Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:18 pm BST

PDB ID	:	6R2Q
Title	:	Structure of the Mtr complex
Authors	:	Clarke, T.A.; Edwards, M.J.
Deposited on	:	2019-03-18
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

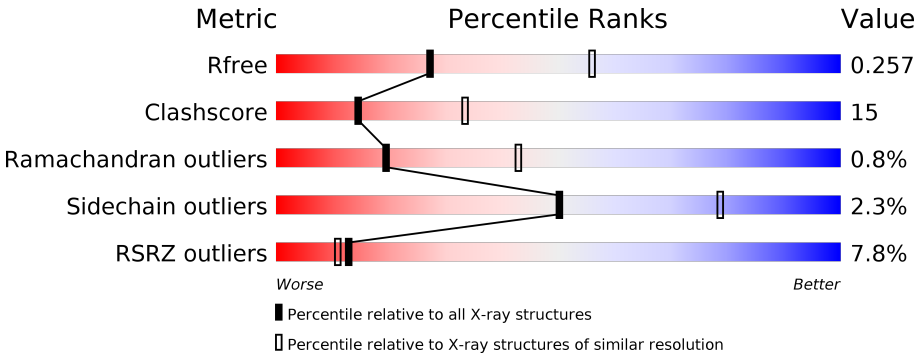
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	333	16% 55% 22% • 20%
2	B	695	8% 64% 27% • 7%
3	C	650	2% 77% 16% • 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	HEC	A	901	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24030 atoms, of which 11567 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	265	3844	1190	1856	381	387	30	0	0	0

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	649	9901	3165	4796	867	1057	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	GLU	ASP	conflict	UNP A0A165K351

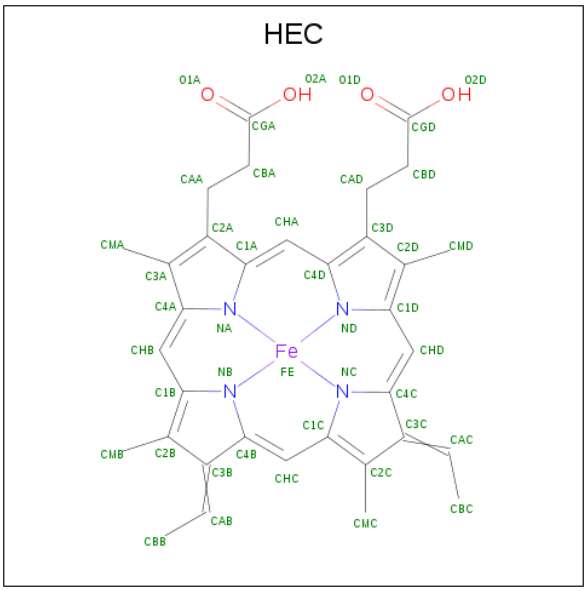
- Molecule 3 is a protein called Decaheme c-type cytochrome, OmcA/MtrC family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	608	8767	2772	4283	781	896	35	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	23	THR	ALA	conflict	UNP A0A379ZX38
C	48	ILE	THR	conflict	UNP A0A379ZX38
C	408	ALA	ASP	conflict	UNP A0A379ZX38

- Molecule 4 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			74	34	1	31	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
4	C	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

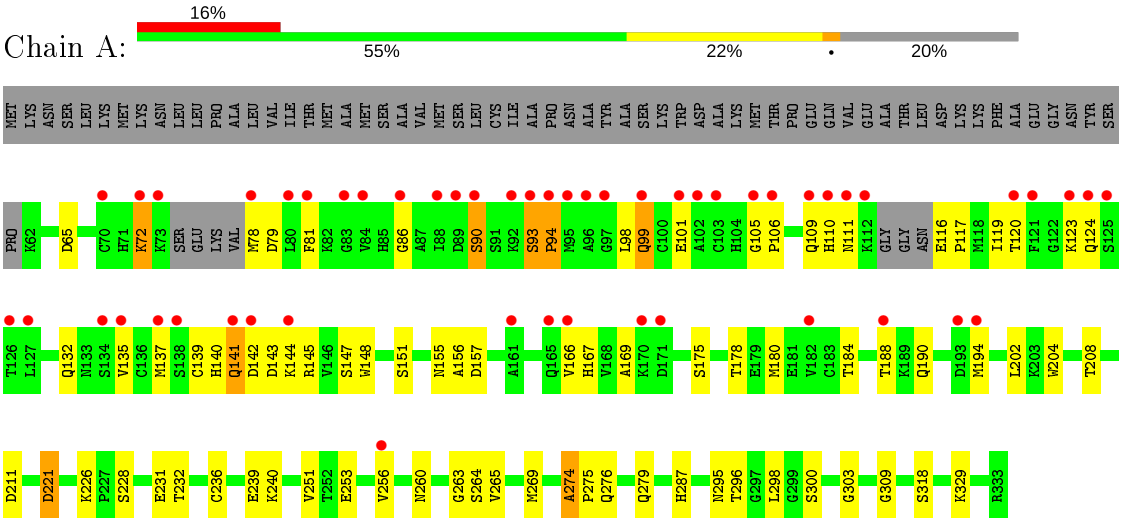
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	13	Total	O	0	0
			13	13		
6	C	8	Total	O	0	0
			8	8		

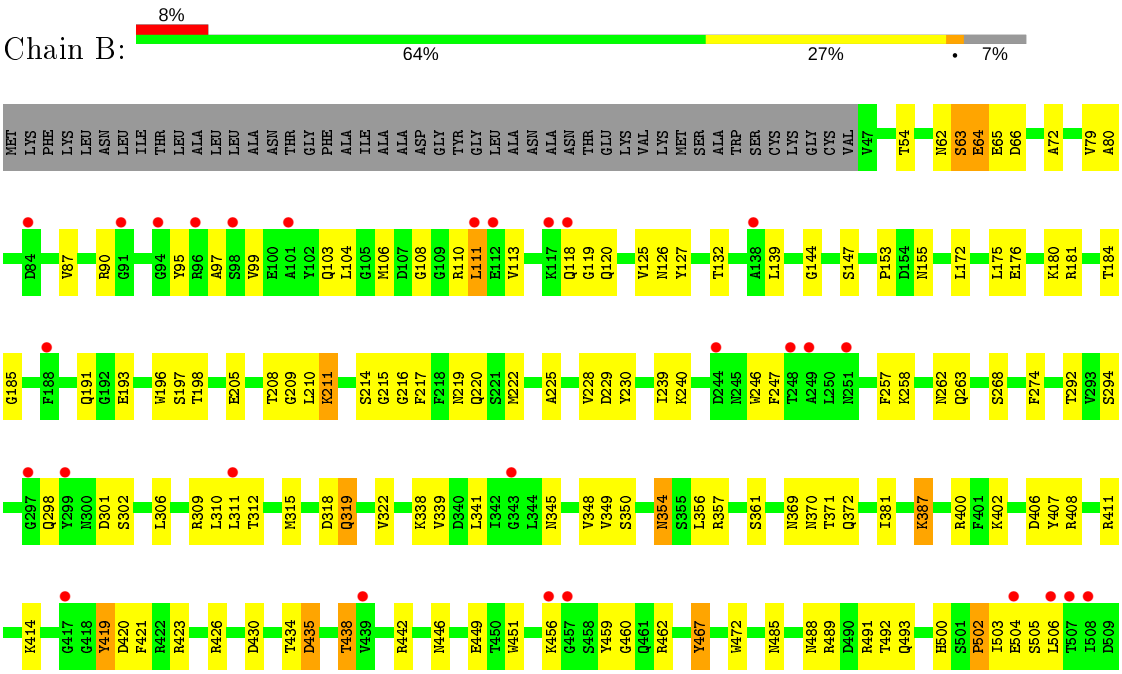
3 Residue-property plots (i)

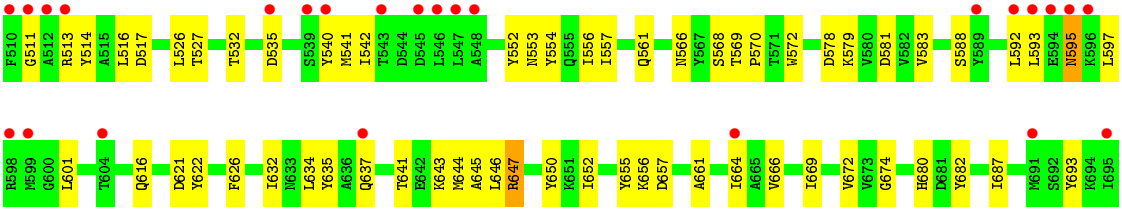
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

