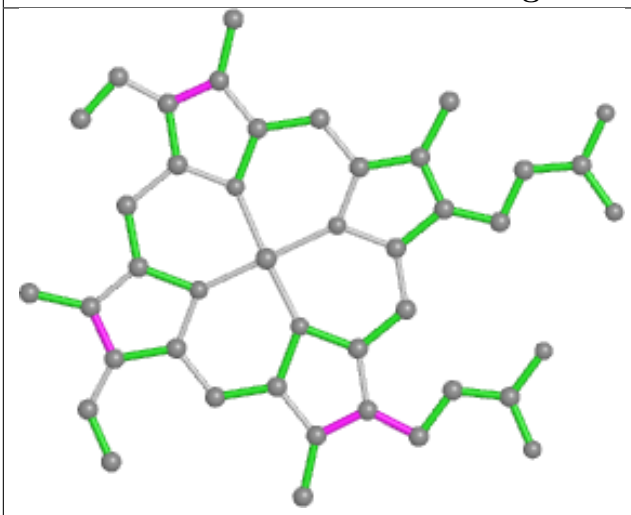


Torsions

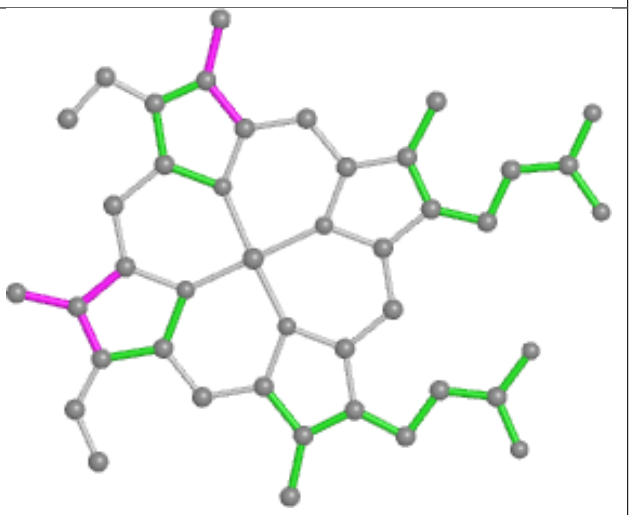


Rings

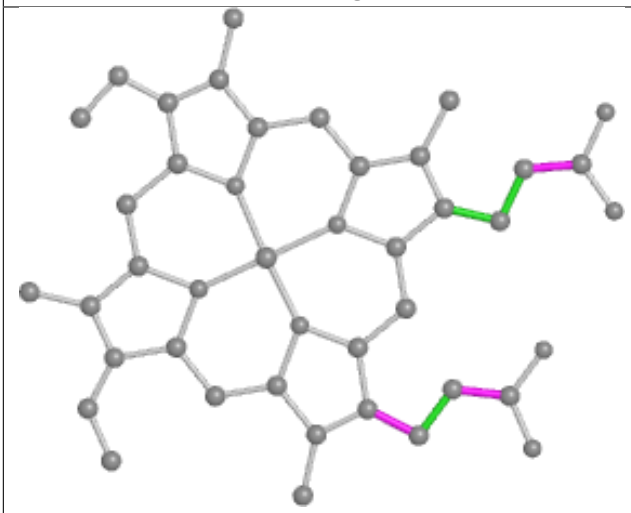
Ligand HEC A 801



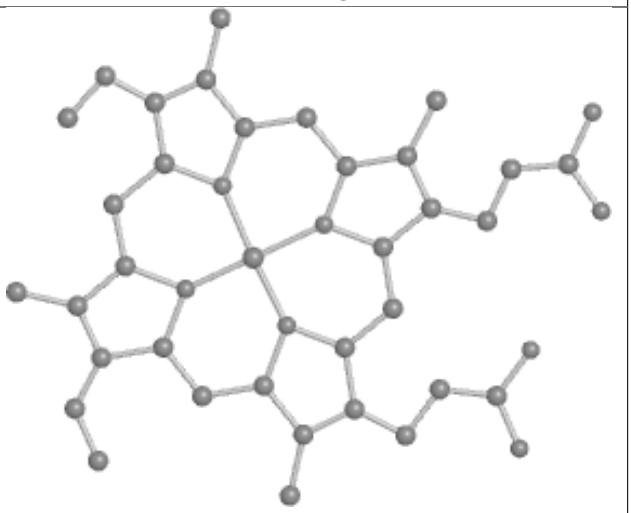
Bond lengths



Bond angles

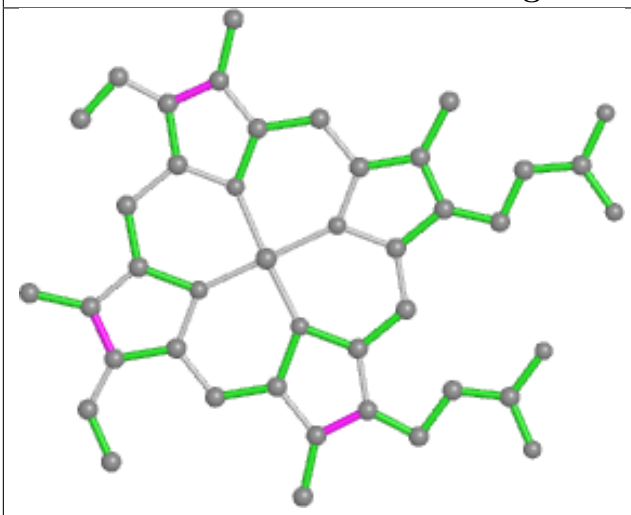


Torsions

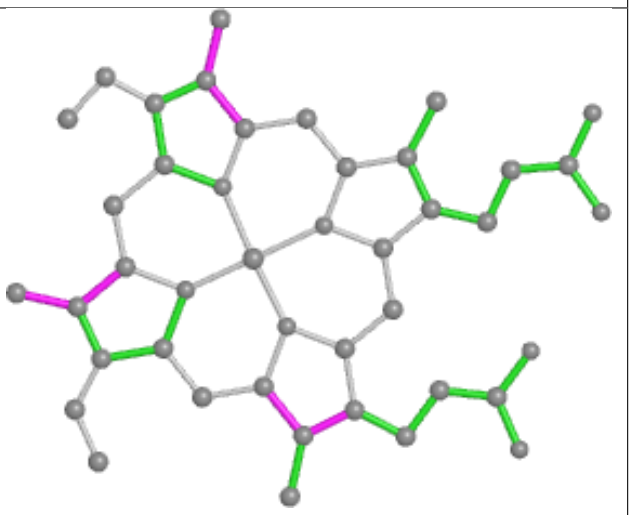


Rings

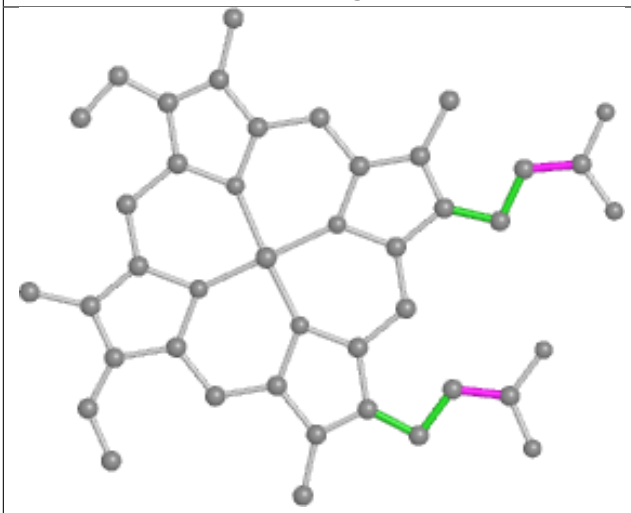
Ligand HEC B 806



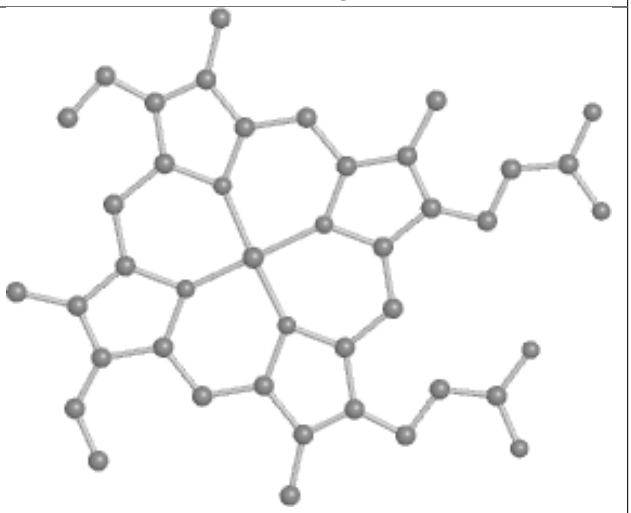
Bond lengths



Bond angles

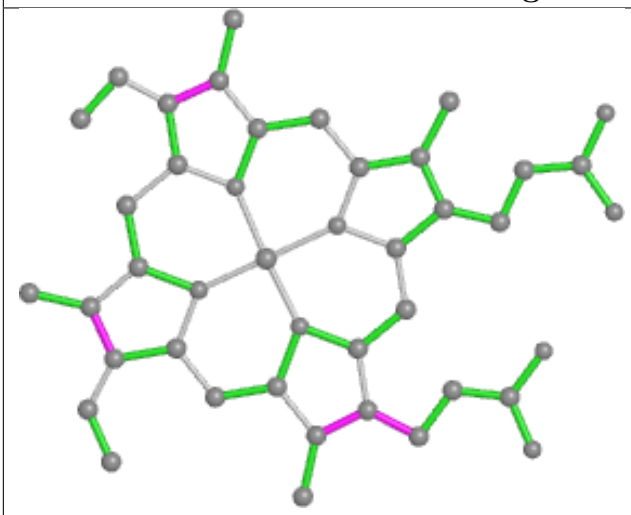


Torsions

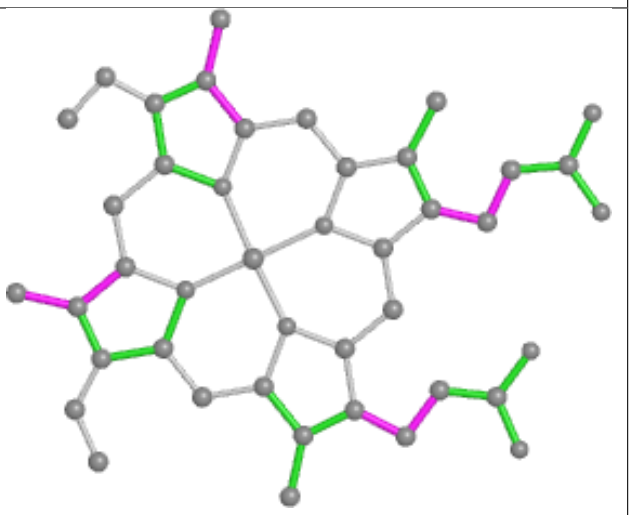


Rings

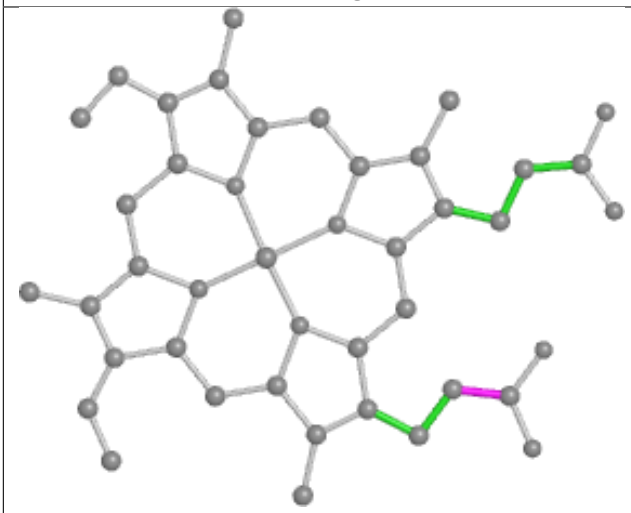
Ligand HEC A 805



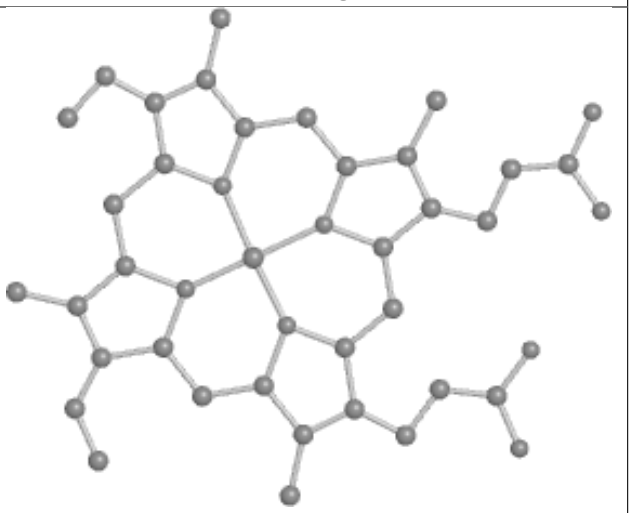
Bond lengths



Bond angles

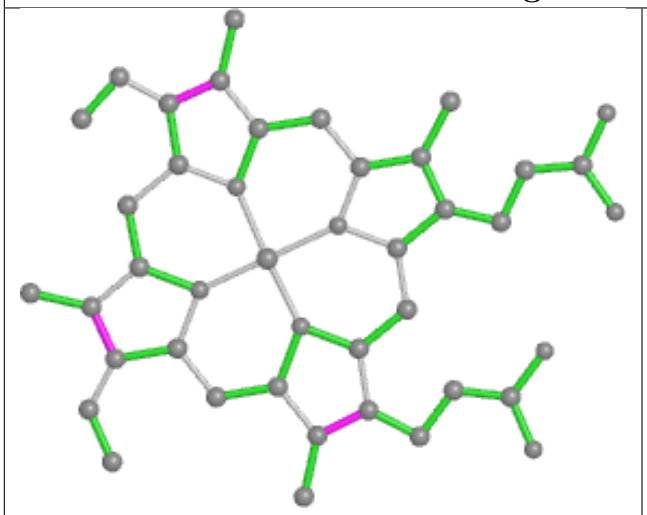


Torsions

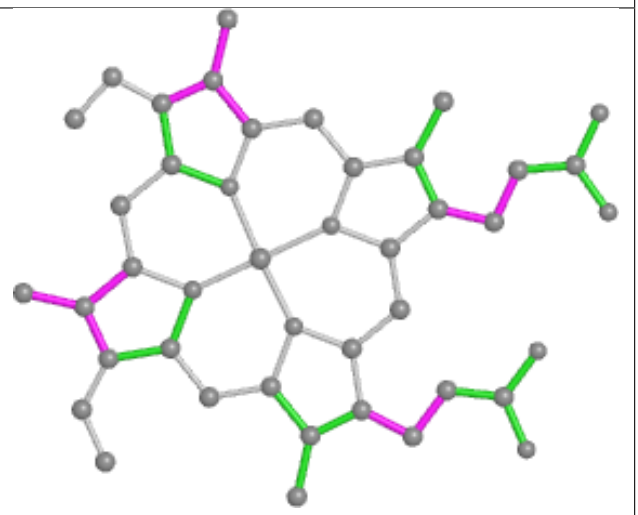


Rings

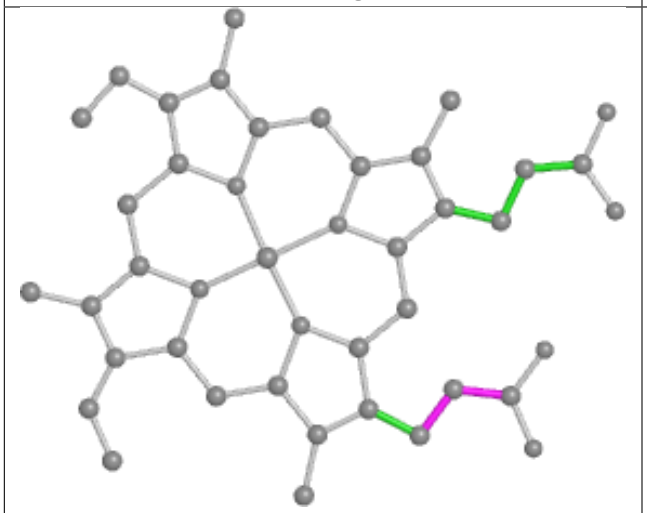
Ligand HEC A 802



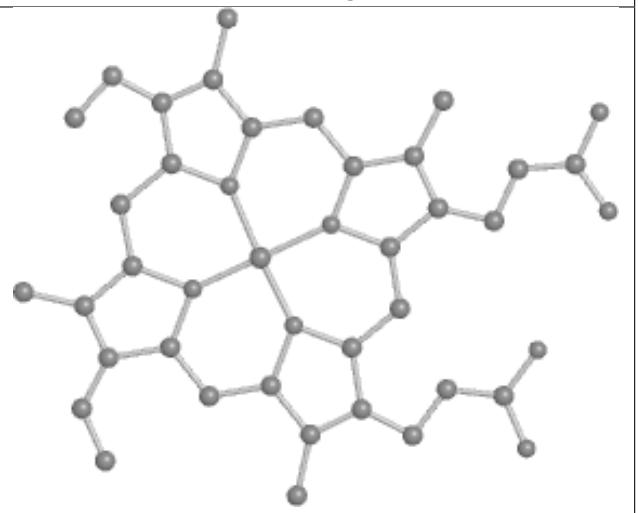
Bond lengths



Bond angles

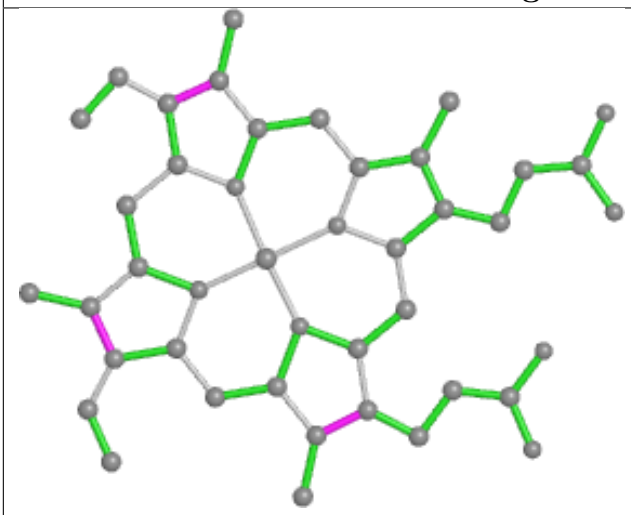


Torsions

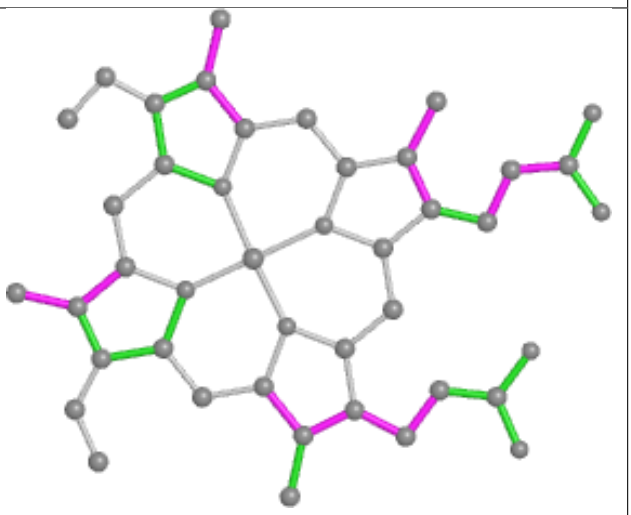


Rings

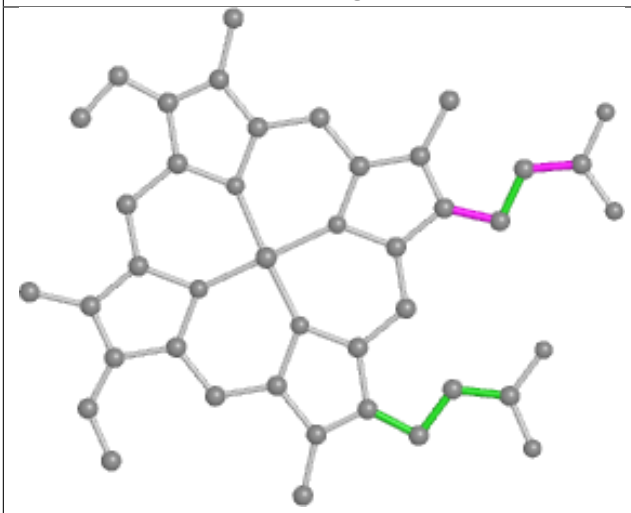
Ligand HEC A 806



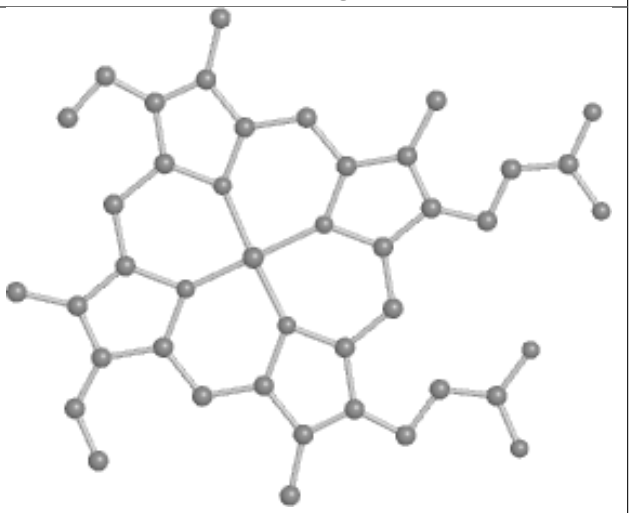
Bond lengths



Bond angles

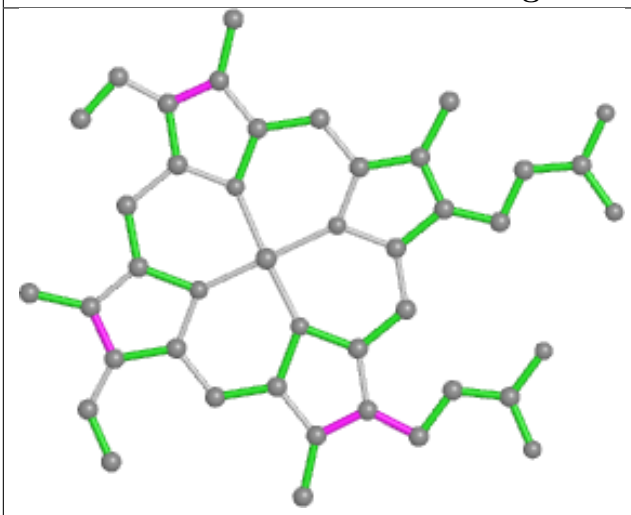


Torsions

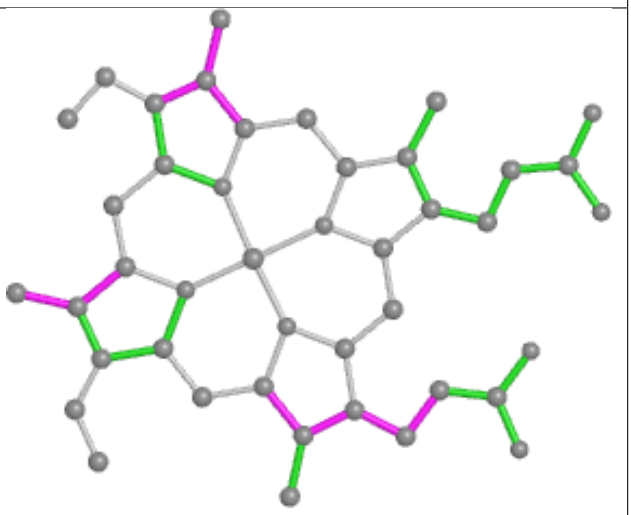


Rings

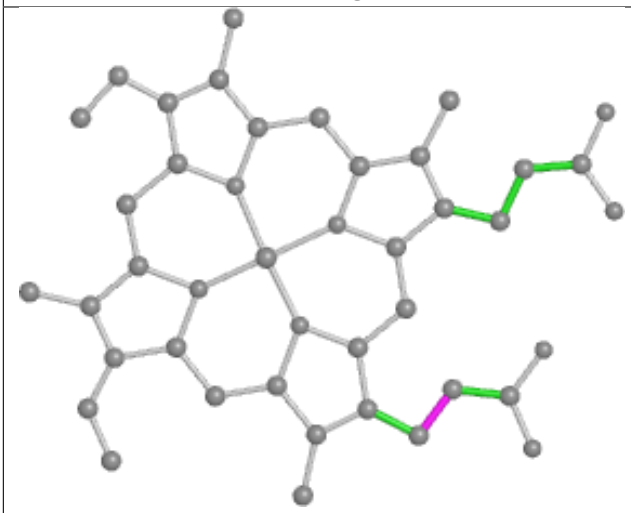
Ligand HEC A 810



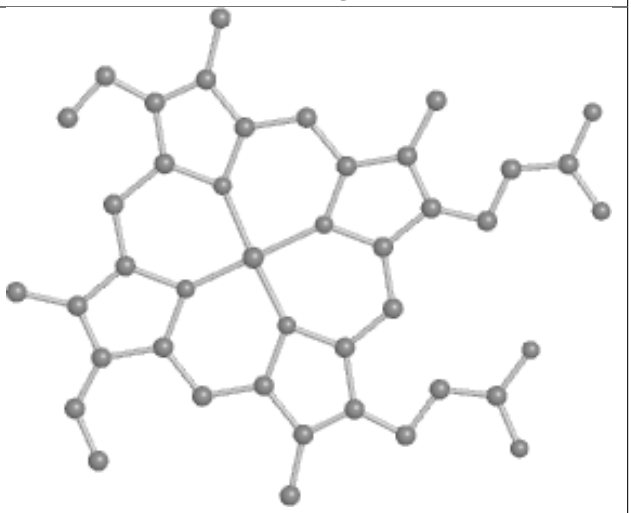
Bond lengths



