Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:24 AM EDT

PDB ID	:	1M1P
Title	:	P21 crystal structure of the tetraheme cytochrome c3 from Shewanella oneidensis MR1
Authors	:	Leys, D.; Meyer, T.E.; Tsapin, A.I.; Nealson, K.H.; Cusanovich, M.A.; Van Beeumen, J.J.
Deposited on	:	2002-06-20
Resolution	:	1.55 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:

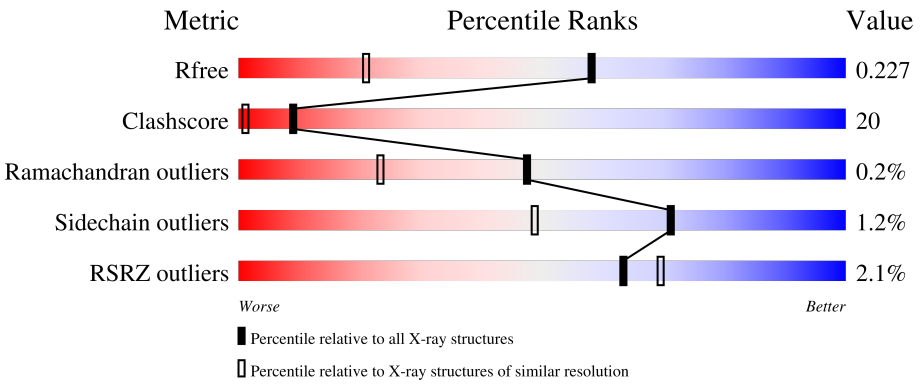
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	91	86% 10% • •
1	B	91	% 87% 11% •
1	C	91	3% 76% 16% • 5%
1	D	91	% 74% 20% • 5%

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Mol	Chain	Length	Quality of chain
1	E	91	2% 84% 12%
1	F	91	4% 84% 12%

2 Entry composition (i)

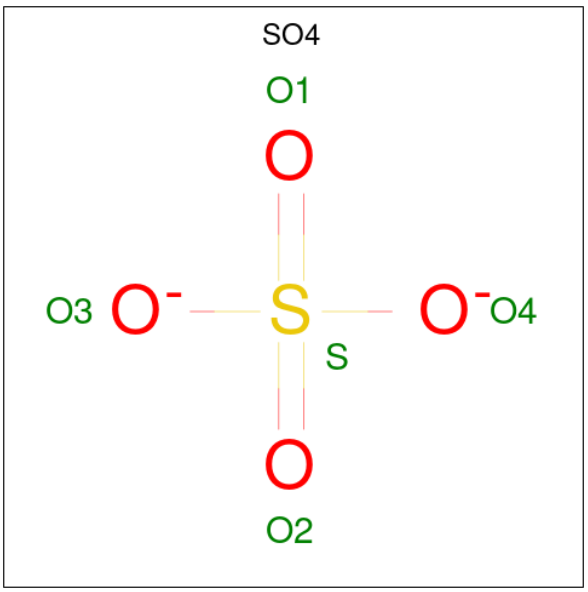
There are 4 unique types of molecules in this entry. The entry contains 5963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Small tetraheme cytochrome c.

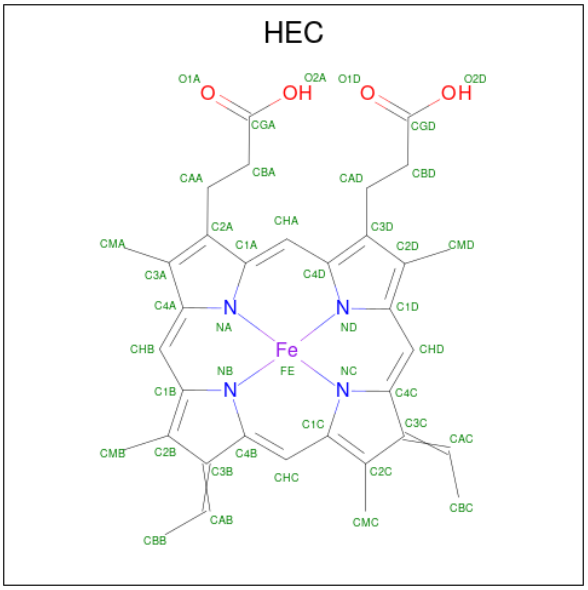
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	88	622	370	116	126	10	0	0	1
1	B	89	632	374	118	130	10	0	0	0
1	C	86	618	368	115	125	10	0	0	0
1	D	86	613	365	113	125	10	0	0	0
1	E	88	636	377	117	132	10	0	0	0
1	F	88	629	373	116	130	10	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	A	1	5	4	1		0	0
			Total	O	S			
2	B	1	5	4	1		0	0
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	F	1	5	4	1		0	0

- Molecule 3 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		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	E	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	F	1	43	34	1	4	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	195	195	195	0	0
			Total	O		
4	B	198	198	198	0	0
			Total	O		
4	C	167	167	167	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	207	207	207	0	0
			Total	O		
4	E	215	215	215	0	0
			Total	O		
4	F	179	179	179	0	0

3 Residue-property plots (i)

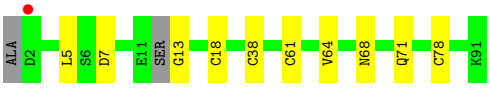
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Small tetraheme cytochrome c

Chain A:

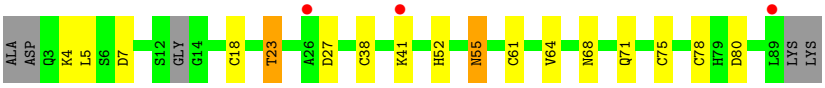
• Molecule 1: Small tetraheme cytochrome c

Chain B:



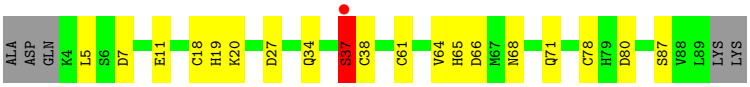
• Molecule 1: Small tetraheme cytochrome c

Chain C:



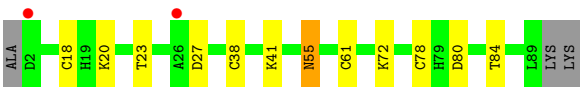
• Molecule 1: Small tetraheme cytochrome c

Chain D:



• Molecule 1: Small tetraheme cytochrome c

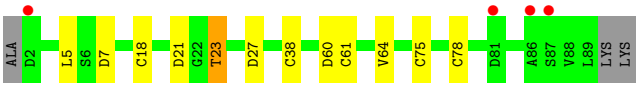
Chain E:



• Molecule 1: Small tetraheme cytochrome c

Chain F:

4%
84%
12%


ALA
D2
L5
S6
D7
C18
D21
G22
T23
D27
C38
D60
C61
V64
C75
C78
D81
A86
S87
V88
L89
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.69Å 34.01Å 108.31Å 90.00° 110.49° 90.00°	Depositor
Resolution (Å)	14.92 – 1.55 14.93 – 1.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (14.92-1.55) 94.7 (14.93-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.173 , 0.211 0.175 , 0.227	Depositor DCC
R_{free} test set	234 reflections (0.26%)	wwPDB-VP
Wilson B-factor (Å^2)	13.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5963	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.76% 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: HEC, SO4