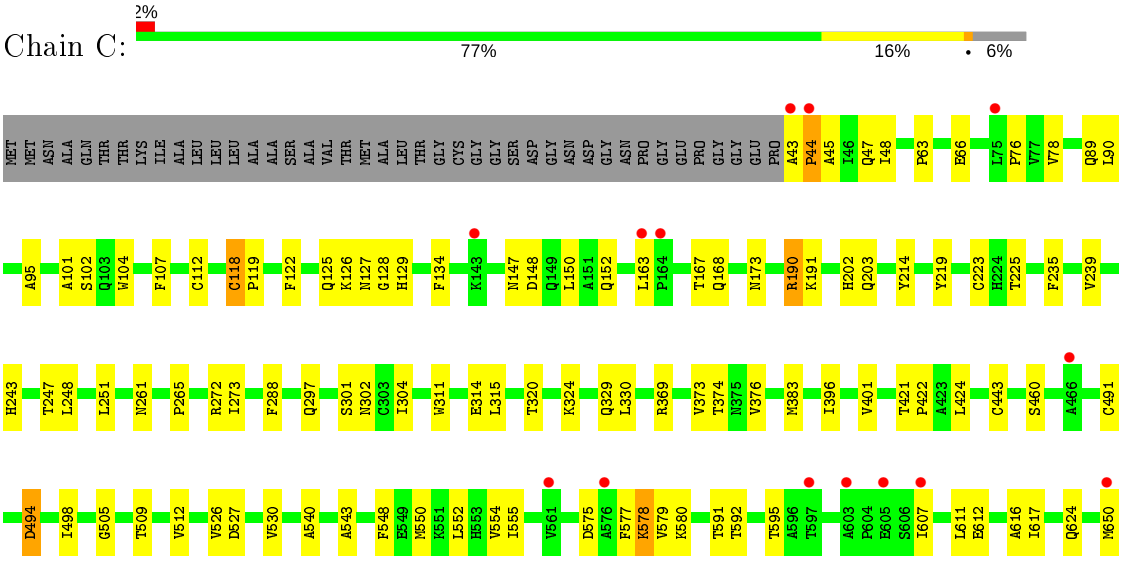


- Molecule 2: Uncharacterized protein





• Molecule 3: Decaheme c-type cytochrome, OmcA/MtrC family



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.04Å 234.16Å 99.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.25 – 2.70 117.08 – 2.70	Depositor EDS
% Data completeness (in resolution range)	72.8 (73.25-2.70) 72.9 (117.08-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.257 0.225 , 0.257	Depositor DCC
R_{free} test set	2472 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	24030	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/2030	0.82	0/2735
2	B	0.50	0/5202	0.89	12/7055 (0.2%)
3	C	0.47	2/4575 (0.0%)	0.80	3/6225 (0.0%)
All	All	0.49	2/11807 (0.0%)	0.85	15/16015 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	314	GLU	CB-CG	6.18	1.63	1.52
3	C	443	CYS	CB-SG	-5.72	1.72	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	229	ASP	CB-CG-OD1	9.38	126.74	118.30
2	B	211	LYS	CD-CE-NZ	-6.66	96.38	111.70
2	B	407	TYR	CB-CG-CD2	-6.51	117.09	121.00
2	B	229	ASP	CB-CG-OD2	-6.42	112.53	118.30
2	B	435	ASP	CB-CG-OD1	-6.38	112.55	118.30
2	B	435	ASP	CB-CG-OD2	6.37	124.03	118.30
2	B	407	TYR	CB-CG-CD1	6.21	124.72	121.00
3	C	555	ILE	CG1-CB-CG2	-5.59	99.10	111.40
2	B	211	LYS	CA-CB-CG	-5.54	101.20	113.40
2	B	175	LEU	CB-CG-CD2	-5.43	101.76	111.00
2	B	176	GLU	CA-CB-CG	5.40	125.27	113.40
3	C	66	GLU	CB-CA-C	-5.34	99.71	110.40
3	C	579	VAL	CG1-CB-CG2	-5.29	102.44	110.90
2	B	111	LEU	CB-CG-CD2	-5.10	102.33	111.00
2	B	647	ARG	CD-NE-CZ	5.10	130.74	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1988	1856	1856	89	0
2	B	5105	4796	4796	167	0
3	C	4484	4283	4280	70	0
4	A	430	315	307	57	0
4	C	430	317	312	44	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	1	0	0	0	0
6	B	13	0	0	3	0
6	C	8	0	0	0	0
All	All	12463	11567	11551	370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (370) 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)
3:C:617:ILE:HD13	3:C:624:GLN:HG2	1.42	1.01
1:A:253:GLU:OE1	2:B:426:ARG:NH2	2.00	0.94
2:B:113:VAL:HG22	2:B:125:VAL:HG22	1.48	0.93
1:A:188:THR:HG21	2:B:535:ASP:OD2	1.72	0.90
2:B:361:SER:OG	2:B:402:LYS:HG3	1.70	0.90
2:B:632:ILE:HD11	2:B:652:ILE:HG13	1.52	0.90
2:B:493:GLN:OE1	2:B:513:ARG:NH1	2.05	0.89
2:B:489:ARG:NH1	2:B:517:ASP:OD1	2.08	0.87
1:A:145:ARG:NH1	4:A:904:HEC:O2A	2.07	0.86
2:B:292:THR:OG1	2:B:311:LEU:HD11	1.78	0.83
2:B:556:ILE:HD12	2:B:556:ILE:O	1.80	0.81
4:A:908:HEC:HBA2	2:B:211:LYS:HZ2	1.43	0.81
4:A:901:HEC:HMB1	4:A:901:HEC:HBB3	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:PRO:HD2	2:B:506:LEU:HD11	1.64	0.80
3:C:617:ILE:CD1	3:C:624:GLN:HG2	2.11	0.80
4:A:909:HEC:HMB1	4:A:909:HEC:HBB3	1.62	0.79
1:A:98:LEU:O	1:A:101:GLU:HB3	1.83	0.79
2:B:506:LEU:HB3	2:B:540:TYR:HD1	1.46	0.78
4:C:803:HEC:HBC3	4:C:803:HEC:HMC1	1.64	0.77
3:C:611:LEU:O	3:C:616:ALA:HB3	1.83	0.77
4:A:901:HEC:HMC1	4:A:901:HEC:HBC3	1.66	0.77
4:A:907:HEC:O2D	2:B:181:ARG:NH2	2.18	0.77
3:C:104:TRP:HB2	3:C:225:THR:HG21	1.66	0.77
4:C:808:HEC:HBB3	4:C:808:HEC:HMB1	1.67	0.77
4:A:910:HEC:HBB3	4:A:910:HEC:HMB1	1.66	0.76
4:C:809:HEC:HBC3	4:C:809:HEC:HMC1	1.68	0.75
2:B:632:ILE:HD12	2:B:632:ILE:O	1.87	0.75
2:B:635:TYR:CD1	2:B:647:ARG:NH2	2.55	0.75
2:B:669:ILE:HB	2:B:672:VAL:HG22	1.70	0.74
4:A:905:HEC:HMC1	4:A:905:HEC:HBC3	1.68	0.74
2:B:657:ASP:OD1	2:B:680:HIS:N	2.21	0.74
1:A:296:THR:HG23	1:A:298:LEU:H	1.53	0.74
4:C:807:HEC:HBC3	4:C:807:HEC:HMC1	1.69	0.73
4:A:902:HEC:HBB3	4:A:902:HEC:HMB1	1.70	0.73
4:C:807:HEC:HMB1	4:C:807:HEC:CBB	2.18	0.73
1:A:155:ASN:O	2:B:414:LYS:NZ	2.16	0.72
2:B:459:TYR:CD1	2:B:492:THR:HG22	2.25	0.71
1:A:101:GLU:HA	1:A:106:PRO:HD2	1.72	0.71
1:A:296:THR:HG21	3:C:95:ALA:O	1.90	0.70
4:A:907:HEC:HBC3	4:A:907:HEC:HMC1	1.73	0.70
4:A:910:HEC:HMC1	4:A:910:HEC:HBC3	1.72	0.70
2:B:556:ILE:HG22	2:B:579:LYS:HB2	1.74	0.70
3:C:575:ASP:HA	3:C:578:LYS:NZ	2.07	0.69
4:A:908:HEC:O2A	2:B:211:LYS:NZ	2.21	0.69
2:B:430:ASP:HB3	2:B:467:TYR:CE1	2.27	0.69
3:C:101:ALA:HB2	3:C:273:ILE:HG21	1.75	0.69
4:A:904:HEC:HMC1	4:A:904:HEC:HBC3	1.74	0.68
1:A:116:GLU:N	1:A:119:ILE:HD12	2.08	0.68
4:C:806:HEC:HBB3	4:C:806:HEC:HMB1	1.76	0.68
2:B:645:ALA:C	2:B:646:LEU:HD23	2.15	0.67
1:A:265:VAL:HG11	2:B:578:ASP:HB3	1.78	0.65
2:B:645:ALA:O	2:B:646:LEU:HD23	1.96	0.65
1:A:202:LEU:HD23	1:A:208:THR:HA	1.77	0.65
1:A:239:GLU:HG3	1:A:240:LYS:HG2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:810:HEC:HBB3	4:C:810:HEC:HMB1	1.78	0.65
3:C:552:LEU:HD12	4:C:808:HEC:HMD2	1.79	0.65
1:A:81:PHE:HB3	1:A:86:GLY:HA3	1.79	0.65
2:B:315:MET:HG3	2:B:341:LEU:HD11	1.77	0.65
2:B:113:VAL:CG2	2:B:125:VAL:HG22	2.23	0.65
1:A:274:ALA:HB1	1:A:275:PRO:HD3	1.79	0.64
2:B:80:ALA:HB1	2:B:106:MET:CE	2.28	0.64
2:B:451:TRP:CE3	2:B:500:HIS:HB2	2.32	0.63
2:B:650:TYR:HD1	2:B:687:ILE:HG22	1.62	0.63
3:C:247:THR:OG1	4:C:806:HEC:O2D	2.16	0.63
2:B:144:GLY:O	2:B:147:SER:HB3	1.99	0.63
2:B:506:LEU:C	2:B:506:LEU:HD12	2.18	0.63
2:B:595:ASN:O	2:B:597:LEU:N	2.31	0.63
4:C:805:HEC:HMB1	4:C:805:HEC:CBB	2.29	0.62
1:A:166:VAL:HG22	4:A:902:HEC:HMD2	1.82	0.62
1:A:264:SER:HB3	1:A:269:MET:HA	1.80	0.62
3:C:575:ASP:HA	3:C:578:LYS:HZ1	1.64	0.62
2:B:110:ARG:HG3	2:B:110:ARG:HH11	1.65	0.62
4:A:908:HEC:CBB	4:A:908:HEC:HMB1	2.30	0.61
3:C:577:PHE:HA	3:C:580:LYS:HD2	1.82	0.61
2:B:64:GLU:OE2	2:B:682:TYR:HB2	2.00	0.61
2:B:552:TYR:HD1	2:B:583:VAL:HG12	1.66	0.61
4:A:908:HEC:CGA	2:B:211:LYS:HZ1	2.13	0.61
2:B:644:MET:HE2	2:B:693:TYR:HD1	1.66	0.61
1:A:145:ARG:HH12	4:A:904:HEC:CGA	2.13	0.61
2:B:459:TYR:HD1	2:B:492:THR:HG22	1.62	0.60
2:B:655:TYR:HB3	2:B:682:TYR:CE1	2.35	0.60
4:C:809:HEC:HBB3	4:C:809:HEC:HMB1	1.82	0.60
4:A:910:HEC:HAC	2:B:219:ASN:HA	1.83	0.60
4:A:904:HEC:HMC1	4:A:904:HEC:CBC	2.32	0.60
1:A:132:GLN:O	1:A:135:VAL:HG12	2.02	0.59
3:C:248:LEU:HG	3:C:491:CYS:O	2.02	0.59
1:A:295:ASN:HB2	2:B:621:ASP:O	2.03	0.58
4:A:907:HEC:HAD2	2:B:132:THR:HG21	1.85	0.58
2:B:247:PHE:CD1	2:B:298:GLN:HB3	2.39	0.58
1:A:221:ASP:CG	2:B:400:ARG:NH1	2.57	0.58
1:A:274:ALA:CB	1:A:275:PRO:CD	2.82	0.58
1:A:228:SER:O	1:A:232:THR:HG22	2.03	0.58
4:A:906:HEC:HMB1	4:A:906:HEC:HBB3	1.86	0.58
4:C:803:HEC:HBB3	4:C:803:HEC:HMB1	1.84	0.58
4:A:905:HEC:HBB3	4:A:905:HEC:HMB1	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:ILE:HD12	2:B:506:LEU:HD21	1.86	0.58
2:B:181:ARG:HG2	2:B:205:GLU:OE2	2.04	0.57
2:B:387:LYS:NZ	6:B:803:HOH:O	2.37	0.57
3:C:422:PRO:O	3:C:424:LEU:HD12	2.04	0.57
2:B:632:ILE:C	2:B:632:ILE:HD12	2.24	0.57
1:A:90:SER:HB2	2:B:119:GLY:HA3	1.87	0.56
1:A:93:SER:HB3	1:A:94:PRO:HD3	1.87	0.56
1:A:228:SER:OG	1:A:231:GLU:OE2	2.18	0.56
2:B:601:LEU:HD23	2:B:634:LEU:HD23	1.88	0.56
4:C:806:HEC:CBB	4:C:806:HEC:HMB1	2.35	0.56
2:B:506:LEU:HB3	2:B:540:TYR:CD1	2.34	0.56
4:A:908:HEC:CGA	2:B:211:LYS:NZ	2.69	0.56
2:B:381:ILE:HG12	4:C:805:HEC:HBC2	1.88	0.56
3:C:125:GLN:HB2	3:C:127:ASN:OD1	2.06	0.56
4:A:903:HEC:HHD	4:A:903:HEC:HBC3	1.88	0.55
2:B:311:LEU:HD12	2:B:312:THR:N	2.21	0.55
1:A:228:SER:OG	1:A:231:GLU:HG2	2.06	0.55
2:B:514:TYR:HD1	2:B:532:THR:HG22	1.71	0.55
1:A:226:LYS:HG3	1:A:232:THR:HA	1.89	0.55
4:C:810:HEC:CBB	4:C:810:HEC:HMB1	2.37	0.55
2:B:449:GLU:HB3	2:B:451:TRP:HD1	1.71	0.54
4:A:909:HEC:CBB	4:A:909:HEC:HMB1	2.36	0.54
3:C:301:SER:OG	3:C:302:ASN:ND2	2.41	0.54
2:B:306:LEU:HG	2:B:348:VAL:HG12	1.89	0.54
1:A:93:SER:HB3	1:A:94:PRO:CD	2.37	0.54
1:A:329:LYS:HE3	4:A:909:HEC:O2A	2.07	0.54
3:C:540:ALA:HB1	3:C:543:ALA:HB3	1.89	0.54
1:A:226:LYS:HB2	1:A:232:THR:HB	1.89	0.54
1:A:265:VAL:CG1	2:B:578:ASP:HB3	2.38	0.54
3:C:90:LEU:HB2	3:C:104:TRP:CZ3	2.43	0.54
1:A:99:GLN:O	1:A:101:GLU:N	2.41	0.53
1:A:101:GLU:CA	1:A:106:PRO:HD2	2.38	0.53
1:A:157:ASP:OD1	2:B:408:ARG:NH1	2.36	0.53
1:A:81:PHE:CZ	1:A:167:HIS:CE1	2.97	0.53
2:B:274:PHE:CG	4:C:805:HEC:HMD2	2.43	0.53
2:B:503:ILE:HG22	2:B:504:GLU:O	2.08	0.53
2:B:108:GLY:O	2:B:110:ARG:NH1	2.41	0.53
1:A:236:CYS:O	2:B:181:ARG:NH1	2.41	0.53
2:B:381:ILE:HD11	4:C:805:HEC:CBC	2.39	0.53
1:A:211:ASP:HB3	4:A:907:HEC:HBC2	1.91	0.53
1:A:116:GLU:HB3	1:A:117:PRO:HD3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:MET:SD	1:A:141:GLN:HG3	2.49	0.53
1:A:251:VAL:HA	4:A:908:HEC:HMC2	1.90	0.53
3:C:112:CYS:SG	3:C:122:PHE:HB2	2.50	0.52
4:A:902:HEC:HMD1	4:A:902:HEC:HBD1	1.92	0.52
2:B:87:VAL:HG22	2:B:99:VAL:HG22	1.91	0.52
3:C:45:ALA:HB1	3:C:168:GLN:HB2	1.90	0.52
4:A:901:HEC:CBB	4:A:901:HEC:HMB1	2.37	0.52
2:B:228:VAL:HG23	2:B:230:TYR:CE1	2.45	0.52
2:B:656:LYS:HA	2:B:680:HIS:O	2.10	0.52
1:A:296:THR:HG23	1:A:298:LEU:N	2.23	0.52
3:C:329:GLN:O	3:C:330:LEU:HD23	2.09	0.52
4:C:801:HEC:HMB1	4:C:801:HEC:HBB3	1.91	0.52
4:A:910:HEC:HMD1	4:A:910:HEC:HBD1	1.90	0.52
2:B:641:THR:O	2:B:643:LYS:N	2.42	0.52
4:A:910:HEC:CBB	4:A:910:HEC:HMB1	2.38	0.52
3:C:78:VAL:HG13	3:C:126:LYS:HA	1.90	0.52
3:C:297:GLN:HE22	4:C:805:HEC:HMC2	1.73	0.52
3:C:421:THR:OG1	3:C:424:LEU:HD11	2.10	0.52
4:A:908:HEC:HBA2	2:B:211:LYS:NZ	2.19	0.51
3:C:311:TRP:CD1	3:C:315:LEU:HD23	2.46	0.51
4:C:802:HEC:HMB1	4:C:802:HEC:CBB	2.41	0.51
2:B:459:TYR:HD1	2:B:492:THR:CG2	2.23	0.51
4:C:808:HEC:HBC3	4:C:808:HEC:HMC1	1.93	0.51
3:C:102:SER:O	3:C:190:ARG:NH1	2.44	0.51
2:B:263:GLN:OE1	2:B:322:VAL:HG22	2.11	0.50
2:B:666:VAL:HG13	2:B:674:GLY:O	2.11	0.50
3:C:248:LEU:HD23	4:C:801:HEC:HAC	1.92	0.50
1:A:260:ASN:ND2	1:A:263:GLY:O	2.44	0.50
3:C:125:GLN:OE1	3:C:129:HIS:HB2	2.11	0.50
1:A:101:GLU:HA	1:A:106:PRO:CD	2.40	0.50
2:B:632:ILE:HD11	2:B:652:ILE:CG1	2.34	0.50
3:C:373:VAL:HG21	4:C:807:HEC:HBC3	1.93	0.50
4:A:906:HEC:HMC1	4:A:906:HEC:CBC	2.41	0.50
1:A:253:GLU:OE1	2:B:426:ARG:HD3	2.11	0.50
2:B:197:SER:OG	2:B:240:LYS:HG3	2.12	0.50
4:A:905:HEC:HBA1	4:A:905:HEC:HHA	1.93	0.50
2:B:572:TRP:HB3	2:B:616:GLN:HB2	1.94	0.49
2:B:426:ARG:HH12	2:B:434:THR:HG21	1.77	0.49
1:A:137:MET:CE	4:A:904:HEC:HBB3	2.42	0.49
2:B:637:GLN:HB3	2:B:647:ARG:HB2	1.94	0.49
1:A:137:MET:HG3	1:A:141:GLN:OE1	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:906:HEC:HMB1	4:A:906:HEC:CBB	2.43	0.49
4:C:804:HEC:HBC3	4:C:804:HEC:HHD	1.94	0.49
2:B:246:TRP:HA	2:B:298:GLN:O	2.13	0.49
2:B:423:ARG:NH1	2:B:435:ASP:OD2	2.45	0.49
1:A:274:ALA:CB	1:A:275:PRO:HD3	2.43	0.49
4:A:908:HEC:CBA	2:B:211:LYS:HZ2	2.20	0.49
4:C:802:HEC:HMC1	4:C:802:HEC:CBC	2.43	0.49
3:C:297:GLN:NE2	4:C:805:HEC:HMC2	2.28	0.49
4:C:810:HEC:HBC3	4:C:810:HEC:HMC1	1.95	0.49
1:A:105:GLY:C	1:A:120:THR:HG23	2.34	0.48
1:A:106:PRO:HA	1:A:120:THR:OG1	2.12	0.48
2:B:103:GLN:HG2	2:B:106:MET:HG3	1.95	0.48
3:C:63:PRO:HD2	3:C:134:PHE:HB2	1.95	0.48
1:A:110:HIS:O	1:A:111:ASN:HB3	2.14	0.48
1:A:190:GLN:HB3	1:A:194:MET:HE2	1.96	0.48
1:A:72:LYS:HB3	1:A:78:MET:CE	2.43	0.48
3:C:272:ARG:HH11	3:C:272:ARG:HG3	1.79	0.48
3:C:612:GLU:OE1	3:C:616:ALA:O	2.31	0.48
4:A:907:HEC:CBB	4:A:907:HEC:HMB1	2.44	0.48
3:C:320:THR:HG22	3:C:324:LYS:HE2	1.94	0.48
4:C:808:HEC:CBB	4:C:808:HEC:HMB1	2.42	0.48
1:A:148:TRP:O	1:A:151:SER:HB3	2.14	0.48
2:B:110:ARG:HG3	2:B:110:ARG:NH1	2.28	0.48
2:B:215:GLY:O	2:B:222:MET:HE3	2.14	0.48
2:B:257:PHE:O	2:B:258:LYS:HD3	2.13	0.48
2:B:506:LEU:HD12	2:B:506:LEU:O	2.13	0.48
2:B:592:LEU:HB3	2:B:593:LEU:HD22	1.95	0.48
2:B:505:SER:HB2	2:B:541:MET:HG2	1.95	0.48
2:B:644:MET:HE2	2:B:693:TYR:CD1	2.47	0.48
3:C:288:PHE:HB3	3:C:297:GLN:HB2	1.96	0.48
3:C:591:THR:HG22	3:C:592:THR:O	2.14	0.48
1:A:93:SER:CB	1:A:94:PRO:HD3	2.44	0.48
2:B:153:PRO:HB2	2:B:155:ASN:OD1	2.14	0.48
1:A:144:LYS:HD2	4:A:904:HEC:O2A	2.14	0.48
2:B:622:TYR:N	2:B:622:TYR:CD1	2.82	0.48
2:B:419:TYR:OH	2:B:421:PHE:HB2	2.14	0.47
4:C:805:HEC:HHD	4:C:805:HEC:CBC	2.44	0.47
4:A:901:HEC:HMC1	4:A:901:HEC:CBC	2.41	0.47
2:B:557:ILE:N	2:B:557:ILE:HD12	2.29	0.47
1:A:79:ASP:N	1:A:79:ASP:OD1	2.47	0.47
2:B:294:SER:HA	2:B:310:LEU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PHE:CE1	1:A:167:HIS:CE1	3.03	0.47
2:B:139:LEU:HB3	2:B:172:LEU:HB3	1.97	0.47
1:A:329:LYS:NZ	2:B:472:TRP:O	2.42	0.47
2:B:566:ASN:ND2	2:B:568:SER:HB3	2.30	0.47
2:B:635:TYR:HB2	2:B:647:ARG:NH2	2.29	0.47
3:C:239:VAL:HG13	3:C:243:HIS:CE1	2.49	0.47
1:A:101:GLU:CB	1:A:106:PRO:HD2	2.45	0.47
4:A:904:HEC:HHA	4:A:904:HEC:HBD2	1.96	0.47
4:A:905:HEC:CBB	4:A:905:HEC:HMB1	2.45	0.47
2:B:208:THR:HA	2:B:228:VAL:O	2.14	0.47
2:B:339:VAL:HG22	2:B:369:ASN:HA	1.97	0.47
2:B:420:ASP:HB2	2:B:438:THR:HG23	1.97	0.47
1:A:175:SER:HB2	1:A:178:THR:CG2	2.44	0.46
4:C:806:HEC:CHA	4:C:806:HEC:HBA2	2.44	0.46
1:A:124:GLN:HE22	1:A:135:VAL:HG11	1.81	0.46
2:B:301:ASP:OD1	2:B:302:SER:N	2.48	0.46
1:A:274:ALA:HB1	1:A:275:PRO:CD	2.44	0.46
2:B:370:ASN:HA	6:B:810:HOH:O	2.15	0.46
2:B:459:TYR:CD1	2:B:492:THR:CG2	2.96	0.46
1:A:124:GLN:O	4:A:902:HEC:HAD1	2.16	0.46
1:A:180:MET:O	1:A:184:THR:HG23	2.15	0.46
1:A:275:PRO:O	1:A:279:GLN:HG3	2.16	0.46
2:B:442:ARG:NH1	2:B:456:LYS:NZ	2.64	0.46
2:B:79:VAL:HG23	2:B:79:VAL:O	2.14	0.46
1:A:137:MET:HE1	4:A:904:HEC:HBB3	1.98	0.46
1:A:318:SER:HB2	2:B:214:SER:HB2	1.98	0.46
2:B:354:ASN:ND2	2:B:354:ASN:O	2.34	0.46
3:C:243:HIS:HB3	3:C:251:LEU:HD13	1.98	0.46
1:A:157:ASP:CG	2:B:408:ARG:HH12	2.17	0.46
3:C:369:ARG:HA	3:C:401:VAL:O	2.16	0.46
2:B:216:GLY:HA3	2:B:220:GLN:O	2.15	0.45
2:B:462:ARG:O	2:B:488:ASN:HA	2.15	0.45
1:A:296:THR:HG22	1:A:300:SER:H	1.81	0.45
4:C:804:HEC:CBC	4:C:804:HEC:HHD	2.46	0.45
3:C:650:MET:SD	4:C:810:HEC:HAC	2.56	0.45
4:C:802:HEC:HMB1	4:C:802:HEC:HBB3	1.99	0.45
1:A:140:HIS:O	1:A:142:ASP:N	2.49	0.45
3:C:550:MET:O	3:C:554:VAL:HG23	2.17	0.45
2:B:210:LEU:HD23	2:B:225:ALA:HB1	1.99	0.45
2:B:63:SER:OG	2:B:64:GLU:HA	2.17	0.45
3:C:191:LYS:HB2	3:C:265:PRO:HD2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:595:THR:HG23	3:C:611:LEU:HD22	1.99	0.45
3:C:147:ASN:HB3	3:C:150:LEU:HG	1.99	0.44
2:B:449:GLU:HB3	2:B:451:TRP:CD1	2.51	0.44
4:A:908:HEC:CBA	2:B:211:LYS:NZ	2.79	0.44
3:C:526:VAL:HG23	3:C:548:PHE:HE2	1.82	0.44
1:A:303:GLY:O	2:B:664:ILE:HD13	2.17	0.44
2:B:228:VAL:HG23	2:B:230:TYR:CZ	2.52	0.44
3:C:173:ASN:HD21	3:C:214:TYR:HA	1.81	0.44
3:C:320:THR:O	3:C:324:LYS:HG3	2.18	0.44
2:B:62:ASN:OD1	2:B:63:SER:N	2.50	0.44
3:C:118:CYS:HA	3:C:119:PRO:HD3	1.83	0.44
4:C:807:HEC:CBC	4:C:807:HEC:HMC1	2.45	0.44
1:A:93:SER:CB	1:A:94:PRO:CD	2.95	0.44
2:B:196:TRP:HA	2:B:240:LYS:O	2.18	0.44
1:A:256:VAL:O	1:A:256:VAL:HG23	2.18	0.44
3:C:223:CYS:HB2	4:C:802:HEC:HBC3	1.81	0.44
3:C:311:TRP:NE1	3:C:315:LEU:HD23	2.33	0.44
1:A:109:GLN:HA	1:A:120:THR:CB	2.48	0.44
1:A:109:GLN:HA	1:A:120:THR:OG1	2.18	0.44
3:C:498:ILE:O	3:C:505:GLY:HA2	2.18	0.44
2:B:274:PHE:CD2	4:C:805:HEC:HMD2	2.53	0.44
2:B:446:ASN:O	2:B:446:ASN:OD1	2.36	0.43
4:A:907:HEC:CBC	4:A:907:HEC:HMC1	2.46	0.43
2:B:505:SER:O	2:B:540:TYR:HA	2.17	0.43
3:C:89:GLN:HG3	3:C:152:GLN:NE2	2.34	0.43
2:B:309:ARG:HB3	2:B:345:ASN:HB2	2.01	0.43
2:B:569:THR:HB	2:B:570:PRO:HD2	2.00	0.43
1:A:137:MET:HE1	4:A:904:HEC:CBB	2.49	0.43
1:A:156:ALA:HB1	4:A:905:HEC:HMD2	2.00	0.43
1:A:98:LEU:HB3	1:A:101:GLU:HG2	2.01	0.43
2:B:554:TYR:HD2	2:B:581:ASP:OD1	2.02	0.43
3:C:202:HIS:O	3:C:203:GLN:HB2	2.18	0.43
4:C:805:HEC:HBB2	4:C:805:HEC:HMB1	1.99	0.43
2:B:442:ARG:HB2	2:B:456:LYS:HB2	2.01	0.43
4:A:903:HEC:CBB	4:A:903:HEC:HMB1	2.49	0.43
2:B:64:GLU:HG2	2:B:66:ASP:H	1.83	0.43
2:B:349:VAL:CG1	2:B:357:ARG:HD2	2.49	0.43
2:B:438:THR:HA	2:B:460:GLY:HA2	2.01	0.43
2:B:540:TYR:CG	2:B:541:MET:N	2.87	0.43
2:B:669:ILE:HB	2:B:672:VAL:CG2	2.46	0.43
2:B:118:GLN:OE1	2:B:118:GLN:O	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:GLU:CD	2:B:193:GLU:H	2.21	0.43
2:B:198:THR:HG22	2:B:239:ILE:HG13	2.01	0.43
2:B:65:GLU:HG3	2:B:65:GLU:O	2.18	0.43
3:C:43:ALA:HB3	3:C:44:PRO:HD3	2.01	0.43
2:B:371:THR:HG22	2:B:372:GLN:N	2.35	0.42
2:B:485:ASN:OD1	2:B:485:ASN:N	2.52	0.42
3:C:248:LEU:HD23	4:C:801:HEC:CAC	2.47	0.42
3:C:509:THR:O	3:C:512:VAL:HG22	2.17	0.42
4:C:801:HEC:HMC1	4:C:801:HEC:HBC3	2.01	0.42
4:A:902:HEC:HHD	4:A:902:HEC:HBC2	2.00	0.42
1:A:204:TRP:NE1	2:B:72:ALA:HA	2.33	0.42
4:A:903:HEC:HBB3	4:A:903:HEC:HMB1	2.01	0.42
4:A:909:HEC:HAC	4:A:909:HEC:HMC1	1.87	0.42
2:B:209:GLY:O	2:B:210:LEU:HD12	2.20	0.42
4:A:905:HEC:HMC1	4:A:905:HEC:CBC	2.43	0.42
2:B:356:LEU:C	2:B:356:LEU:HD12	2.39	0.42
2:B:95:TYR:CE1	2:B:97:ALA:HB2	2.55	0.42
3:C:460:SER:OG	3:C:505:GLY:HA3	2.20	0.42
1:A:110:HIS:HB3	1:A:120:THR:O	2.19	0.42
2:B:356:LEU:O	2:B:356:LEU:HD12	2.19	0.42
3:C:527:ASP:O	3:C:530:VAL:HG22	2.19	0.42
2:B:381:ILE:CD1	4:C:805:HEC:CBC	2.98	0.42
1:A:287:HIS:HB3	3:C:304:ILE:HG23	2.01	0.42
4:C:806:HEC:HMC1	4:C:806:HEC:CBC	2.50	0.42
2:B:111:LEU:HD23	2:B:111:LEU:C	2.40	0.42
3:C:76:PRO:HB3	3:C:128:GLY:HA3	2.01	0.42
2:B:127:TYR:HD1	2:B:184:THR:HG22	1.84	0.42
2:B:506:LEU:CD1	2:B:506:LEU:C	2.85	0.42
3:C:63:PRO:HB2	3:C:134:PHE:CD1	2.55	0.42
3:C:494:ASP:N	3:C:494:ASP:OD1	2.53	0.41
4:C:802:HEC:HBC3	4:C:802:HEC:HMC1	2.02	0.41
1:A:90:SER:HB3	2:B:118:GLN:HG3	2.02	0.41
3:C:163:LEU:HD12	3:C:167:THR:HB	2.01	0.41
3:C:47:GLN:O	3:C:48:ILE:HD13	2.20	0.41
4:C:802:HEC:HHA	4:C:802:HEC:HBA1	2.02	0.41
2:B:104:LEU:HD12	2:B:111:LEU:HB2	2.02	0.41
2:B:406:ASP:HB3	2:B:414:LYS:HE2	2.02	0.41
3:C:374:THR:HB	3:C:396:ILE:HB	2.02	0.41
3:C:617:ILE:HD13	3:C:624:GLN:CG	2.30	0.41
4:A:903:HEC:HHD	4:A:903:HEC:CBC	2.49	0.41
2:B:64:GLU:CD	2:B:64:GLU:H	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:910:HEC:CGD	6:B:803:HOH:O	2.68	0.41
2:B:209:GLY:C	2:B:210:LEU:HD12	2.41	0.41
2:B:217:PHE:CE2	2:B:268:SER:HB2	2.55	0.41
2:B:80:ALA:HB1	2:B:106:MET:HE1	1.99	0.41
3:C:607:ILE:HD12	3:C:611:LEU:HD11	2.03	0.41
3:C:607:ILE:HD13	3:C:611:LEU:HD21	2.02	0.41
1:A:194:MET:SD	1:A:202:LEU:HD13	2.60	0.41
2:B:120:GLN:O	2:B:191:GLN:N	2.49	0.41
2:B:361:SER:OG	2:B:402:LYS:CG	2.56	0.41
2:B:491:ARG:HA	2:B:516:LEU:O	2.21	0.41
2:B:493:GLN:HA	2:B:514:TYR:O	2.21	0.41
3:C:376:VAL:HG23	3:C:383:MET:CE	2.51	0.41
1:A:175:SER:CB	1:A:178:THR:HG22	2.51	0.41
1:A:276:GLN:HB3	2:B:561:GLN:OE1	2.21	0.41
1:A:260:ASN:O	1:A:269:MET:HE2	2.21	0.41
2:B:511:GLY:O	2:B:535:ASP:OD1	2.38	0.41
1:A:99:GLN:C	1:A:101:GLU:N	2.73	0.40
2:B:526:LEU:HD12	2:B:527:THR:N	2.36	0.40
2:B:650:TYR:HD1	2:B:687:ILE:CG2	2.32	0.40
1:A:309:GLY:HA2	2:B:661:ALA:HB1	2.02	0.40
3:C:89:GLN:HB2	3:C:107:PHE:CE2	2.56	0.40
3:C:248:LEU:HD12	3:C:248:LEU:HA	1.93	0.40
1:A:143:ASP:OD1	1:A:143:ASP:N	2.55	0.40
4:A:910:HEC:HMC1	4:A:910:HEC:CBC	2.45	0.40
2:B:126:ASN:OD1	2:B:185:GLY:N	2.55	0.40
2:B:262:ASN:OD1	2:B:319:GLN:NE2	2.54	0.40
2:B:318:ASP:OD1	2:B:318:ASP:C	2.60	0.40
2:B:626:PHE:HE1	2:B:656:LYS:HG2	1.86	0.40
4:C:805:HEC:HHD	4:C:805:HEC:HBC2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	259/333 (78%)	216 (83%)	35 (14%)	8 (3%)	4 9
2	B	647/695 (93%)	614 (95%)	30 (5%)	3 (0%)	29 54
3	C	606/650 (93%)	583 (96%)	22 (4%)	1 (0%)	47 73
All	All	1512/1678 (90%)	1413 (94%)	87 (6%)	12 (1%)	19 43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	169	ALA
1	A	274	ALA
1	A	99	GLN
1	A	123	LYS
1	A	141	GLN
1	A	72	LYS
2	B	595	ASN
2	B	542	ILE
2	B	502	PRO
3	C	44	PRO
1	A	94	PRO

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	226/282 (80%)	221 (98%)	5 (2%)	52 79
2	B	552/586 (94%)	536 (97%)	16 (3%)	42 71
3	C	483/511 (94%)	475 (98%)	8 (2%)	60 84
All	All	1261/1379 (91%)	1232 (98%)	29 (2%)	50 78

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	90	SER
1	A	139	CYS
1	A	147	SER
1	A	221	ASP
2	B	54	THR
2	B	63	SER
2	B	64	GLU
2	B	90	ARG
2	B	180	LYS
2	B	319	GLN
2	B	338	LYS
2	B	350	SER
2	B	354	ASN
2	B	387	LYS
2	B	411	ARG
2	B	419	TYR
2	B	438	THR
2	B	467	TYR
2	B	553	ASN
2	B	588	SER
3	C	118	CYS
3	C	148	ASP
3	C	190	ARG
3	C	219	TYR
3	C	235	PHE
3	C	261	ASN
3	C	494	ASP
3	C	578	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	297	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
4	HEC	C	803	3	26,50,50	2.53	4 (15%)	18,82,82	2.08	6 (33%)
4	HEC	C	805	3	26,50,50	2.78	6 (23%)	18,82,82	3.11	5 (27%)
4	HEC	A	905	1	26,50,50	2.33	4 (15%)	18,82,82	1.66	3 (16%)
4	HEC	C	809	3	26,50,50	2.40	8 (30%)	18,82,82	2.25	6 (33%)
4	HEC	A	902	1	26,50,50	2.39	8 (30%)	18,82,82	1.59	4 (22%)
4	HEC	C	804	3	26,50,50	2.47	4 (15%)	18,82,82	3.07	7 (38%)
4	HEC	A	906	1	26,50,50	2.25	4 (15%)	18,82,82	3.26	7 (38%)
4	HEC	A	909	1	26,50,50	2.82	5 (19%)	18,82,82	1.58	4 (22%)
4	HEC	A	903	1	26,50,50	2.36	7 (26%)	18,82,82	2.20	6 (33%)
4	HEC	C	810	3	26,50,50	2.22	5 (19%)	18,82,82	2.50	5 (27%)
4	HEC	A	907	1	26,50,50	2.41	3 (11%)	18,82,82	1.95	6 (33%)
4	HEC	C	807	3	26,50,50	2.49	5 (19%)	18,82,82	1.65	4 (22%)
4	HEC	A	908	1	26,50,50	2.37	3 (11%)	18,82,82	2.41	6 (33%)
4	HEC	C	802	3	26,50,50	2.27	5 (19%)	18,82,82	2.59	6 (33%)
4	HEC	A	910	1	26,50,50	2.35	6 (23%)	18,82,82	2.79	6 (33%)
4	HEC	C	806	3	26,50,50	2.43	3 (11%)	18,82,82	2.86	7 (38%)
4	HEC	A	904	1	26,50,50	2.30	5 (19%)	18,82,82	2.16	4 (22%)
4	HEC	C	808	3	26,50,50	2.33	5 (19%)	18,82,82	2.44	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HEC	C	801	3	26,50,50	2.52	6 (23%)	18,82,82	3.30	9 (50%)
4	HEC	A	901	1	26,50,50	2.26	5 (19%)	18,82,82	1.82	6 (33%)

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
4	HEC	C	803	3	-	0/6/54/54	-
4	HEC	C	805	3	-	0/6/54/54	-
4	HEC	A	905	1	-	2/6/54/54	-
4	HEC	C	809	3	-	3/6/54/54	-
4	HEC	A	902	1	-	2/6/54/54	-
4	HEC	C	804	3	-	1/6/54/54	-
4	HEC	A	906	1	-	3/6/54/54	-
4	HEC	A	909	1	-	0/6/54/54	-
4	HEC	A	903	1	-	0/6/54/54	-
4	HEC	C	810	3	-	1/6/54/54	-
4	HEC	A	907	1	-	0/6/54/54	-
4	HEC	C	807	3	-	0/6/54/54	-
4	HEC	A	908	1	-	1/6/54/54	-
4	HEC	C	802	3	-	3/6/54/54	-
4	HEC	A	910	1	-	2/6/54/54	-
4	HEC	C	806	3	-	5/6/54/54	-
4	HEC	A	904	1	-	3/6/54/54	-
4	HEC	C	808	3	-	1/6/54/54	-
4	HEC	C	801	3	-	3/6/54/54	-
4	HEC	A	901	1	-	0/6/54/54	-

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	909	HEC	C3C-C2C	-9.50	1.30	1.40
4	C	805	HEC	C3C-C2C	-8.65	1.31	1.40
4	C	804	HEC	C3C-C2C	-7.72	1.32	1.40
4	C	805	HEC	C3B-C2B	-7.55	1.32	1.40
4	A	909	HEC	C3B-C2B	-7.49	1.32	1.40
4	C	807	HEC	C3C-C2C	-7.37	1.33	1.40
4	C	801	HEC	C3C-C2C	-7.30	1.33	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	806	HEC	C3C-C2C	-7.28	1.33	1.40
4	C	803	HEC	C3B-C2B	-7.07	1.33	1.40
4	A	910	HEC	C3C-C2C	-7.05	1.33	1.40
4	A	907	HEC	C3C-C2C	-7.00	1.33	1.40
4	C	804	HEC	C3B-C2B	-6.99	1.33	1.40
4	C	803	HEC	C3C-C2C	-6.97	1.33	1.40
4	C	808	HEC	C3B-C2B	-6.93	1.33	1.40
4	A	902	HEC	C3C-C2C	-6.78	1.33	1.40
4	A	908	HEC	C3C-C2C	-6.75	1.33	1.40
4	C	801	HEC	C3B-C2B	-6.69	1.33	1.40
4	A	907	HEC	C3B-C2B	-6.67	1.33	1.40
4	C	807	HEC	C3B-C2B	-6.65	1.33	1.40
4	A	908	HEC	C3B-C2B	-6.59	1.33	1.40
4	A	906	HEC	C3B-C2B	-6.56	1.33	1.40
4	A	905	HEC	C3B-C2B	-6.52	1.33	1.40
4	C	809	HEC	C3B-C2B	-6.50	1.34	1.40
4	A	903	HEC	C3C-C2C	-6.40	1.34	1.40
4	C	802	HEC	C3B-C2B	-6.29	1.34	1.40
4	C	806	HEC	C3B-C2B	-6.17	1.34	1.40
4	A	904	HEC	C3C-C2C	-6.15	1.34	1.40
4	A	901	HEC	C3C-C2C	-5.87	1.34	1.40
4	C	810	HEC	C3B-C2B	-5.77	1.34	1.40
4	C	808	HEC	C3C-C2C	-5.65	1.34	1.40
4	A	904	HEC	C3D-C2D	5.59	1.54	1.37
4	C	806	HEC	C3D-C2D	5.52	1.54	1.37
4	A	905	HEC	C3C-C2C	-5.52	1.35	1.40
4	C	809	HEC	C3D-C2D	5.45	1.53	1.37
4	A	910	HEC	C3B-C2B	-5.44	1.35	1.40
4	C	802	HEC	C3C-C2C	-5.41	1.35	1.40
4	C	810	HEC	C3C-C2C	-5.41	1.35	1.40
4	A	906	HEC	C3C-C2C	-5.41	1.35	1.40
4	C	803	HEC	C3D-C2D	5.32	1.53	1.37
4	A	901	HEC	C3B-C2B	-5.31	1.35	1.40
4	A	905	HEC	C3D-C2D	5.26	1.53	1.37
4	A	902	HEC	C3D-C2D	5.25	1.53	1.37
4	C	808	HEC	C3D-C2D	5.25	1.53	1.37
4	A	903	HEC	C3B-C2B	-5.22	1.35	1.40
4	A	910	HEC	C3D-C2D	5.14	1.52	1.37
4	A	904	HEC	C3B-C2B	-5.13	1.35	1.40
4	C	807	HEC	C3D-C2D	5.09	1.52	1.37
4	A	907	HEC	C3D-C2D	5.08	1.52	1.37
4	A	908	HEC	C3D-C2D	5.08	1.52	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	HEC	C3D-C2D	5.07	1.52	1.37
4	A	903	HEC	C3D-C2D	5.05	1.52	1.37
4	C	805	HEC	C3D-C2D	5.04	1.52	1.37
4	C	810	HEC	C3D-C2D	4.99	1.52	1.37
4	A	902	HEC	C3B-C2B	-4.94	1.35	1.40
4	C	809	HEC	C3C-C2C	-4.90	1.35	1.40
4	A	906	HEC	C3D-C2D	4.84	1.52	1.37
4	A	909	HEC	C3D-C2D	4.74	1.51	1.37
4	C	802	HEC	C3D-C2D	4.64	1.51	1.37
4	C	804	HEC	C3D-C2D	4.25	1.50	1.37
4	C	801	HEC	C3D-C2D	4.24	1.50	1.37
4	C	801	HEC	CAA-C2A	3.86	1.59	1.52
4	C	809	HEC	CAA-C2A	3.28	1.58	1.52
4	A	903	HEC	CAD-C3D	2.78	1.56	1.52
4	C	809	HEC	CAD-C3D	2.72	1.56	1.52
4	A	904	HEC	CAD-C3D	2.69	1.56	1.52
4	C	803	HEC	CAD-C3D	2.67	1.56	1.52
4	C	805	HEC	C3C-C4C	2.65	1.47	1.43
4	A	903	HEC	C3C-C4C	2.64	1.47	1.43
4	C	808	HEC	CAD-C3D	2.48	1.55	1.52
4	C	805	HEC	CAA-C2A	2.47	1.56	1.52
4	C	807	HEC	CAA-C2A	2.45	1.56	1.52
4	C	809	HEC	C4D-ND	2.42	1.41	1.36
4	C	805	HEC	C1C-CHC	-2.42	1.34	1.41
4	A	903	HEC	C4D-ND	2.40	1.41	1.36
4	C	802	HEC	CAA-C2A	2.40	1.56	1.52
4	A	902	HEC	CAA-C2A	2.40	1.56	1.52
4	A	902	HEC	C4D-ND	2.37	1.41	1.36
4	A	910	HEC	C1D-ND	2.37	1.41	1.36
4	A	910	HEC	C2A-C3A	-2.35	1.30	1.37
4	A	909	HEC	C3C-C4C	2.34	1.47	1.43
4	C	808	HEC	C4D-CHA	-2.33	1.34	1.41
4	C	810	HEC	CAA-C2A	2.33	1.56	1.52
4	A	902	HEC	CAD-C3D	2.32	1.55	1.52
4	C	802	HEC	CAD-C3D	2.32	1.55	1.52
4	C	801	HEC	C4D-ND	2.30	1.40	1.36
4	A	901	HEC	C3B-C4B	2.26	1.47	1.43
4	A	905	HEC	CAA-C2A	2.21	1.56	1.52
4	A	903	HEC	CAA-C2A	2.20	1.56	1.52
4	A	909	HEC	CAA-C2A	2.20	1.56	1.52
4	A	904	HEC	C1C-CHC	-2.19	1.34	1.41
4	C	801	HEC	C4A-C3A	2.17	1.47	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	810	HEC	CAD-C3D	2.13	1.55	1.52
4	A	902	HEC	C1D-ND	2.11	1.40	1.36
4	C	807	HEC	C4D-ND	2.10	1.40	1.36
4	A	906	HEC	C1C-CHC	-2.10	1.35	1.41
4	C	809	HEC	C1D-ND	2.10	1.40	1.36
4	A	901	HEC	C1D-ND	2.05	1.40	1.36
4	A	902	HEC	C3C-C4C	2.05	1.46	1.43
4	C	804	HEC	C1C-CHC	-2.04	1.35	1.41
4	C	809	HEC	C1A-C2A	2.04	1.47	1.42
4	A	910	HEC	C3B-C4B	2.02	1.46	1.43