Bond angles

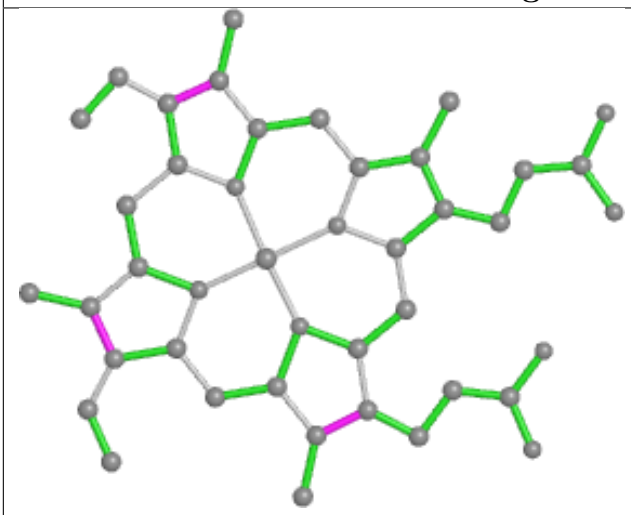


Torsions

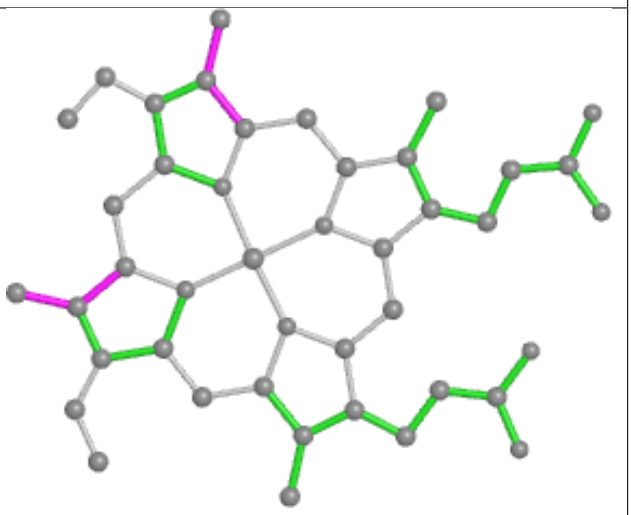


Rings

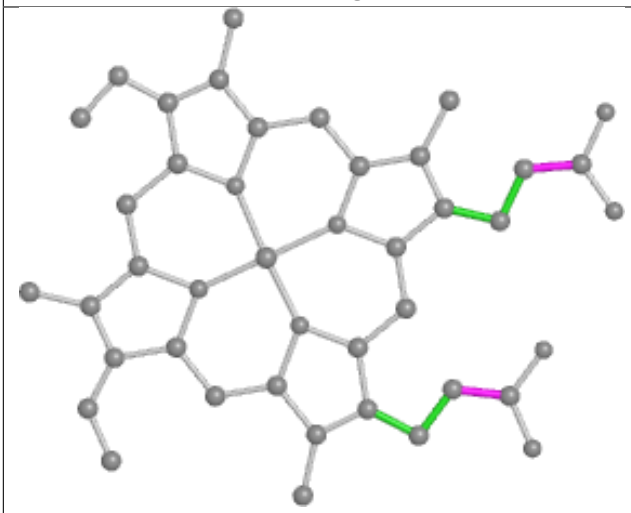
Ligand HEC A 808



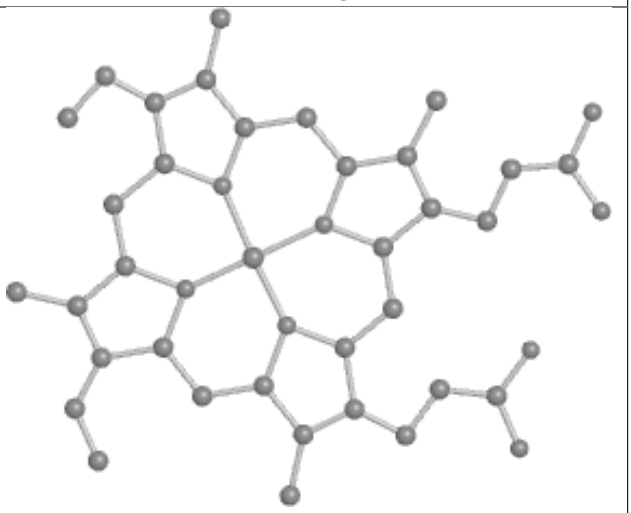
Bond lengths



Bond angles

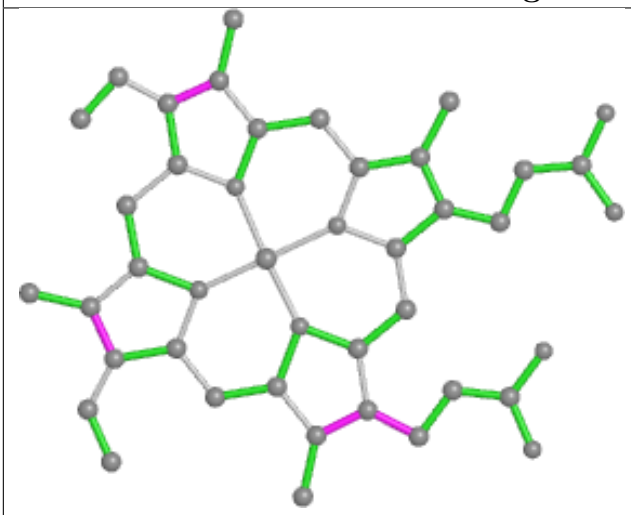


Torsions

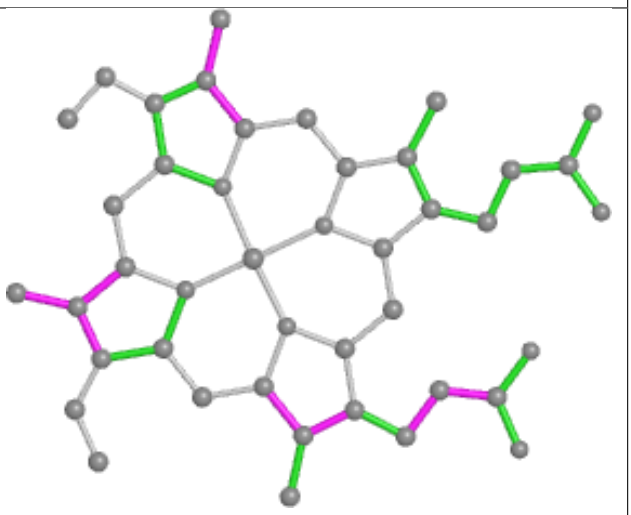


Rings

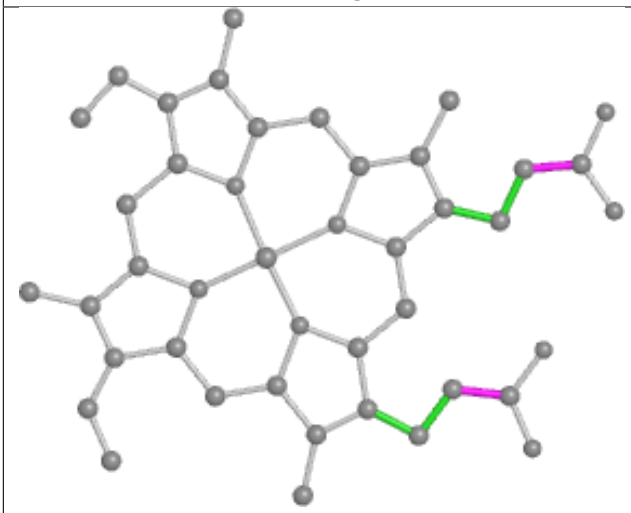
Ligand HEC B 808



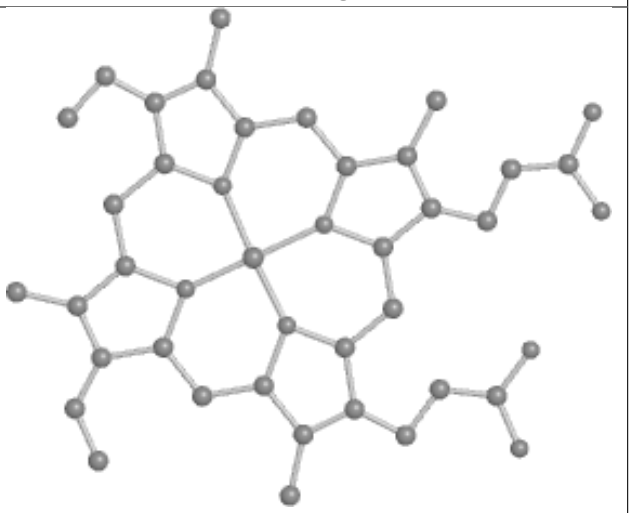
Bond lengths



Bond angles

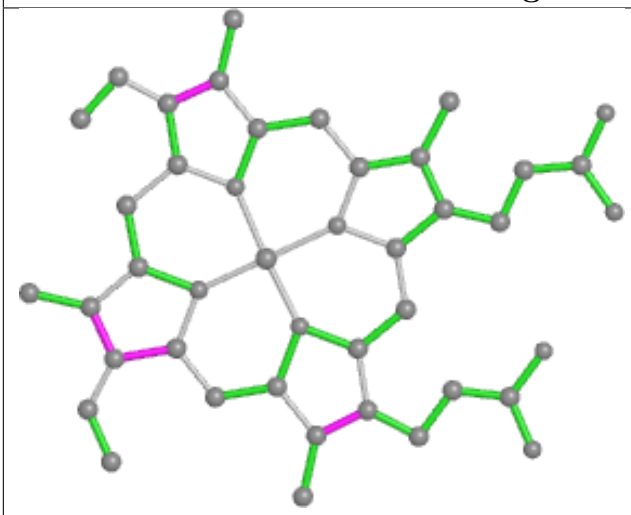


Torsions

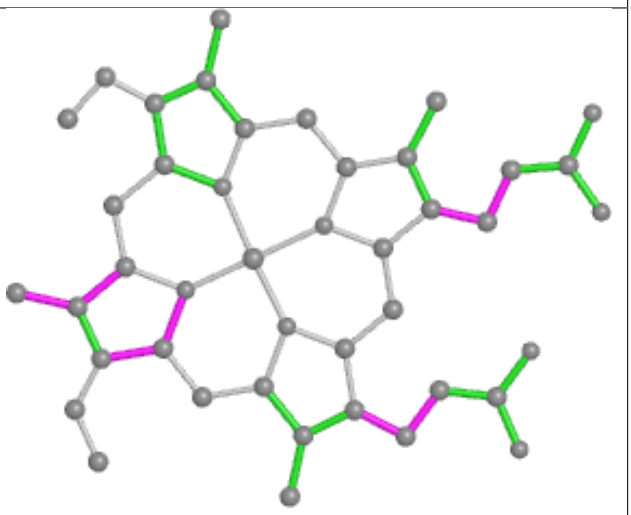


Rings

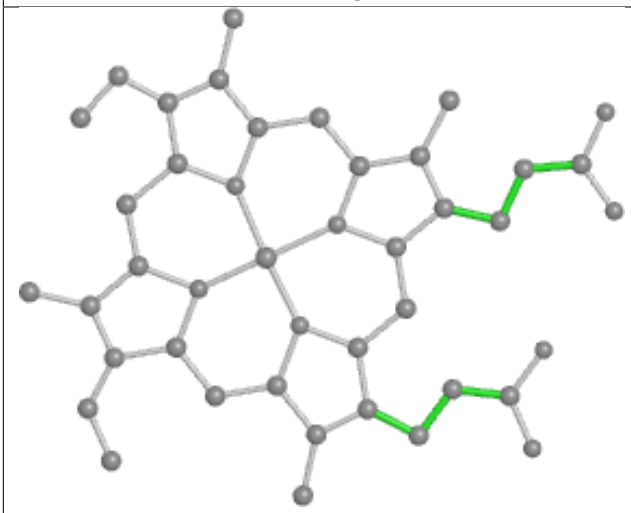
Ligand HEC C 805



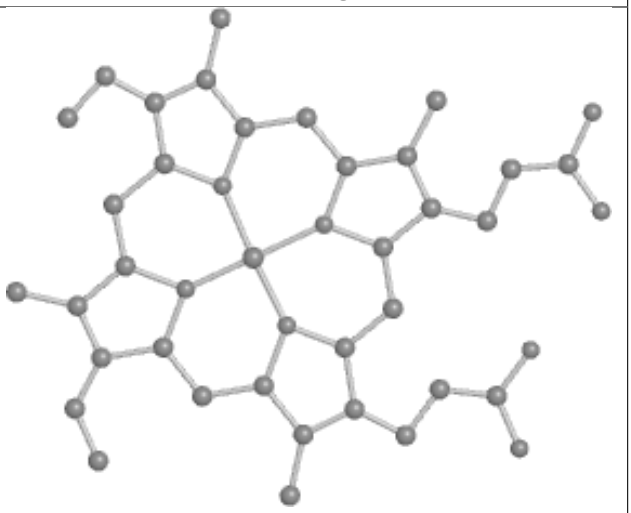
Bond lengths



Bond angles

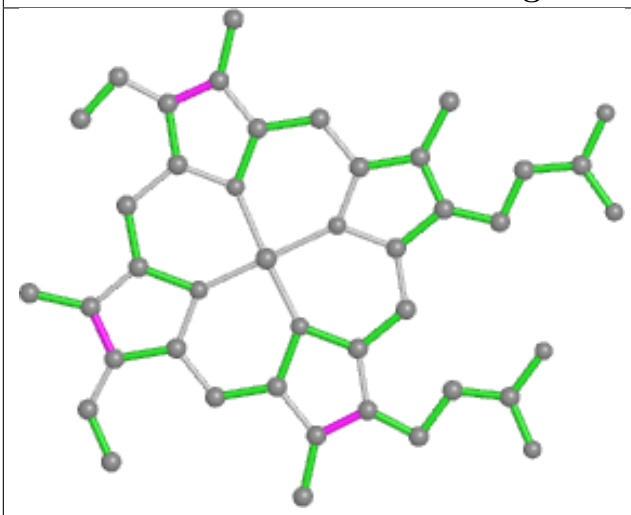


Torsions

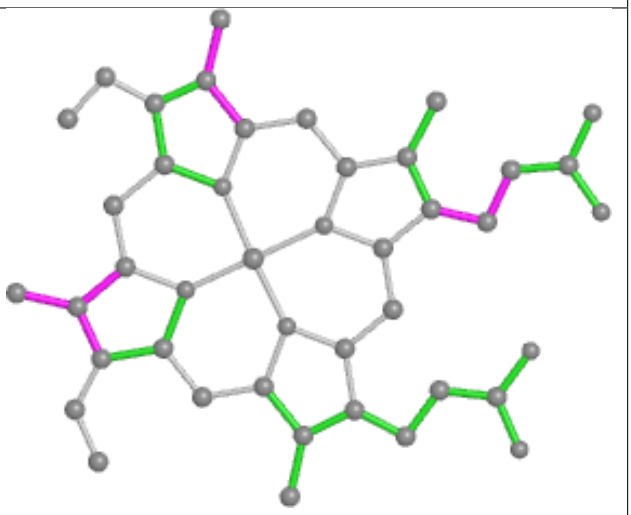


Rings

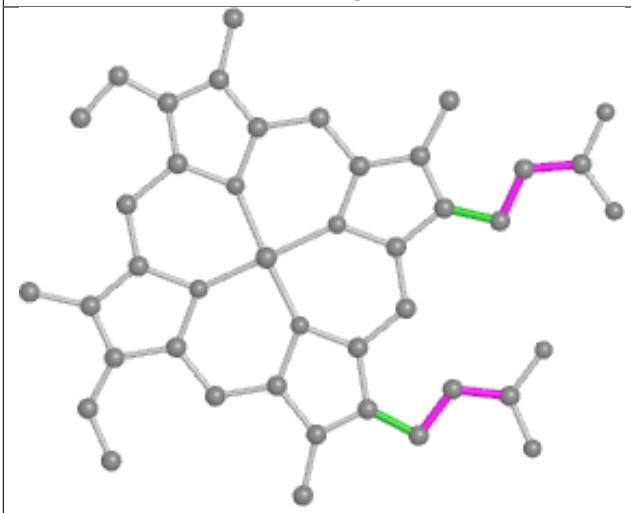
Ligand HEC B 802



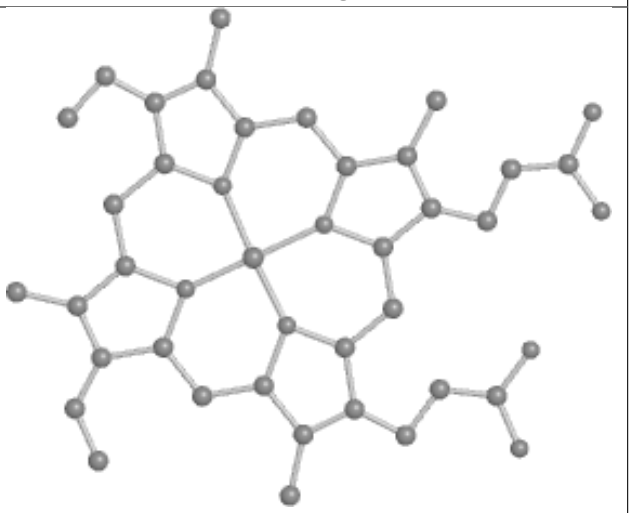
Bond lengths



Bond angles

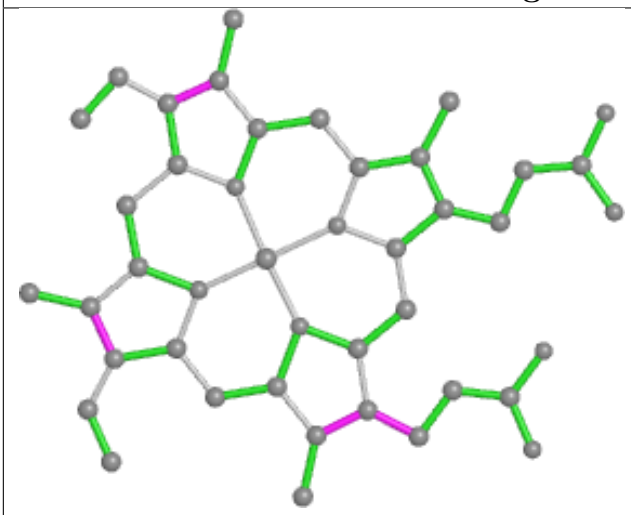


Torsions

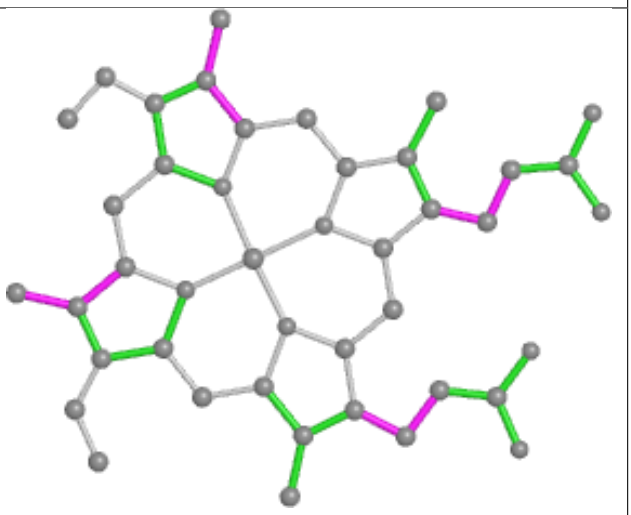


Rings

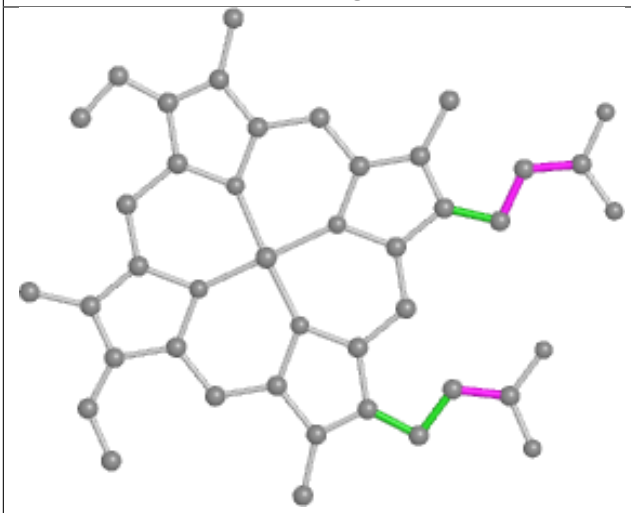
Ligand HEC B 810



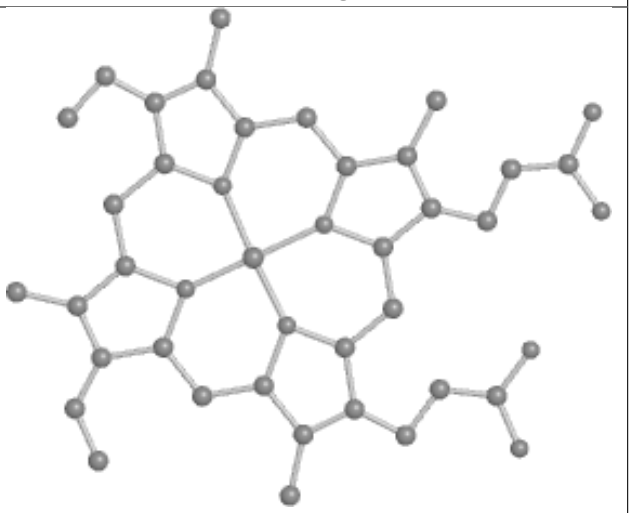
Bond lengths



Bond angles

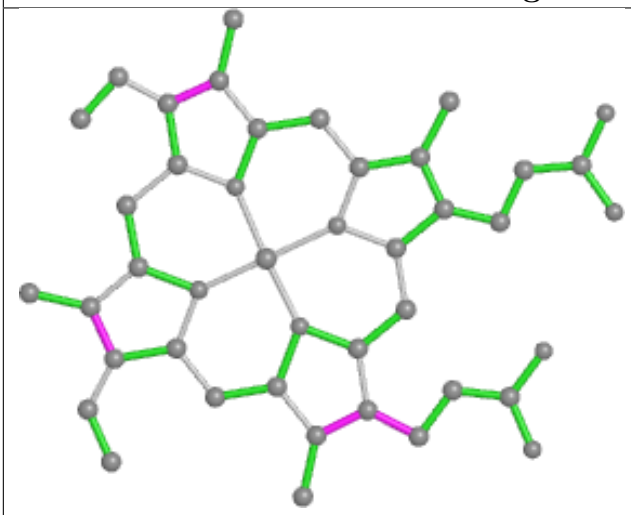


Torsions

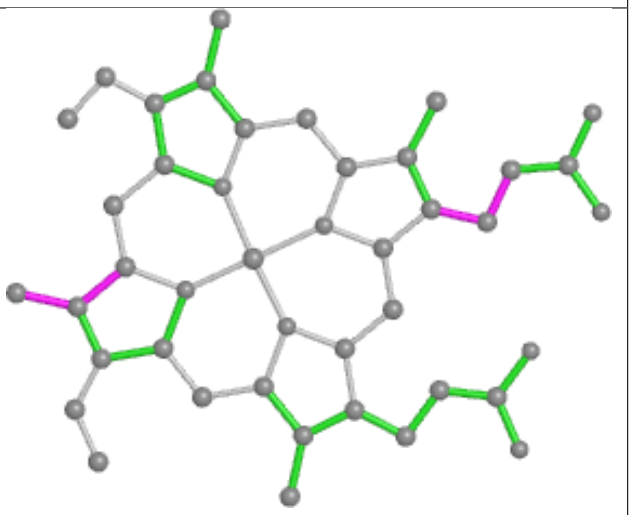


Rings

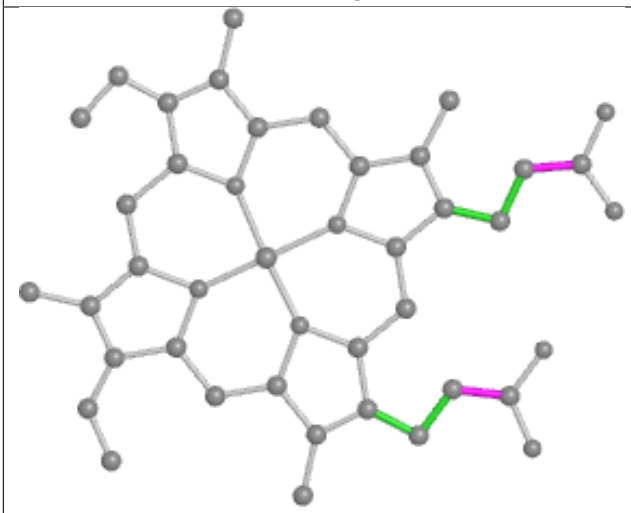
Ligand HEC B 807



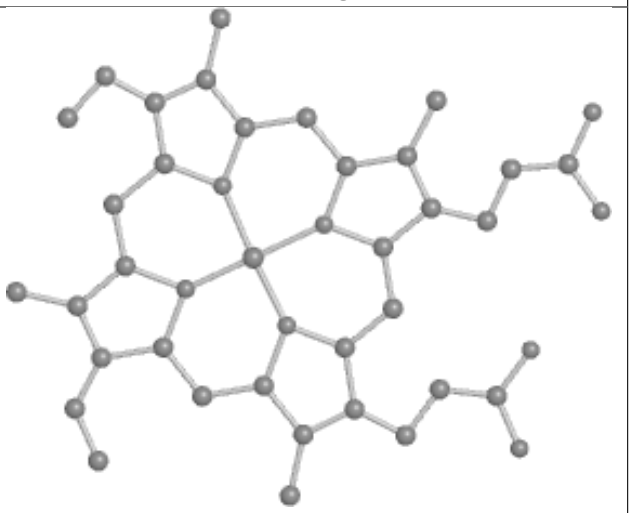