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	0.58	0/635	0.80	1/856 (0.1%)
1	B	0.54	0/644	0.80	1/867 (0.1%)
1	C	0.53	0/630	0.89	3/848 (0.4%)
1	D	0.58	0/626	0.92	4/845 (0.5%)
1	E	0.53	0/649	0.87	2/873 (0.2%)
1	F	0.54	0/642	0.87	5/865 (0.6%)
All	All	0.55	0/3826	0.86	16/5154 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	27	ASP	CB-CG-OD2	8.22	125.70	118.30
1	E	27	ASP	CB-CG-OD2	7.50	125.05	118.30
1	C	80	ASP	CB-CG-OD2	7.44	125.00	118.30
1	D	80	ASP	CB-CG-OD2	6.94	124.55	118.30
1	E	80	ASP	CB-CG-OD2	6.49	124.14	118.30
1	D	66	ASP	CB-CG-OD2	6.37	124.03	118.30
1	C	7	ASP	CB-CG-OD2	6.05	123.74	118.30
1	F	7	ASP	CB-CG-OD2	5.65	123.39	118.30
1	F	60	ASP	CB-CG-OD2	5.50	123.25	118.30
1	D	27	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	27	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	21	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	27	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	7	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	23	THR	CB-CA-C	-5.10	97.84	111.60
1	D	37	SER	CB-CA-C	-5.08	100.44	110.10

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	622	0	544	23	0
1	B	632	0	542	18	0
1	C	618	0	544	28	0
1	D	613	0	531	29	0
1	E	636	0	558	23	0
1	F	629	0	547	23	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	F	5	0	0	0	0
3	A	172	0	124	25	0
3	B	172	0	123	20	0
3	C	172	0	124	25	0
3	D	172	0	123	17	0
3	E	172	0	123	19	1
3	F	172	0	125	26	0
4	A	195	0	0	0	0
4	B	198	0	0	1	0
4	C	167	0	0	3	0
4	D	207	0	0	6	1
4	E	215	0	0	8	0
4	F	179	0	0	0	0
All	All	5963	0	4008	169	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 20.