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	801	HEC	CBA-CAA-C2A	9.24	129.51	112.48
4	A	906	HEC	CBD-CAD-C3D	-9.10	95.71	112.49
4	C	805	HEC	CMC-C2C-C3C	-7.92	116.51	125.82
4	C	802	HEC	CMC-C2C-C1C	-7.48	116.96	128.46
4	C	808	HEC	CMC-C2C-C1C	-7.28	117.27	128.46
4	C	805	HEC	CMC-C2C-C1C	-7.25	117.32	128.46
4	A	906	HEC	CMC-C2C-C1C	-6.89	117.87	128.46
4	C	806	HEC	CMC-C2C-C1C	-6.15	119.01	128.46
4	C	806	HEC	CMB-C2B-C1B	-6.02	119.21	128.46
4	C	804	HEC	CMC-C2C-C1C	-5.84	119.48	128.46
4	C	804	HEC	CBD-CAD-C3D	-5.79	101.82	112.49
4	C	806	HEC	CMB-C2B-C3B	5.73	132.55	125.82
4	C	810	HEC	CBA-CAA-C2A	5.60	122.79	112.48
4	A	903	HEC	CBD-CAD-C3D	5.56	122.75	112.49
4	C	804	HEC	CMC-C2C-C3C	-5.51	119.34	125.82
4	A	908	HEC	CMB-C2B-C1B	-5.46	120.08	128.46
4	A	910	HEC	CMB-C2B-C1B	-5.43	120.11	128.46
4	C	803	HEC	CMC-C2C-C1C	-5.41	120.14	128.46
4	C	810	HEC	CAA-CBA-CGA	5.36	121.66	112.67
4	A	910	HEC	CMB-C2B-C3B	5.14	131.87	125.82
4	A	910	HEC	CAD-CBD-CGD	-4.97	104.33	112.67
4	C	801	HEC	CMC-C2C-C1C	-4.95	120.86	128.46
4	C	809	HEC	CMC-C2C-C1C	-4.82	121.05	128.46
4	A	910	HEC	C1D-C2D-C3D	-4.81	103.65	107.00
4	C	801	HEC	CMC-C2C-C3C	4.81	131.47	125.82
4	A	904	HEC	CMC-C2C-C1C	-4.68	121.27	128.46
4	A	908	HEC	CMB-C2B-C3B	4.56	131.18	125.82
4	C	809	HEC	CMC-C2C-C3C	4.43	131.03	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	809	HEC	CBA-CAA-C2A	4.33	120.46	112.48
4	C	804	HEC	CMB-C2B-C1B	-4.32	121.82	128.46
4	A	904	HEC	CMC-C2C-C3C	4.31	130.89	125.82
4	A	907	HEC	C1D-C2D-C3D	-4.27	104.02	107.00
4	C	805	HEC	CBA-CAA-C2A	4.24	120.29	112.48
4	A	908	HEC	CMC-C2C-C1C	-4.21	122.00	128.46
4	C	804	HEC	CMB-C2B-C3B	4.18	130.74	125.82
4	A	903	HEC	CAD-CBD-CGD	-4.18	105.66	112.67
4	C	802	HEC	CAA-CBA-CGA	4.14	119.62	112.67
4	C	810	HEC	CMC-C2C-C1C	-4.13	122.11	128.46
4	C	807	HEC	CBA-CAA-C2A	4.11	120.04	112.48
4	C	801	HEC	CAD-CBD-CGD	-3.99	105.97	112.67
4	C	804	HEC	CMA-C3A-C2A	3.91	132.31	124.94
4	A	901	HEC	C1D-C2D-C3D	-3.84	104.33	107.00
4	A	906	HEC	CMB-C2B-C1B	-3.79	122.64	128.46
4	A	906	HEC	CBA-CAA-C2A	3.79	119.46	112.48
4	A	907	HEC	CMC-C2C-C1C	-3.66	122.84	128.46
4	C	803	HEC	CMD-C2D-C1D	-3.60	122.92	128.46
4	A	910	HEC	CMC-C2C-C1C	-3.60	122.94	128.46
4	C	804	HEC	CAA-CBA-CGA	-3.59	106.64	112.67
4	C	802	HEC	CMB-C2B-C1B	-3.59	122.94	128.46
4	A	905	HEC	CMB-C2B-C1B	-3.59	122.95	128.46
4	C	810	HEC	CMC-C2C-C3C	3.56	130.01	125.82
4	A	904	HEC	CMB-C2B-C1B	-3.55	123.00	128.46
4	C	810	HEC	CMB-C2B-C1B	-3.52	123.05	128.46
4	C	808	HEC	CMB-C2B-C1B	-3.52	123.05	128.46
4	C	808	HEC	CBA-CAA-C2A	-3.52	105.99	112.48
4	A	903	HEC	CMB-C2B-C1B	-3.51	123.08	128.46
4	A	909	HEC	CBD-CAD-C3D	-3.49	106.06	112.49
4	A	902	HEC	CBA-CAA-C2A	3.45	118.83	112.48
4	A	905	HEC	CMC-C2C-C1C	-3.43	123.19	128.46
4	A	907	HEC	CMB-C2B-C1B	-3.34	123.33	128.46
4	C	805	HEC	CMB-C2B-C1B	-3.32	123.36	128.46
4	C	806	HEC	CAD-CBD-CGD	-3.29	107.15	112.67
4	A	908	HEC	CMC-C2C-C3C	3.29	129.68	125.82
4	A	906	HEC	CAA-CBA-CGA	3.27	118.15	112.67
4	A	901	HEC	CMB-C2B-C1B	-3.20	123.55	128.46
4	C	801	HEC	CMB-C2B-C1B	-3.16	123.61	128.46
4	C	801	HEC	CAA-CBA-CGA	3.14	117.94	112.67
4	C	801	HEC	C1D-C2D-C3D	-3.08	104.85	107.00
4	A	902	HEC	CMB-C2B-C1B	-3.06	123.76	128.46
4	C	807	HEC	C1D-C2D-C3D	-2.88	104.99	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	806	HEC	C1D-C2D-C3D	-2.88	104.99	107.00
4	A	910	HEC	CBA-CAA-C2A	-2.87	107.19	112.48
4	C	803	HEC	CMD-C2D-C3D	2.87	130.35	124.94
4	A	908	HEC	CBA-CAA-C2A	-2.87	107.19	112.48
4	C	807	HEC	CMB-C2B-C1B	-2.85	124.08	128.46
4	C	802	HEC	CMD-C2D-C1D	2.82	132.80	128.46
4	A	907	HEC	CAA-CBA-CGA	-2.80	107.97	112.67
4	A	903	HEC	CMC-C2C-C1C	-2.77	124.21	128.46
4	A	901	HEC	CMC-C2C-C1C	-2.77	124.21	128.46
4	A	909	HEC	CMC-C2C-C3C	-2.72	122.62	125.82
4	C	803	HEC	CMB-C2B-C1B	-2.72	124.29	128.46
4	C	809	HEC	CMB-C2B-C1B	-2.66	124.38	128.46
4	C	806	HEC	CMD-C2D-C3D	2.65	129.94	124.94
4	A	904	HEC	CMD-C2D-C1D	-2.64	124.41	128.46
4	C	803	HEC	CAA-CBA-CGA	-2.64	108.25	112.67
4	A	901	HEC	CAD-CBD-CGD	-2.63	108.26	112.67
4	A	909	HEC	C1D-C2D-C3D	-2.63	105.17	107.00
4	C	801	HEC	CMA-C3A-C2A	2.62	129.89	124.94
4	C	805	HEC	C3C-C4C-NC	-2.59	106.05	110.94
4	C	808	HEC	CMB-C2B-C3B	2.50	128.76	125.82
4	C	802	HEC	CMD-C2D-C3D	-2.47	120.28	124.94
4	A	905	HEC	CAD-CBD-CGD	-2.46	108.54	112.67
4	C	806	HEC	CMD-C2D-C1D	-2.42	124.75	128.46
4	C	807	HEC	CMC-C2C-C1C	-2.42	124.75	128.46
4	A	902	HEC	CMC-C2C-C3C	-2.39	123.01	125.82
4	C	802	HEC	CMC-C2C-C3C	2.38	128.62	125.82
4	A	903	HEC	C3C-C4C-NC	-2.35	106.51	110.94
4	A	906	HEC	CMB-C2B-C3B	2.29	128.51	125.82
4	A	907	HEC	CMD-C2D-C3D	2.26	129.21	124.94
4	C	801	HEC	CAA-C2A-C3A	2.25	133.70	127.25
4	C	803	HEC	CBA-CAA-C2A	2.23	116.59	112.48
4	C	809	HEC	CAA-CBA-CGA	2.23	116.41	112.67
4	A	901	HEC	CAA-CBA-CGA	-2.22	108.95	112.67
4	A	909	HEC	CMB-C2B-C1B	-2.15	125.17	128.46
4	C	809	HEC	CAD-CBD-CGD	2.10	116.19	112.67
4	A	902	HEC	CAD-C3D-C2D	-2.08	121.26	127.25
4	A	907	HEC	CAD-C3D-C2D	2.08	133.23	127.25
4	C	808	HEC	CAA-CBA-CGA	2.07	116.15	112.67
4	A	906	HEC	C1D-C2D-C3D	-2.04	105.58	107.00
4	A	908	HEC	CMD-C2D-C1D	-2.03	125.35	128.46
4	A	901	HEC	CBD-CAD-C3D	-2.01	108.78	112.49
4	A	903	HEC	CMB-C2B-C3B	2.00	128.18	125.82

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	HEC	C3A-C2A-CAA-CBA
4	A	902	HEC	C4D-C3D-CAD-CBD
4	C	804	HEC	C2A-CAA-CBA-CGA
4	C	806	HEC	C1A-C2A-CAA-CBA
4	C	806	HEC	C3A-C2A-CAA-CBA
4	C	806	HEC	C2D-C3D-CAD-CBD
4	C	806	HEC	C4D-C3D-CAD-CBD
4	C	806	HEC	C3D-CAD-CBD-CGD
4	C	809	HEC	C1A-C2A-CAA-CBA
4	C	809	HEC	C3A-C2A-CAA-CBA
4	C	809	HEC	C2A-CAA-CBA-CGA
4	A	905	HEC	C1A-C2A-CAA-CBA
4	A	905	HEC	C3A-C2A-CAA-CBA
4	C	810	HEC	C2A-CAA-CBA-CGA
4	A	904	HEC	C2D-C3D-CAD-CBD
4	A	904	HEC	C4D-C3D-CAD-CBD
4	C	802	HEC	C3A-C2A-CAA-CBA
4	C	802	HEC	C3D-CAD-CBD-CGD
4	A	910	HEC	C2D-C3D-CAD-CBD
4	C	801	HEC	C1A-C2A-CAA-CBA
4	A	906	HEC	C1A-C2A-CAA-CBA
4	A	906	HEC	C3A-C2A-CAA-CBA
4	A	908	HEC	C4D-C3D-CAD-CBD
4	C	802	HEC	C1A-C2A-CAA-CBA
4	A	910	HEC	C4D-C3D-CAD-CBD
4	C	801	HEC	C3A-C2A-CAA-CBA
4	C	801	HEC	C4D-C3D-CAD-CBD
4	A	906	HEC	C2A-CAA-CBA-CGA
4	A	904	HEC	C3D-CAD-CBD-CGD
4	C	808	HEC	C2A-CAA-CBA-CGA

There are no ring outliers.

20 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	803	HEC	2	0
4	C	805	HEC	11	0
4	A	905	HEC	6	0
4	C	809	HEC	2	0
4	A	902	HEC	5	0

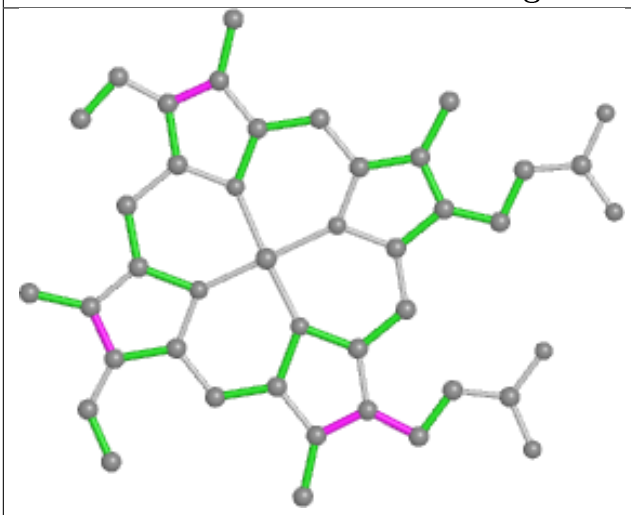
Continued on next page...

Continued from previous page...

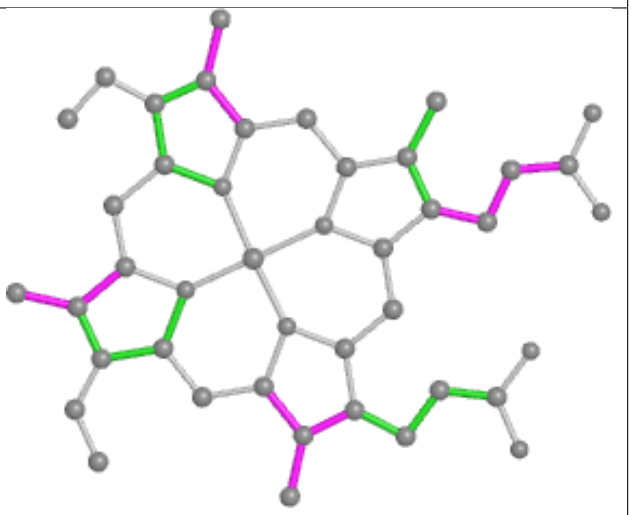
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	804	HEC	2	0
4	A	906	HEC	3	0
4	A	909	HEC	4	0
4	A	903	HEC	4	0
4	C	810	HEC	4	0
4	A	907	HEC	6	0
4	C	807	HEC	4	0
4	A	908	HEC	9	0
4	C	802	HEC	6	0
4	A	910	HEC	7	0
4	C	806	HEC	5	0
4	A	904	HEC	9	0
4	C	808	HEC	4	0
4	C	801	HEC	4	0
4	A	901	HEC	4	0

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.