Bond lengths



Bond angles

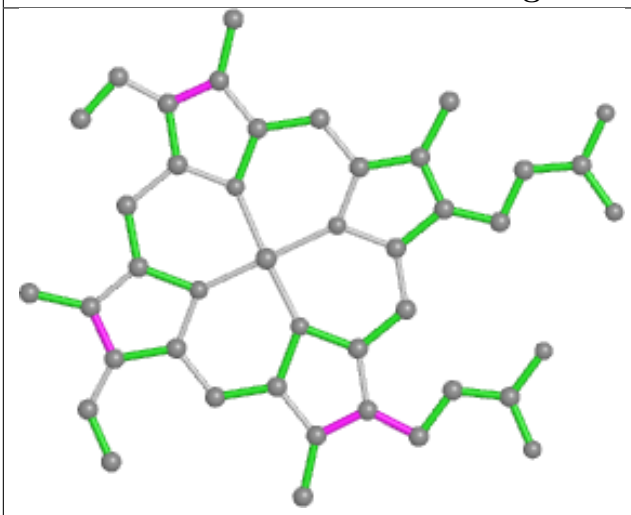


Torsions

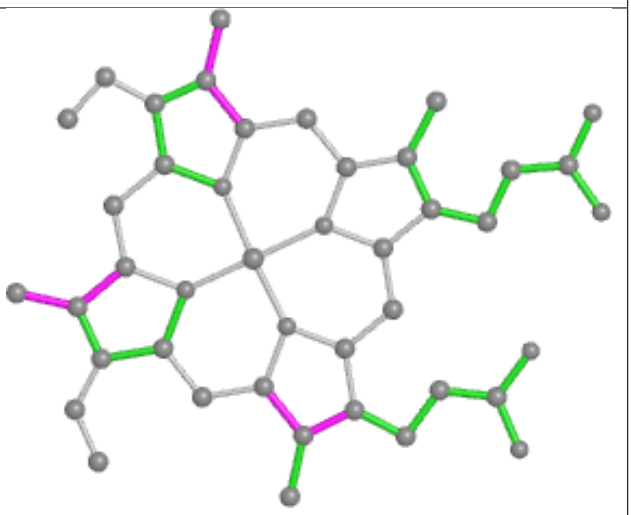


Rings

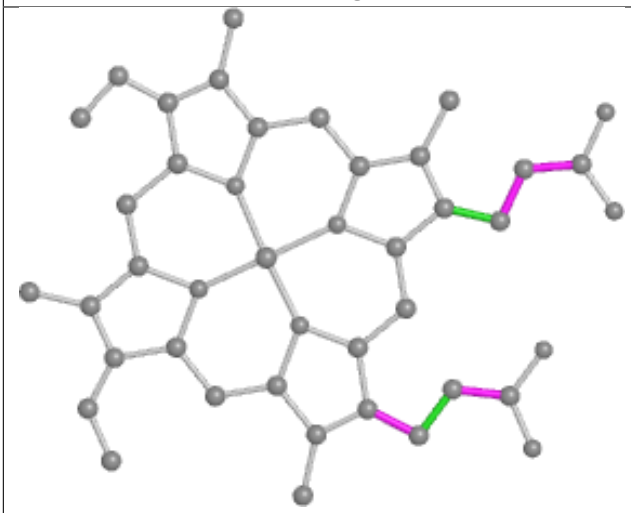
Ligand HEC B 804



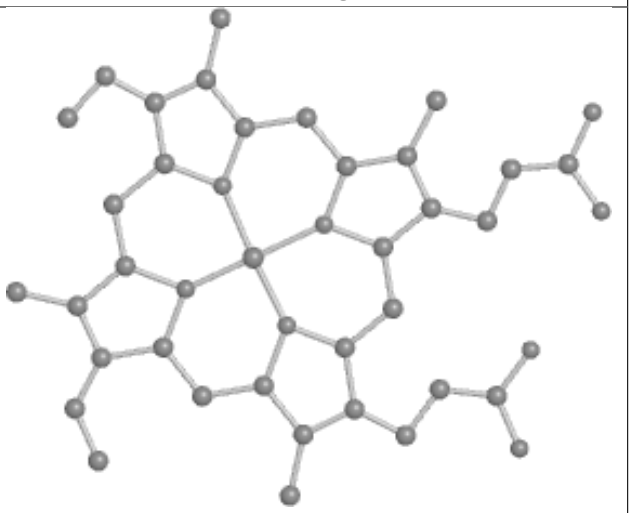
Bond lengths



Bond angles

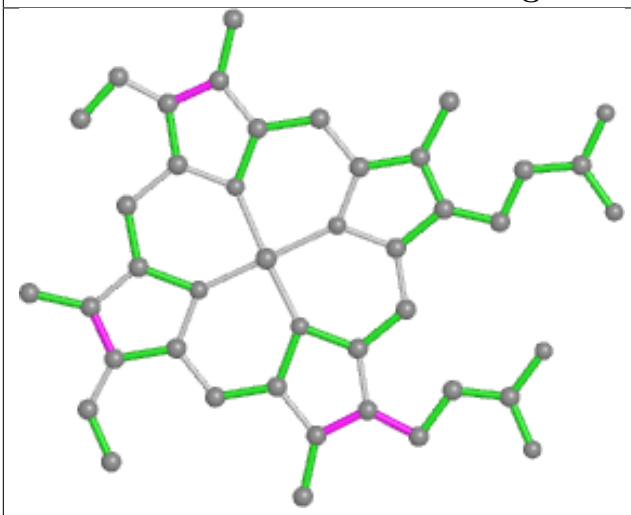


Torsions

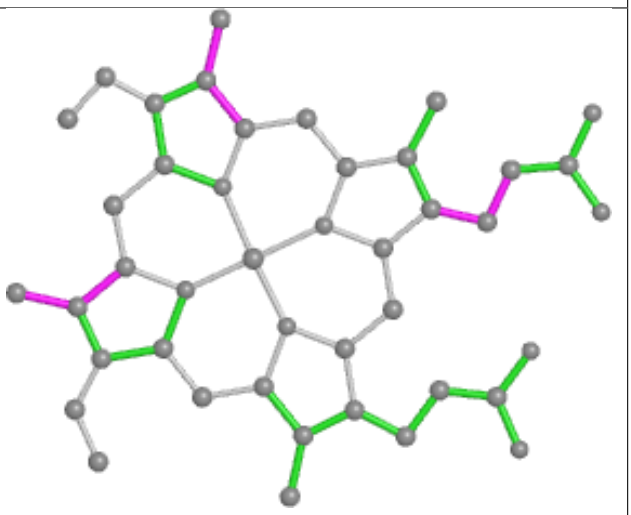


Rings

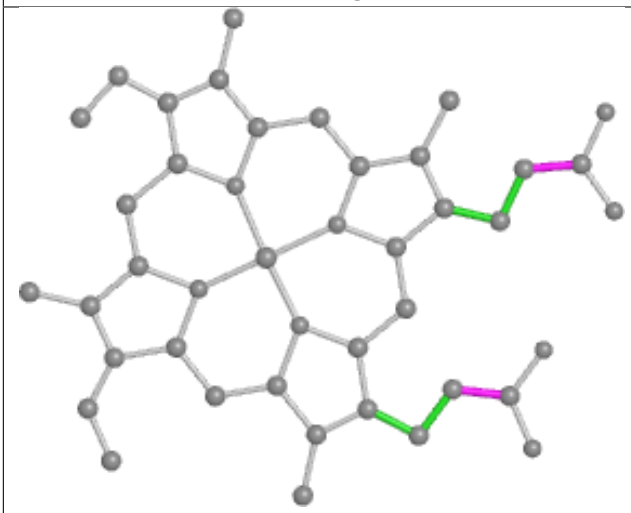
Ligand HEC A 807



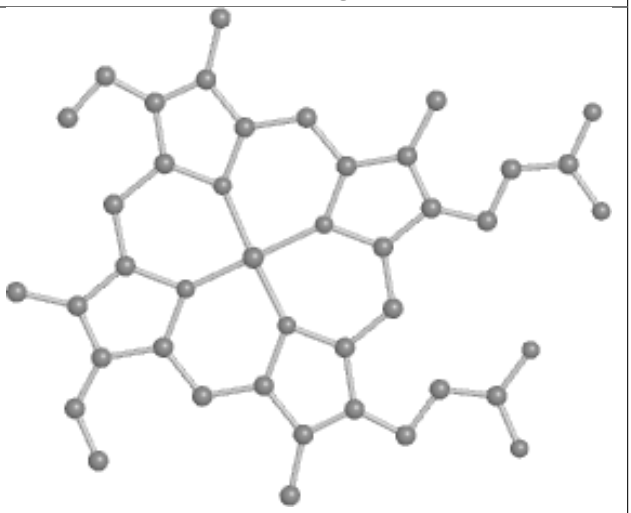
Bond lengths



Bond angles

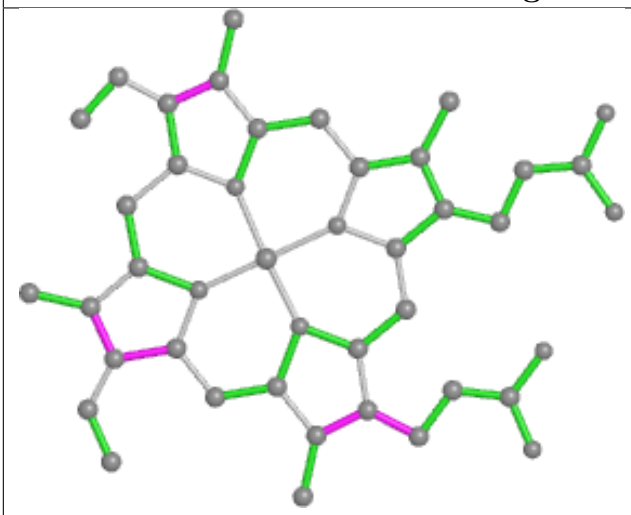


Torsions

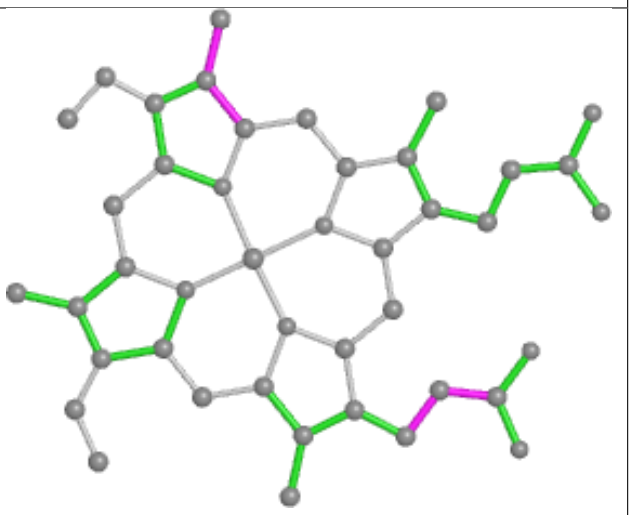


Rings

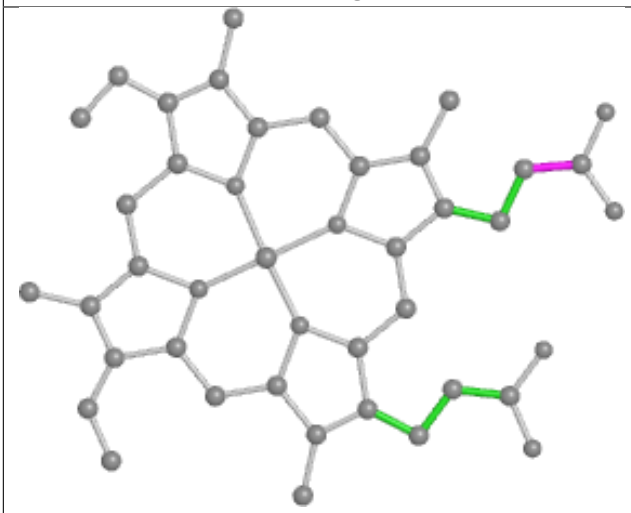
Ligand HEC B 805



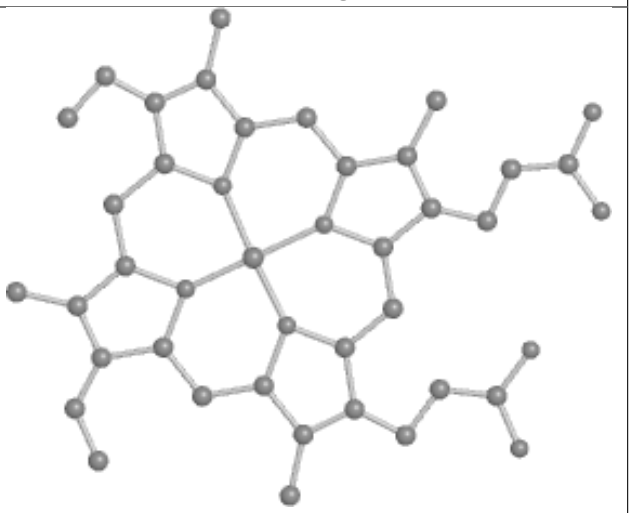
Bond lengths



Bond angles

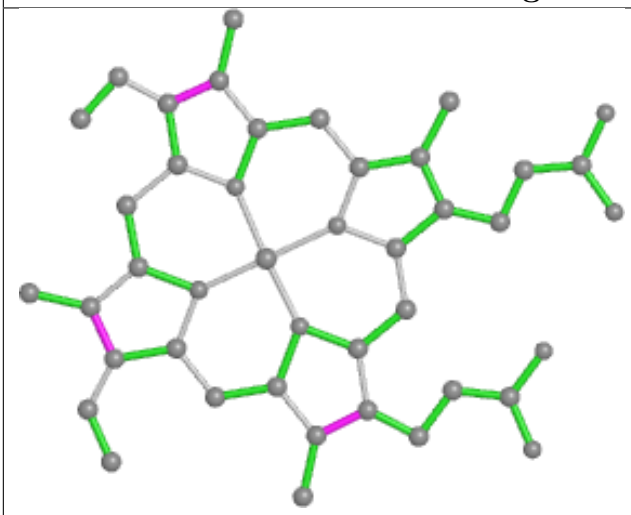


Torsions

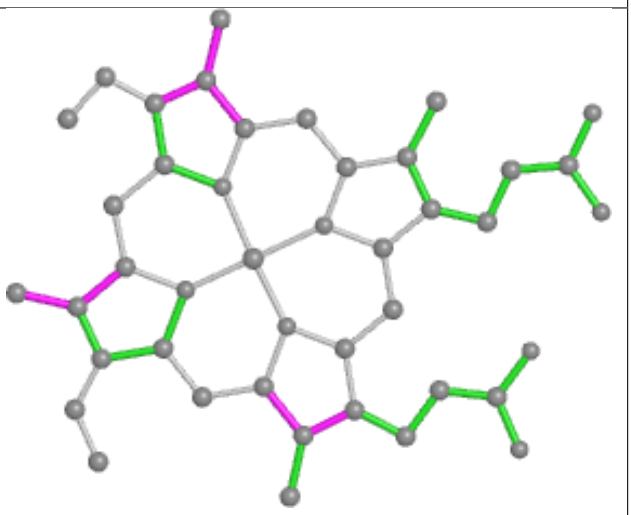


Rings

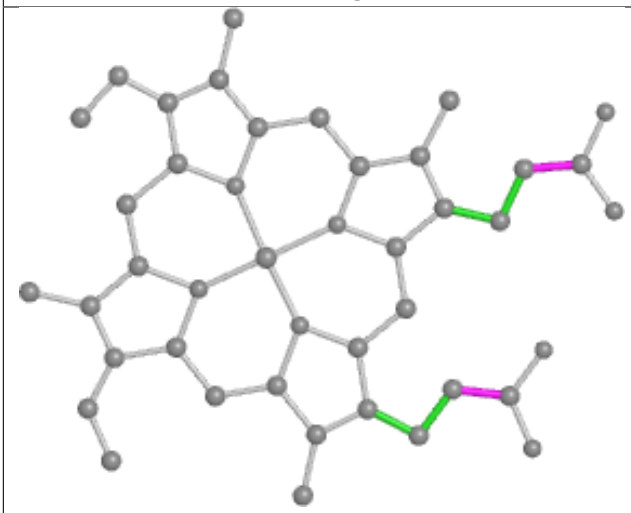
Ligand HEC C 806



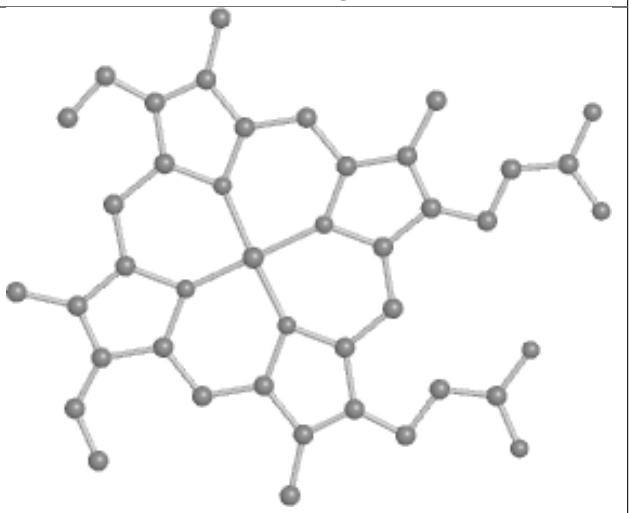
Bond lengths



Bond angles

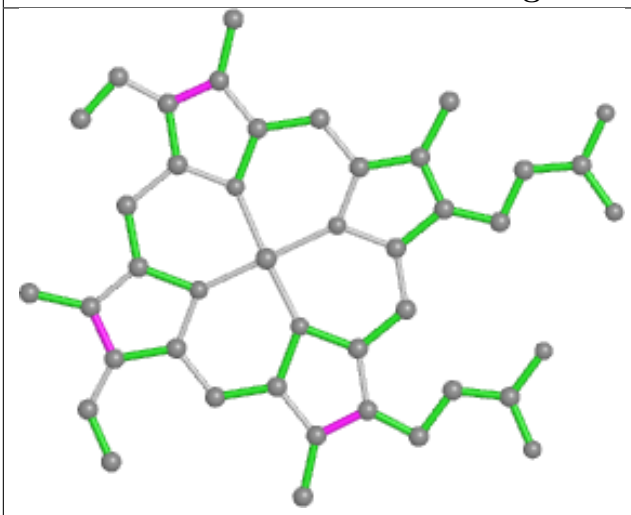


Torsions

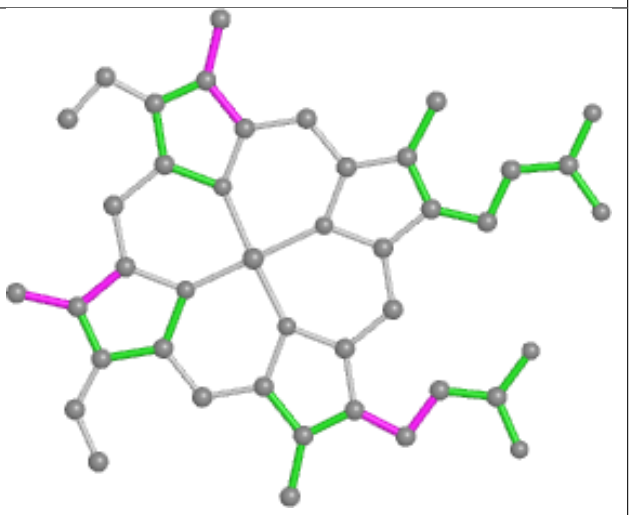


Rings

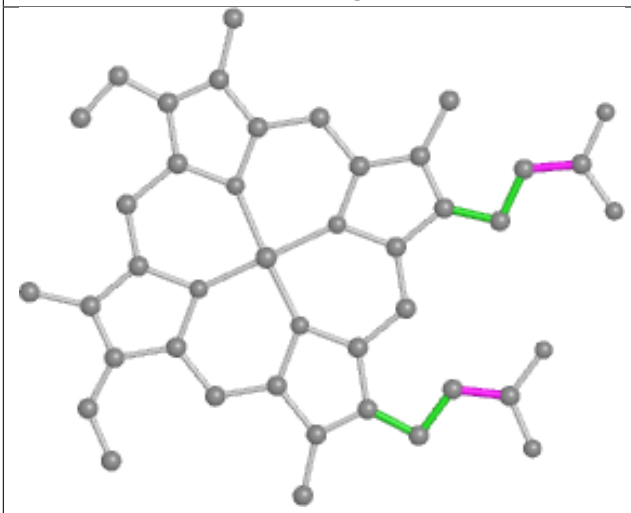
Ligand HEC B 809



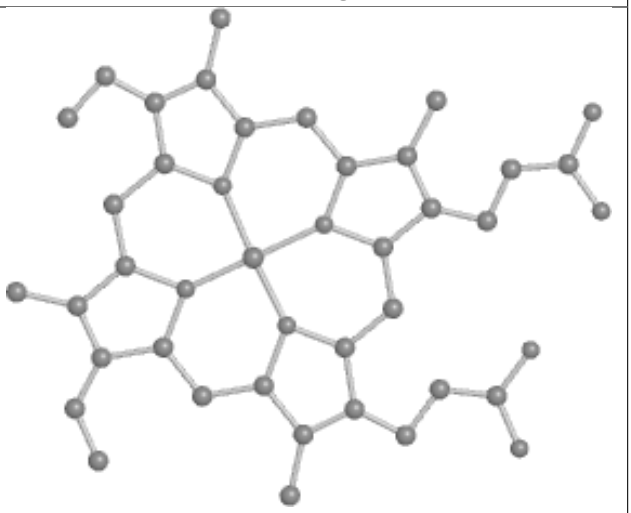
Bond lengths



Bond angles

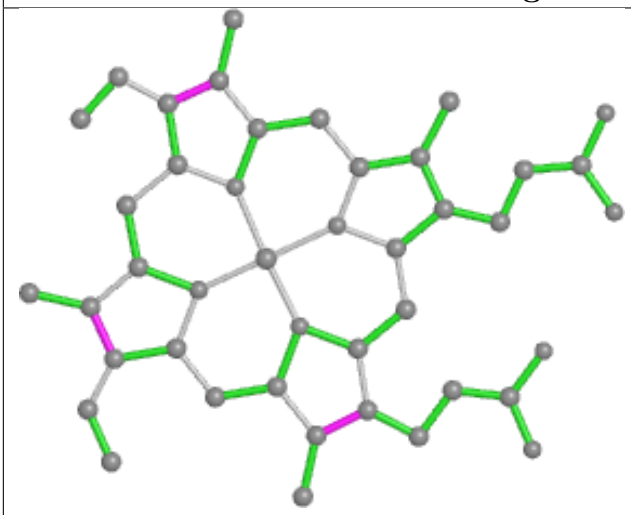


Torsions

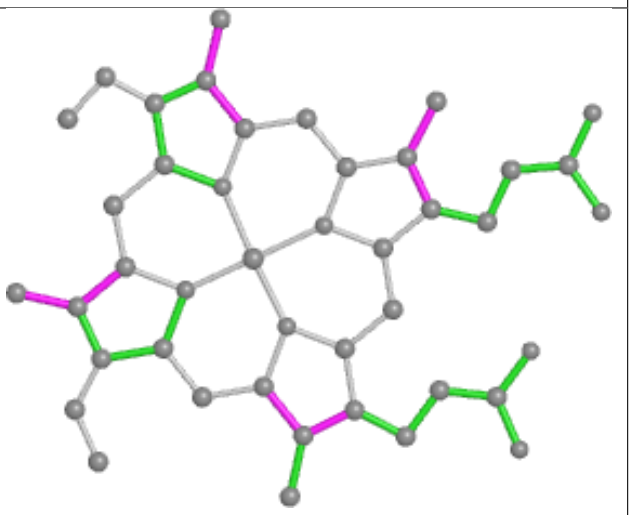


Rings

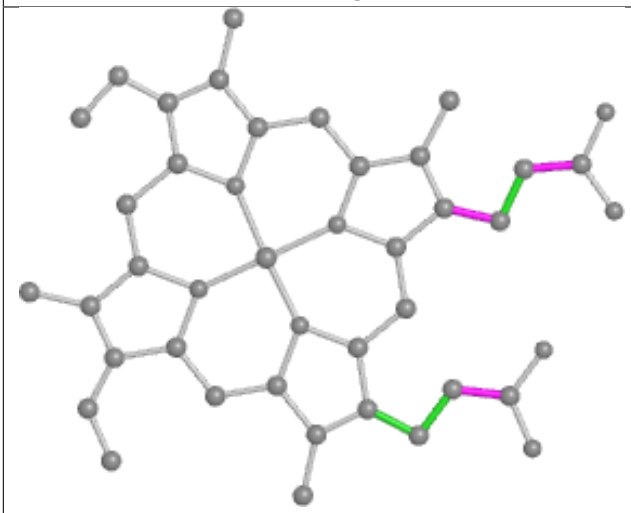
Ligand HEC B 801