All (169) 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:78:CYS:SG	3:C:804:HEC:CAC	2.11	1.39
1:E:61:CYS:SG	3:E:803:HEC:CAC	2.12	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:CYS:SG	3:C:804:HEC:HAC	1.63	1.36
1:D:18:CYS:SG	3:D:801:HEC:CAC	2.14	1.36
1:A:38:CYS:SG	3:A:802:HEC:CAC	2.15	1.35
1:F:61:CYS:SG	3:F:803:HEC:CAC	2.13	1.35
1:F:75:CYS:SG	3:F:804:HEC:HAB	1.64	1.35
1:C:61:CYS:SG	3:C:803:HEC:CAC	2.15	1.35
1:A:18:CYS:SG	3:A:801:HEC:CAC	2.13	1.35
1:A:61:CYS:SG	3:A:803:HEC:CAC	2.17	1.32
1:F:18:CYS:SG	3:F:801:HEC:CAC	2.18	1.31
1:F:78:CYS:SG	3:F:804:HEC:CAC	2.18	1.30
1:B:18:CYS:SG	3:B:801:HEC:CAC	2.18	1.30
1:F:78:CYS:SG	3:F:804:HEC:HAC	1.73	1.29
1:D:38:CYS:SG	3:D:802:HEC:CAC	2.22	1.28
1:E:18:CYS:SG	3:E:801:HEC:CAC	2.21	1.28
1:D:87:SER:CB	4:D:824:HOH:O	1.80	1.24
1:C:18:CYS:SG	3:C:801:HEC:CAC	2.25	1.23
1:D:37:SER:CA	4:D:986:HOH:O	1.84	1.23
1:D:38:CYS:SG	3:D:802:HEC:HAC	1.79	1.21
1:A:78:CYS:SG	3:A:804:HEC:HAC	1.74	1.21
1:E:61:CYS:SG	3:E:803:HEC:HAC	1.78	1.20
1:E:38:CYS:SG	3:E:802:HEC:CAC	2.32	1.18
1:D:18:CYS:SG	3:D:801:HEC:HAC	1.81	1.18
1:F:38:CYS:SG	3:F:802:HEC:CAC	2.32	1.17
1:D:61:CYS:SG	3:D:803:HEC:HAC	1.76	1.17
1:F:61:CYS:SG	3:F:803:HEC:HAC	1.78	1.16
1:A:18:CYS:SG	3:A:801:HEC:HAC	1.81	1.16
1:B:61:CYS:SG	3:B:803:HEC:HAC	1.78	1.15
1:C:61:CYS:SG	3:C:803:HEC:HAC	1.82	1.15
1:D:37:SER:CB	4:D:986:HOH:O	1.92	1.14
1:C:38:CYS:SG	3:C:802:HEC:CAC	2.36	1.12
1:E:84:THR:HG22	4:E:860:HOH:O	0.97	1.12
1:B:38:CYS:SG	3:B:802:HEC:CAC	2.44	1.04
1:F:18:CYS:SG	3:F:801:HEC:HAC	1.94	1.04
1:A:61:CYS:SG	3:A:803:HEC:HAC	1.95	1.04
1:D:34:GLN:O	1:D:37:SER:CB	2.07	1.03
1:B:18:CYS:SG	3:B:801:HEC:HAC	1.99	1.01
1:A:38:CYS:SG	3:A:802:HEC:HAC	1.98	1.00
1:B:61:CYS:HG	3:B:803:HEC:HAC	1.26	0.99
1:F:61:CYS:HG	3:F:803:HEC:HAC	1.24	0.99
1:E:18:CYS:SG	3:E:801:HEC:HAC	2.01	0.97
1:D:34:GLN:O	1:D:37:SER:HB2	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:HIS:O	4:D:970:HOH:O	1.85	0.95
1:C:18:CYS:SG	3:C:801:HEC:HAC	2.05	0.94
1:D:37:SER:HA	4:D:986:HOH:O	1.47	0.93
1:C:78:CYS:HG	3:C:804:HEC:HAC	1.08	0.89
1:C:38:CYS:SG	3:C:802:HEC:HAC	2.14	0.88
1:D:34:GLN:O	1:D:37:SER:HB3	1.73	0.87
1:E:84:THR:CG2	4:E:860:HOH:O	1.67	0.87
1:E:55:ASN:HB2	4:E:952:HOH:O	1.74	0.86
1:A:18:CYS:HG	3:A:801:HEC:HAC	1.41	0.82
1:D:18:CYS:HG	3:D:801:HEC:HAC	1.42	0.81
1:F:78:CYS:HG	3:F:804:HEC:HAC	1.42	0.81
1:B:5:LEU:HD23	1:B:64:VAL:HG12	1.70	0.72
1:E:78:CYS:SG	3:E:804:HEC:CBC	2.78	0.71
1:F:38:CYS:SG	3:F:802:HEC:CBC	2.77	0.71
1:C:18:CYS:HG	3:C:801:HEC:HAC	1.55	0.71
1:A:38:CYS:SG	3:A:802:HEC:CBC	2.77	0.70
1:E:38:CYS:SG	3:E:802:HEC:HAC	2.32	0.70
1:F:38:CYS:SG	3:F:802:HEC:HAC	2.32	0.70
1:B:61:CYS:SG	3:B:803:HEC:CBC	2.81	0.69
1:B:18:CYS:SG	3:B:801:HEC:CBC	2.81	0.68
1:D:78:CYS:SG	3:D:804:HEC:CBC	2.79	0.68
1:E:38:CYS:SG	3:E:802:HEC:CBC	2.82	0.68
1:A:61:CYS:SG	3:A:803:HEC:CBC	2.82	0.67
1:C:61:CYS:HG	3:C:803:HEC:HAC	1.58	0.66
1:D:78:CYS:SG	3:D:804:HEC:C3C	2.82	0.66
1:D:61:CYS:SG	3:D:803:HEC:CBC	2.81	0.65
1:A:38:CYS:SG	3:A:802:HEC:C3C	2.85	0.65
1:B:78:CYS:SG	3:B:804:HEC:C3C	2.82	0.65
1:C:41:LYS:HD3	4:C:1232:HOH:O	1.95	0.65
1:A:78:CYS:SG	3:A:804:HEC:CBC	2.84	0.65
1:B:61:CYS:SG	3:B:803:HEC:C3C	2.86	0.64
1:E:18:CYS:SG	3:E:801:HEC:CBC	2.84	0.64
1:A:75:CYS:SG	3:A:804:HEC:CBB	2.82	0.64
1:F:61:CYS:SG	3:F:803:HEC:C3C	2.86	0.64
1:C:75:CYS:SG	3:C:804:HEC:C3B	2.85	0.64
1:C:78:CYS:SG	3:C:804:HEC:C3C	2.85	0.64
1:B:38:CYS:SG	3:B:802:HEC:CBC	2.85	0.64
1:A:52:HIS:HA	1:A:55:ASN:HD21	1.63	0.63
1:E:78:CYS:SG	3:E:804:HEC:C3C	2.85	0.63
1:F:75:CYS:SG	3:F:804:HEC:C3B	2.87	0.63
1:C:61:CYS:SG	3:C:803:HEC:C3C	2.86	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:CYS:SG	3:F:801:HEC:CBC	2.84	0.62
1:C:75:CYS:SG	3:C:804:HEC:CBB	2.84	0.62
1:E:38:CYS:SG	3:E:802:HEC:C3C	2.87	0.62
1:F:18:CYS:SG	3:F:801:HEC:C3C	2.87	0.62
1:C:18:CYS:SG	3:C:801:HEC:CBC	2.86	0.62
1:A:78:CYS:SG	3:A:804:HEC:C3C	2.86	0.62
1:C:5:LEU:HD23	1:C:64:VAL:HG12	1.82	0.62
1:E:61:CYS:SG	3:E:803:HEC:C3C	2.85	0.62
1:A:18:CYS:SG	3:A:801:HEC:CBC	2.86	0.62
1:B:78:CYS:SG	3:B:804:HEC:CBC	2.86	0.61
1:A:18:CYS:SG	3:A:801:HEC:C3C	2.87	0.61
1:E:72:LYS:HD3	4:E:887:HOH:O	2.00	0.61
1:D:61:CYS:SG	3:D:803:HEC:C3C	2.86	0.61
1:A:75:CYS:SG	3:A:804:HEC:C3B	2.86	0.61
1:D:38:CYS:SG	3:D:802:HEC:C3C	2.89	0.61
1:E:18:CYS:SG	3:E:801:HEC:C3C	2.88	0.61
1:A:61:CYS:SG	3:A:803:HEC:C3C	2.89	0.61
3:F:802:HEC:HBB3	3:F:802:HEC:HMB1	1.81	0.61
1:F:78:CYS:SG	3:F:804:HEC:C3C	2.89	0.60
1:A:61:CYS:HG	3:A:803:HEC:HAC	1.66	0.60
1:D:18:CYS:SG	3:D:801:HEC:C3C	2.89	0.60
1:B:18:CYS:SG	3:B:801:HEC:C3C	2.89	0.60
1:D:18:CYS:SG	3:D:801:HEC:CBC	2.88	0.59
1:E:61:CYS:SG	3:E:803:HEC:CBC	2.88	0.59
1:F:75:CYS:CB	3:F:804:HEC:HAB	2.32	0.58
3:D:802:HEC:HMB1	3:D:802:HEC:HBB3	1.86	0.58
1:C:38:CYS:SG	3:C:802:HEC:C3C	2.93	0.57
3:E:801:HEC:HBD2	4:E:978:HOH:O	2.04	0.57
1:F:38:CYS:SG	3:F:802:HEC:C3C	2.94	0.56
3:E:802:HEC:HMB1	3:E:802:HEC:HBB3	1.88	0.56
1:F:75:CYS:SG	3:F:804:HEC:CBB	2.87	0.56
1:C:18:CYS:SG	3:C:801:HEC:C3C	2.94	0.56
3:C:802:HEC:HMB1	3:C:802:HEC:HBB3	1.88	0.56
1:F:5:LEU:HD23	1:F:64:VAL:HG12	1.88	0.56
3:C:803:HEC:HMB1	3:C:803:HEC:HBB3	1.89	0.55
1:B:38:CYS:SG	3:B:802:HEC:C3C	2.94	0.55
3:B:802:HEC:HMB1	3:B:802:HEC:HBB3	1.88	0.55
1:C:61:CYS:SG	3:C:803:HEC:CBC	2.90	0.55
3:D:804:HEC:HMC1	3:D:804:HEC:HBC3	1.89	0.55
3:A:802:HEC:HMB1	3:A:802:HEC:HBB3	1.88	0.54
1:C:38:CYS:HG	3:C:802:HEC:HAC	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:HIS:HA	1:C:55:ASN:HD21	1.75	0.52
3:F:802:HEC:HBC3	3:F:802:HEC:HMC1	1.92	0.52
3:E:802:HEC:HMC1	3:E:802:HEC:HBC3	1.92	0.50
1:D:5:LEU:HD23	1:D:64:VAL:HG12	1.93	0.49
3:C:804:HEC:HMC1	3:C:804:HEC:HBC3	1.93	0.49
1:C:68:ASN:H	1:C:71:GLN:NE2	2.11	0.49
3:C:801:HEC:HMC1	3:C:801:HEC:HBC3	1.95	0.49
1:C:4:LYS:HG3	4:C:1283:HOH:O	2.12	0.48
1:A:5:LEU:HD23	1:A:64:VAL:HG12	1.95	0.48
1:B:38:CYS:SG	3:B:802:HEC:HBC3	2.52	0.48
1:D:37:SER:HB3	1:D:38:CYS:H	1.40	0.48
3:A:804:HEC:HBC3	3:A:804:HEC:HMC1	1.96	0.48
1:B:13:GLY:N	4:B:1227:HOH:O	2.46	0.47
3:B:804:HEC:HMC1	3:B:804:HEC:HBC3	1.95	0.47
1:F:38:CYS:SG	3:F:802:HEC:HBC3	2.54	0.47
1:C:23:THR:HG23	4:C:1260:HOH:O	2.14	0.47
1:B:5:LEU:HD11	3:B:802:HEC:HBA1	1.97	0.47
3:E:803:HEC:HBB3	3:E:803:HEC:HMB1	1.95	0.46
1:D:68:ASN:H	1:D:71:GLN:HE21	1.62	0.46
1:A:64:VAL:HG21	3:A:801:HEC:CHD	2.45	0.46
3:A:802:HEC:HMC1	3:A:802:HEC:HBC3	1.97	0.46
1:D:20:LYS:HB3	1:D:20:LYS:HE3	1.75	0.46
3:D:803:HEC:HMB1	3:D:803:HEC:HBB3	1.99	0.44
1:A:52:HIS:HA	1:A:55:ASN:ND2	2.30	0.44
1:E:41:LYS:HD2	4:E:967:HOH:O	2.18	0.43
1:C:68:ASN:H	1:C:71:GLN:HE21	1.63	0.43
1:F:61:CYS:SG	3:F:803:HEC:CBC	2.92	0.43
3:F:801:HEC:HBC3	3:F:801:HEC:HMC1	2.00	0.43
1:E:41:LYS:HB2	1:E:41:LYS:HZ2	1.84	0.43
1:E:23:THR:HG23	4:E:1003:HOH:O	2.18	0.43
3:B:801:HEC:HBB3	3:B:801:HEC:HMB1	2.00	0.42
1:D:20:LYS:NZ	4:D:915:HOH:O	2.52	0.42
1:C:78:CYS:SG	3:C:804:HEC:CBC	2.96	0.42
1:E:38:CYS:SG	3:E:802:HEC:HBC3	2.59	0.42
3:B:802:HEC:HHA	3:B:802:HEC:HBA2	2.02	0.41
1:D:7:ASP:O	1:D:11:GLU:HG3	2.20	0.41
1:B:68:ASN:H	1:B:71:GLN:NE2	2.18	0.41
1:E:20:LYS:HD3	4:E:921:HOH:O	2.19	0.41
3:A:803:HEC:HMB1	3:A:803:HEC:HBB3	2.03	0.41
1:D:68:ASN:H	1:D:71:GLN:NE2	2.19	0.41
3:F:804:HEC:HMC1	3:F:804:HEC:HBC3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:801:HEC:HMC1	3:B:801:HEC:HBC3	2.03	0.41
1:D:19:HIS:CE1	3:D:801:HEC:ND	2.89	0.40
3:A:804:HEC:HMB1	3:A:804:HEC:HBB3	2.02	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)
3:E:804:HEC:CMA	4:D:830:HOH:O[2_556]	2.08	0.12