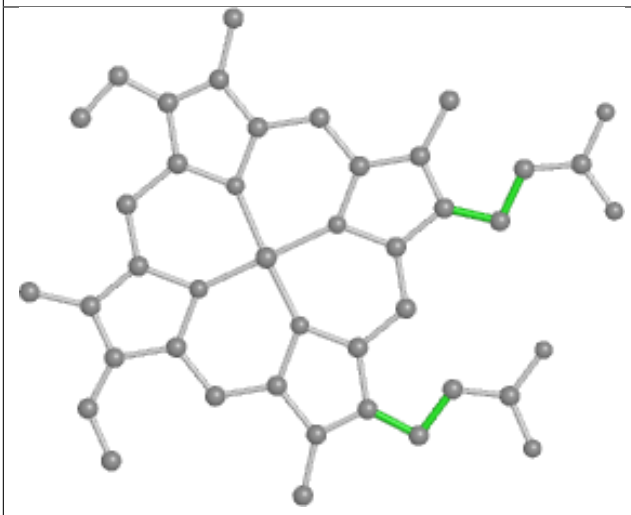
Ligand HEC C 803



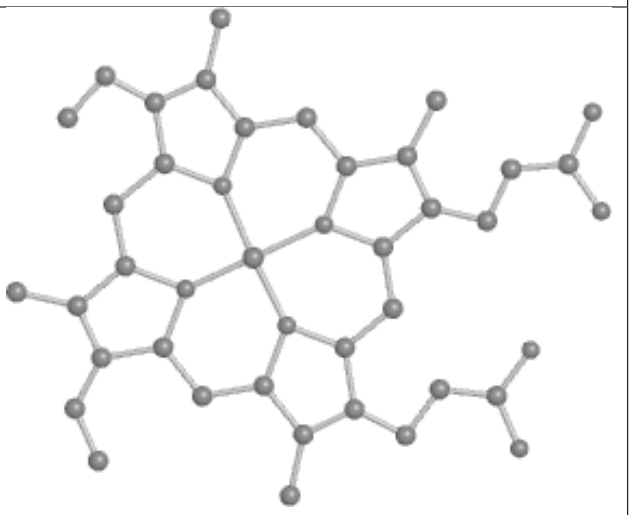
Bond lengths



Bond angles

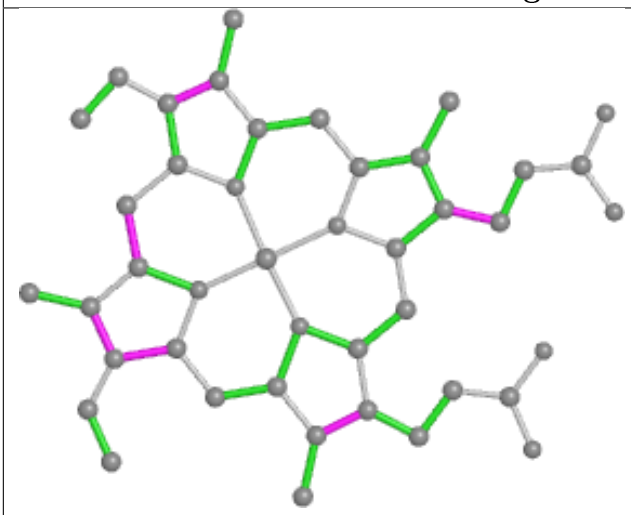


Torsions

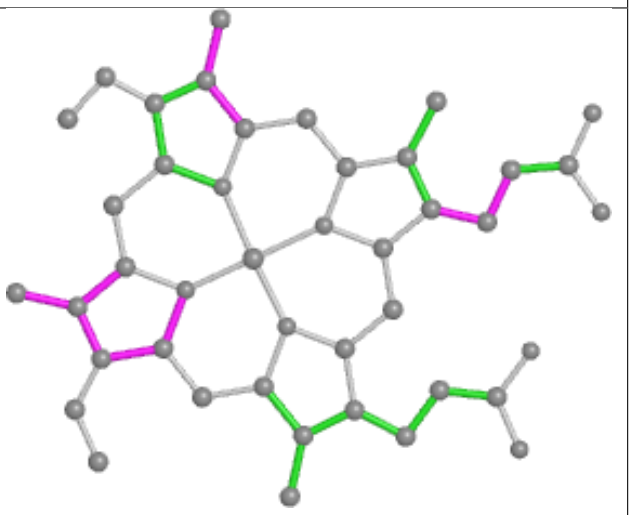


Rings

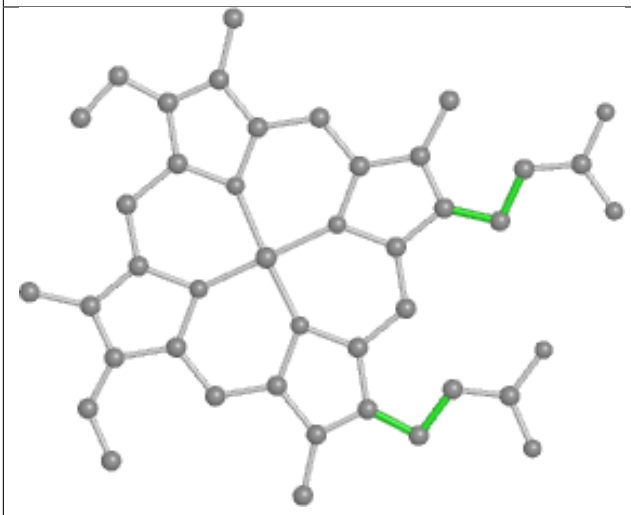
Ligand HEC C 805



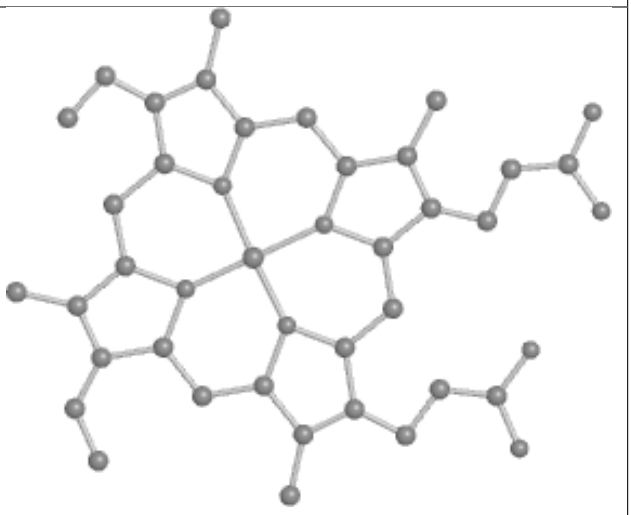
Bond lengths



Bond angles

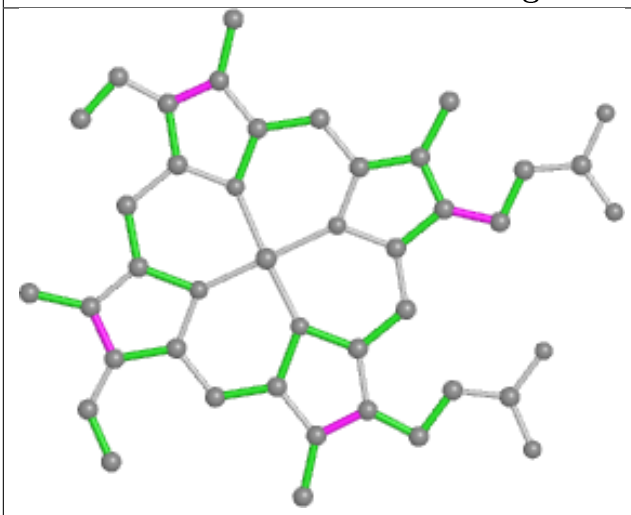


Torsions

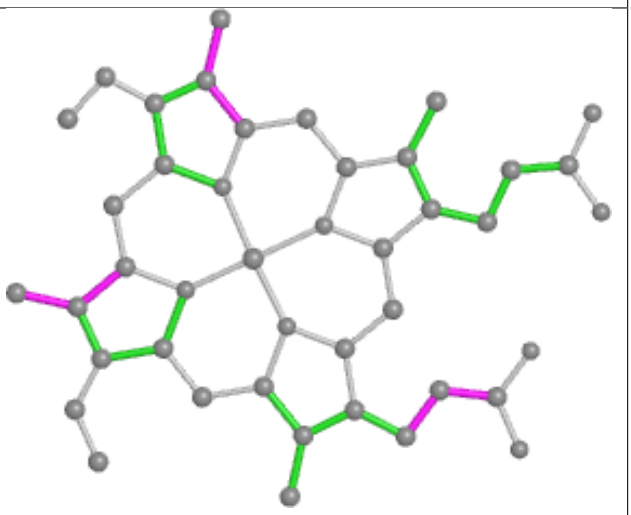


Rings

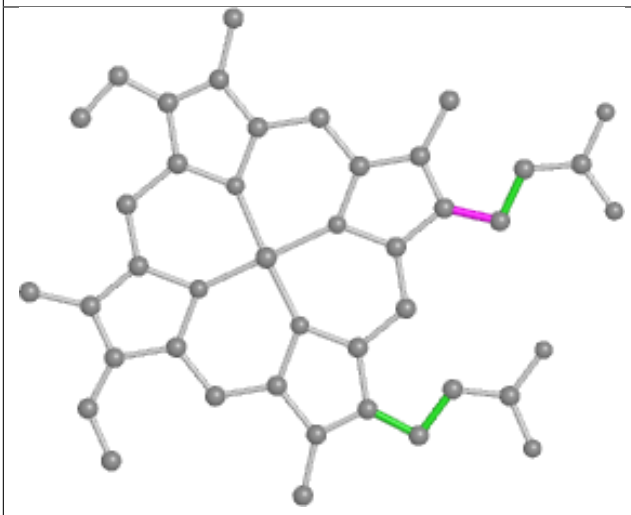
Ligand HEC A 905



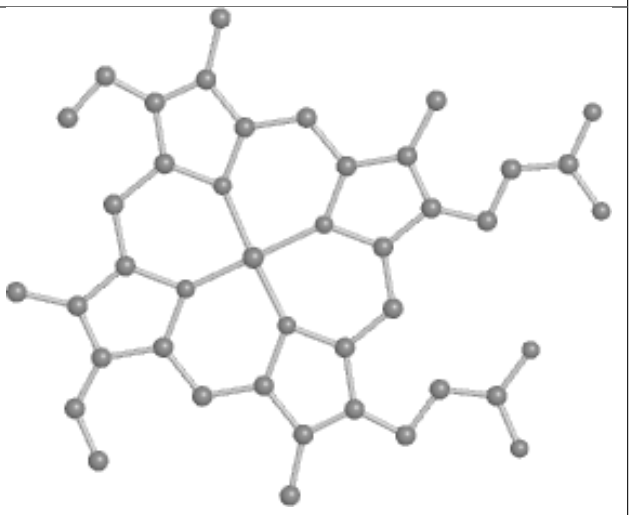
Bond lengths



Bond angles

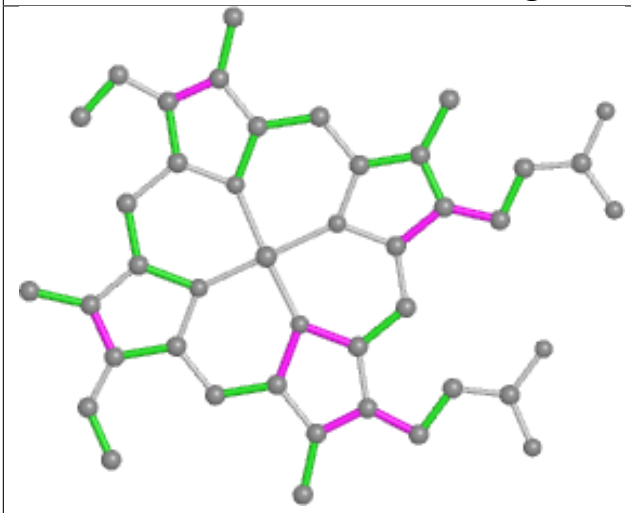


Torsions

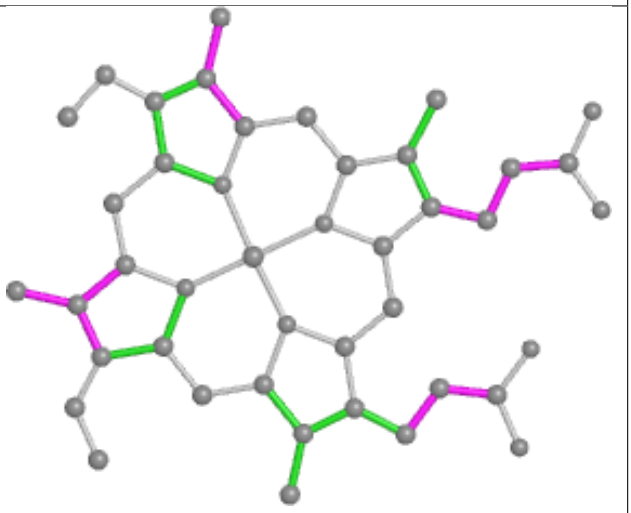


Rings

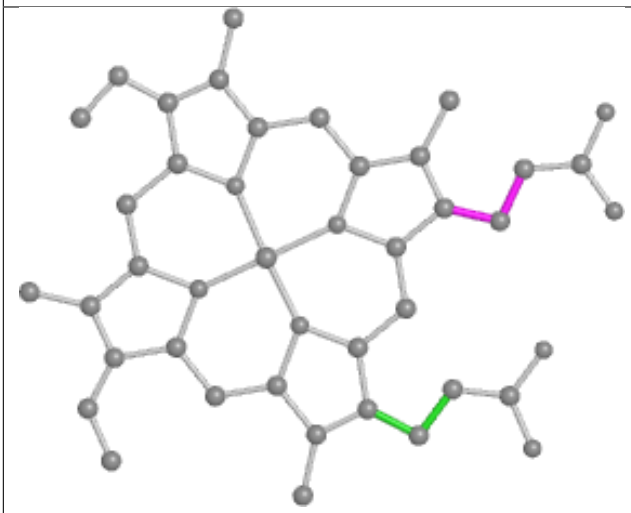
Ligand HEC C 809



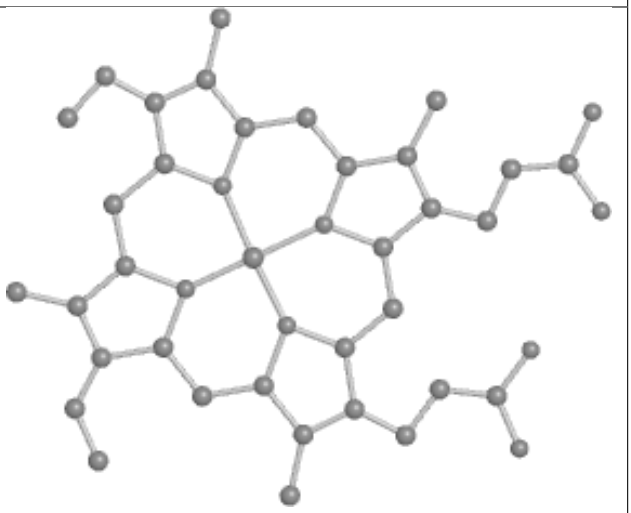
Bond lengths



Bond angles

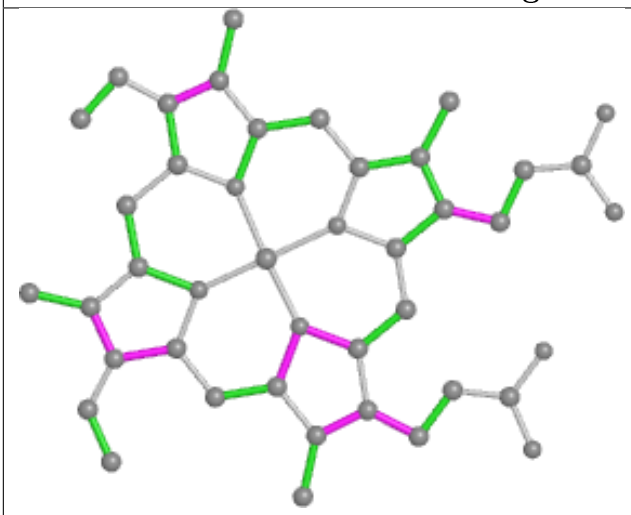


Torsions

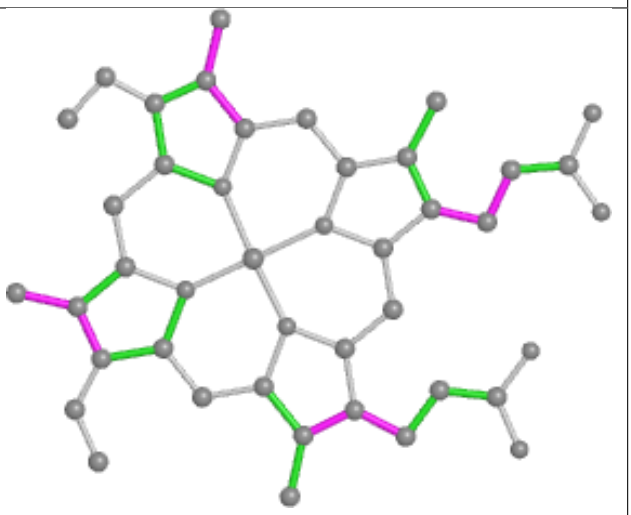


Rings

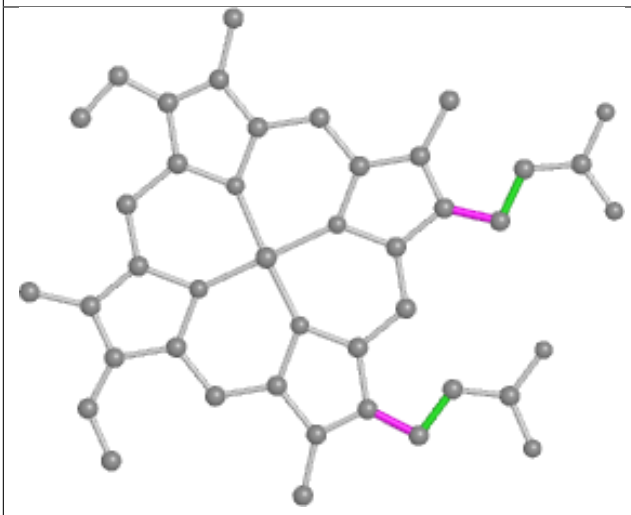
Ligand HEC A 902



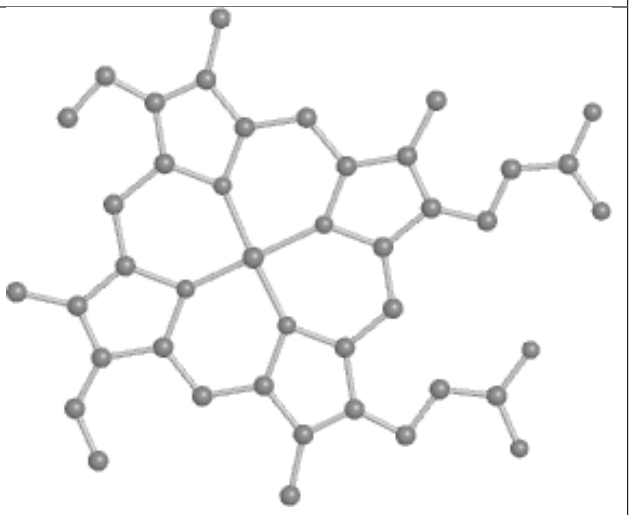
Bond lengths



Bond angles

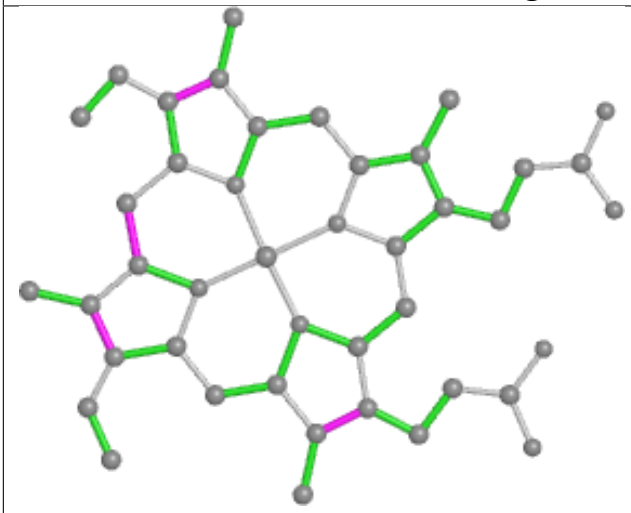


Torsions

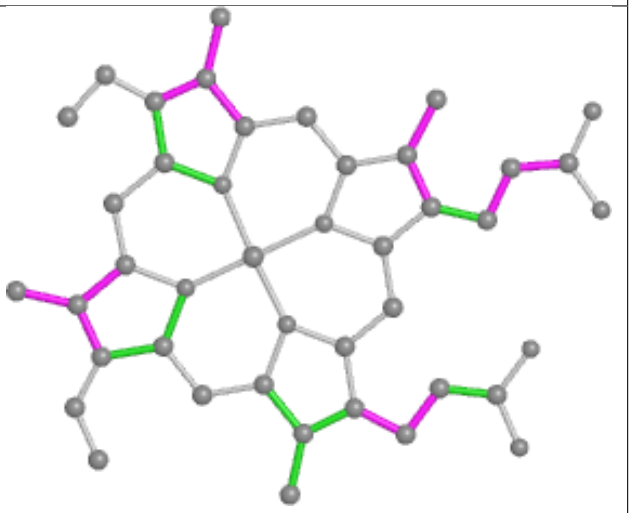


Rings

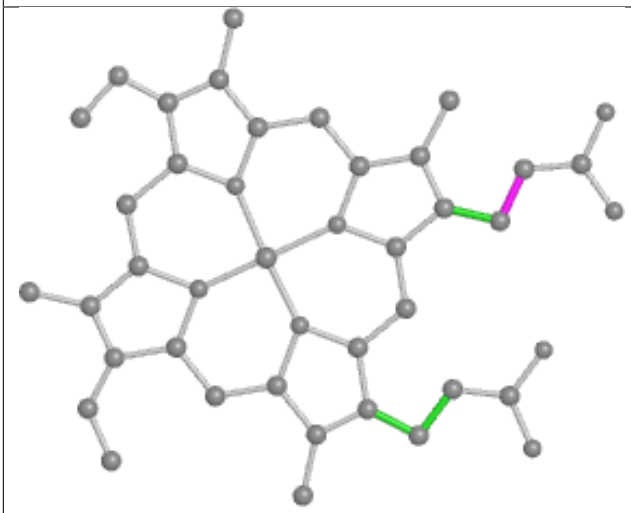
Ligand HEC C 804



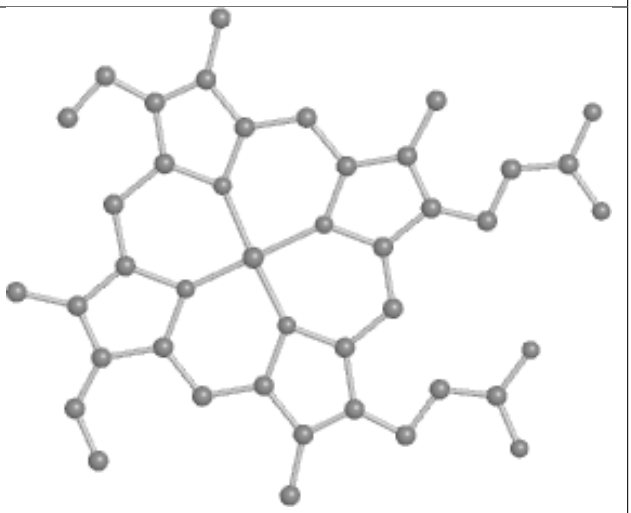
Bond lengths



Bond angles

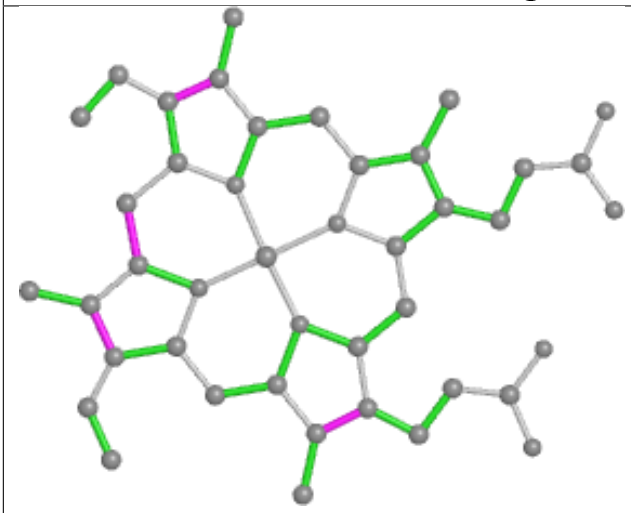


Torsions

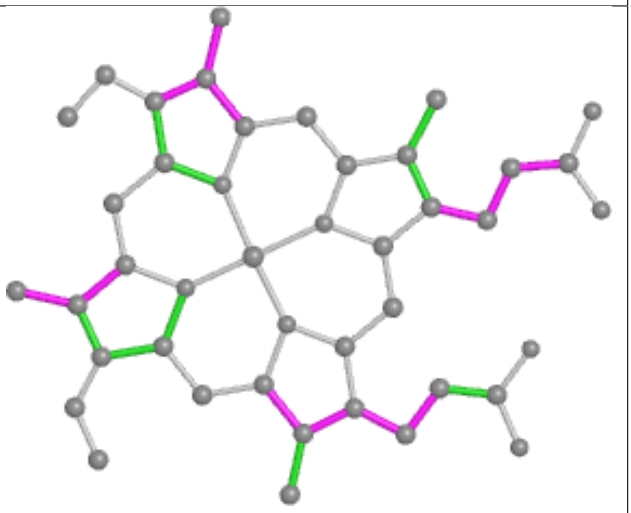


Rings

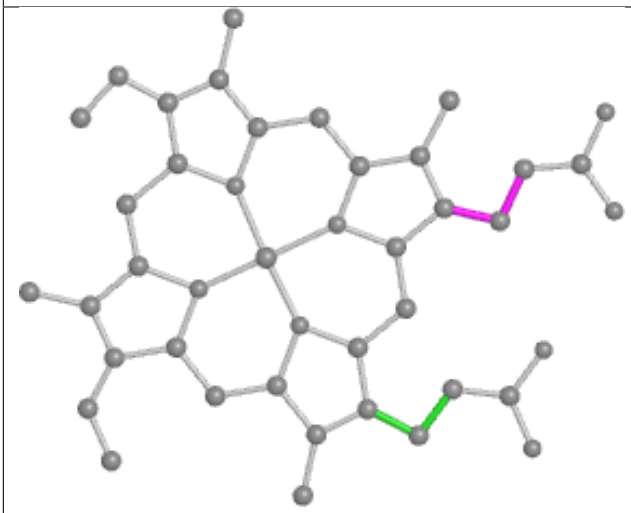
Ligand HEC A 906



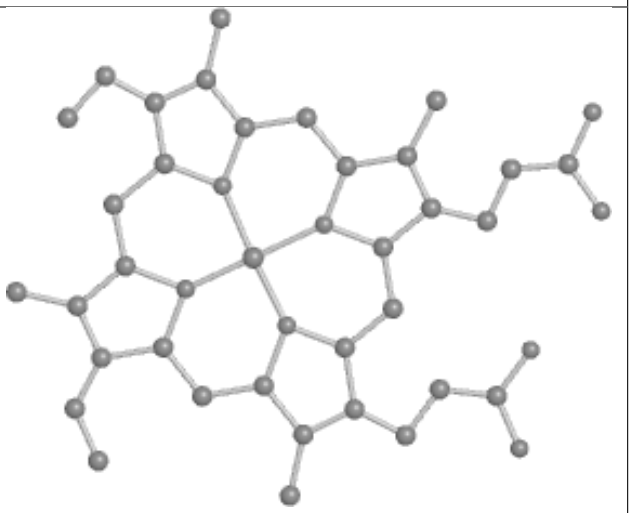
Bond lengths



Bond angles

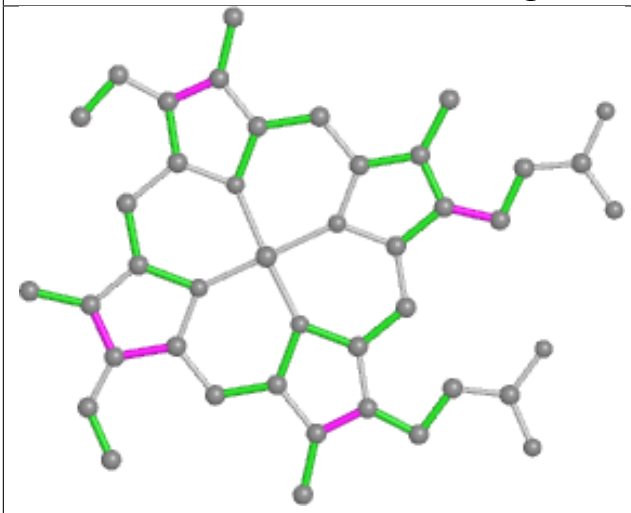


Torsions

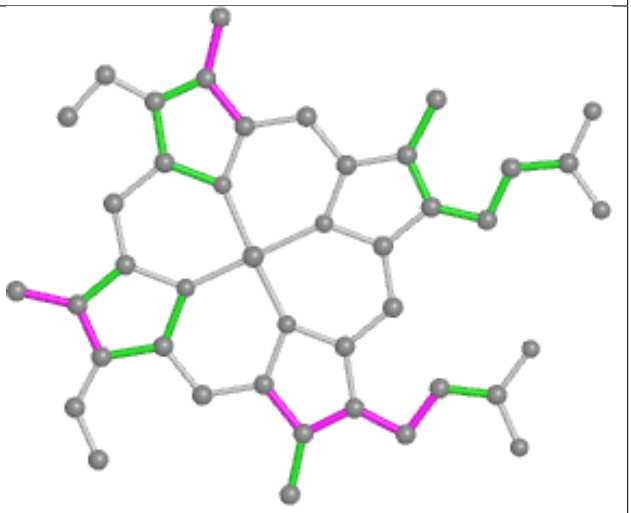


Rings

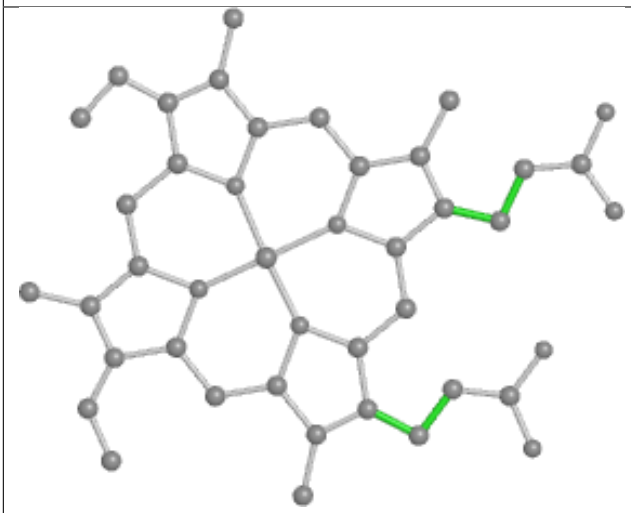
Ligand HEC A 909



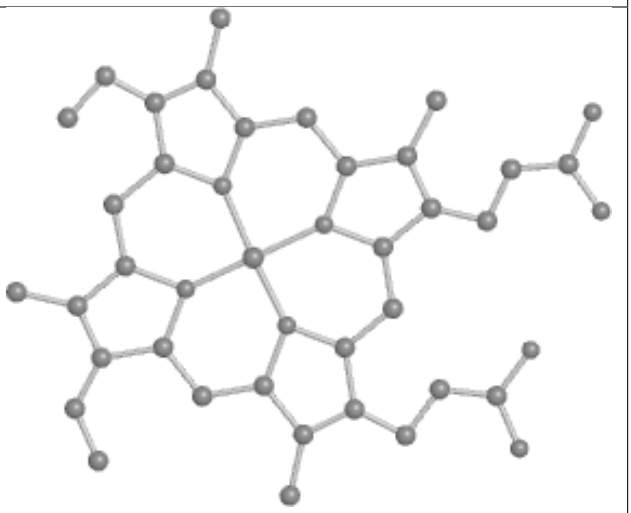
Bond lengths



Bond angles

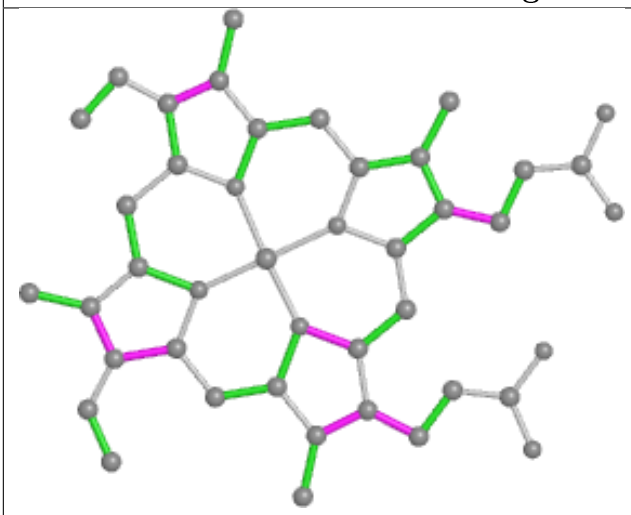


Torsions

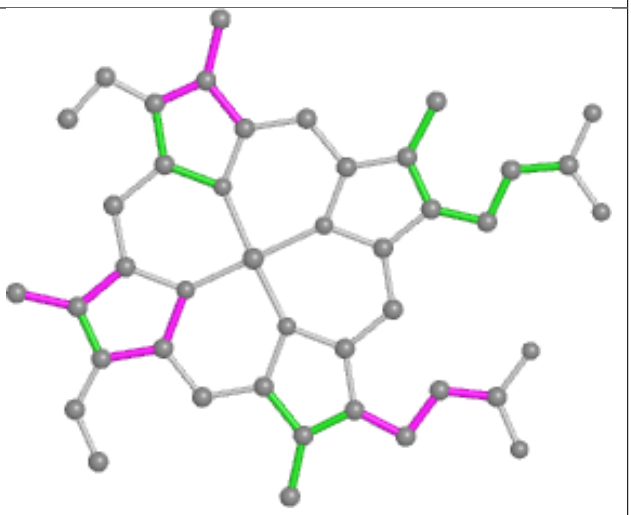


Rings

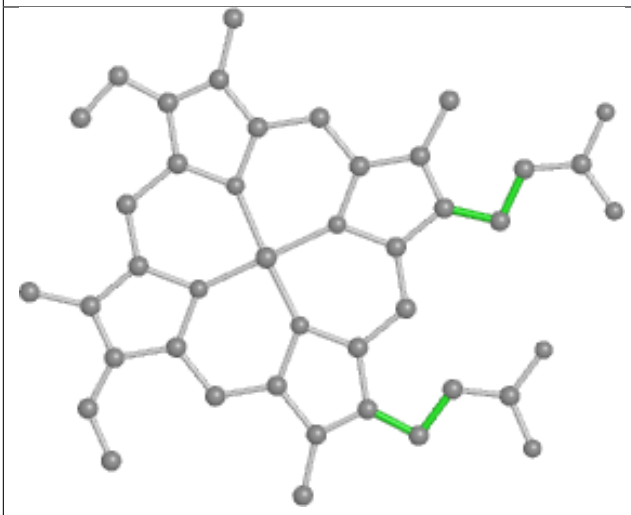
Ligand HEC A 903



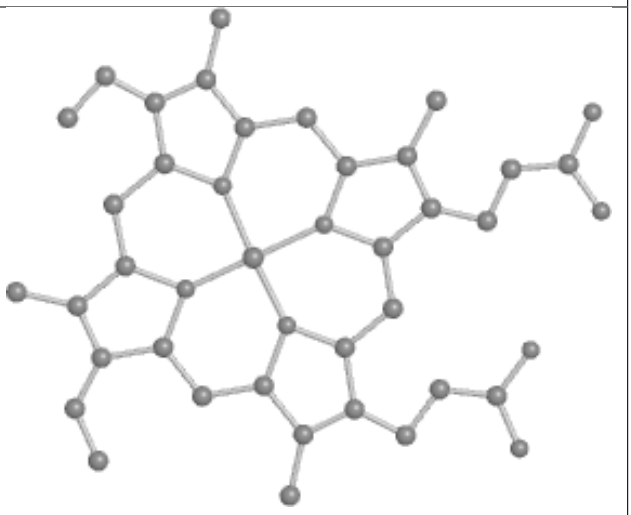
Bond lengths



Bond angles

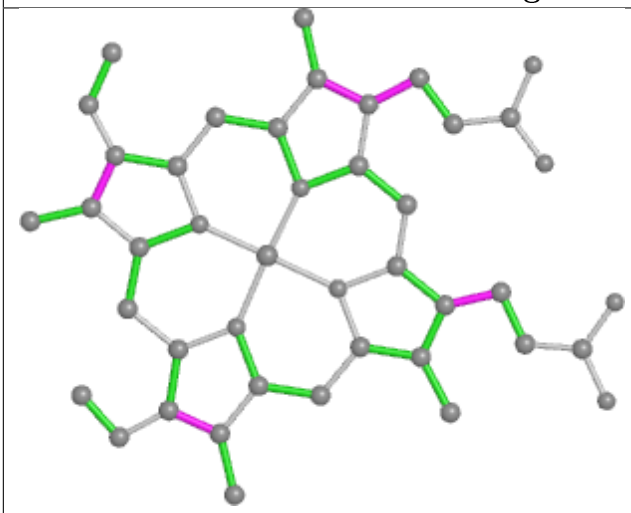


Torsions

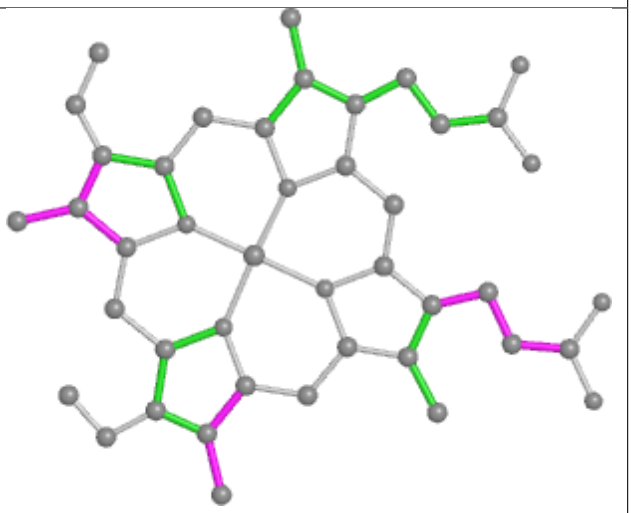


Rings

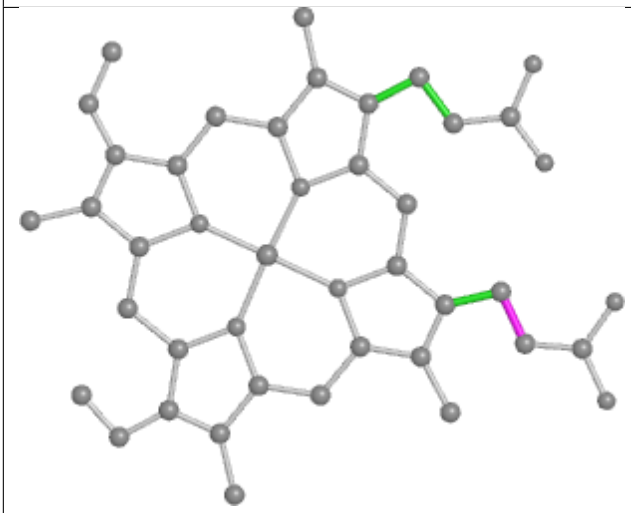
Ligand HEC C 810



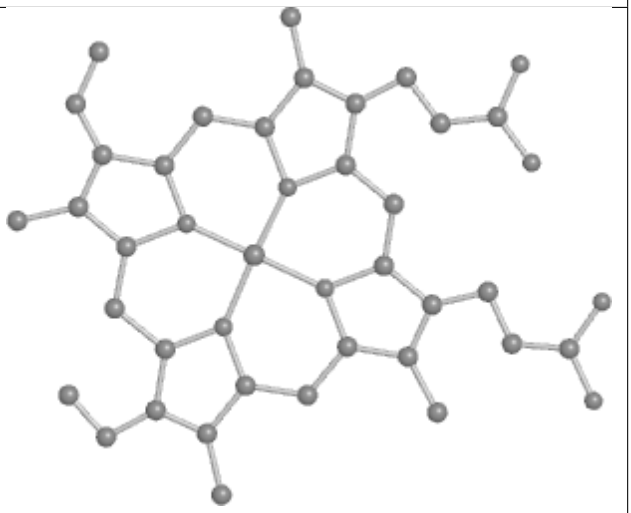
Bond lengths



Bond angles

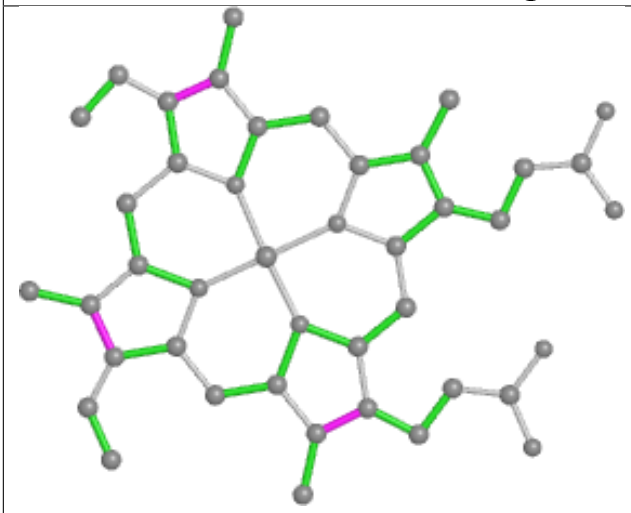


Torsions

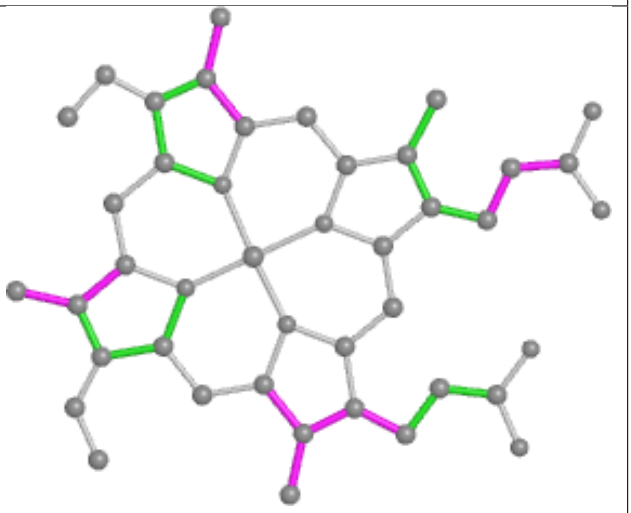


Rings

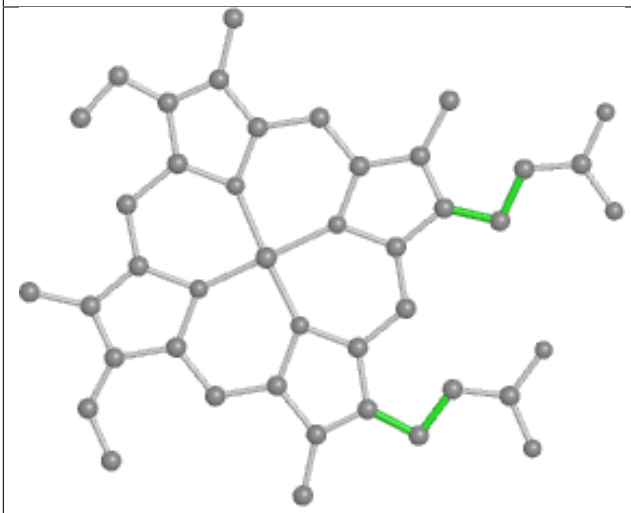
Ligand HEC A 907



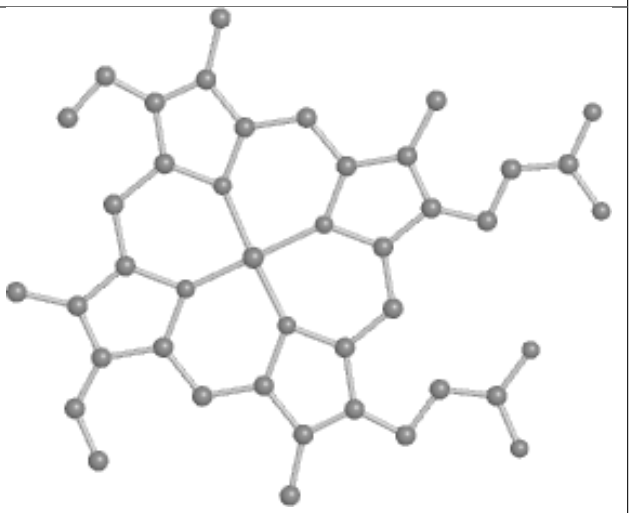
Bond lengths



Bond angles

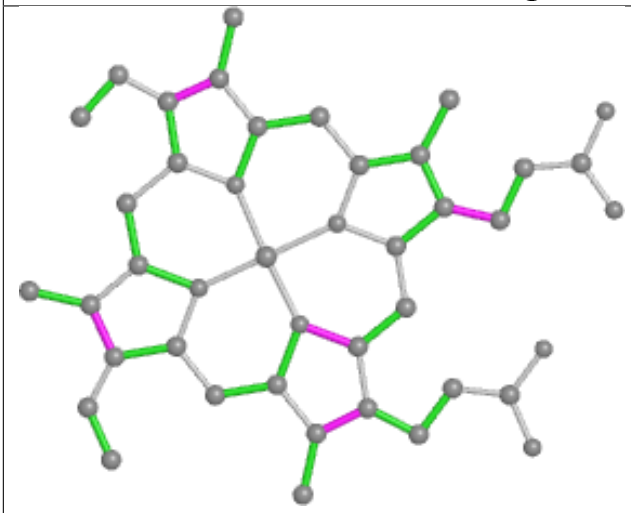


Torsions

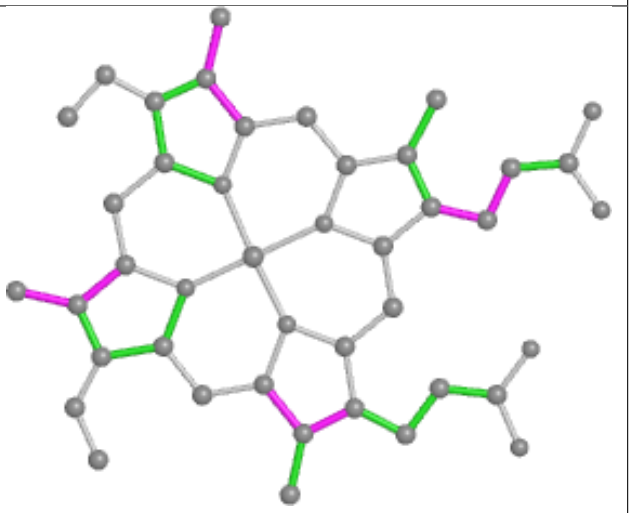


Rings

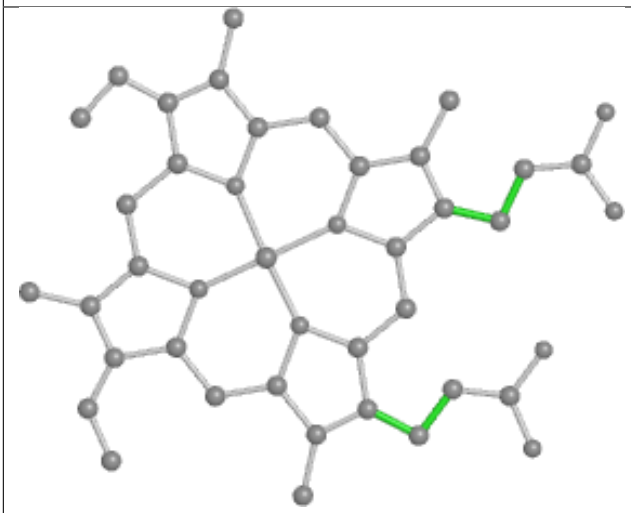
Ligand HEC C 807



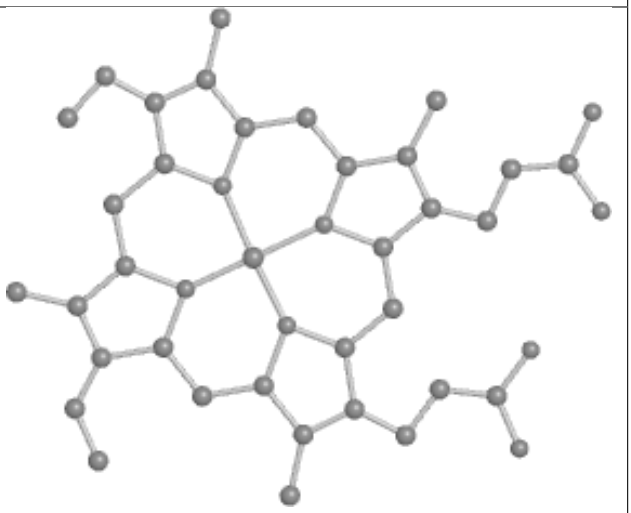
Bond lengths



Bond angles