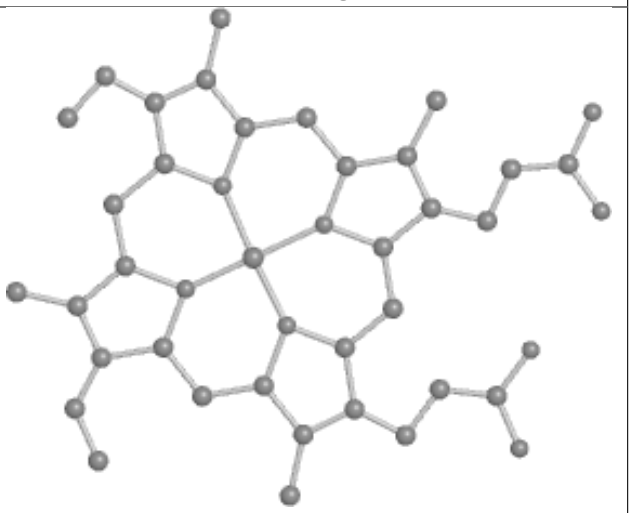
Bond lengths



Bond angles

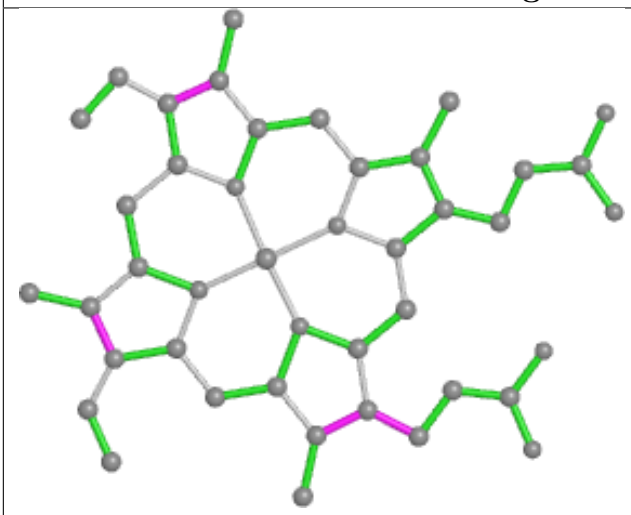


Torsions

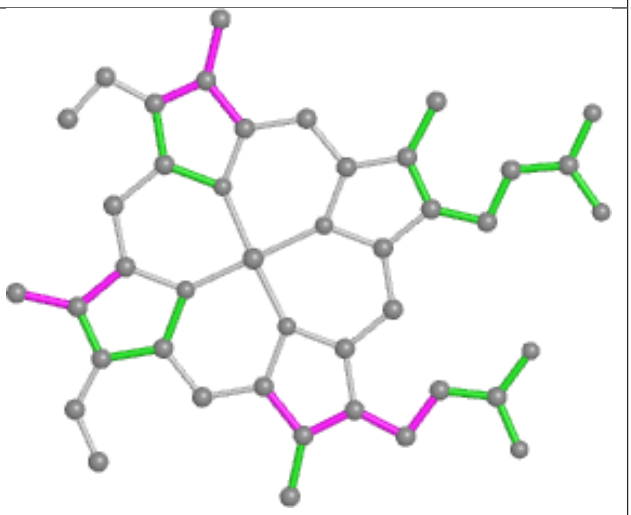


Rings

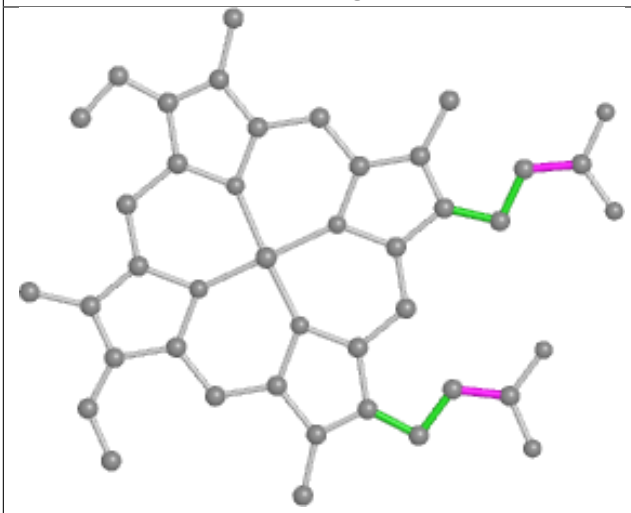
Ligand HEC C 809



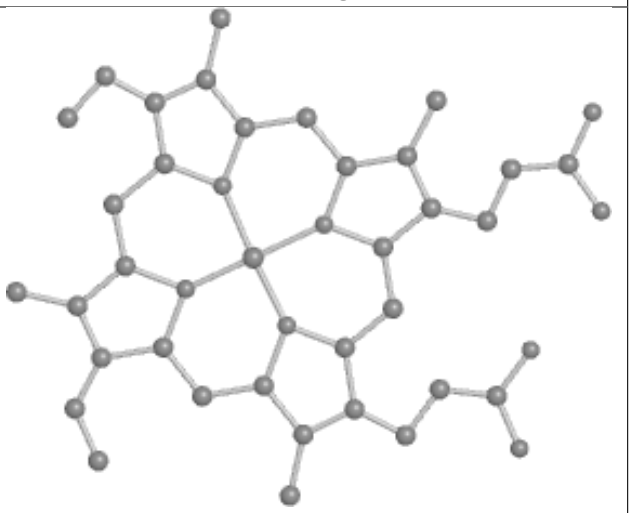
Bond lengths



Bond angles

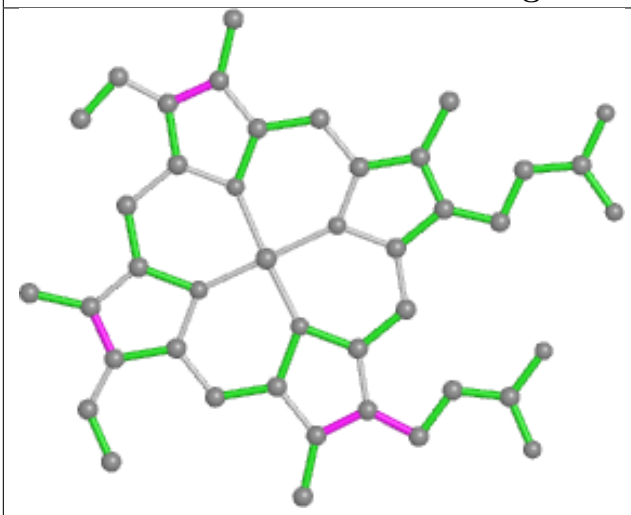


Torsions

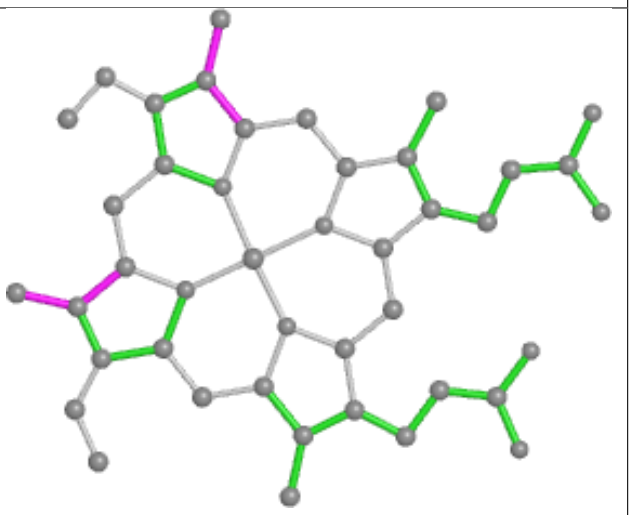


Rings

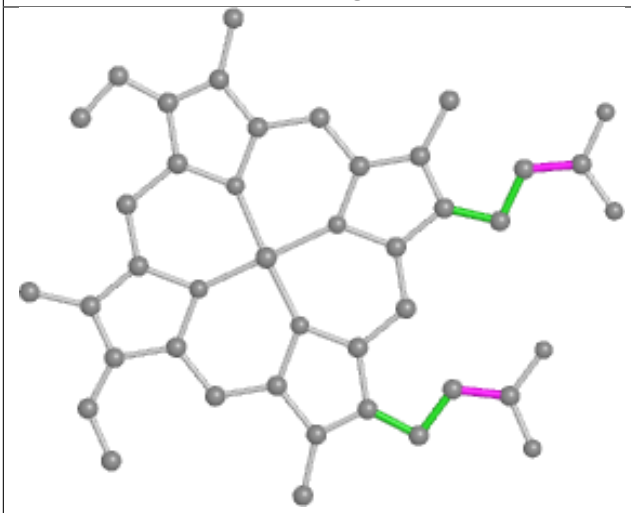
Ligand HEC C 807



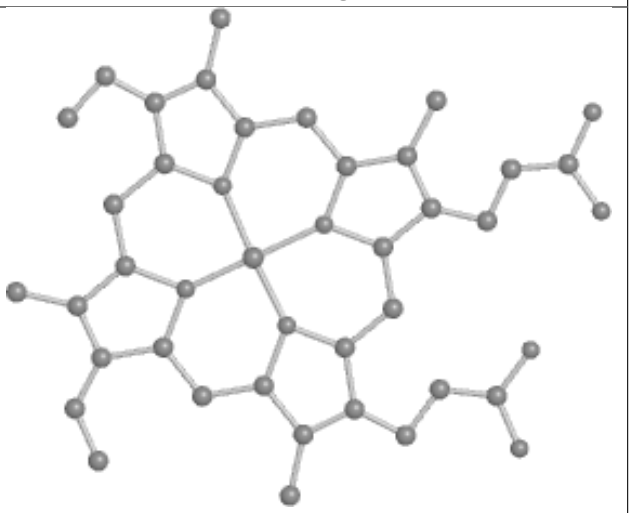
Bond lengths



Bond angles

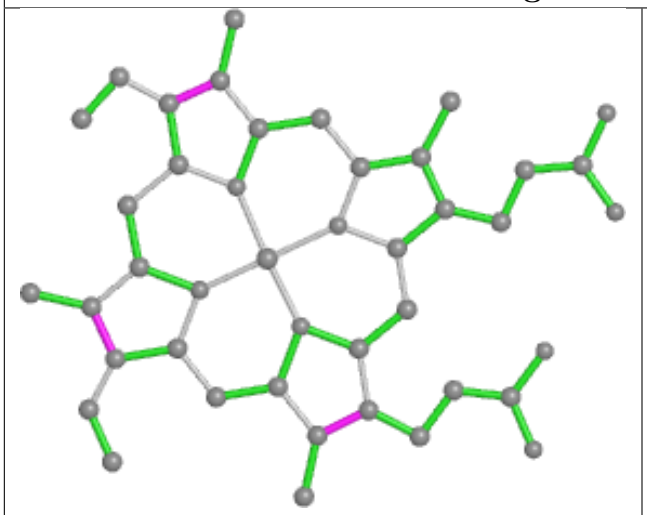


Torsions

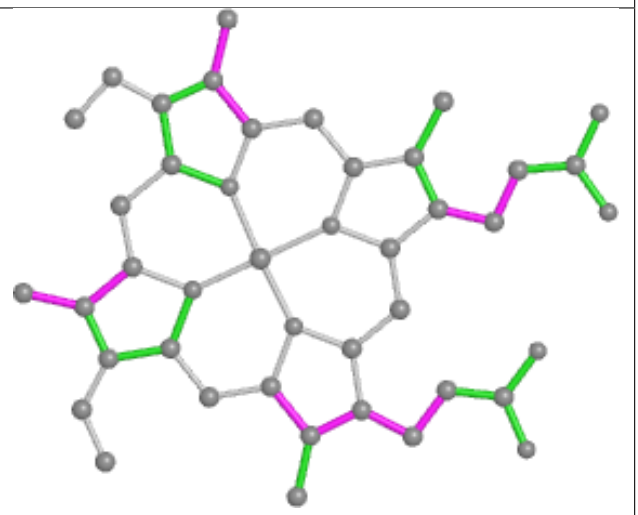


Rings

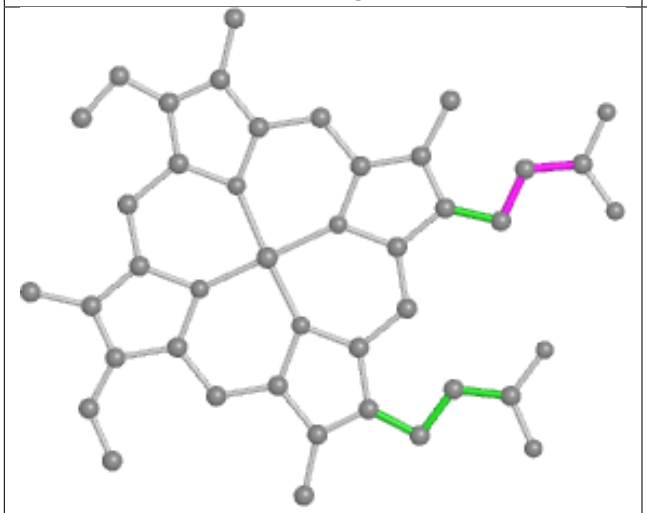
Ligand HEC C 801



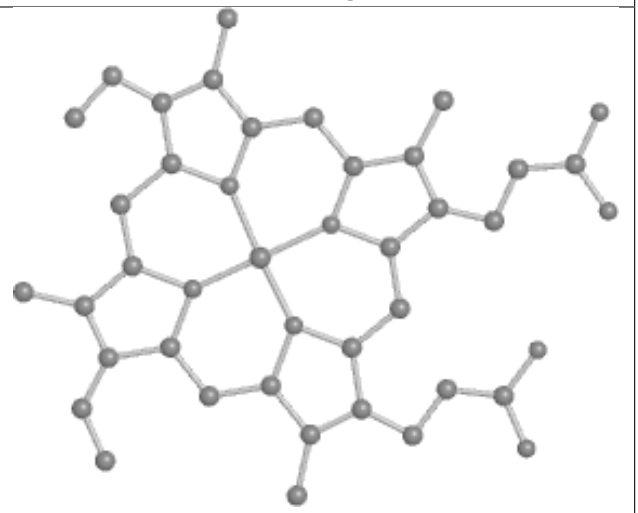
Bond lengths



Bond angles

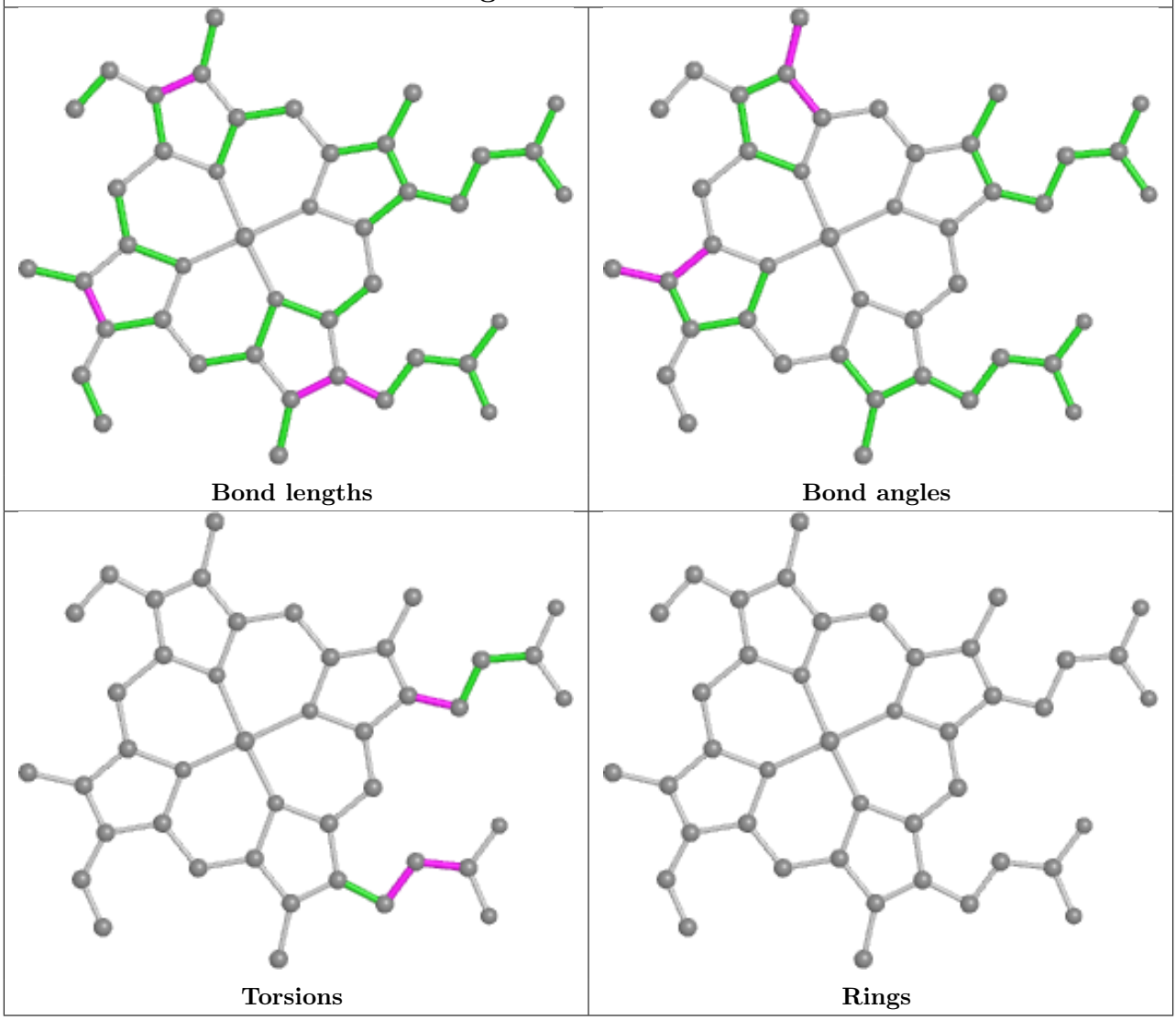


Torsions



Rings

Ligand HEC C 804



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.23	0 100 100	38, 48, 63, 89	0
1	B	608/608 (100%)	-0.21	2 (0%) 94 96	38, 49, 65, 113	0
1	C	604/608 (99%)	-0.02	17 (2%) 53 60	38, 54, 93, 112	0
All	All	1817/1824 (99%)	-0.15	19 (1%) 82 86	38, 50, 78, 113	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	650	MET	6.3
1	C	122	PHE	3.3
1	C	140	ALA	3.2
1	C	169	VAL	3.1
1	B	43	ALA	2.9
1	C	74	ASP	2.9
1	C	115	ALA	2.8
1	C	163	LEU	2.8
1	C	168	GLN	2.6
1	C	119	PRO	2.5
1	C	255	GLN	2.4
1	C	154	VAL	2.4
1	C	155	LEU	2.4
1	C	68	THR	2.4
1	B	166	GLY	2.3