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	86/91 (94%)	85 (99%)	1 (1%)	0	100	100
1	B	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
1	C	82/91 (90%)	80 (98%)	2 (2%)	0	100	100
1	D	84/91 (92%)	82 (98%)	1 (1%)	1 (1%)	13	2
1	E	86/91 (94%)	85 (99%)	1 (1%)	0	100	100
1	F	86/91 (94%)	86 (100%)	0	0	100	100
All	All	509/546 (93%)	501 (98%)	7 (1%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	37	SER

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	66/74 (89%)	65 (98%)	1 (2%)	65	37
1	B	67/74 (90%)	67 (100%)	0	100	100
1	C	67/74 (90%)	65 (97%)	2 (3%)	41	12
1	D	65/74 (88%)	65 (100%)	0	100	100
1	E	70/74 (95%)	69 (99%)	1 (1%)	67	41
1	F	68/74 (92%)	67 (98%)	1 (2%)	65	37
All	All	403/444 (91%)	398 (99%)	5 (1%)	71	49

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	C	23	THR
1	C	55	ASN
1	E	55	ASN
1	F	23	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	B	71	GLN
1	C	55	ASN
1	C	71	GLN
1	D	71	GLN
1	E	71	GLN
1	F	71	GLN

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)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEC	D	804	1	32,50,50	1.96	7 (21%)	24,82,82	1.57	5 (20%)
2	SO4	C	1162	-	4,4,4	0.25	0	6,6,6	0.52	0
3	HEC	F	802	1	32,50,50	1.91	6 (18%)	24,82,82	1.56	5 (20%)
3	HEC	D	803	1	32,50,50	2.35	10 (31%)	24,82,82	1.91	8 (33%)
3	HEC	A	803	1	32,50,50	1.96	7 (21%)	24,82,82	1.56	5 (20%)
3	HEC	B	801	1	32,50,50	2.41	8 (25%)	24,82,82	1.46	4 (16%)
3	HEC	A	801	1	32,50,50	2.13	7 (21%)	24,82,82	2.06	7 (29%)
3	HEC	E	803	1	32,50,50	2.09	7 (21%)	24,82,82	1.87	8 (33%)
3	HEC	F	803	1	32,50,50	2.28	6 (18%)	24,82,82	1.81	8 (33%)
3	HEC	E	804	1	32,50,50	2.16	8 (25%)	24,82,82	1.34	3 (12%)
3	HEC	C	802	1	32,50,50	2.21	7 (21%)	24,82,82	1.58	4 (16%)
3	HEC	B	804	1	32,50,50	2.22	6 (18%)	24,82,82	1.40	4 (16%)
2	SO4	B	1165	-	4,4,4	0.26	0	6,6,6	0.41	0
3	HEC	C	804	1	32,50,50	2.30	7 (21%)	24,82,82	1.30	3 (12%)
3	HEC	B	803	1	32,50,50	2.45	7 (21%)	24,82,82	1.86	5 (20%)
3	HEC	D	802	1	32,50,50	2.47	9 (28%)	24,82,82	1.82	4 (16%)
3	HEC	E	802	1	32,50,50	2.45	7 (21%)	24,82,82	1.99	4 (16%)
2	SO4	A	1164	-	4,4,4	0.11	0	6,6,6	0.36	0
3	HEC	C	803	1	32,50,50	2.21	6 (18%)	24,82,82	1.94	7 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEC	A	804	1	32,50,50	2.25	7 (21%)	24,82,82	1.46	4 (16%)
3	HEC	D	801	1	32,50,50	2.28	7 (21%)	24,82,82	1.83	10 (41%)
3	HEC	C	801	1	32,50,50	2.43	5 (15%)	24,82,82	1.46	5 (20%)
3	HEC	F	801	1	32,50,50	2.09	7 (21%)	24,82,82	1.72	5 (20%)
3	HEC	B	802	1	32,50,50	2.16	8 (25%)	24,82,82	1.54	4 (16%)
3	HEC	E	801	1	32,50,50	2.27	7 (21%)	24,82,82	1.66	4 (16%)
3	HEC	F	804	1	32,50,50	2.27	6 (18%)	24,82,82	1.44	2 (8%)
3	HEC	A	802	1	32,50,50	2.25	5 (15%)	24,82,82	1.48	3 (12%)
2	SO4	F	1163	-	4,4,4	0.13	0	6,6,6	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	D	804	1	-	2/10/54/54	-
3	HEC	F	802	1	-	2/10/54/54	-
3	HEC	D	803	1	-	4/10/54/54	-
3	HEC	A	803	1	-	2/10/54/54	-
3	HEC	B	801	1	-	4/10/54/54	-
3	HEC	A	801	1	-	3/10/54/54	-
3	HEC	E	803	1	-	2/10/54/54	-
3	HEC	F	803	1	-	4/10/54/54	-
3	HEC	E	804	1	-	4/10/54/54	-
3	HEC	C	802	1	-	2/10/54/54	-
3	HEC	B	804	1	-	4/10/54/54	-
3	HEC	C	804	1	-	4/10/54/54	-
3	HEC	B	803	1	-	3/10/54/54	-
3	HEC	D	802	1	-	4/10/54/54	-
3	HEC	E	802	1	-	2/10/54/54	-
3	HEC	C	803	1	-	2/10/54/54	-
3	HEC	A	804	1	-	5/10/54/54	-
3	HEC	D	801	1	-	5/10/54/54	-
3	HEC	C	801	1	-	4/10/54/54	-
3	HEC	F	801	1	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	B	802	1	-	5/10/54/54	-
3	HEC	E	801	1	-	3/10/54/54	-
3	HEC	F	804	1	-	2/10/54/54	-
3	HEC	A	802	1	-	2/10/54/54	-