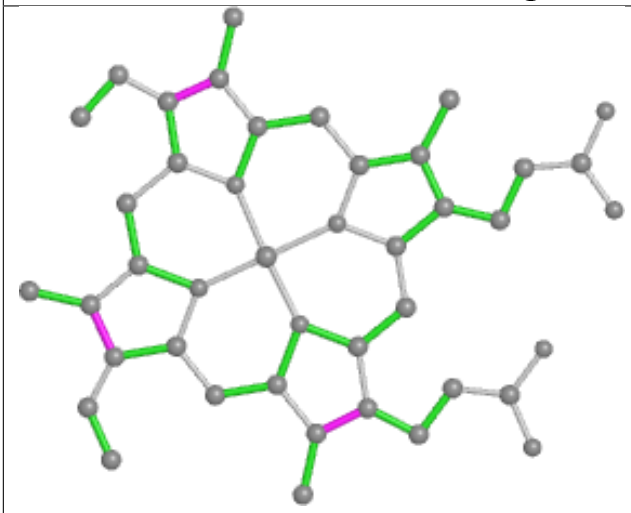


Torsions

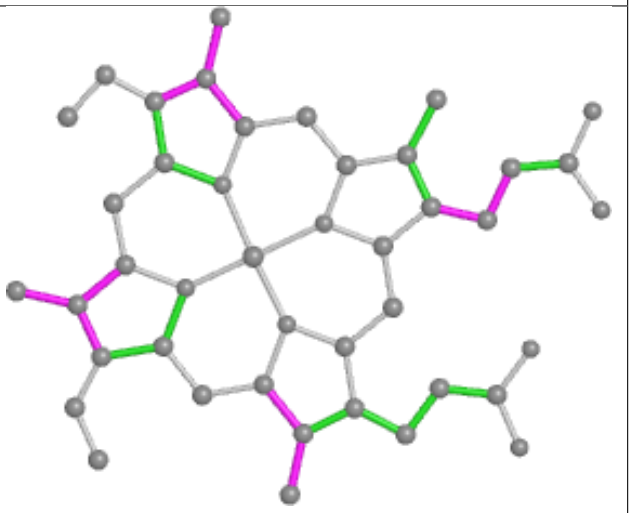


Rings

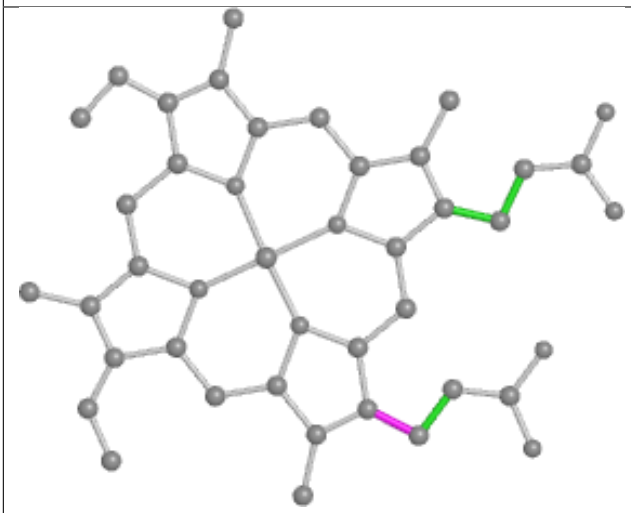
Ligand HEC A 908



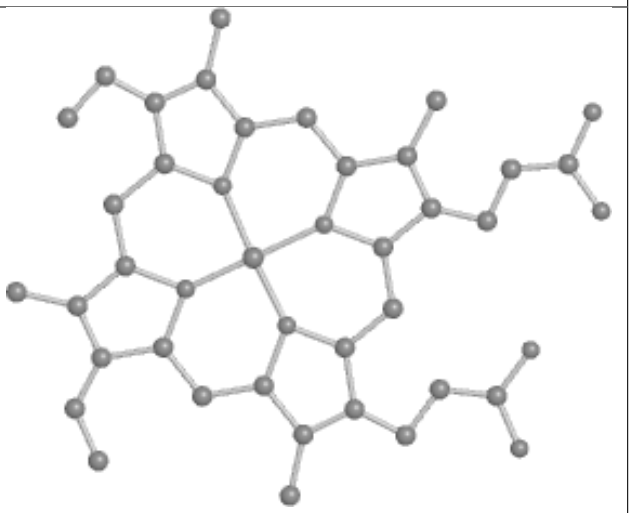
Bond lengths



Bond angles

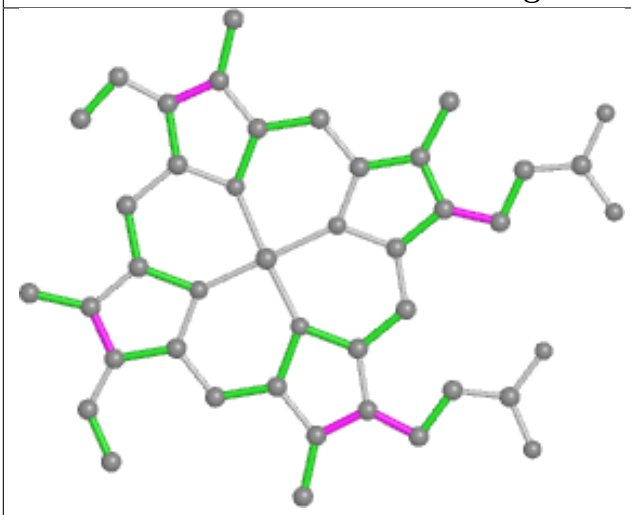


Torsions

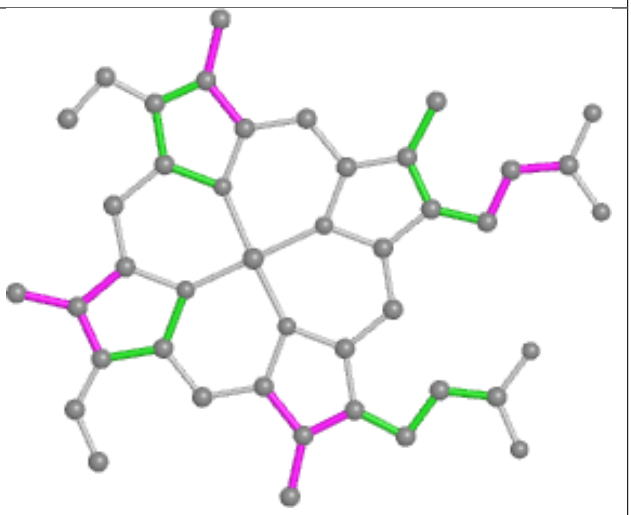


Rings

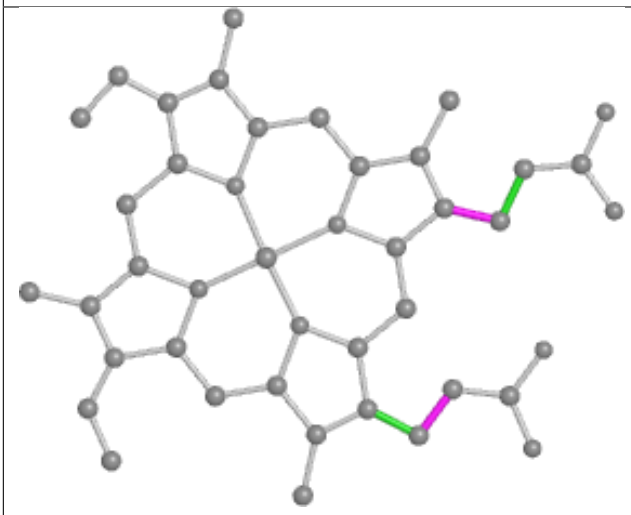
Ligand HEC C 802



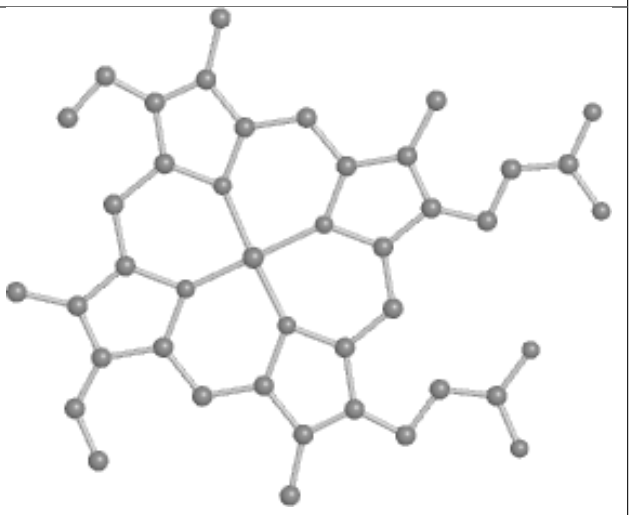
Bond lengths



Bond angles

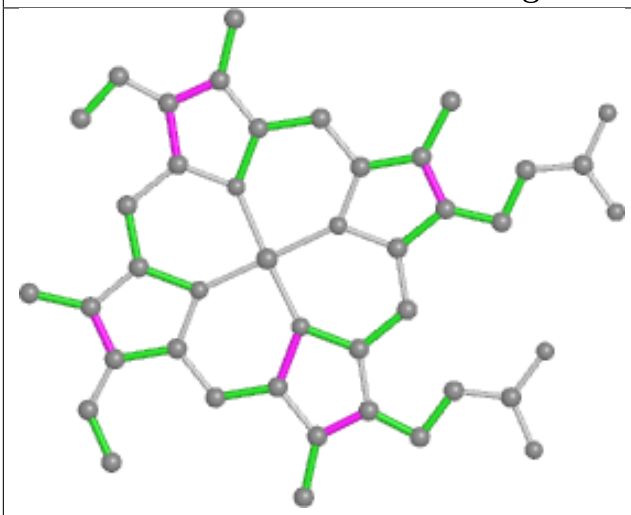


Torsions

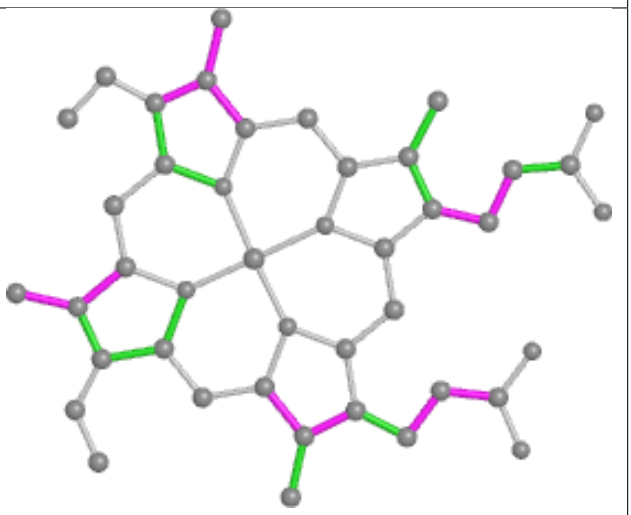


Rings

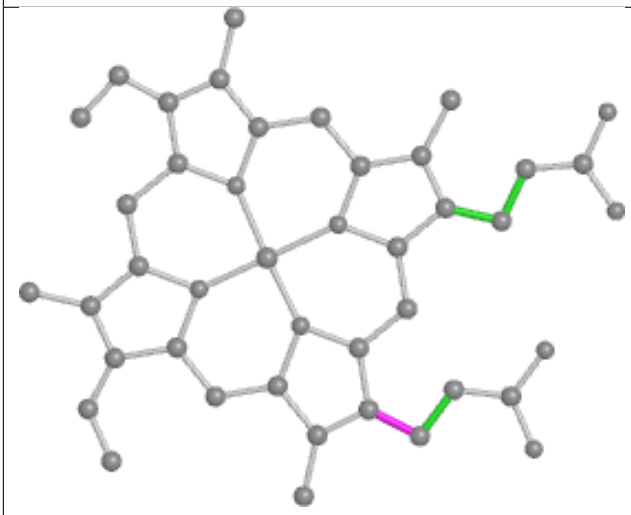
Ligand HEC A 910



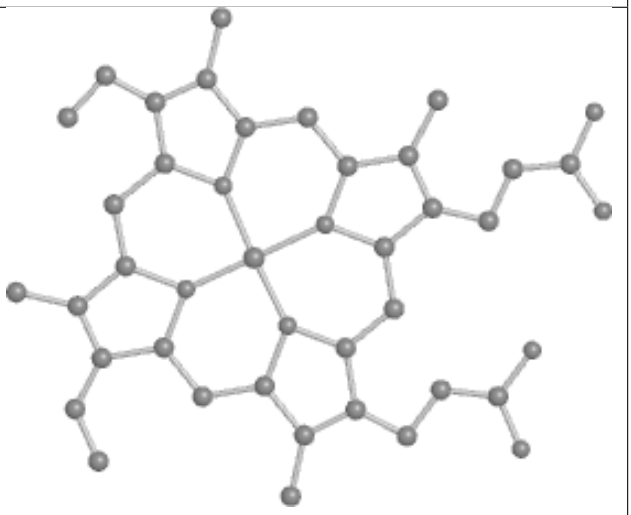
Bond lengths



Bond angles

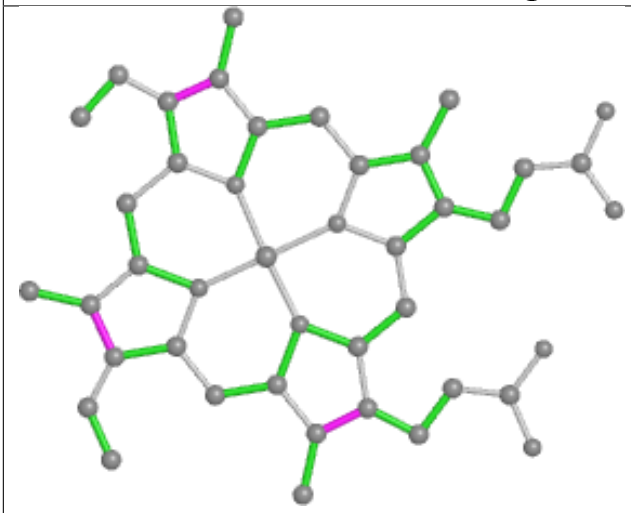


Torsions

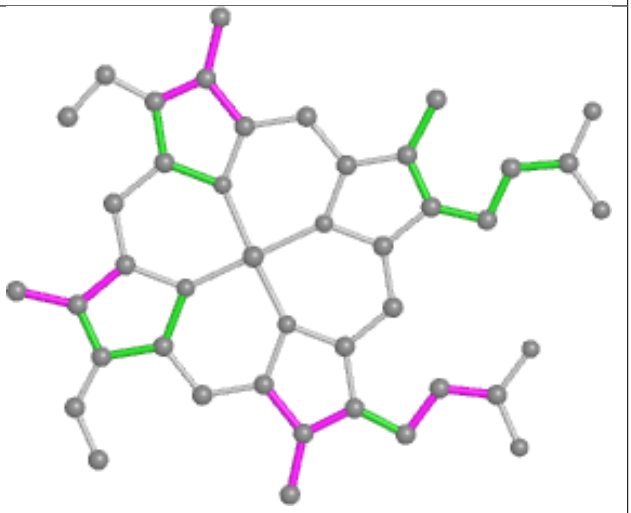


Rings

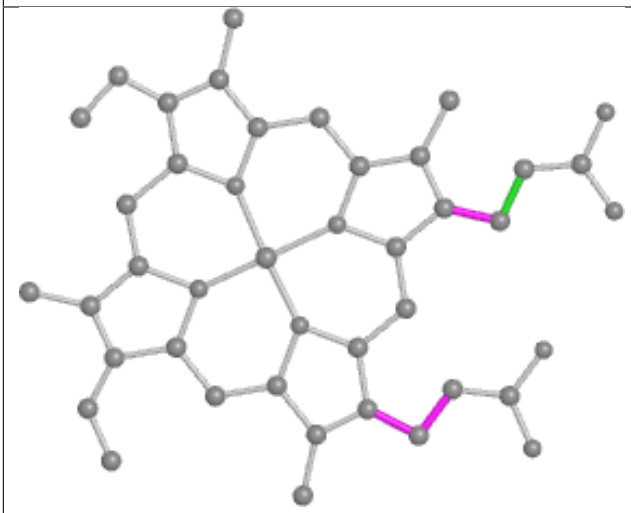
Ligand HEC C 806



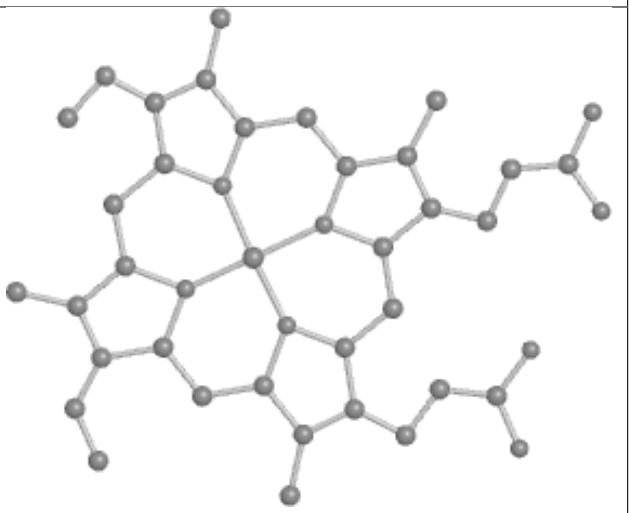
Bond lengths



Bond angles

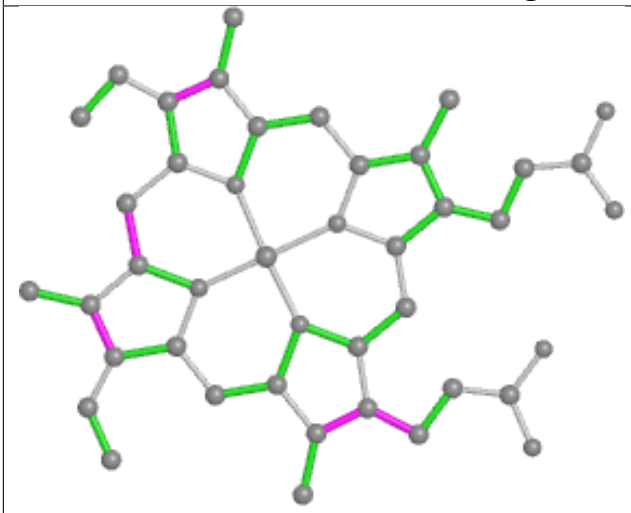


Torsions

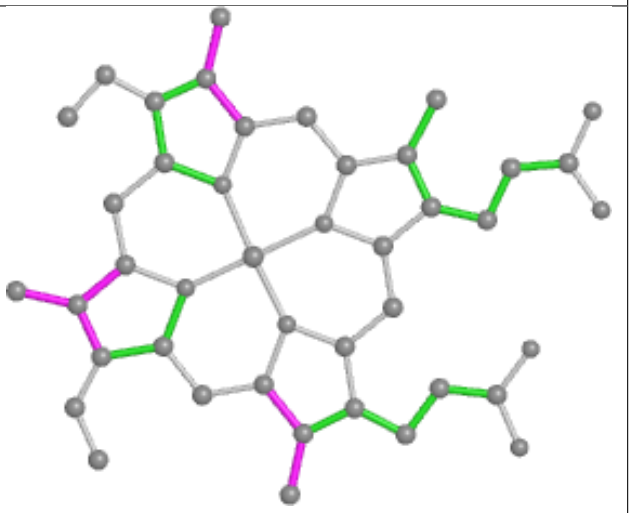


Rings

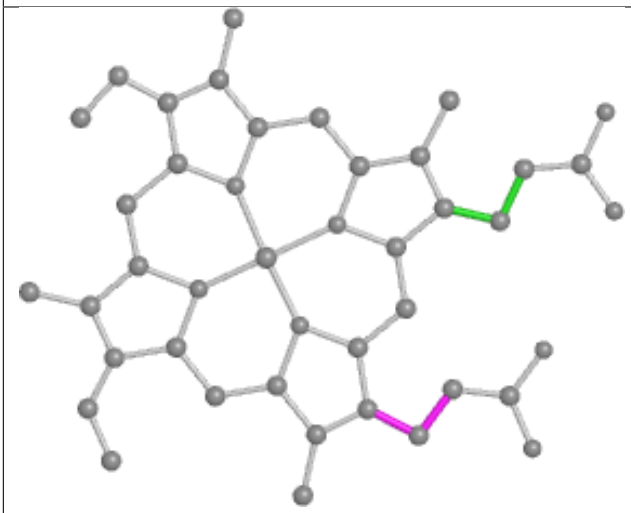
Ligand HEC A 904



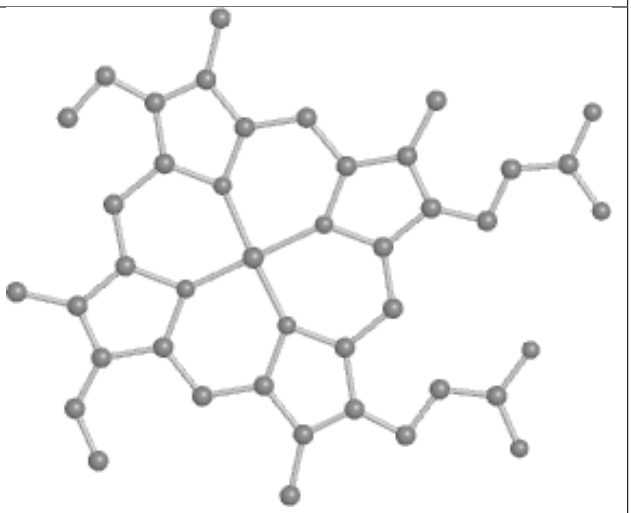
Bond lengths



Bond angles

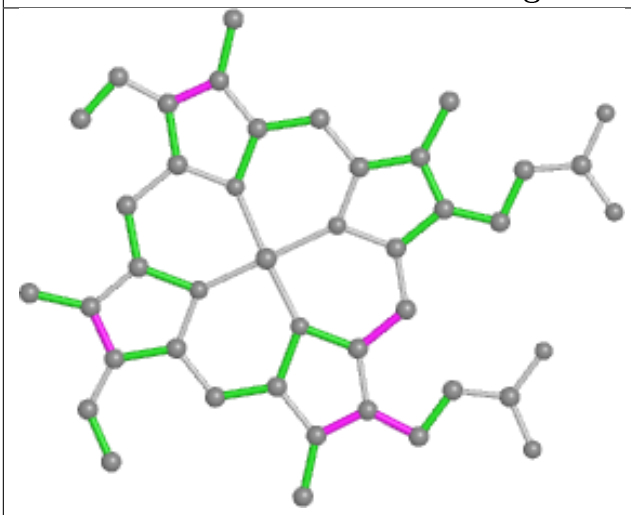


Torsions

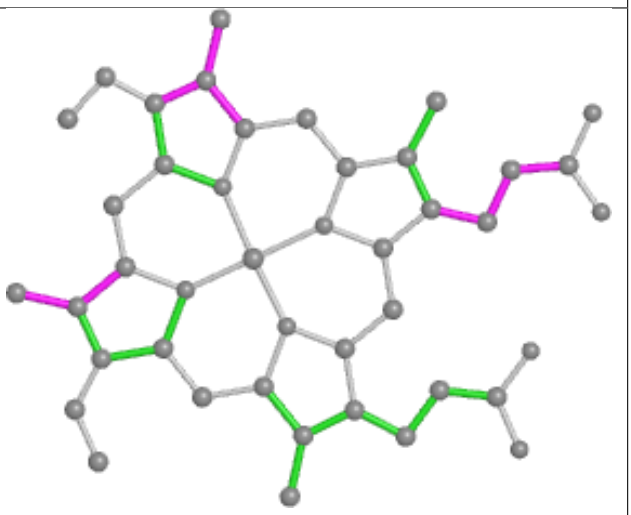


Rings

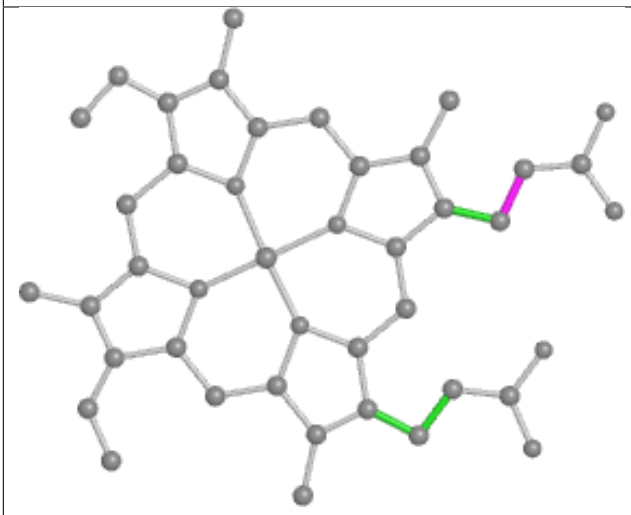
Ligand HEC C 808



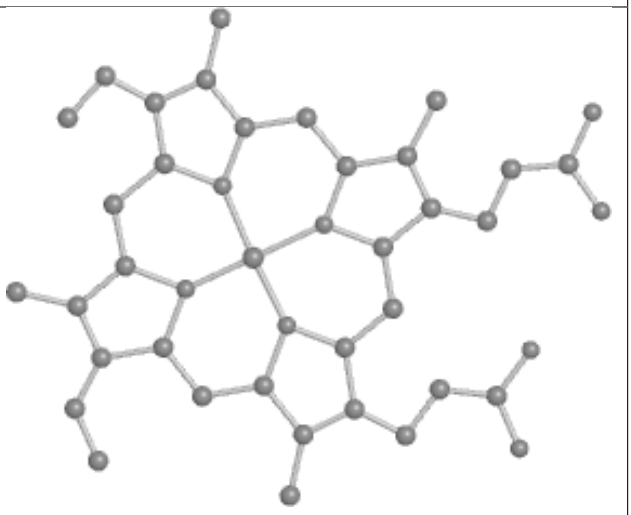
Bond lengths



Bond angles

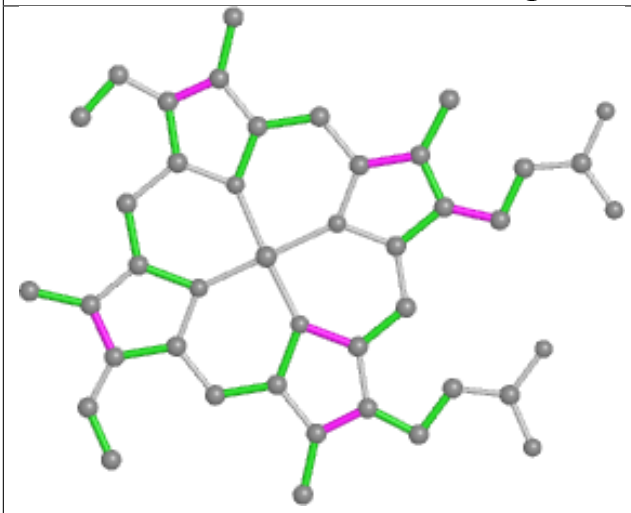


Torsions

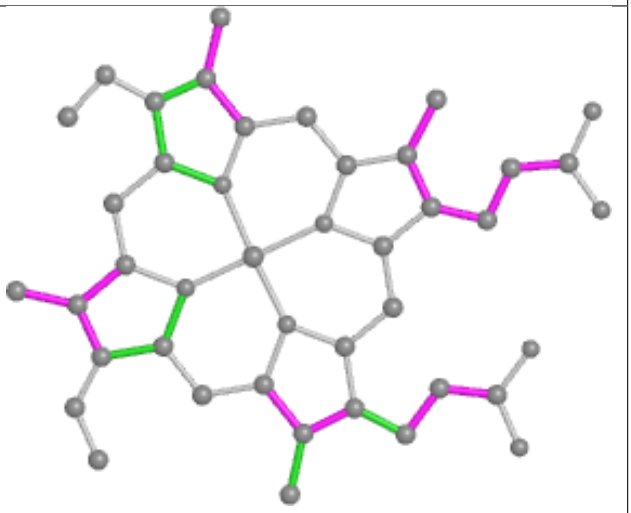


Rings

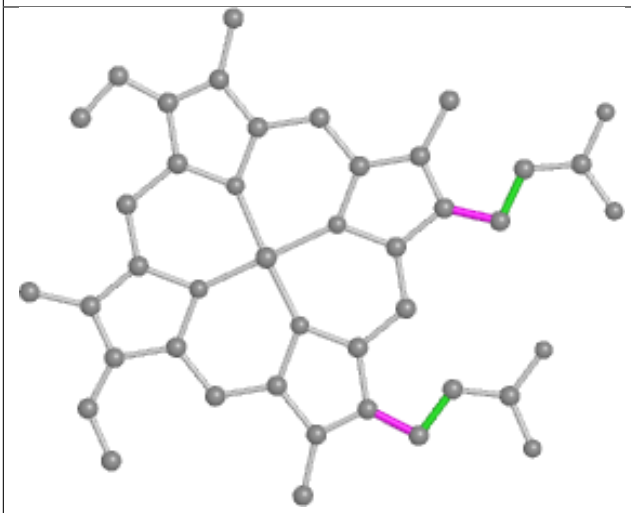
Ligand HEC C 801



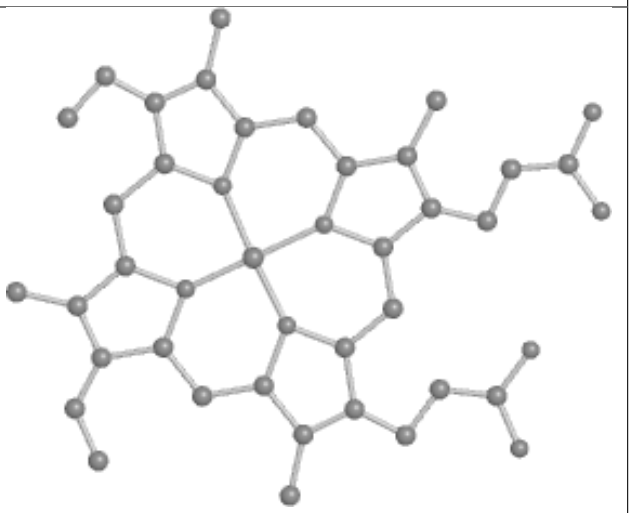
Bond lengths



Bond angles

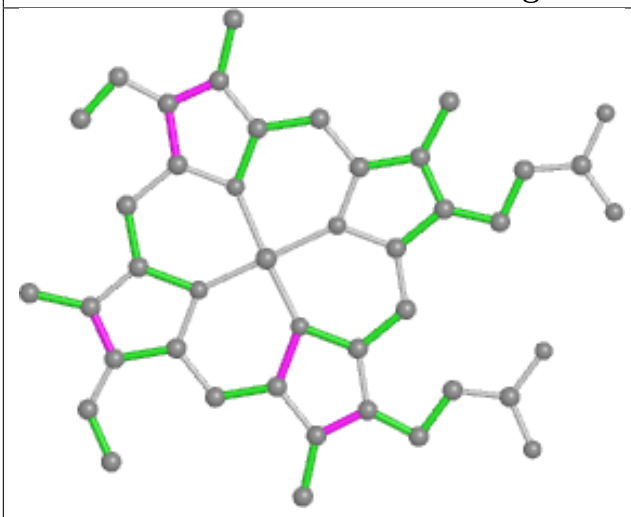


Torsions

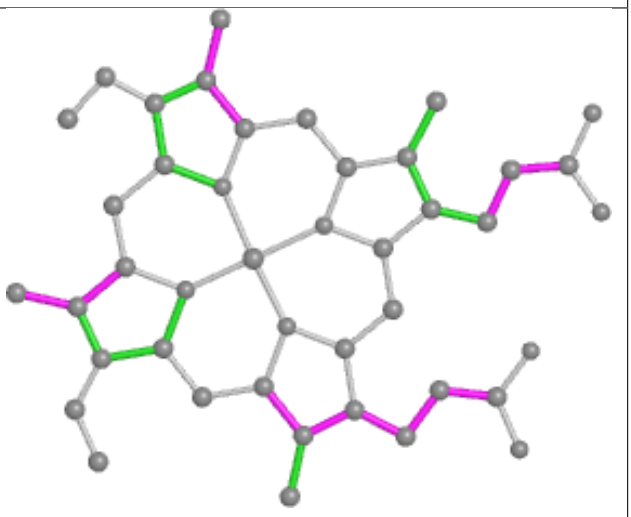


Rings

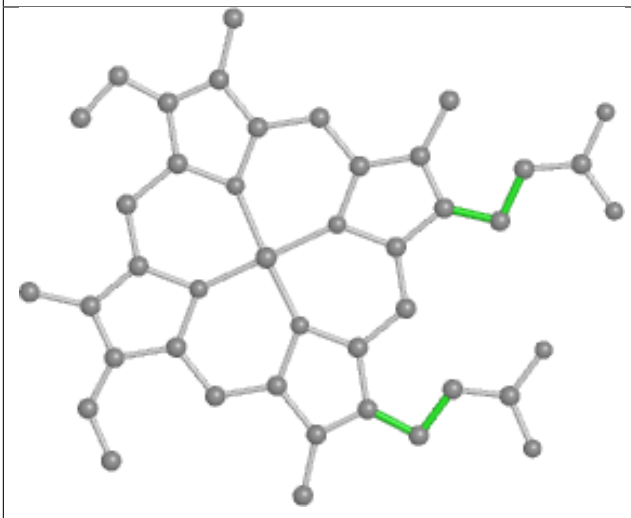
Ligand HEC A 901



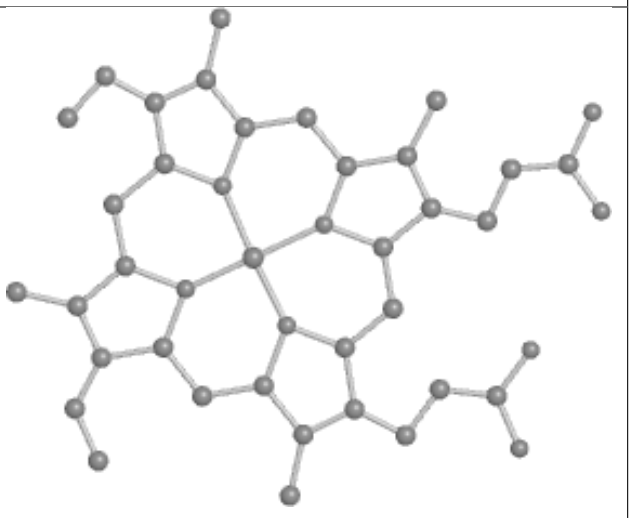
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	265/333 (79%)	1.34	52 (19%)	1	0	20, 55, 137, 169	0
2	B	649/695 (93%)	0.67	53 (8%)	11	9	22, 54, 96, 158	0
3	C	608/650 (93%)	0.52	14 (2%)	60	62	20, 48, 93, 129	0
All	All	1522/1678 (90%)	0.73	119 (7%)	13	11	20, 51, 107, 169	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	ALA	13.4
1	A	89	ASP	11.8
1	A	95	MET	11.0
3	C	43	ALA	9.8
2	B	593	LEU	8.5
1	A	101	GLU	8.2
1	A	165	GLN	7.6
2	B	543	THR	7.0
1	A	194	MET	6.9
1	A	102	ALA	6.8
3	C	163	LEU	6.7
2	B	594	GLU	6.1
2	B	540	TYR	5.9
1	A	105	GLY	5.8
2	B	592	LEU	5.7
1	A	106	PRO	5.6
1	A	123	LYS	5.5
1	A	83	GLY	5.2
2	B	112	GLU	5.2
1	A	81	PHE	5.1
2	B	535	ASP	5.1
1	A	166	VAL	5.1
1	A	94	PRO	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	161	ALA	5.0
1	A	70	CYS	4.8
1	A	84	VAL	4.7
3	C	44	PRO	4.6
2	B	546	LEU	4.3
3	C	143	LYS	4.2
1	A	126	THR	4.2
1	A	99	GLN	4.1