1	C	117	THR	2.3
1	C	164	PRO	2.1
1	C	118	CYS	2.1
1	C	65	VAL	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 monosaccharides 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	0.82	0.48	83,83,83,83	0
4	EDO	A	814	4/4	0.86	0.25	58,58,64,64	0
3	CA	C	813	1/1	0.87	0.07	80,80,80,80	0
3	CA	B	812	1/1	0.88	0.44	77,77,77,77	0
3	CA	A	812	1/1	0.94	0.07	77,77,77,77	0
2	HEC	C	805	43/43	0.94	0.13	51,60,66,73	0
4	EDO	A	813	4/4	0.94	0.18	51,52,53,56	0
3	CA	B	813	1/1	0.94	0.04	81,81,81,81	0
2	HEC	C	802	43/43	0.95	0.15	50,56,70,78	0
2	HEC	A	802	43/43	0.95	0.17	41,46,66,80	0
2	HEC	A	804	43/43	0.95	0.14	34,48,67,72	0
2	HEC	C	806	43/43	0.96	0.14	31,42,49,53	0
2	HEC	A	806	43/43	0.96	0.16	36,41,53,59	0
2	HEC	B	802	43/43	0.96	0.15	41,48,66,73	0
2	HEC	B	806	43/43	0.96	0.13	37,43,52,54	0
2	HEC	C	801	43/43	0.96	0.13	38,49,60,66	0
2	HEC	A	801	43/43	0.96	0.14	36,44,63,69	0
2	HEC	C	804	43/43	0.96	0.14	45,52,70,80	0
2	HEC	A	805	43/43	0.96	0.13	41,51,63,66	0
2	HEC	B	801	43/43	0.97	0.12	35,41,55,63	0
2	HEC	A	808	43/43	0.97	0.11	34,39,45,46	0
2	HEC	C	803	43/43	0.97	0.11	44,48,56,58	0
2	HEC	B	804	43/43	0.97	0.15	36,42,70,78	0
2	HEC	B	805	43/43	0.97	0.13	38,44,53,62	0
2	HEC	A	809	43/43	0.97	0.14	37,44,59,65	0
2	HEC	C	809	43/43	0.97	0.13	31,39,54,61	0
2	HEC	C	807	43/43	0.98	0.11	35,41,45,46	0

Continued on next page...

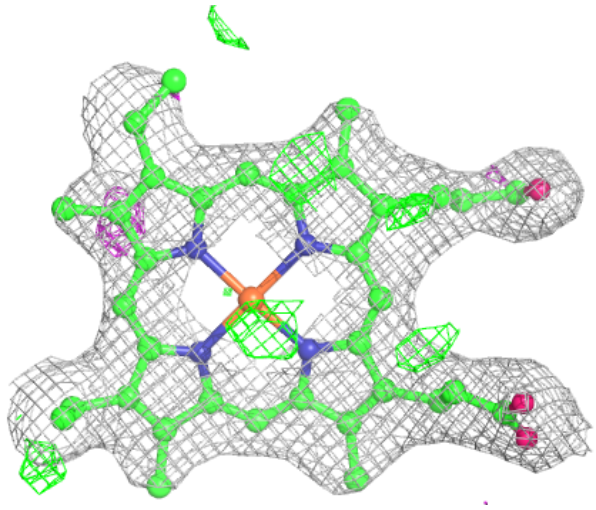
Continued from previous page...