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	HEC	C2B-C3B	-7.97	1.32	1.40
3	D	802	HEC	C2B-C3B	-7.77	1.32	1.40
3	B	803	HEC	C2B-C3B	-7.76	1.32	1.40
3	B	801	HEC	C2B-C3B	-7.70	1.32	1.40
3	E	802	HEC	C3C-C2C	-7.45	1.33	1.40
3	D	803	HEC	C3C-C2C	-7.02	1.33	1.40
3	E	802	HEC	C2B-C3B	-6.89	1.33	1.40
3	A	802	HEC	C2B-C3B	-6.88	1.33	1.40
3	E	803	HEC	C2B-C3B	-6.69	1.33	1.40
3	A	801	HEC	C2B-C3B	-6.59	1.33	1.40
3	C	804	HEC	C2B-C3B	-6.38	1.34	1.40
3	D	801	HEC	C2B-C3B	-6.36	1.34	1.40
3	B	804	HEC	C3C-C2C	-6.24	1.34	1.40
3	C	803	HEC	C2B-C3B	-6.23	1.34	1.40
3	F	803	HEC	C2B-C3B	-6.22	1.34	1.40
3	D	802	HEC	C3C-C2C	-6.21	1.34	1.40
3	F	804	HEC	C2B-C3B	-6.16	1.34	1.40
3	C	801	HEC	C3C-C2C	-6.07	1.34	1.40
3	F	803	HEC	C3C-C2C	-6.02	1.34	1.40
3	C	804	HEC	C3C-C2C	-5.94	1.34	1.40
3	C	802	HEC	C2B-C3B	-5.90	1.34	1.40
3	A	804	HEC	C3C-C2C	-5.86	1.34	1.40
3	B	803	HEC	C3C-C2C	-5.81	1.34	1.40
3	D	803	HEC	C2B-C3B	-5.78	1.34	1.40
3	E	801	HEC	C2B-C3B	-5.74	1.34	1.40
3	D	804	HEC	C2B-C3B	-5.63	1.34	1.40
3	A	804	HEC	C2B-C3B	-5.60	1.34	1.40
3	A	802	HEC	C3C-C2C	-5.60	1.34	1.40
3	B	801	HEC	C3C-C2C	-5.57	1.34	1.40
3	B	804	HEC	C2B-C3B	-5.55	1.35	1.40
3	C	803	HEC	C3C-C2C	-5.51	1.35	1.40
3	D	801	HEC	C3C-C2C	-5.49	1.35	1.40
3	E	801	HEC	C3C-C2C	-5.49	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	804	HEC	C3C-C2C	-5.40	1.35	1.40
3	E	804	HEC	C2B-C3B	-5.38	1.35	1.40
3	E	804	HEC	C3C-C2C	-5.38	1.35	1.40
3	C	802	HEC	C3D-C2D	5.37	1.53	1.37
3	F	801	HEC	C3C-C2C	-5.35	1.35	1.40
3	E	801	HEC	C3D-C2D	5.12	1.52	1.37
3	B	802	HEC	C3C-C2C	-5.09	1.35	1.40
3	F	802	HEC	C3C-C2C	-5.08	1.35	1.40
3	A	804	HEC	C3D-C2D	5.00	1.52	1.37
3	F	804	HEC	C3D-C2D	4.97	1.52	1.37
3	C	802	HEC	C3C-C2C	-4.94	1.35	1.40
3	B	802	HEC	C3D-C2D	4.93	1.52	1.37
3	B	802	HEC	C2B-C3B	-4.86	1.35	1.40
3	D	803	HEC	C3D-C2D	4.84	1.52	1.37
3	A	803	HEC	C3C-C2C	-4.81	1.35	1.40
3	B	803	HEC	C3D-C2D	4.80	1.51	1.37
3	E	802	HEC	C3D-C2D	4.79	1.51	1.37
3	F	801	HEC	C2B-C3B	-4.78	1.35	1.40
3	B	801	HEC	C3D-C2D	4.76	1.51	1.37
3	C	804	HEC	C3D-C2D	4.76	1.51	1.37
3	D	802	HEC	C3D-C2D	4.74	1.51	1.37
3	F	803	HEC	C3D-C2D	4.62	1.51	1.37
3	B	804	HEC	C3D-C2D	4.54	1.51	1.37
3	A	801	HEC	C3D-C2D	4.54	1.51	1.37
3	D	801	HEC	C3D-C2D	4.51	1.51	1.37
3	F	801	HEC	C3D-C2D	4.49	1.51	1.37
3	D	804	HEC	C3D-C2D	4.48	1.51	1.37
3	C	801	HEC	C3D-C2D	4.44	1.50	1.37
3	A	803	HEC	C2B-C3B	-4.40	1.36	1.40
3	F	802	HEC	C3D-C2D	4.34	1.50	1.37
3	F	802	HEC	C2B-C3B	-4.27	1.36	1.40
3	E	803	HEC	C3D-C2D	4.24	1.50	1.37
3	C	803	HEC	C3D-C2D	4.22	1.50	1.37
3	A	801	HEC	C3C-C2C	-4.22	1.36	1.40
3	E	804	HEC	C3D-C2D	4.20	1.50	1.37
3	A	802	HEC	C3D-C2D	4.17	1.50	1.37
3	B	802	HEC	CBC-CAC	-4.16	1.33	1.49
3	C	802	HEC	CBC-CAC	-4.07	1.34	1.49
3	C	801	HEC	CBC-CAC	-4.02	1.34	1.49
3	A	803	HEC	C3D-C2D	3.90	1.49	1.37
3	E	801	HEC	CBC-CAC	-3.90	1.34	1.49
3	C	804	HEC	CBC-CAC	-3.86	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	HEC	CBC-CAC	-3.85	1.35	1.49
3	C	803	HEC	CBC-CAC	-3.76	1.35	1.49
3	B	803	HEC	CBC-CAC	-3.75	1.35	1.49
3	E	803	HEC	C3C-C2C	-3.72	1.36	1.40
3	F	804	HEC	CBC-CAC	-3.71	1.35	1.49
3	F	804	HEC	CBB-CAB	-3.68	1.35	1.49
3	B	801	HEC	CBC-CAC	-3.67	1.35	1.49
3	C	804	HEC	CBB-CAB	-3.67	1.35	1.49
3	C	801	HEC	CBB-CAB	-3.64	1.35	1.49
3	F	803	HEC	CBC-CAC	-3.59	1.36	1.49
3	A	802	HEC	CBC-CAC	-3.58	1.36	1.49
3	A	804	HEC	CBC-CAC	-3.55	1.36	1.49
3	D	801	HEC	CBC-CAC	-3.54	1.36	1.49
3	F	801	HEC	CBC-CAC	-3.52	1.36	1.49
3	B	804	HEC	CBC-CAC	-3.50	1.36	1.49
3	E	802	HEC	CBC-CAC	-3.46	1.36	1.49
3	B	804	HEC	CBB-CAB	-3.42	1.36	1.49
3	E	803	HEC	CBC-CAC	-3.37	1.36	1.49
3	D	803	HEC	CBC-CAC	-3.36	1.36	1.49
3	A	804	HEC	CBB-CAB	-3.36	1.36	1.49
3	A	801	HEC	CBC-CAC	-3.35	1.36	1.49
3	D	801	HEC	CBB-CAB	-3.30	1.37	1.49
3	A	803	HEC	CBC-CAC	-3.28	1.37	1.49
3	B	803	HEC	CBB-CAB	-3.23	1.37	1.49
3	E	804	HEC	CBC-CAC	-3.20	1.37	1.49
3	B	801	HEC	CBB-CAB	-3.20	1.37	1.49
3	D	804	HEC	C3C-C2C	-3.18	1.37	1.40
3	A	801	HEC	CBB-CAB	-3.15	1.37	1.49
3	F	802	HEC	CBC-CAC	-3.14	1.37	1.49
3	D	803	HEC	CBB-CAB	-3.11	1.37	1.49
3	E	803	HEC	CBB-CAB	-3.09	1.37	1.49
3	F	803	HEC	CBB-CAB	-3.02	1.38	1.49
3	D	804	HEC	CBB-CAB	-3.02	1.38	1.49
3	E	801	HEC	CBB-CAB	-3.01	1.38	1.49
3	E	804	HEC	CBB-CAB	-3.01	1.38	1.49
3	D	802	HEC	CBB-CAB	-3.01	1.38	1.49
3	E	802	HEC	CBB-CAB	-3.00	1.38	1.49
3	A	803	HEC	CBB-CAB	-2.95	1.38	1.49
3	D	804	HEC	CBC-CAC	-2.92	1.38	1.49
3	C	803	HEC	CBB-CAB	-2.83	1.38	1.49
3	B	802	HEC	CBB-CAB	-2.78	1.39	1.49
3	A	803	HEC	CAA-C2A	2.77	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	HEC	C1D-ND	2.73	1.41	1.36
3	F	801	HEC	CBB-CAB	-2.63	1.39	1.49
3	C	803	HEC	C1D-ND	2.62	1.41	1.36
3	C	802	HEC	CBB-CAB	-2.57	1.39	1.49
3	D	803	HEC	C1B-NB	2.57	1.41	1.36
3	B	801	HEC	CAD-C3D	2.51	1.55	1.52
3	F	803	HEC	CAA-C2A	2.50	1.56	1.52
3	B	802	HEC	CAD-C3D	2.47	1.55	1.52
3	E	803	HEC	CAA-C2A	2.45	1.56	1.52
3	E	804	HEC	C1D-ND	2.44	1.41	1.36
3	B	802	HEC	CAA-C2A	2.42	1.56	1.52
3	E	802	HEC	CAD-C3D	2.39	1.55	1.52
3	B	803	HEC	CAA-C2A	2.36	1.56	1.52
3	E	801	HEC	CAA-C2A	2.32	1.56	1.52
3	E	803	HEC	C4D-ND	2.32	1.40	1.36
3	F	802	HEC	CBB-CAB	-2.32	1.40	1.49
3	A	802	HEC	CBB-CAB	-2.30	1.40	1.49
3	E	804	HEC	CAA-C2A	2.29	1.56	1.52
3	B	803	HEC	C4B-C3B	2.27	1.47	1.43
3	D	801	HEC	CAD-C3D	2.26	1.55	1.52
3	D	803	HEC	CMB-C2B	2.25	1.56	1.51
3	D	802	HEC	C1B-NB	2.25	1.40	1.36
3	F	801	HEC	C1D-ND	2.24	1.40	1.36
3	A	804	HEC	CAD-C3D	2.23	1.55	1.52
3	B	802	HEC	C4D-ND	2.19	1.40	1.36
3	E	801	HEC	CAD-C3D	2.19	1.55	1.52
3	D	803	HEC	CMA-C3A	2.18	1.56	1.51
3	D	804	HEC	C1C-NC	2.18	1.40	1.36
3	D	803	HEC	C1D-ND	2.18	1.40	1.36
3	B	804	HEC	CAD-C3D	2.16	1.55	1.52
3	A	804	HEC	C4D-ND	2.14	1.40	1.36
3	F	802	HEC	CAA-C2A	2.14	1.56	1.52
3	D	802	HEC	CMD-C2D	2.11	1.56	1.51
3	D	802	HEC	CAD-C3D	2.11	1.55	1.52
3	A	801	HEC	CAA-C2A	2.10	1.55	1.52
3	B	801	HEC	CAA-C2A	2.10	1.55	1.52
3	C	804	HEC	CAA-C2A	2.10	1.55	1.52
3	A	801	HEC	C3C-C4C	2.10	1.46	1.43
3	E	802	HEC	C1D-ND	2.09	1.40	1.36
3	E	804	HEC	C1C-NC	2.09	1.40	1.36
3	F	801	HEC	CMD-C2D	2.09	1.56	1.51