2	B	504	GLU	4.0
2	B	598	ARG	4.0
1	A	137	MET	4.0
1	A	120	THR	3.9
2	B	507	THR	3.8
1	A	103	CYS	3.8
1	A	144	LYS	3.7
2	B	510	PHE	3.7
1	A	141	GLN	3.6
1	A	93	SER	3.5
1	A	72	LYS	3.5
2	B	637	GLN	3.5
1	A	109	GLN	3.4
2	B	547	LEU	3.4
1	A	78	MET	3.4
1	A	170	LYS	3.4
1	A	86	GLY	3.4
2	B	589	TYR	3.3
2	B	343	GLY	3.3
1	A	92	LYS	3.3
2	B	456	LYS	3.2
2	B	664	ILE	3.2
2	B	595	ASN	3.2
3	C	164	PRO	3.2
1	A	138	SER	3.2
2	B	101	ALA	3.1
2	B	513	ARG	3.1
2	B	512	ALA	3.1
1	A	256	VAL	3.1
1	A	142	ASP	3.1
1	A	193	ASP	3.1
2	B	299	TYR	3.0
1	A	171	ASP	3.0
2	B	111	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	695	ILE	2.9
2	B	244	ASP	2.9
3	C	607	ILE	2.9
3	C	650	MET	2.9
2	B	691	MET	2.9
1	A	73	LYS	2.9
3	C	75	LEU	2.8
2	B	548	ALA	2.8
2	B	96	ARG	2.8
2	B	84	ASP	2.8
1	A	134	SER	2.8
2	B	506	LEU	2.8
1	A	125	SER	2.7
3	C	605	GLU	2.7
1	A	90	SER	2.7
3	C	603	ALA	2.7
1	A	124	GLN	2.7
1	A	110	HIS	2.7
1	A	182	VAL	2.6
2	B	248	THR	2.6
1	A	111	ASN	2.6
2	B	539	SER	2.6
3	C	576	ALA	2.6
2	B	138	ALA	2.5
1	A	127	LEU	2.5
1	A	97	GLY	2.5
2	B	251	ASN	2.5
2	B	249	ALA	2.5
2	B	417	GLY	2.5
2	B	545	ASP	2.4
2	B	91	GLY	2.4
2	B	599	MET	2.4
2	B	508	ILE	2.4
3	C	466	ALA	2.4
1	A	80	LEU	2.3
2	B	98	SER	2.3
3	C	597	THR	2.3
1	A	188	THR	2.3
2	B	117	LYS	2.3
2	B	118	GLN	2.3
1	A	88	ILE	2.2
2	B	457	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	311	LEU	2.2
2	B	188	PHE	2.2
1	A	121	PHE	2.2
2	B	439	VAL	2.2
1	A	112	LYS	2.2
3	C	561	VAL	2.2
2	B	94	GLY	2.1
2	B	297	GLY	2.1
2	B	596	LYS	2.1
1	A	135	VAL	2.1
2	B	511	GLY	2.0
2	B	604	THR	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	HEC	A	901	43/43	0.70	0.47	107,155,190,192	0
4	HEC	A	902	43/43	0.88	0.42	73,116,143,154	0
4	HEC	A	903	43/43	0.89	0.32	58,100,125,126	0
5	CA	C	812	1/1	0.92	0.18	52,52,52,52	0
4	HEC	A	904	43/43	0.94	0.30	50,77,110,115	0
4	HEC	C	809	43/43	0.95	0.25	29,53,104,130	0
4	HEC	C	810	43/43	0.95	0.25	46,67,101,116	0
4	HEC	A	905	43/43	0.96	0.25	39,56,72,90	0
4	HEC	A	906	43/43	0.96	0.29	29,43,73,87	0
4	HEC	A	907	43/43	0.96	0.24	20,35,59,71	0
5	CA	B	701	1/1	0.96	0.24	47,47,47,47	0

Continued on next page...

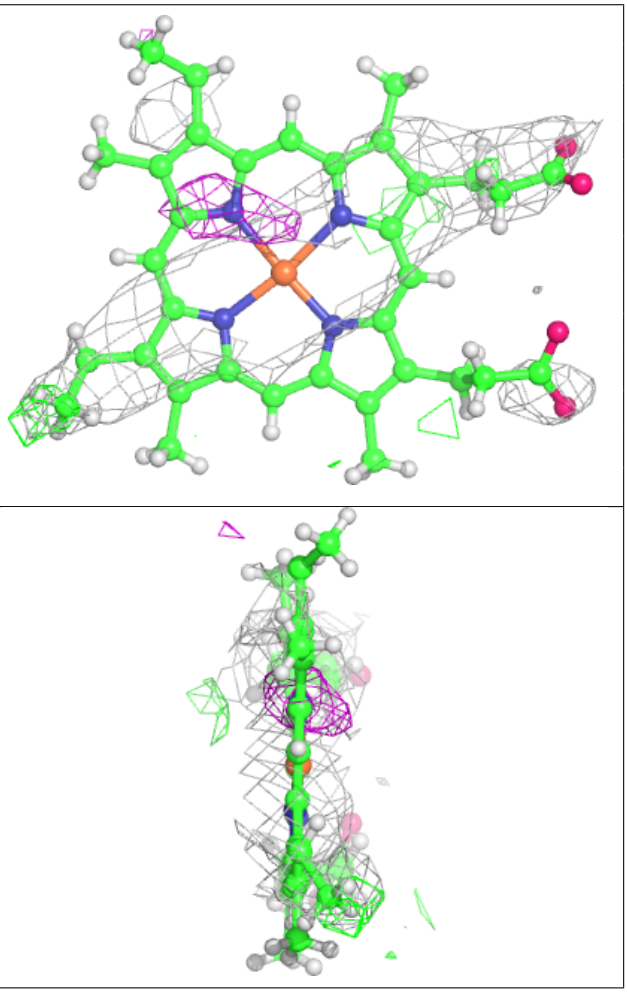
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HEC	C	805	43/43	0.96	0.23	10,23,43,59	0
4	HEC	C	804	43/43	0.96	0.23	10,26,49,71	0
4	HEC	C	801	43/43	0.96	0.24	12,31,51,94	0
4	HEC	C	806	43/43	0.97	0.25	18,33,56,97	0
4	HEC	C	803	43/43	0.97	0.20	12,27,37,44	0
4	HEC	C	808	43/43	0.97	0.22	16,35,55,56	0
4	HEC	C	807	43/43	0.97	0.24	16,30,57,100	0
4	HEC	A	908	43/43	0.97	0.23	13,31,57,64	0
4	HEC	A	910	43/43	0.97	0.21	11,29,45,48	0
4	HEC	A	909	43/43	0.97	0.22	16,30,45,50	0
5	CA	C	811	1/1	0.98	0.22	52,52,52,52	0
4	HEC	C	802	43/43	0.98	0.21	22,39,52,72	0
5	CA	B	702	1/1	0.99	0.17	28,28,28,28	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.