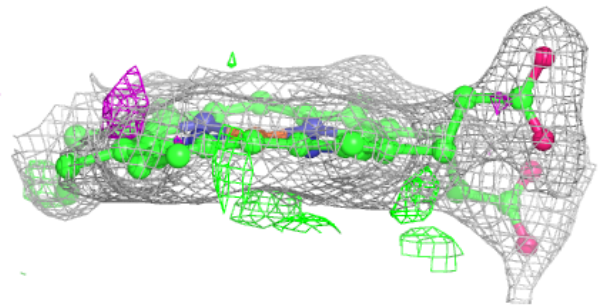
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	C	808	43/43	0.98	0.12	35,41,44,47	0
2	HEC	B	809	43/43	0.98	0.14	34,42,58,71	0
2	HEC	C	810	43/43	0.98	0.14	33,39,52,62	0
2	HEC	B	810	43/43	0.98	0.13	37,43,58,64	0
2	HEC	B	803	43/43	0.98	0.12	35,41,46,50	0
2	HEC	A	810	43/43	0.98	0.12	37,45,52,57	0
2	HEC	A	803	43/43	0.98	0.12	35,42,44,47	0
2	HEC	A	807	43/43	0.98	0.12	32,40,45,50	0
2	HEC	B	807	43/43	0.98	0.13	34,41,45,49	0
2	HEC	B	808	43/43	0.98	0.12	35,40,43,46	0
3	CA	B	811	1/1	0.99	0.09	45,45,45,45	0
3	CA	C	811	1/1	0.99	0.09	47,47,47,47	0
3	CA	A	811	1/1	0.99	0.12	47,47,47,47	0

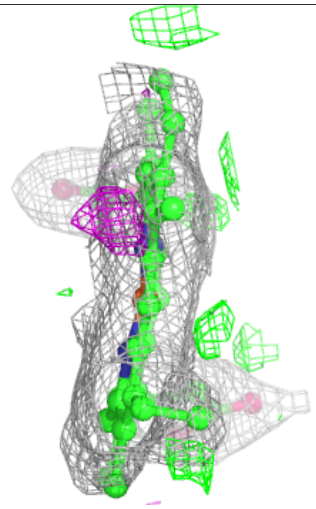
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC C 805:

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

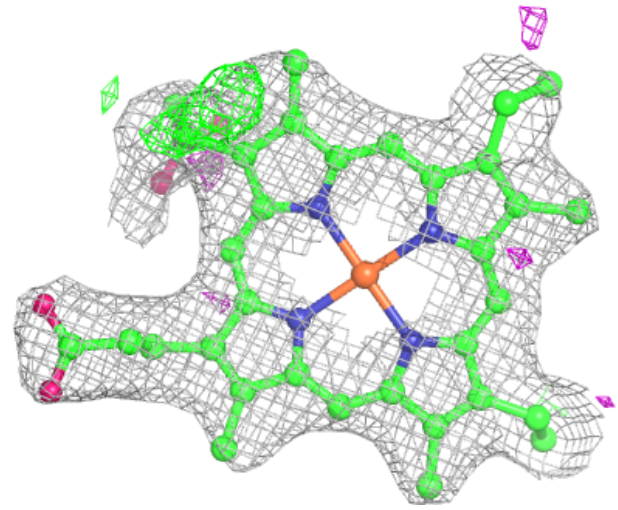


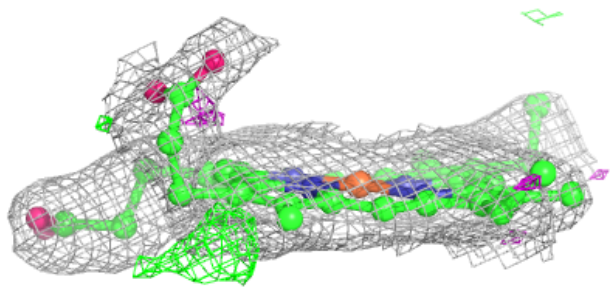


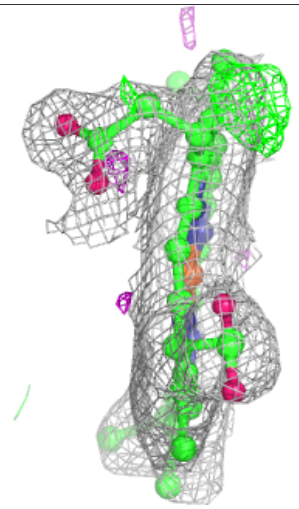


Electron density around HEC C 802:

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

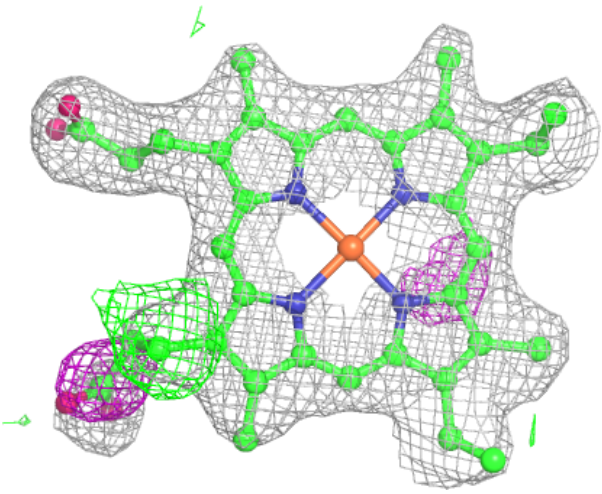


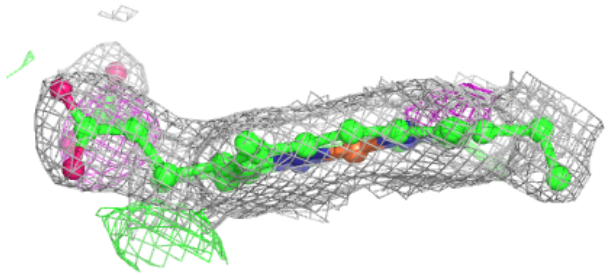


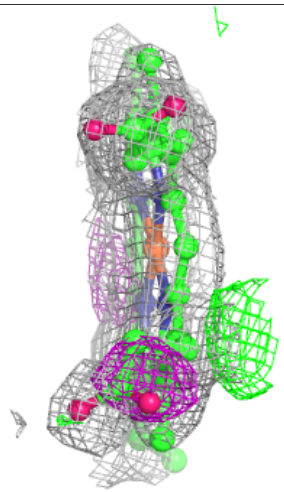


Electron density around HEC A 802:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

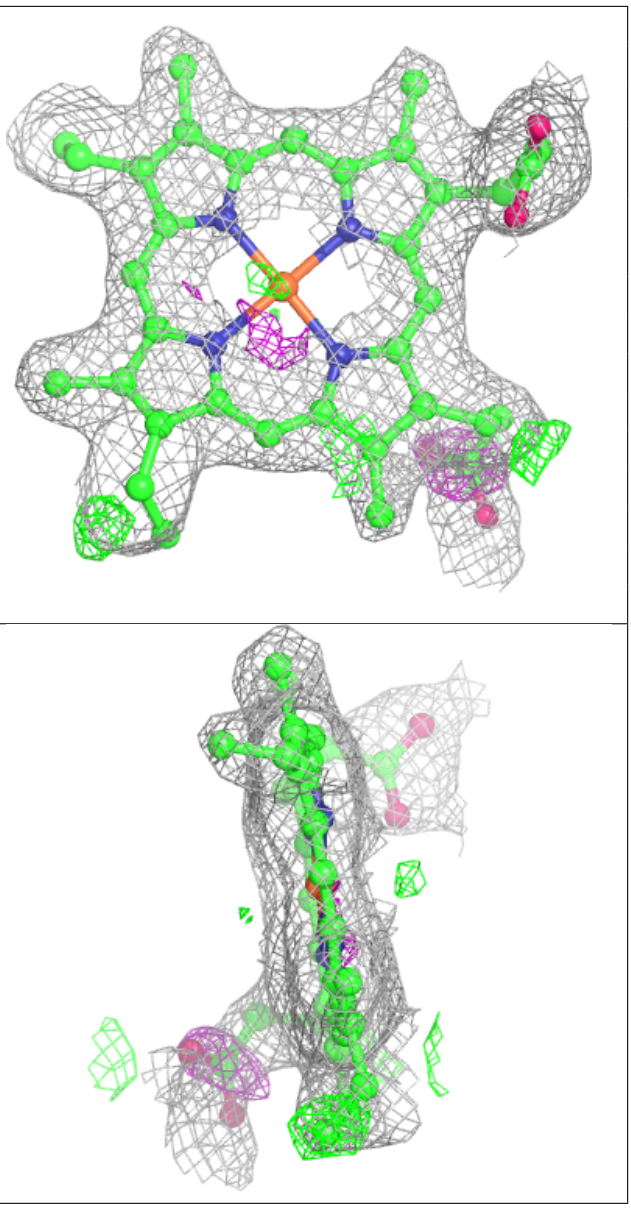






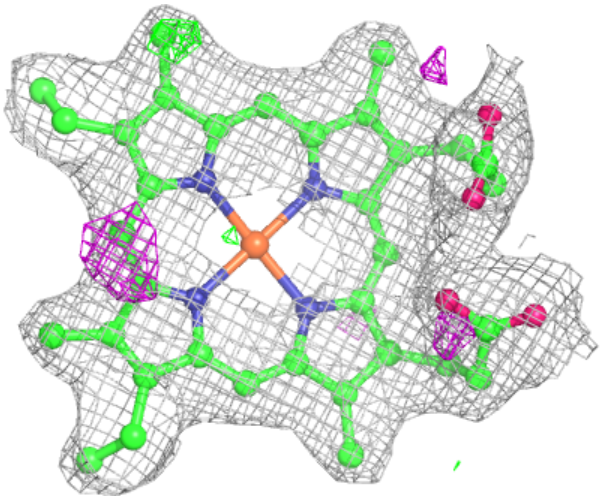
Electron density around HEC A 804:

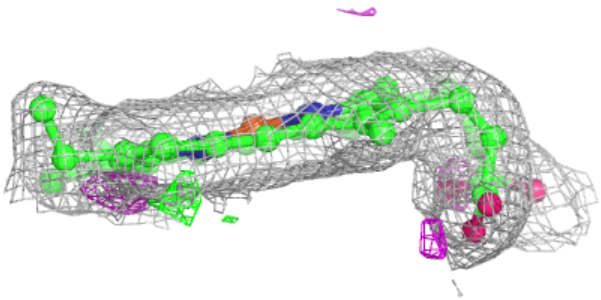
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

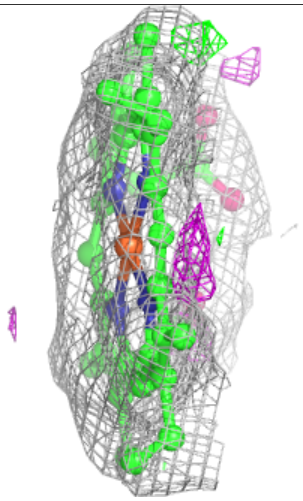


Electron density around HEC C 806:

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

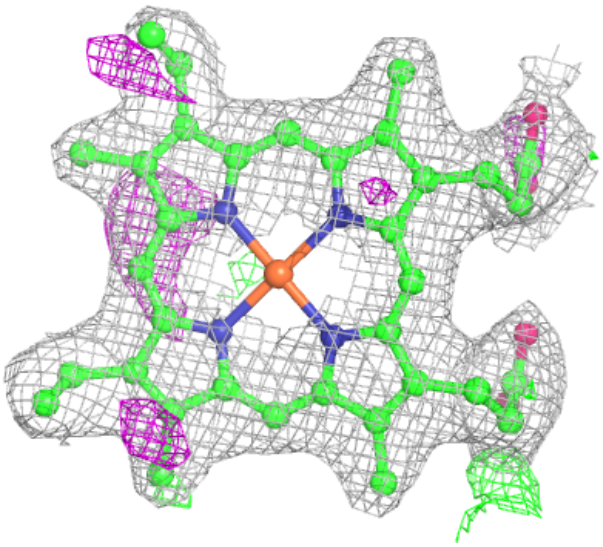


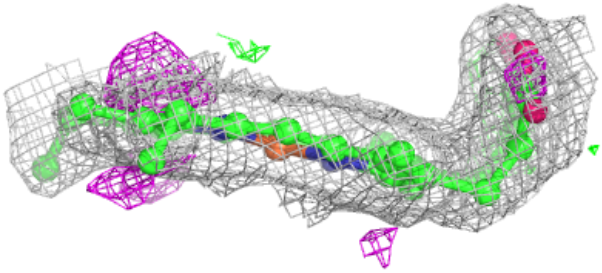


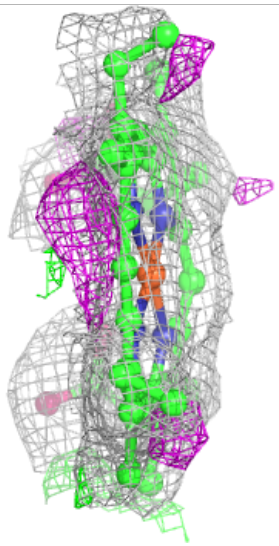


Electron density around HEC A 806:

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

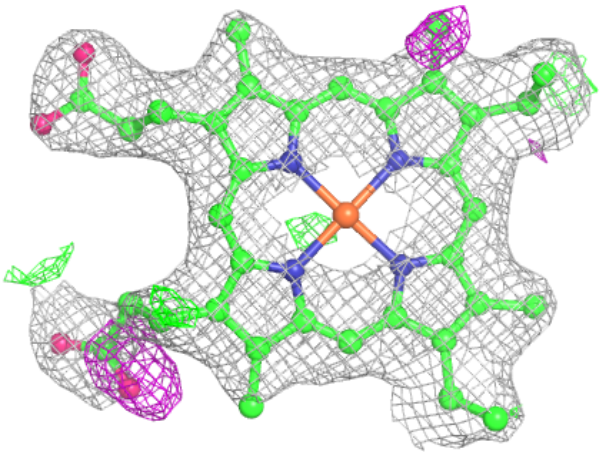


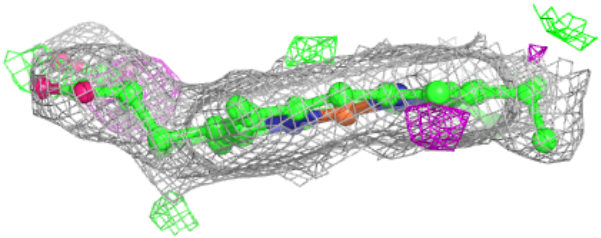


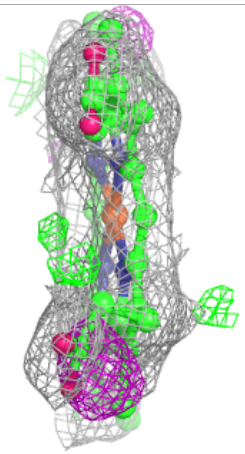


Electron density around HEC B 802:

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

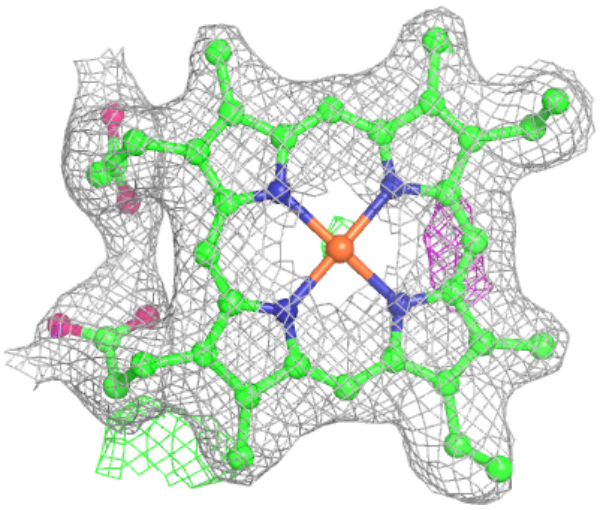


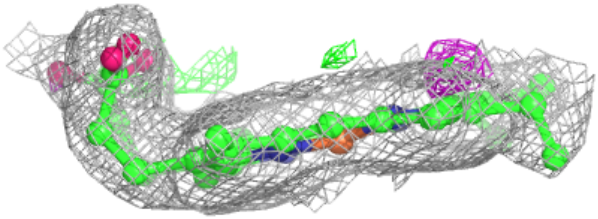


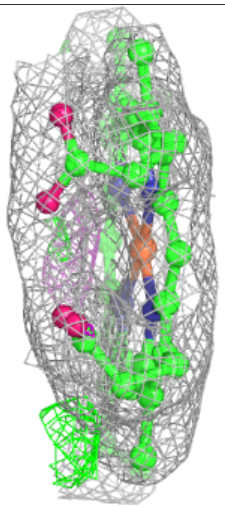


Electron density around HEC B 806:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

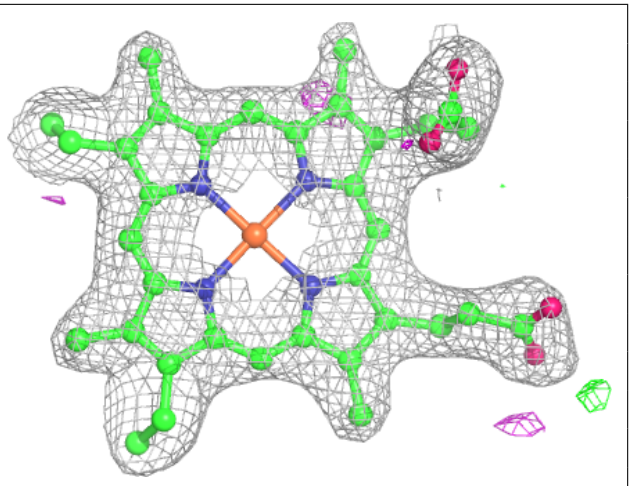


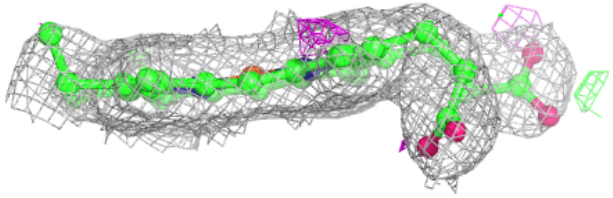


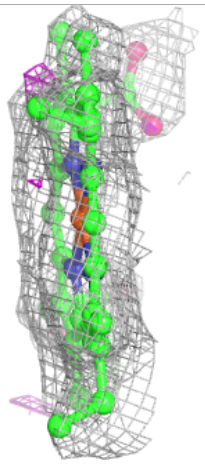


Electron density around HEC C 801:

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

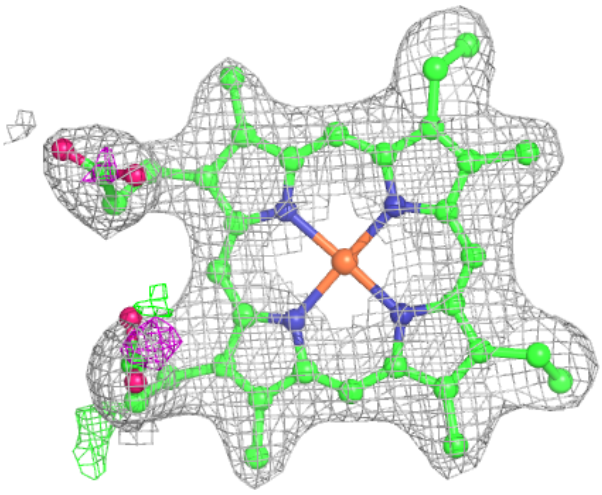


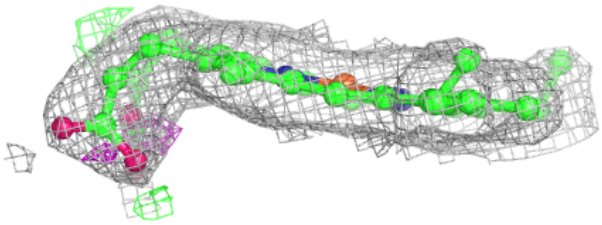


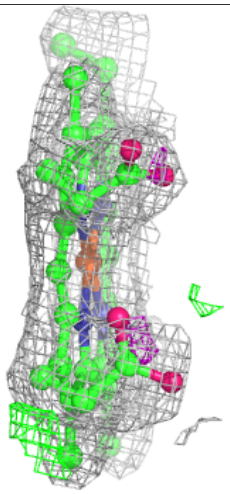


Electron density around HEC A 801:

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

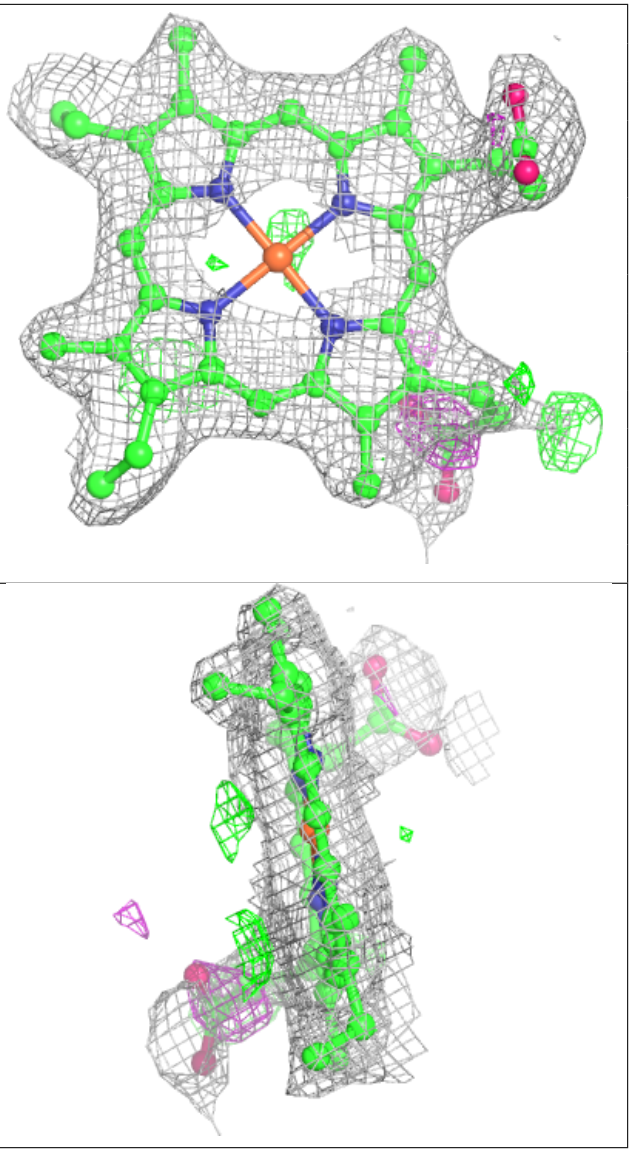






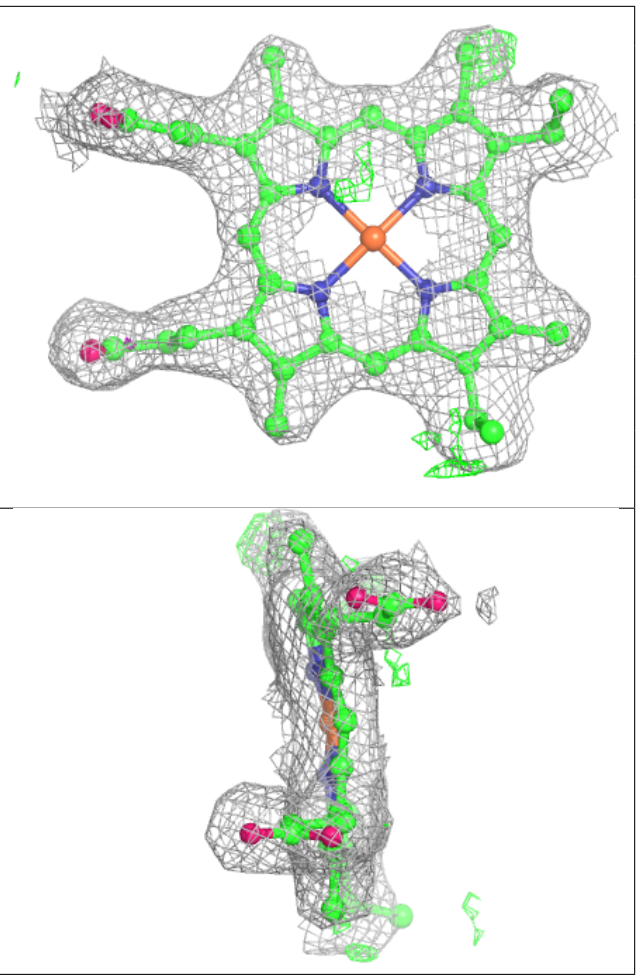
Electron density around HEC C 804:

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



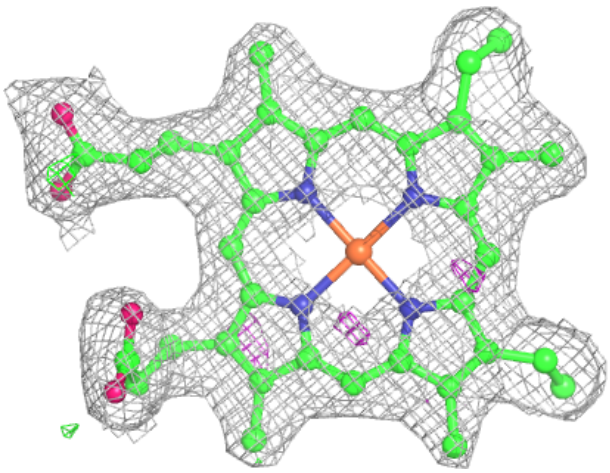
Electron density around HEC A 805:

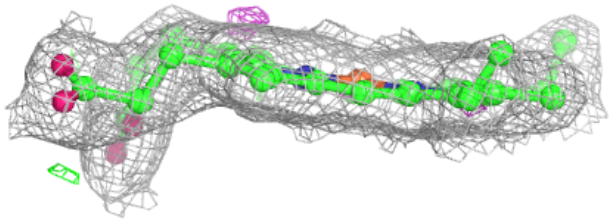
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

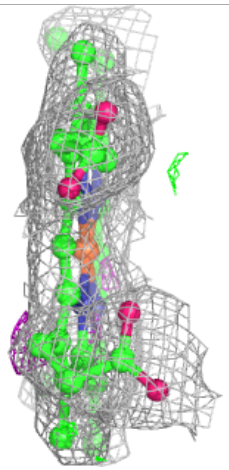


Electron density around HEC B 801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

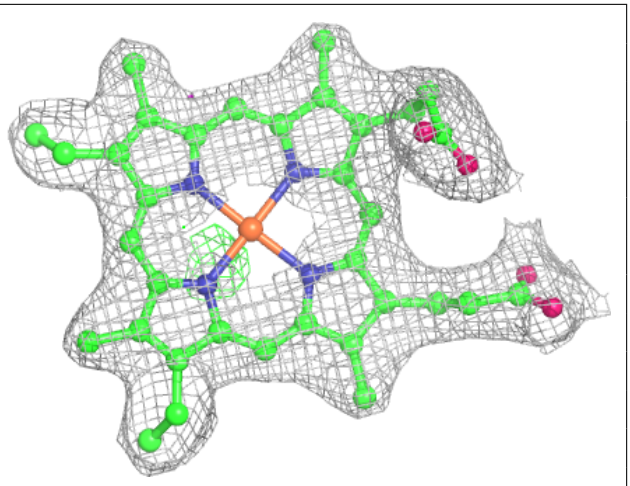


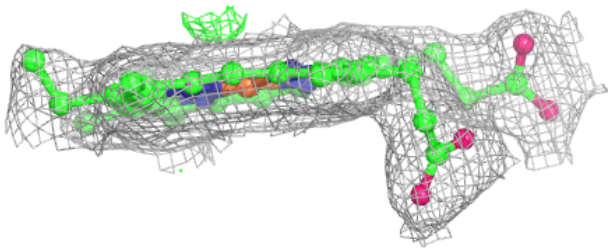


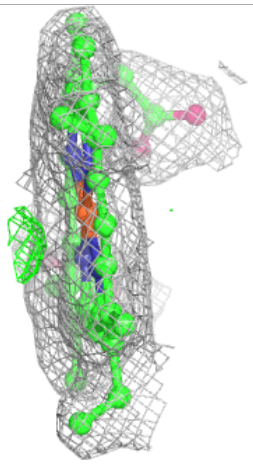


Electron density around HEC A 808:

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

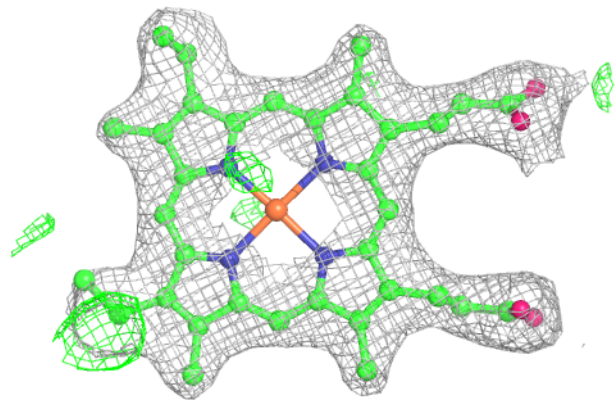


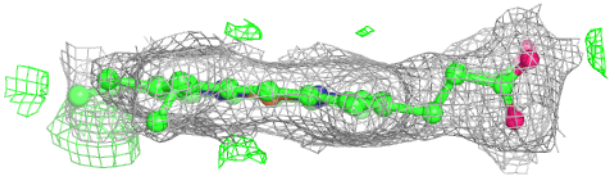


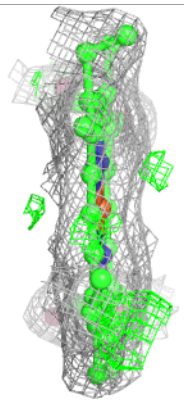


Electron density around HEC C 803:

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

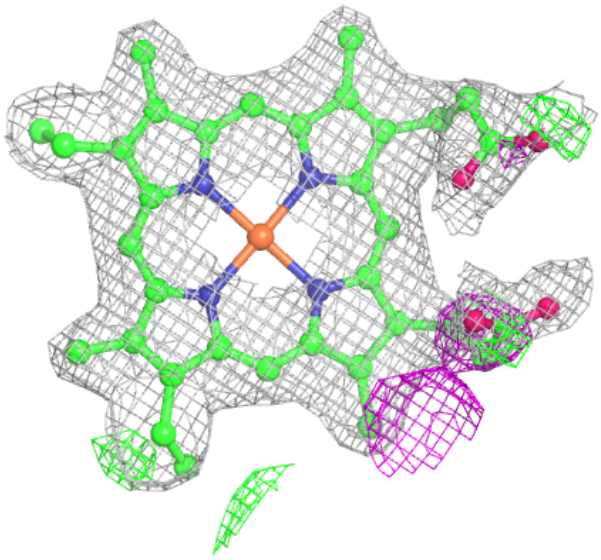


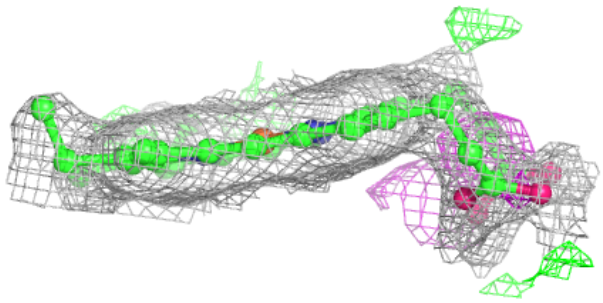


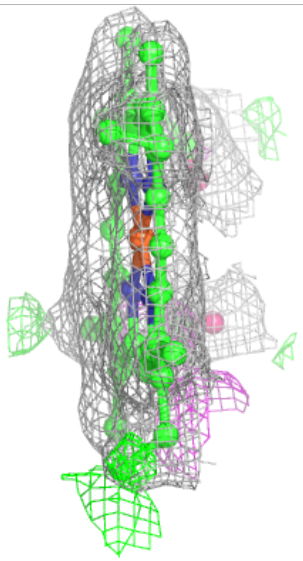


Electron density around HEC B 804:

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

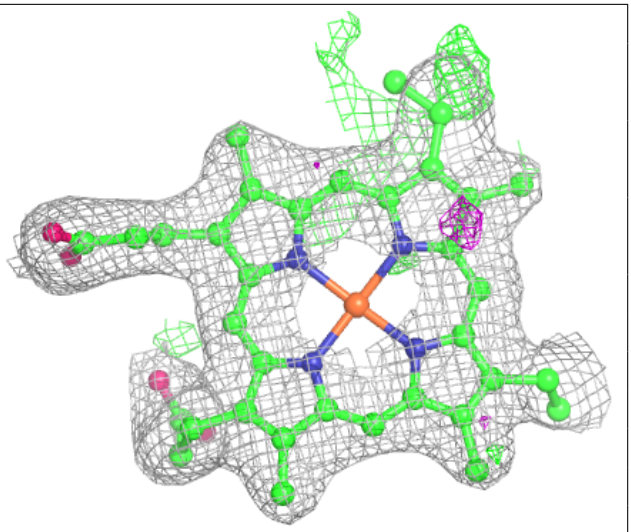


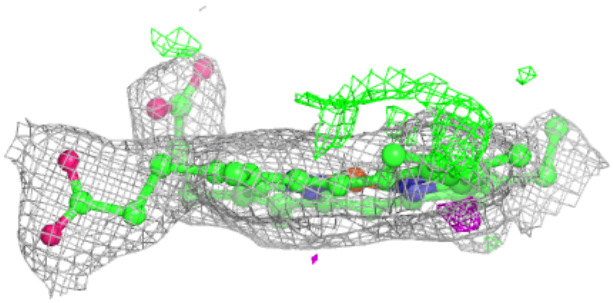




Electron density around HEC B 805:

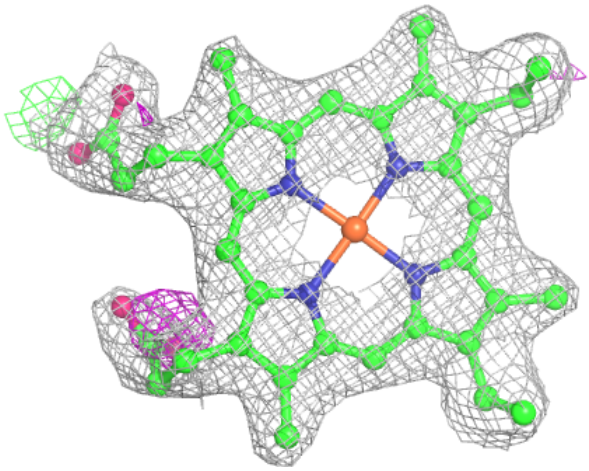
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

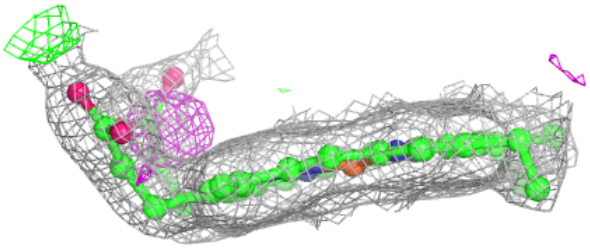


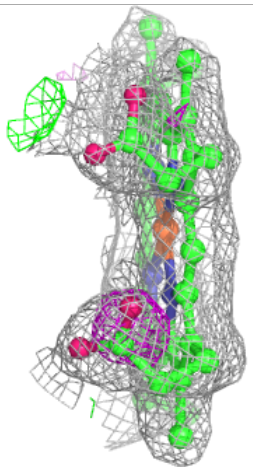


Electron density around HEC A 809:

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

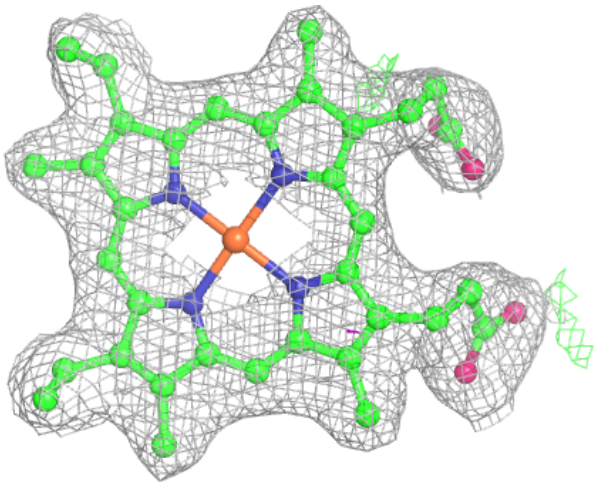


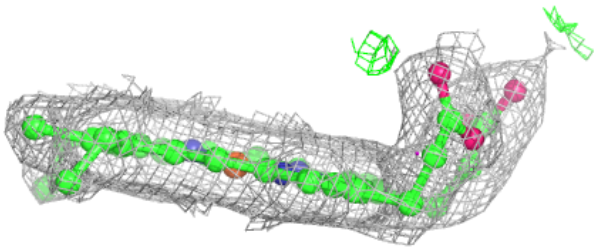


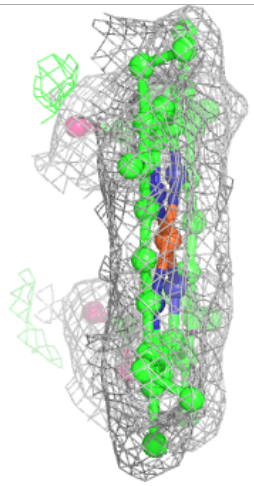


Electron density around HEC C 809:

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

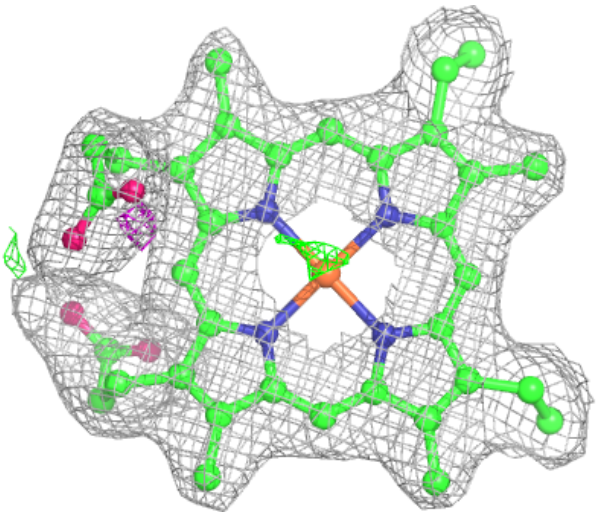


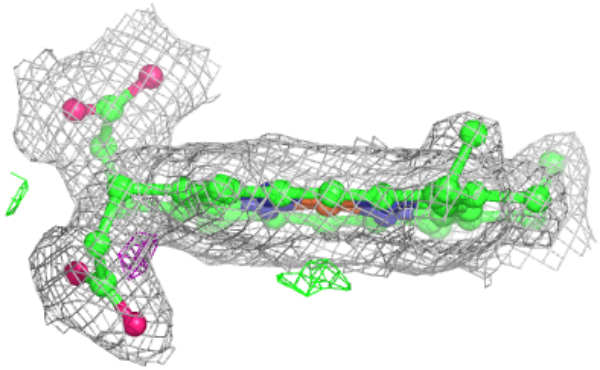


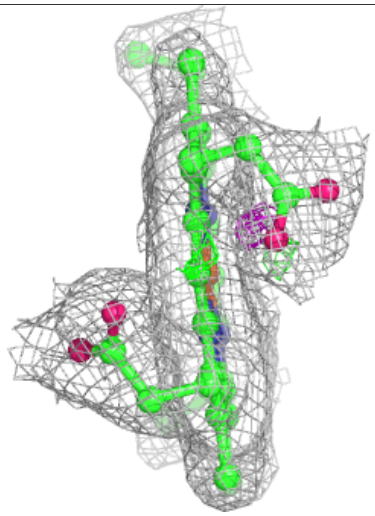


Electron density around HEC C 807:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