3	D	803	HEC	CAA-C2A	2.08	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	801	HEC	CAA-C2A	2.08	1.55	1.52
3	D	804	HEC	C4D-ND	2.07	1.40	1.36
3	C	804	HEC	CAD-C3D	2.05	1.55	1.52
3	A	803	HEC	CAD-C3D	2.03	1.55	1.52
3	B	801	HEC	C1D-ND	2.01	1.40	1.36
3	C	802	HEC	CAD-C3D	2.00	1.55	1.52
3	C	802	HEC	CAA-C2A	2.00	1.55	1.52
3	F	804	HEC	CAD-C3D	2.00	1.55	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	802	HEC	CBD-CAD-C3D	-5.01	104.08	112.62
3	A	801	HEC	CMC-C2C-C1C	-4.98	120.81	128.46
3	B	803	HEC	CBA-CAA-C2A	-4.69	104.70	112.60
3	D	803	HEC	CMB-C2B-C1B	-4.45	121.63	128.46
3	F	804	HEC	CBD-CAD-C3D	-4.37	105.17	112.62
3	E	802	HEC	CMB-C2B-C1B	-4.30	121.86	128.46
3	A	801	HEC	CBA-CAA-C2A	4.06	119.45	112.60
3	E	801	HEC	CMB-C2B-C1B	-4.04	122.25	128.46
3	F	803	HEC	CMC-C2C-C1C	-4.00	122.31	128.46
3	E	803	HEC	CMB-C2B-C1B	-4.00	122.32	128.46
3	C	803	HEC	CMC-C2C-C1C	-3.98	122.34	128.46
3	F	801	HEC	CMB-C2B-C1B	-3.98	122.34	128.46
3	A	802	HEC	CMB-C2B-C1B	-3.96	122.38	128.46
3	D	802	HEC	CBD-CAD-C3D	-3.92	105.93	112.62
3	A	803	HEC	CMB-C2B-C1B	-3.91	122.46	128.46
3	F	802	HEC	CBD-CAD-C3D	-3.87	106.01	112.62
3	D	803	HEC	CBD-CAD-C3D	-3.82	106.11	112.62
3	B	802	HEC	CMC-C2C-C1C	-3.73	122.72	128.46
3	C	802	HEC	CMB-C2B-C1B	-3.70	122.78	128.46
3	C	803	HEC	CMC-C2C-C3C	3.62	130.08	125.82
3	F	803	HEC	CBD-CAD-C3D	-3.61	106.46	112.62
3	C	802	HEC	CMC-C2C-C1C	-3.60	122.93	128.46
3	C	803	HEC	CBA-CAA-C2A	-3.56	106.61	112.60
3	B	803	HEC	CMB-C2B-C1B	-3.46	123.15	128.46
3	D	802	HEC	CMB-C2B-C1B	-3.45	123.16	128.46
3	B	803	HEC	CMC-C2C-C1C	-3.43	123.19	128.46
3	A	801	HEC	CBD-CAD-C3D	-3.43	106.77	112.62
3	C	803	HEC	CBD-CAD-C3D	-3.40	106.81	112.62
3	E	802	HEC	CMC-C2C-C1C	-3.28	123.42	128.46
3	F	804	HEC	C1D-C2D-C3D	-3.26	104.72	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	803	HEC	CMB-C2B-C1B	-3.26	123.45	128.46
3	D	802	HEC	CMC-C2C-C1C	-3.25	123.47	128.46
3	D	804	HEC	CBD-CAD-C3D	-3.24	107.10	112.62
3	B	803	HEC	CMC-C2C-C3C	3.23	129.62	125.82
3	F	802	HEC	C1D-C2D-C3D	-3.20	104.77	107.00
3	A	802	HEC	CMC-C2C-C1C	-3.20	123.55	128.46
3	F	801	HEC	C1D-C2D-C3D	-3.19	104.77	107.00
3	B	801	HEC	CMC-C2C-C1C	-3.19	123.57	128.46
3	B	804	HEC	CMC-C2C-C1C	-3.14	123.64	128.46
3	F	803	HEC	CMB-C2B-C1B	-3.12	123.66	128.46
3	F	801	HEC	CMB-C2B-C3B	3.08	129.45	125.82
3	F	801	HEC	CMC-C2C-C1C	-3.04	123.79	128.46
3	E	801	HEC	CMC-C2C-C1C	-3.03	123.80	128.46
3	E	803	HEC	CMC-C2C-C1C	-2.99	123.86	128.46
3	F	803	HEC	CMC-C2C-C3C	2.98	129.32	125.82
3	E	804	HEC	CMB-C2B-C1B	-2.96	123.91	128.46
3	D	803	HEC	CMC-C2C-C1C	-2.96	123.92	128.46
3	B	801	HEC	CBA-CAA-C2A	2.95	117.58	112.60
3	D	801	HEC	CAD-CBD-CGD	2.94	122.01	113.76
3	E	803	HEC	CBA-CAA-C2A	-2.92	107.69	112.60
3	A	803	HEC	CMB-C2B-C3B	2.89	129.22	125.82
3	D	801	HEC	CMC-C2C-C1C	-2.85	124.08	128.46
3	D	801	HEC	O2D-CGD-O1D	-2.81	116.29	123.30
3	B	802	HEC	CMC-C2C-C3C	2.79	129.10	125.82
3	D	804	HEC	C1D-C2D-C3D	-2.79	105.06	107.00
3	A	803	HEC	CMC-C2C-C1C	-2.78	124.19	128.46
3	C	801	HEC	CMB-C2B-C1B	-2.76	124.22	128.46
3	D	804	HEC	CMB-C2B-C1B	-2.76	124.22	128.46
3	A	801	HEC	CMC-C2C-C3C	2.76	129.06	125.82
3	E	803	HEC	CMB-C2B-C3B	2.73	129.03	125.82
3	A	803	HEC	CBD-CAD-C3D	-2.72	107.97	112.62
3	F	802	HEC	CMC-C2C-C1C	-2.71	124.31	128.46
3	D	801	HEC	O2D-CGD-CBD	2.70	122.70	114.03
3	D	801	HEC	CBD-CAD-C3D	-2.70	108.02	112.62
3	B	804	HEC	CMB-C2B-C3B	2.69	128.99	125.82
3	B	801	HEC	CMB-C2B-C1B	-2.69	124.33	128.46
3	A	804	HEC	CMC-C2C-C1C	-2.69	124.33	128.46
3	C	804	HEC	CMB-C2B-C1B	-2.68	124.35	128.46
3	E	804	HEC	CMC-C2C-C1C	-2.67	124.36	128.46
3	D	801	HEC	CMC-C2C-C3C	2.64	128.93	125.82
3	E	803	HEC	CMC-C2C-C3C	2.64	128.92	125.82
3	E	803	HEC	CMA-C3A-C2A	2.63	129.90	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	802	HEC	CMB-C2B-C3B	2.62	128.90	125.82
3	C	803	HEC	CMA-C3A-C2A	2.61	129.85	124.94
3	B	804	HEC	CMC-C2C-C3C	2.59	128.87	125.82
3	D	803	HEC	O2A-CGA-CBA	2.59	122.34	114.03
3	B	804	HEC	CMB-C2B-C1B	-2.56	124.53	128.46
3	A	801	HEC	C1D-C2D-C3D	-2.55	105.22	107.00
3	A	801	HEC	CMB-C2B-C1B	-2.50	124.62	128.46
3	D	801	HEC	O1A-CGA-CBA	-2.46	115.17	123.08
3	B	803	HEC	CBD-CAD-C3D	-2.46	108.42	112.62
3	D	802	HEC	CBA-CAA-C2A	-2.46	108.46	112.60
3	E	803	HEC	CBD-CAD-C3D	-2.44	108.46	112.62
3	C	804	HEC	CMC-C2C-C1C	-2.42	124.74	128.46
3	D	801	HEC	CMB-C2B-C1B	-2.40	124.78	128.46
3	E	804	HEC	O1D-CGD-CBD	-2.40	115.38	123.08
3	D	801	HEC	C4C-C3C-C2C	2.38	108.92	106.35
3	F	803	HEC	CMB-C2B-C3B	2.38	128.61	125.82
3	F	802	HEC	CMB-C2B-C1B	-2.36	124.83	128.46
3	D	804	HEC	CMA-C3A-C2A	2.31	129.31	124.94
3	C	802	HEC	CBD-CAD-C3D	-2.31	108.67	112.62
3	F	802	HEC	CAA-CBA-CGA	-2.31	107.29	113.76
3	A	803	HEC	CMC-C2C-C3C	2.31	128.53	125.82
3	B	802	HEC	CBA-CAA-C2A	-2.28	108.77	112.60
3	C	803	HEC	C3B-C4B-NB	-2.24	106.71	110.94
3	D	803	HEC	CMB-C2B-C3B	2.23	128.44	125.82
3	E	801	HEC	O1D-CGD-CBD	-2.22	115.95	123.08
3	D	803	HEC	CMC-C2C-C3C	2.21	128.42	125.82
3	A	804	HEC	C2B-C3B-C4B	2.19	108.72	106.35
3	E	801	HEC	CMC-C2C-C3C	2.18	128.38	125.82
3	D	803	HEC	C4C-C3C-C2C	2.17	108.69	106.35
3	A	801	HEC	O2A-CGA-CBA	2.17	121.00	114.03
3	C	801	HEC	CMC-C2C-C1C	-2.17	125.13	128.46
3	F	803	HEC	C2B-C3B-C4B	2.16	108.68	106.35
3	B	802	HEC	CMB-C2B-C1B	-2.16	125.15	128.46
3	A	804	HEC	C4C-C3C-C2C	2.15	108.67	106.35
3	D	804	HEC	CMC-C2C-C1C	-2.14	125.17	128.46
3	D	801	HEC	O2A-CGA-CBA	2.14	120.90	114.03
3	C	804	HEC	CMB-C2B-C3B	2.13	128.33	125.82
3	E	803	HEC	CAD-CBD-CGD	-2.12	107.81	113.76
3	F	803	HEC	C1D-C2D-C3D	-2.07	105.56	107.00
3	C	801	HEC	CBD-CAD-C3D	-2.07	109.09	112.62
3	A	802	HEC	CMB-C2B-C3B	2.06	128.25	125.82
3	C	801	HEC	O1A-CGA-CBA	-2.05	116.48	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	801	HEC	O2A-CGA-CBA	2.03	120.57	114.03
3	A	804	HEC	C3C-C4C-NC	-2.03	107.11	110.94
3	C	802	HEC	CAD-CBD-CGD	-2.01	108.12	113.76
3	C	801	HEC	CAA-CBA-CGA	-2.01	108.13	113.76
3	F	803	HEC	CAD-CBD-CGD	2.01	119.38	113.76
3	D	803	HEC	O1A-CGA-CBA	-2.00	116.64	123.08
3	B	801	HEC	CMC-C2C-C3C	2.00	128.17	125.82