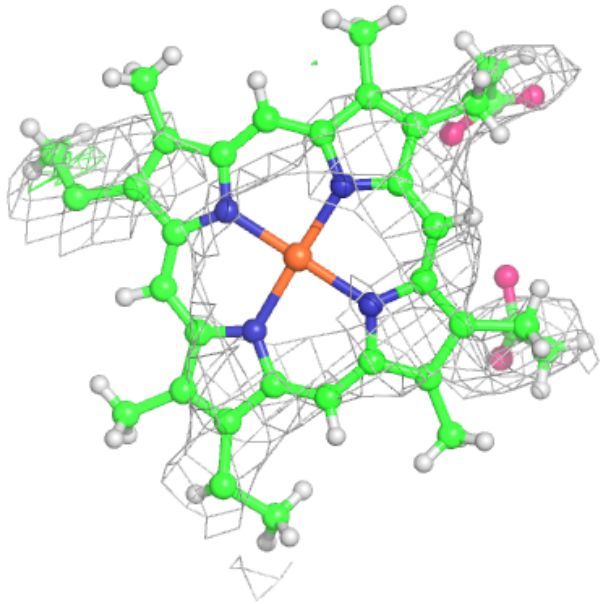
Electron density around HEC A 901:

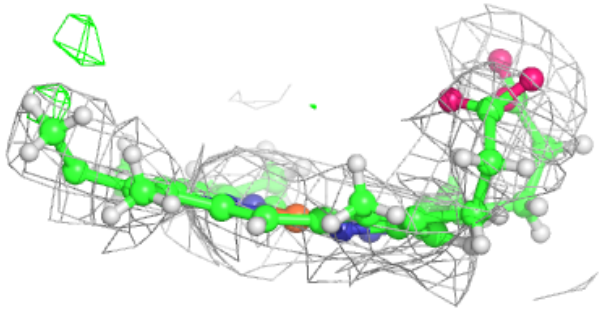
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

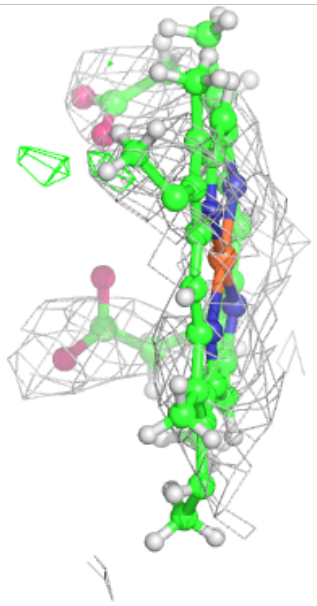


Electron density around HEC A 902:

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

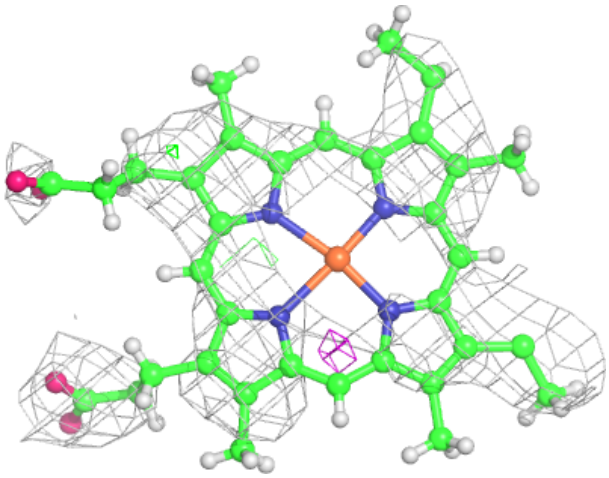


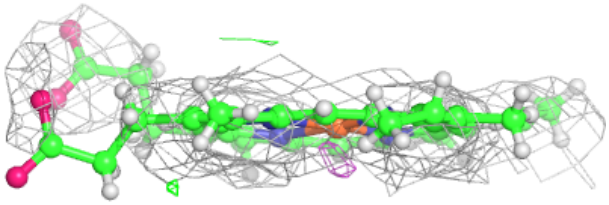


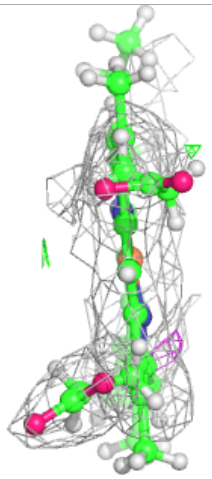


Electron density around HEC A 903:

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

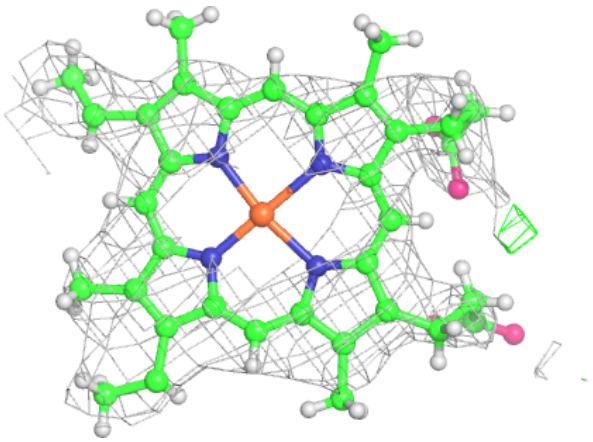


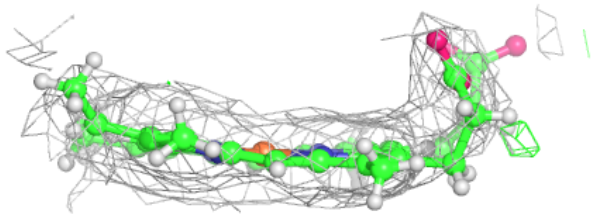


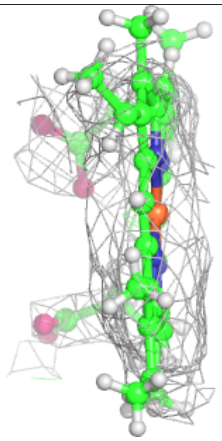


Electron density around HEC A 904:

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

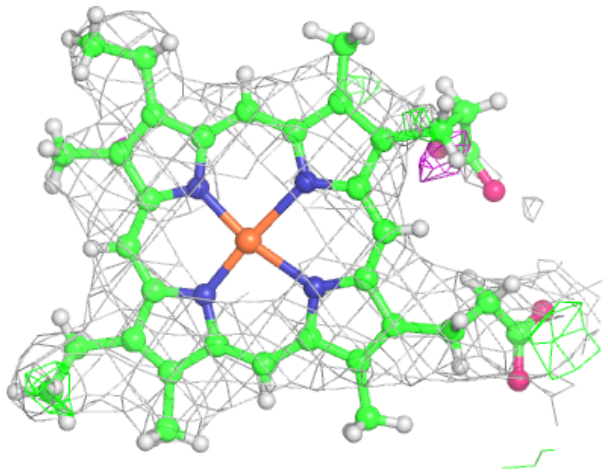


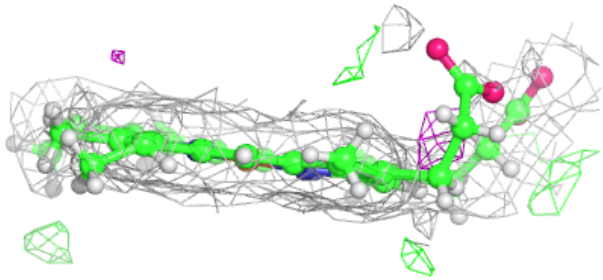


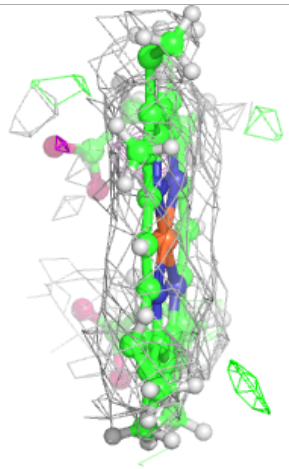


Electron density around HEC C 809:

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

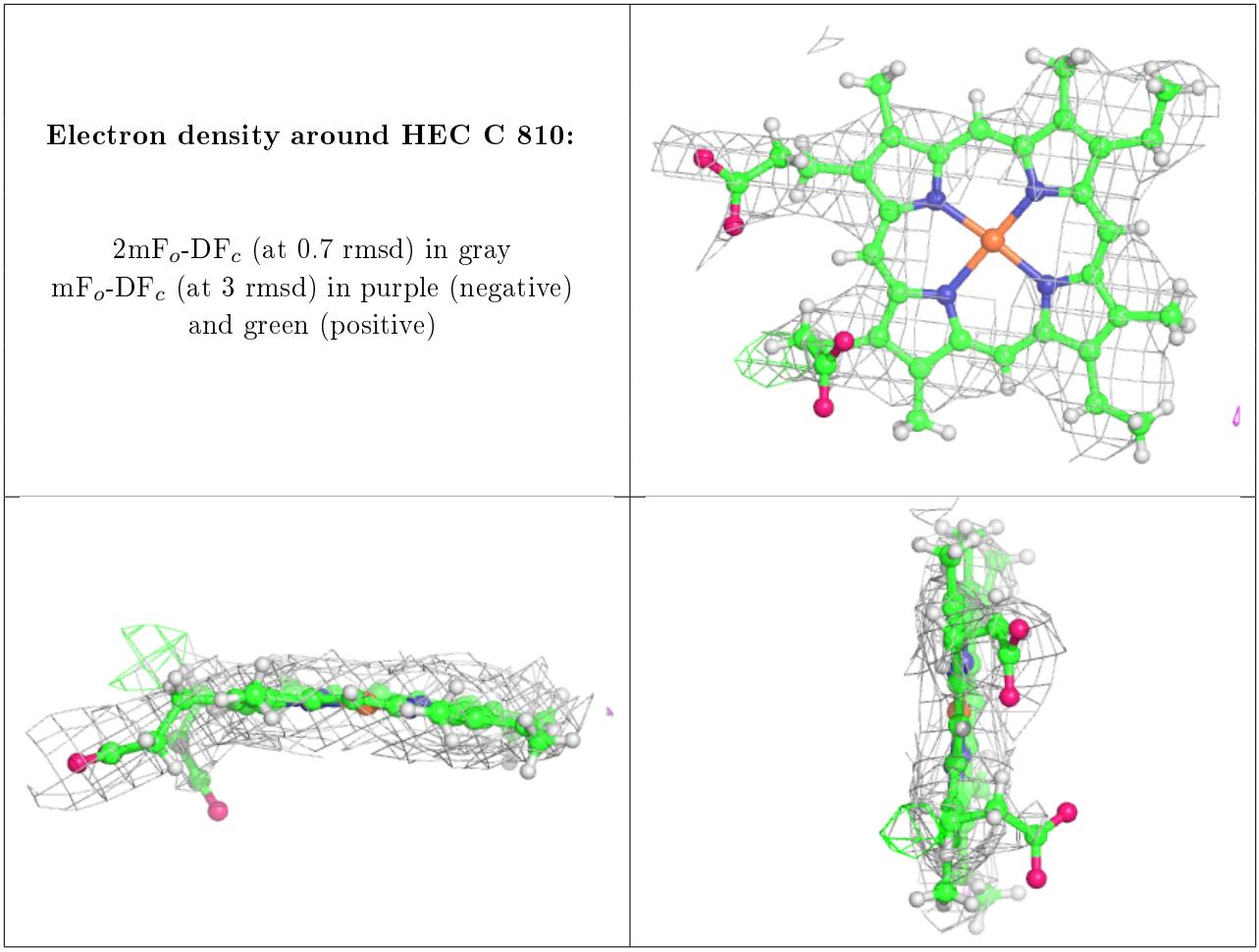






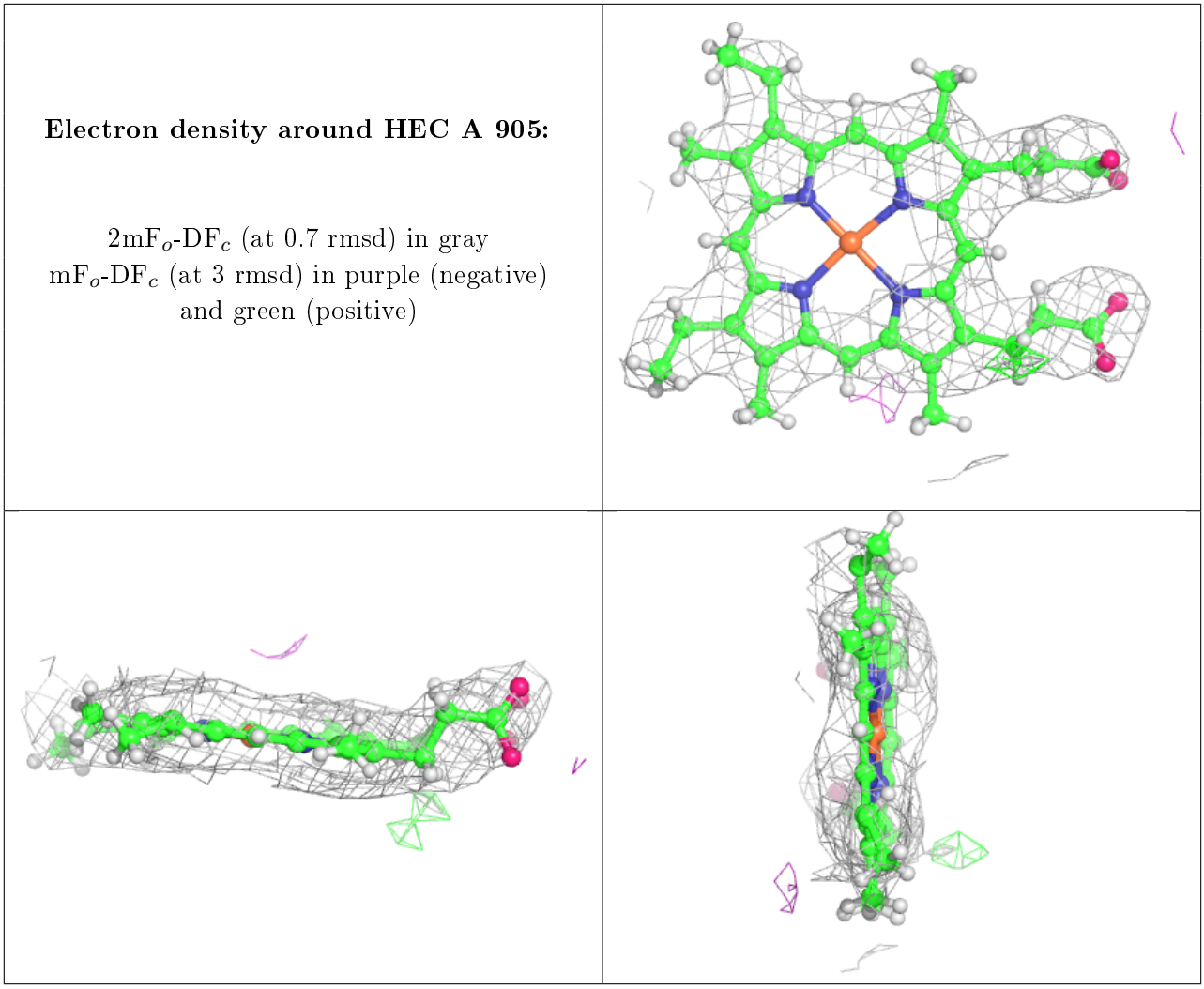
Electron density around HEC C 810:

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



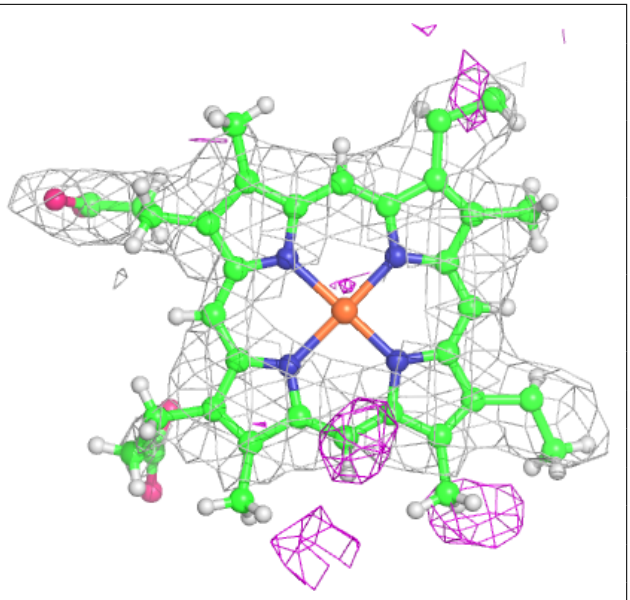
Electron density around HEC A 905:

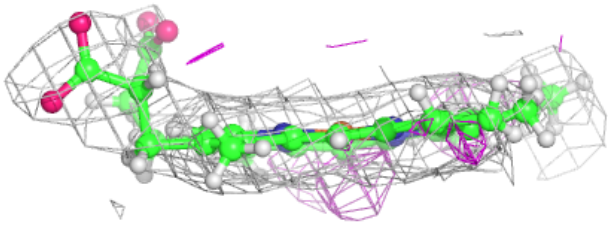
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

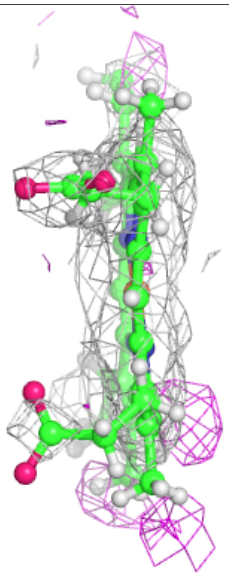


Electron density around HEC A 906:

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

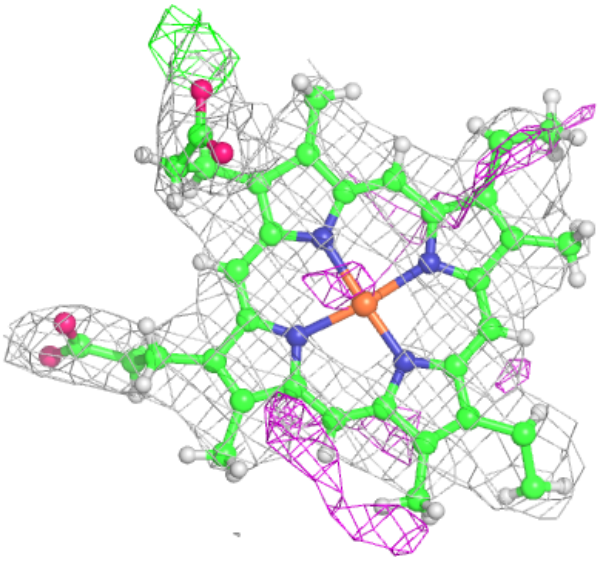


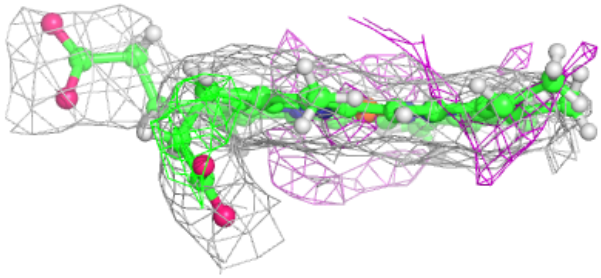


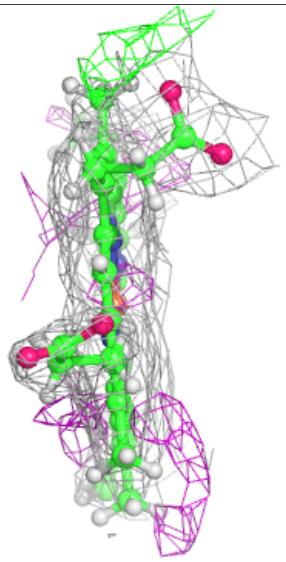


Electron density around HEC A 907:

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

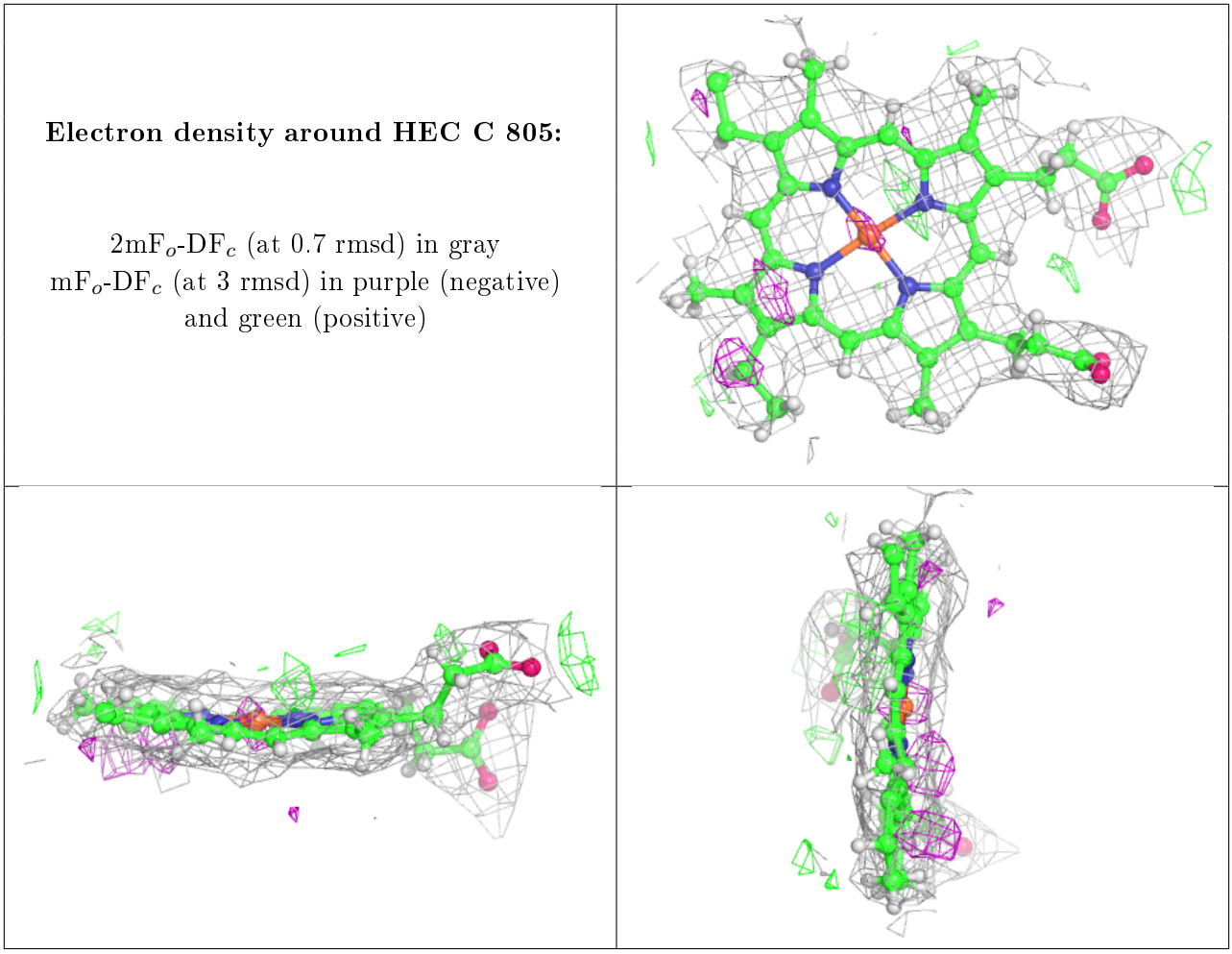






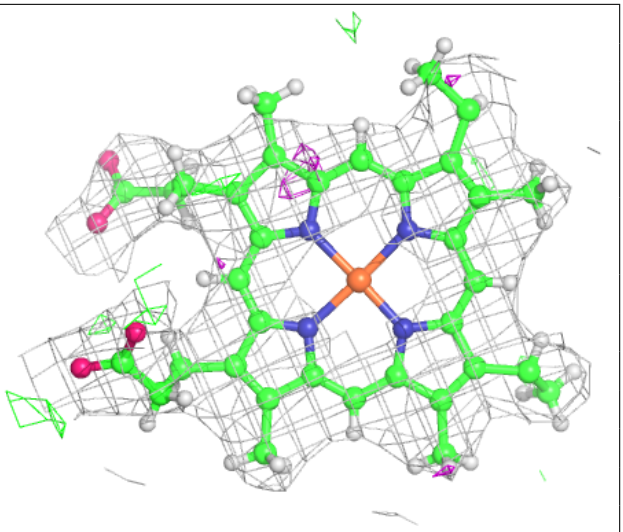
Electron density around HEC C 805:

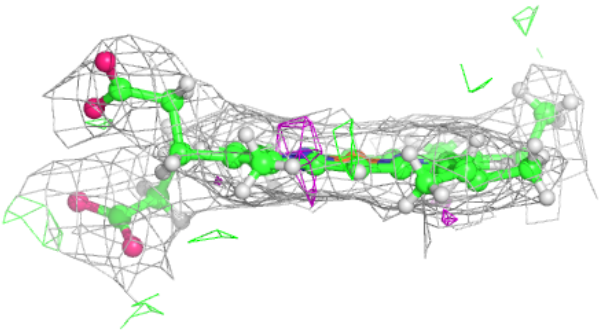
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

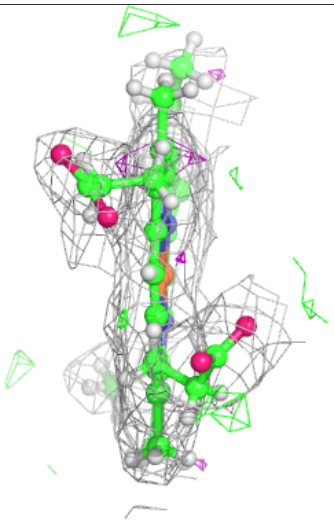


Electron density around HEC C 804:

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

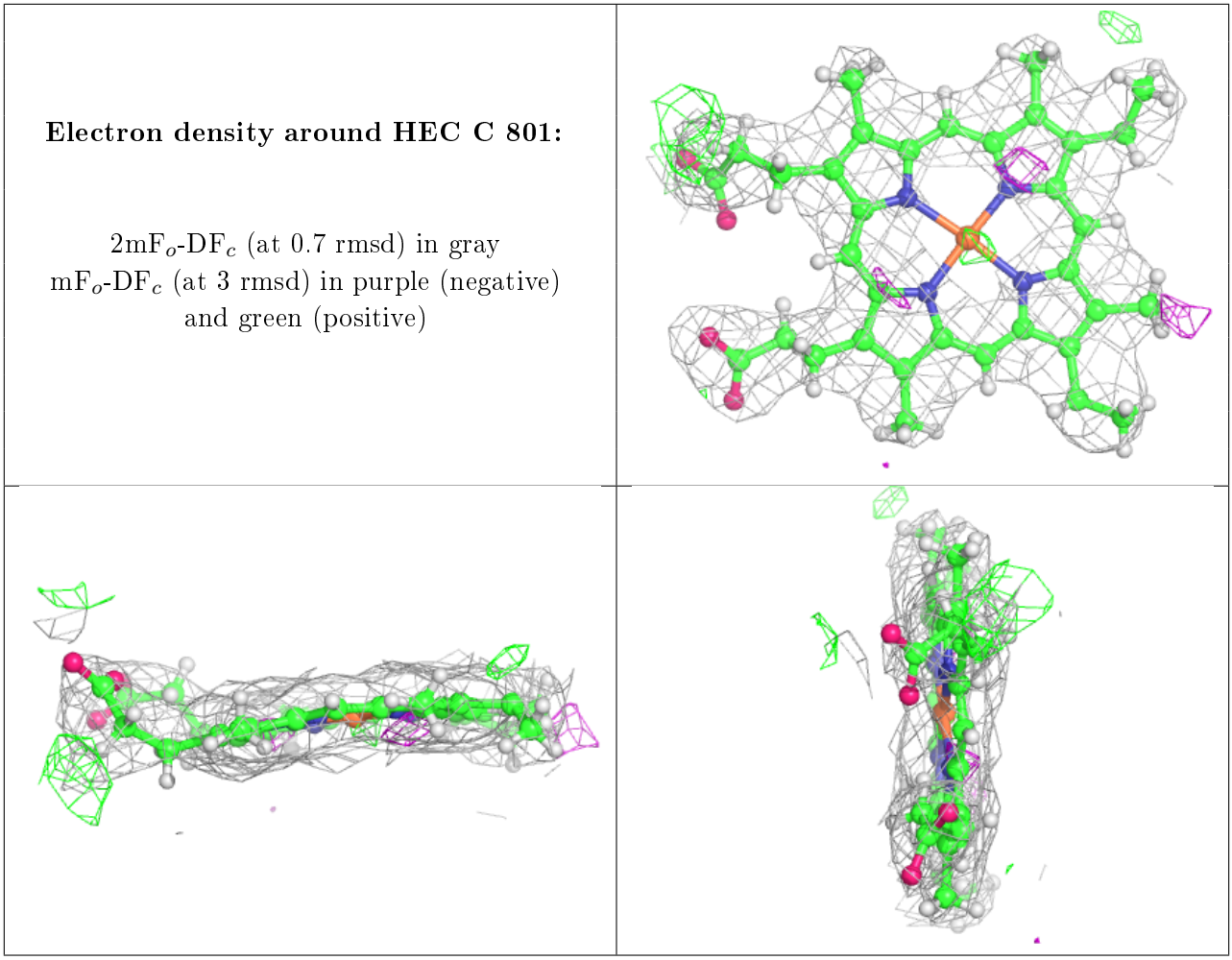






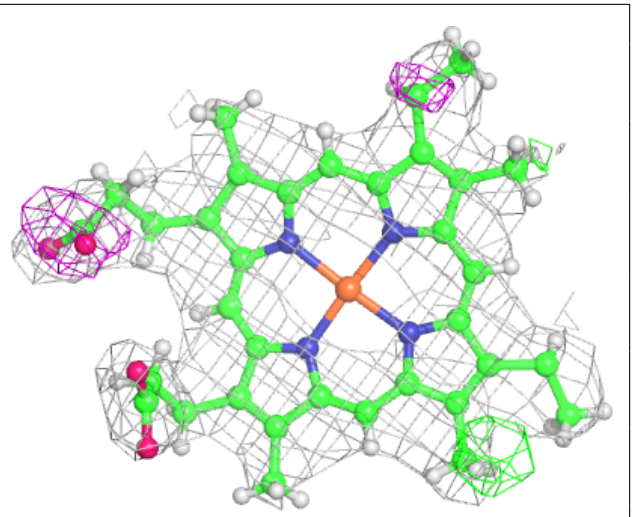
Electron density around HEC C 801:

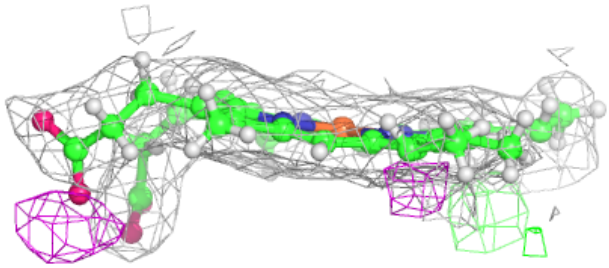
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

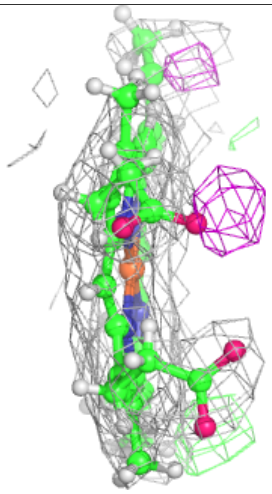


Electron density around HEC C 806:

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

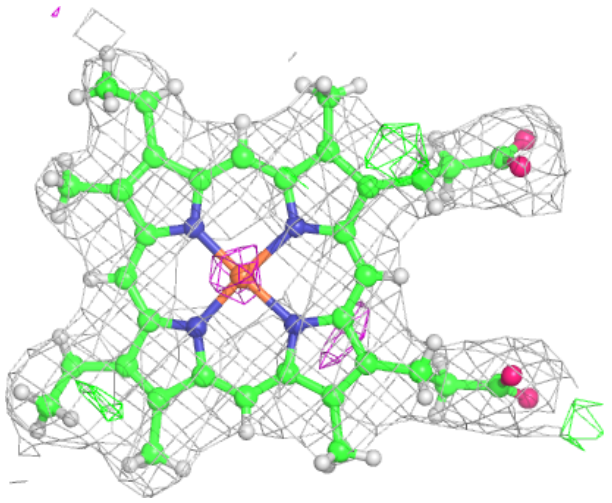


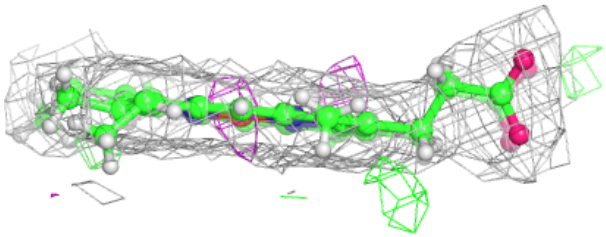


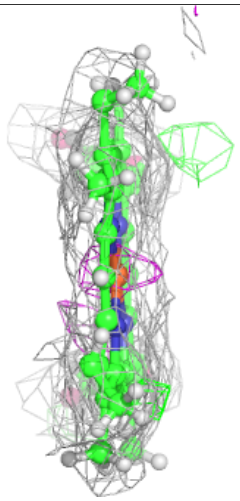


Electron density around HEC C 803:

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

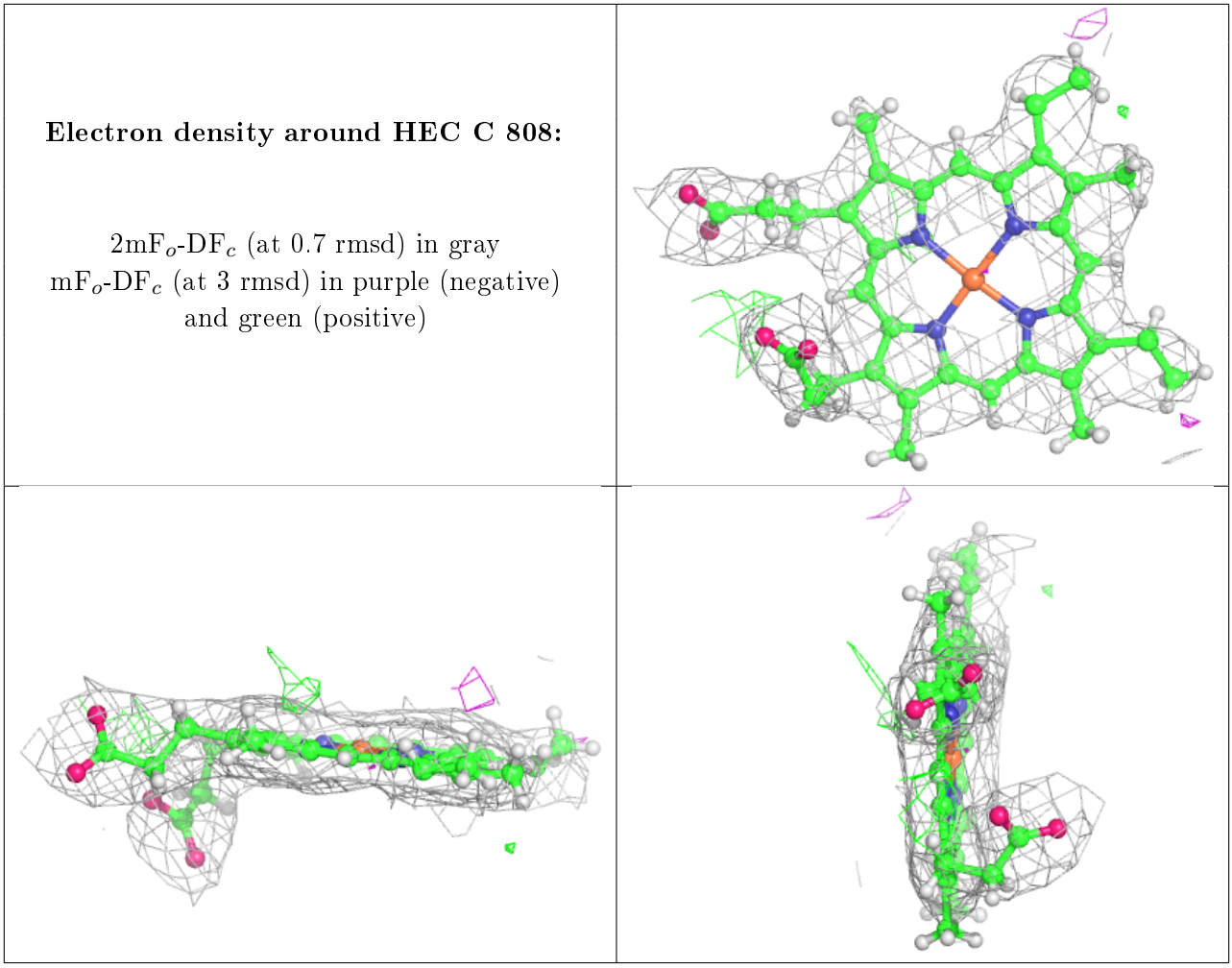






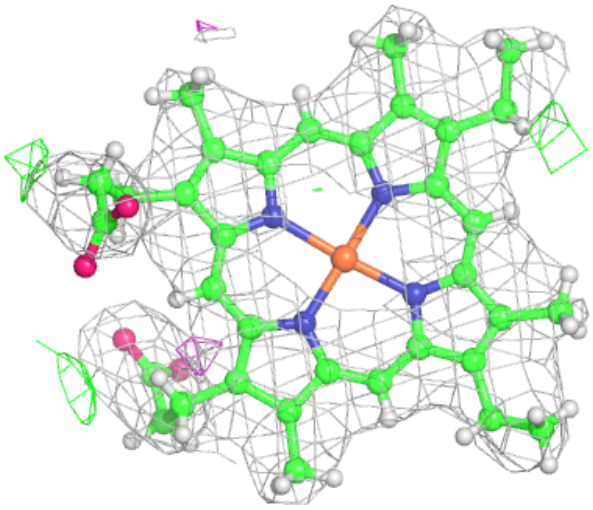
Electron density around HEC C 808:

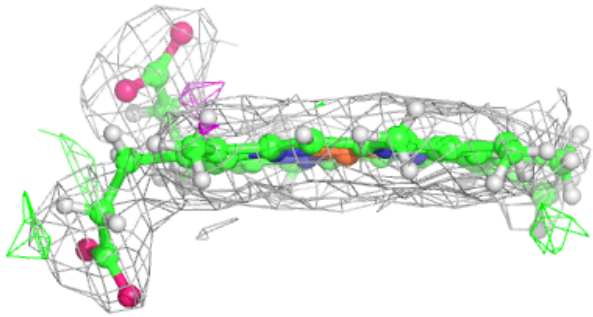
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

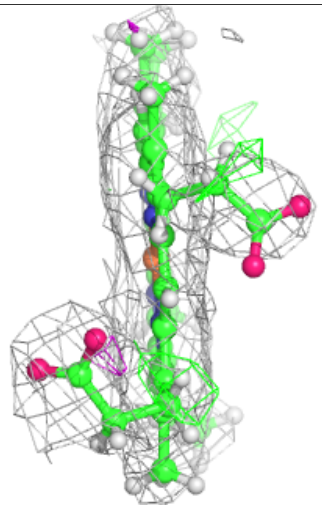


Electron density around HEC C 807:

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

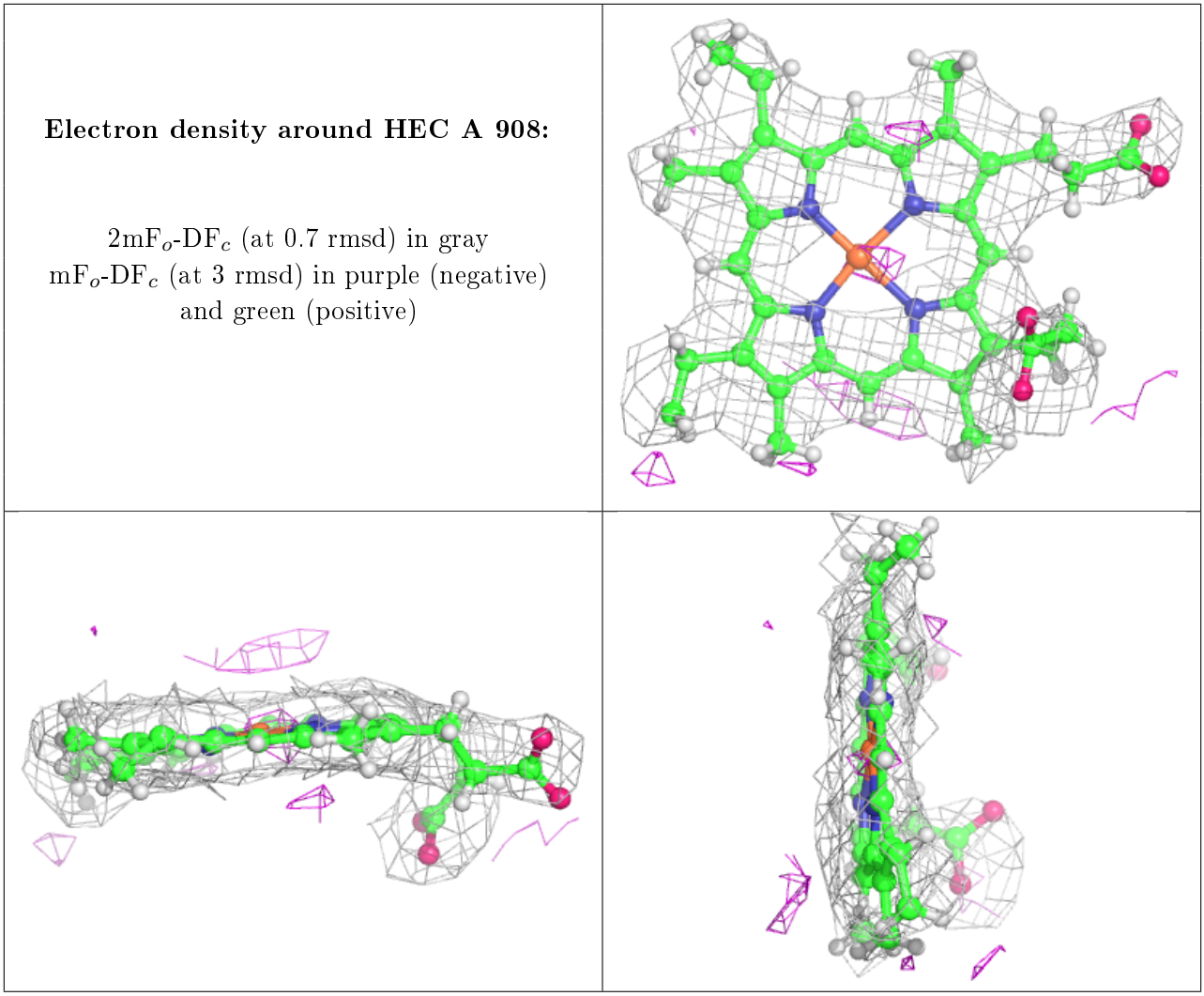






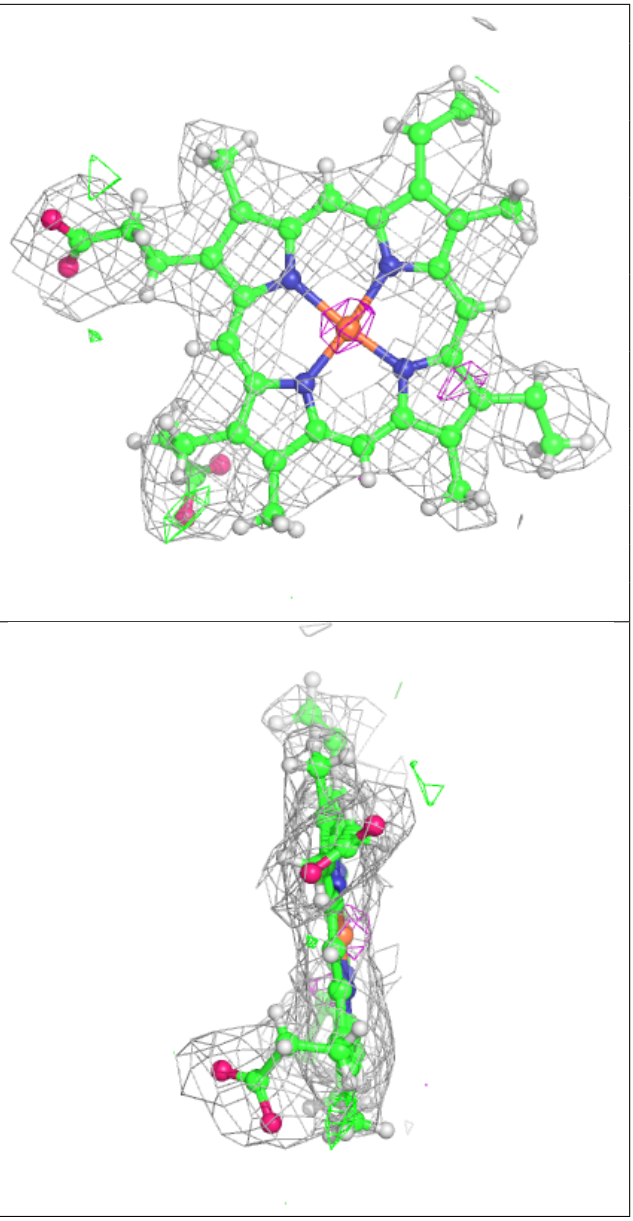
Electron density around HEC A 908:

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



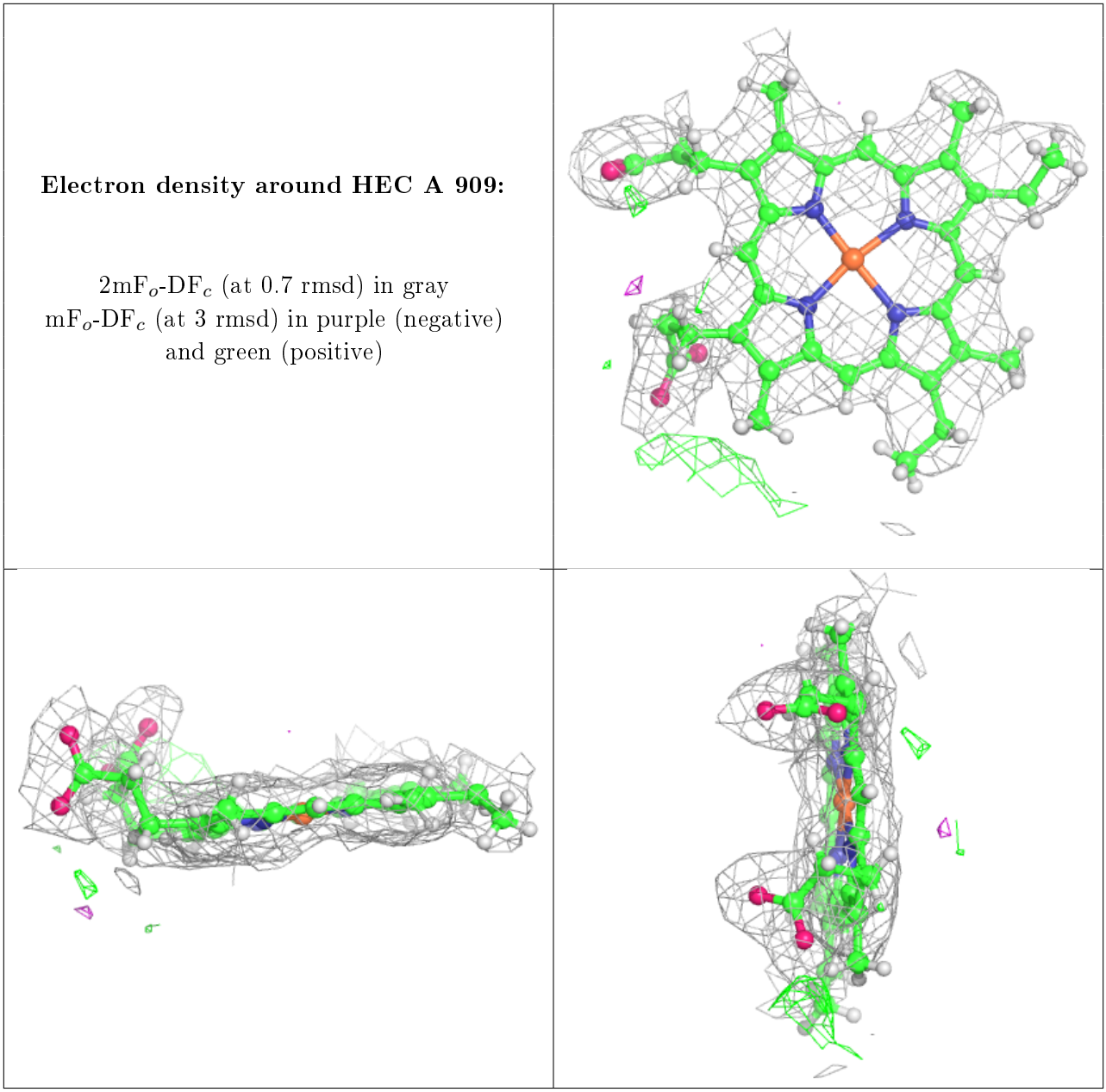
Electron density around HEC A 910:

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



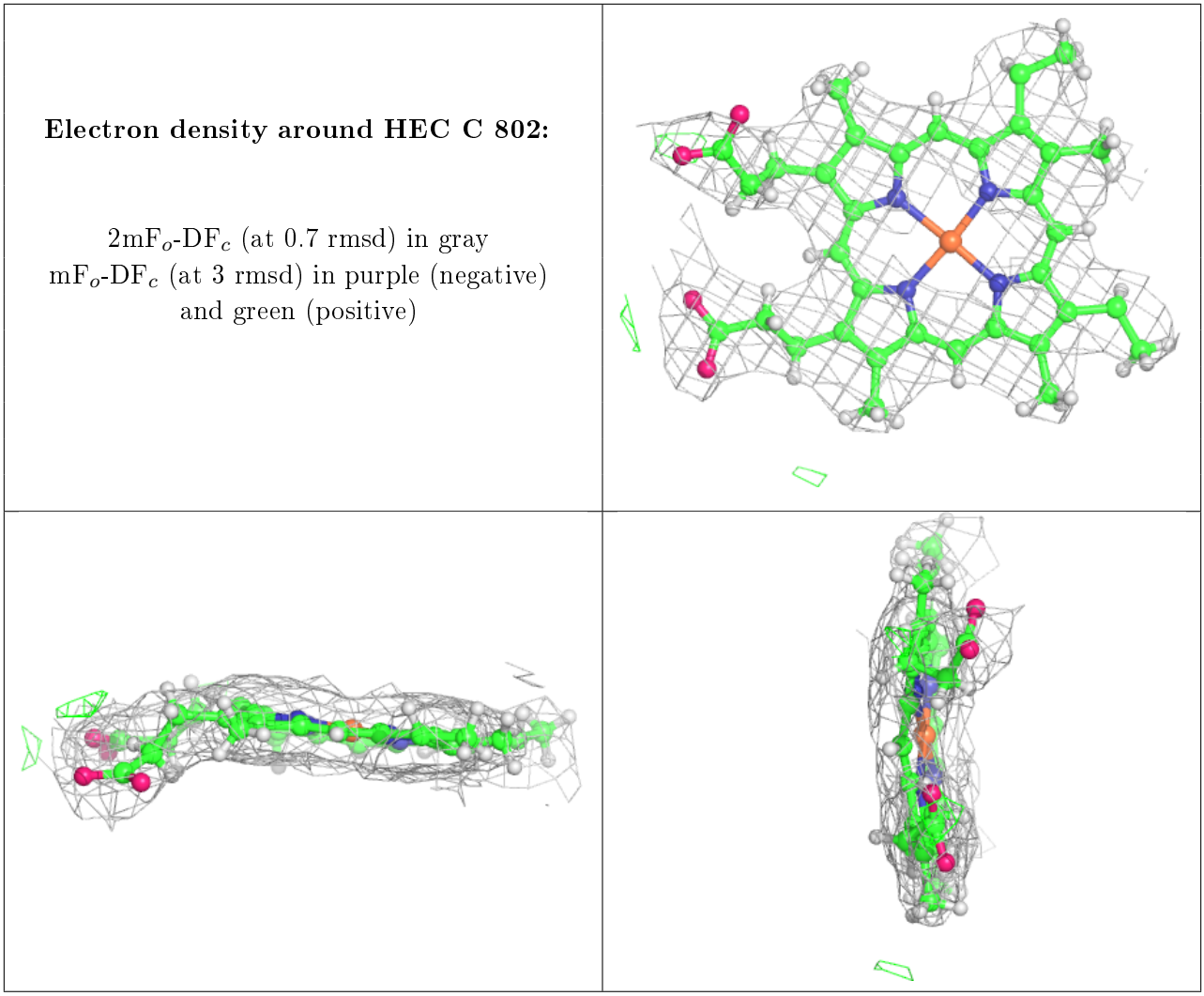
Electron density around HEC A 909:

$2mF_o$-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)



6.5 Other polymers

There are no such residues in this entry.