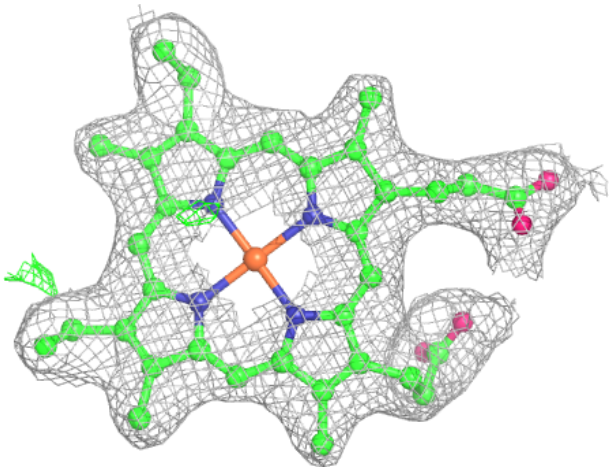


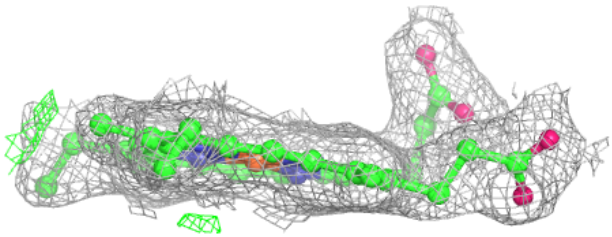


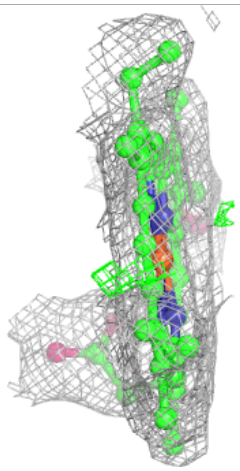


Electron density around HEC C 808:

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

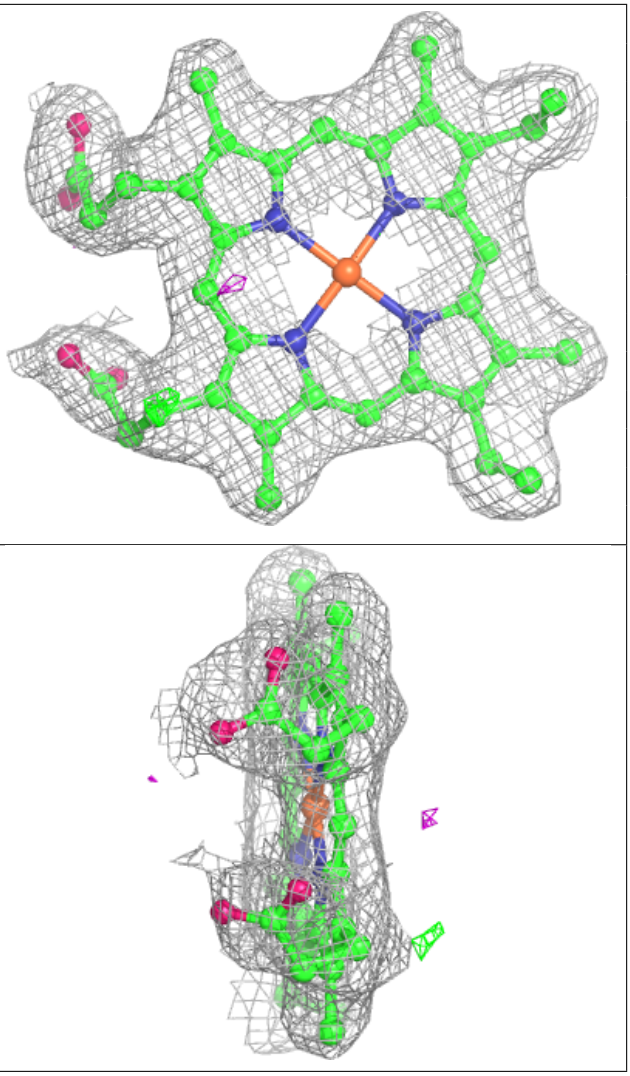






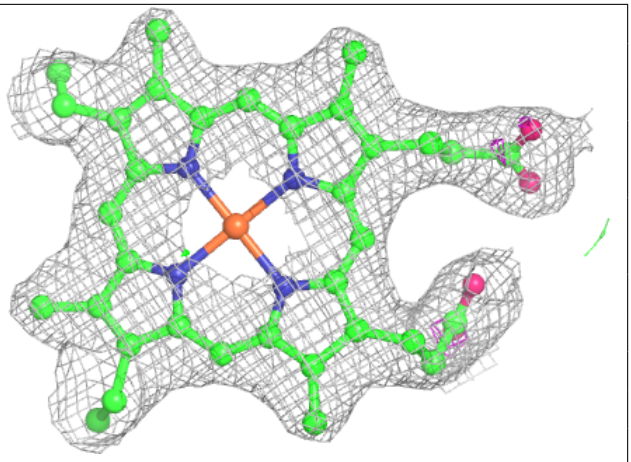
Electron density around HEC B 809:

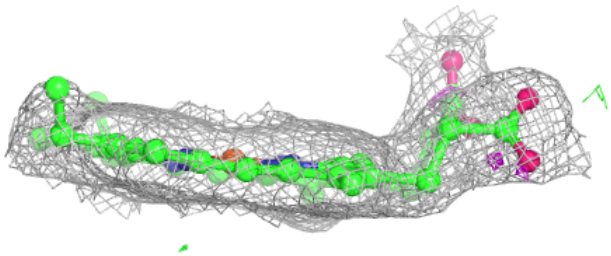
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

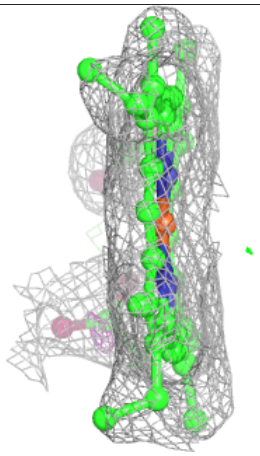


Electron density around HEC C 810:

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

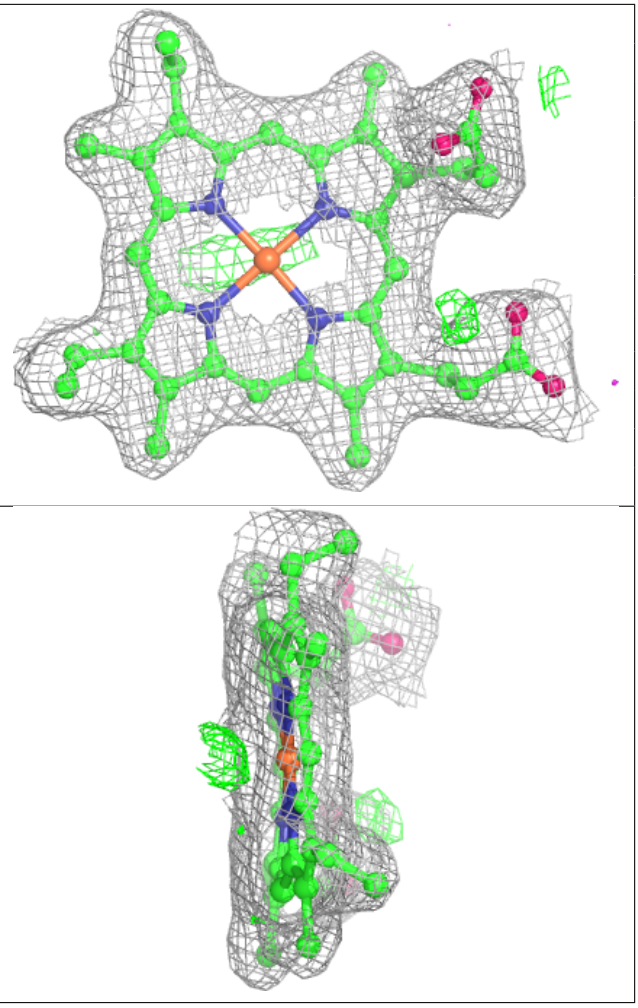






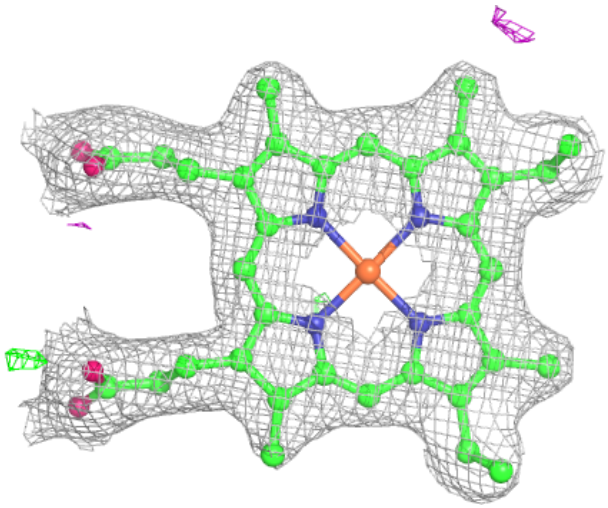
Electron density around HEC B 810:

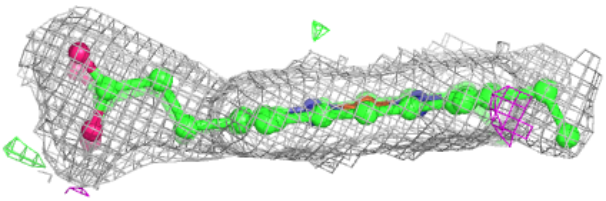
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

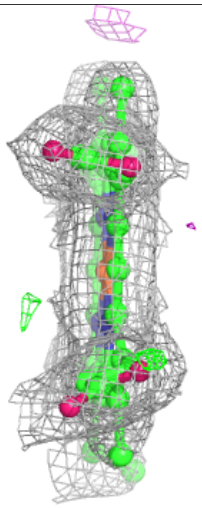


Electron density around HEC B 803:

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

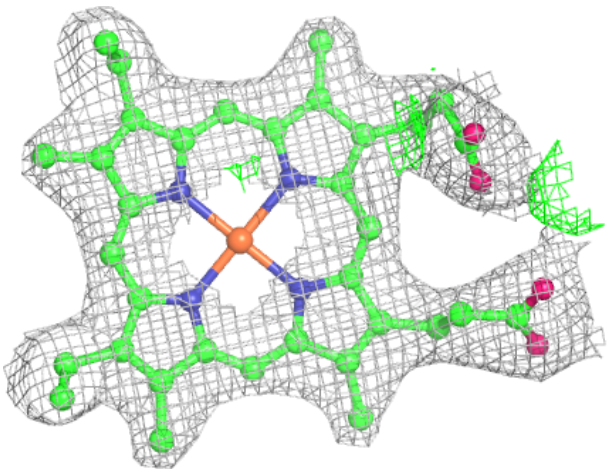


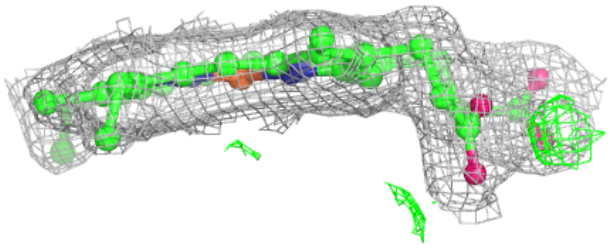


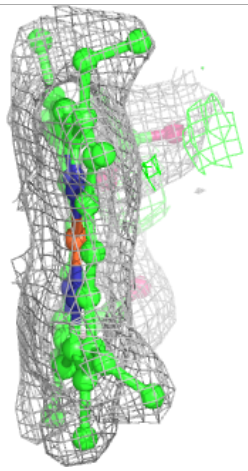


Electron density around HEC A 810:

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

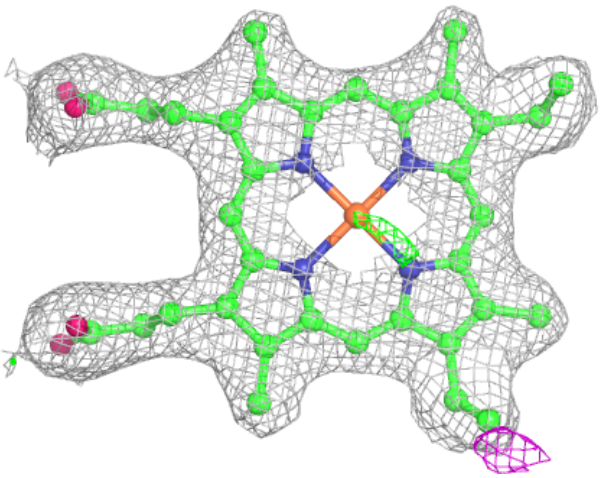


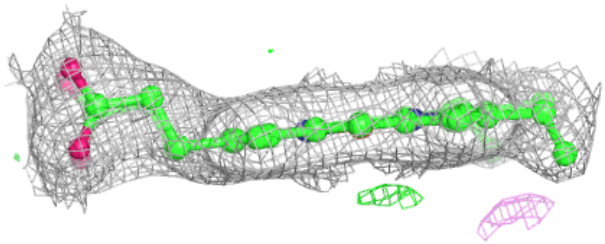


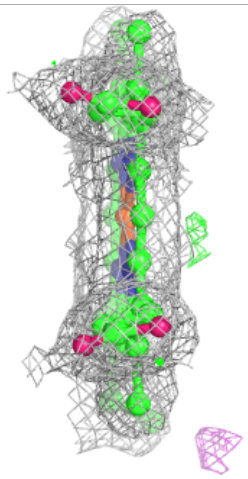


Electron density around HEC A 803:

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

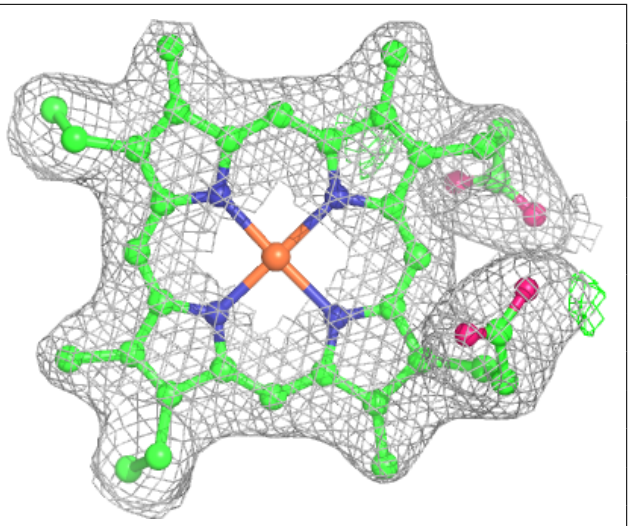


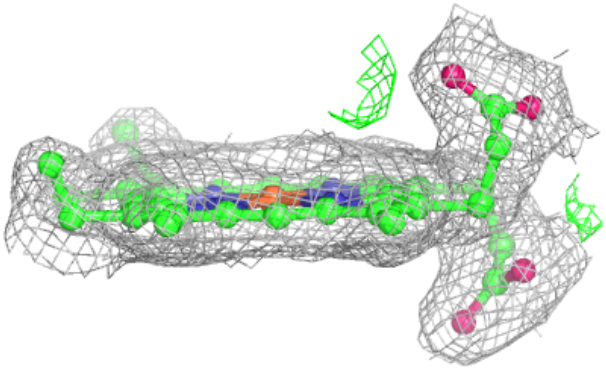




Electron density around HEC A 807:

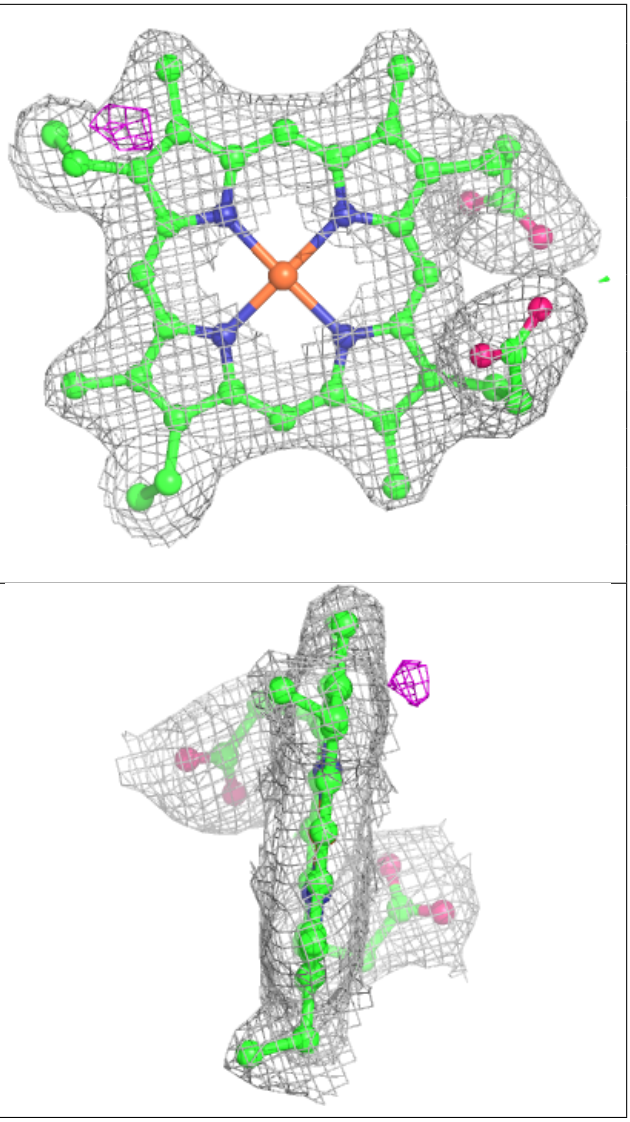
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

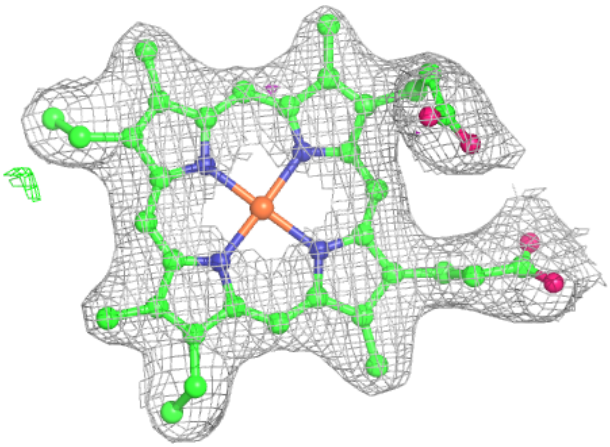
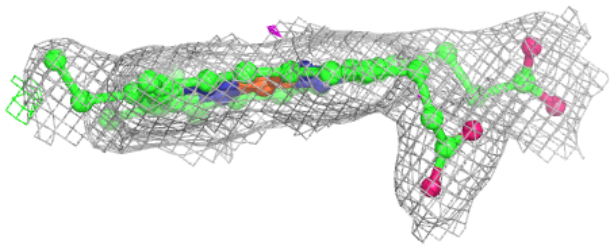
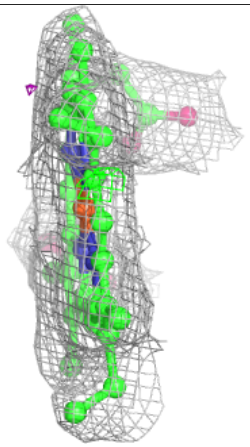




Electron density around HEC B 807:

$2mF_o$-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 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.