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	HEC	C3D-CAD-CBD-CGD
3	D	801	HEC	C3D-CAD-CBD-CGD
3	B	803	HEC	C2A-CAA-CBA-CGA
3	B	801	HEC	C3D-CAD-CBD-CGD
3	A	804	HEC	C3D-CAD-CBD-CGD
3	E	801	HEC	C4D-C3D-CAD-CBD
3	B	804	HEC	CAA-CBA-CGA-O2A
3	F	804	HEC	CAA-CBA-CGA-O2A
3	D	803	HEC	CAA-CBA-CGA-O1A
3	E	804	HEC	CAD-CBD-CGD-O1D
3	D	802	HEC	CAA-CBA-CGA-O1A
3	C	804	HEC	CAA-CBA-CGA-O1A
3	C	804	HEC	CAA-CBA-CGA-O2A
3	D	802	HEC	CAD-CBD-CGD-O2D
3	F	804	HEC	CAA-CBA-CGA-O1A
3	C	802	HEC	CAA-CBA-CGA-O2A
3	A	804	HEC	CAA-CBA-CGA-O1A
3	A	804	HEC	CAD-CBD-CGD-O2D
3	C	804	HEC	CAD-CBD-CGD-O1D
3	D	801	HEC	CAD-CBD-CGD-O1D
3	F	801	HEC	CAA-CBA-CGA-O1A
3	B	802	HEC	CAA-CBA-CGA-O1A
3	C	801	HEC	CAA-CBA-CGA-O1A
3	D	802	HEC	CAD-CBD-CGD-O1D
3	B	801	HEC	CAD-CBD-CGD-O1D
3	B	801	HEC	CAD-CBD-CGD-O2D
3	C	801	HEC	CAA-CBA-CGA-O2A
3	C	802	HEC	CAA-CBA-CGA-O1A
3	D	803	HEC	CAA-CBA-CGA-O2A
3	A	804	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
3	B	804	HEC	CAA-CBA-CGA-O1A
3	E	804	HEC	CAD-CBD-CGD-O2D
3	B	802	HEC	CAA-CBA-CGA-O2A
3	B	802	HEC	CAD-CBD-CGD-O2D
3	D	802	HEC	CAA-CBA-CGA-O2A
3	D	803	HEC	CAD-CBD-CGD-O2D
3	F	802	HEC	CAA-CBA-CGA-O1A
3	D	801	HEC	CAD-CBD-CGD-O2D
3	F	802	HEC	CAA-CBA-CGA-O2A
3	A	804	HEC	CAA-CBA-CGA-O2A
3	A	802	HEC	CAA-CBA-CGA-O1A
3	A	802	HEC	CAA-CBA-CGA-O2A
3	F	801	HEC	CAA-CBA-CGA-O2A
3	E	803	HEC	CAD-CBD-CGD-O2D
3	C	804	HEC	CAD-CBD-CGD-O2D
3	D	801	HEC	CAA-CBA-CGA-O2A
3	C	801	HEC	CAD-CBD-CGD-O2D
3	D	803	HEC	CAD-CBD-CGD-O1D
3	F	803	HEC	CAD-CBD-CGD-O2D
3	E	804	HEC	CAA-CBA-CGA-O2A
3	D	804	HEC	CAA-CBA-CGA-O2A
3	E	802	HEC	CAA-CBA-CGA-O1A
3	A	801	HEC	CAD-CBD-CGD-O2D
3	B	802	HEC	CAD-CBD-CGD-O1D
3	E	802	HEC	CAA-CBA-CGA-O2A
3	E	804	HEC	CAA-CBA-CGA-O1A
3	F	803	HEC	CAA-CBA-CGA-O2A
3	B	803	HEC	CAD-CBD-CGD-O2D
3	B	804	HEC	CAD-CBD-CGD-O2D
3	C	803	HEC	CAD-CBD-CGD-O2D
3	F	803	HEC	CAD-CBD-CGD-O1D
3	A	803	HEC	CAD-CBD-CGD-O2D
3	C	801	HEC	CAD-CBD-CGD-O1D
3	C	803	HEC	CAD-CBD-CGD-O1D
3	E	801	HEC	CAD-CBD-CGD-O2D
3	E	803	HEC	CAD-CBD-CGD-O1D
3	F	803	HEC	CAA-CBA-CGA-O1A
3	B	803	HEC	CAD-CBD-CGD-O1D
3	A	801	HEC	CAD-CBD-CGD-O1D
3	D	804	HEC	CAA-CBA-CGA-O1A
3	A	803	HEC	CAD-CBD-CGD-O1D
3	D	801	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	B	804	HEC	CAD-CBD-CGD-O1D
3	A	801	HEC	C3D-CAD-CBD-CGD
3	E	801	HEC	CAD-CBD-CGD-O1D
3	B	801	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

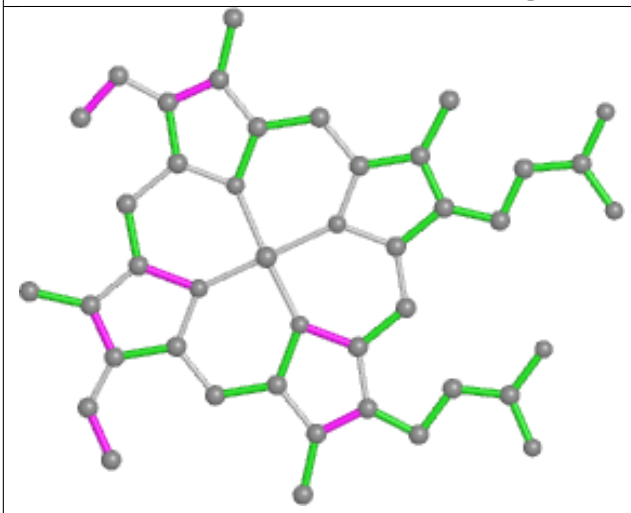
24 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	804	HEC	3	0
3	F	802	HEC	7	0
3	D	803	HEC	4	0
3	A	803	HEC	6	0
3	B	801	HEC	6	0
3	A	801	HEC	6	0
3	E	803	HEC	5	0
3	F	803	HEC	5	0
3	E	804	HEC	2	1
3	C	802	HEC	5	0
3	B	804	HEC	3	0
3	C	804	HEC	8	0
3	B	803	HEC	4	0
3	D	802	HEC	4	0
3	E	802	HEC	7	0
3	C	803	HEC	6	0
3	A	804	HEC	7	0
3	D	801	HEC	6	0
3	C	801	HEC	6	0
3	F	801	HEC	5	0
3	B	802	HEC	7	0
3	E	801	HEC	5	0
3	F	804	HEC	9	0
3	A	802	HEC	6	0

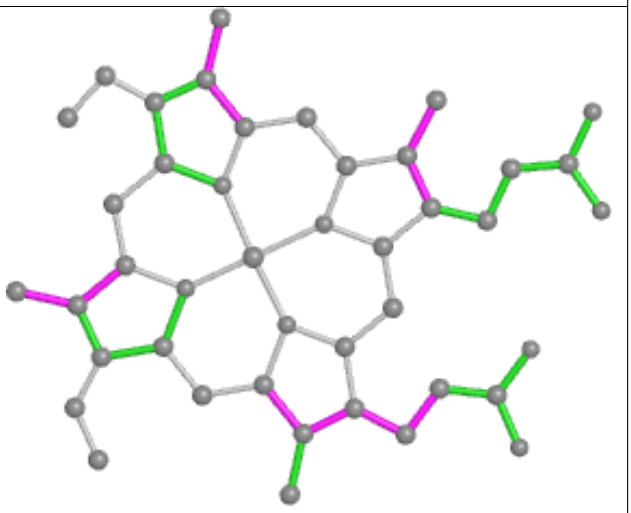
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

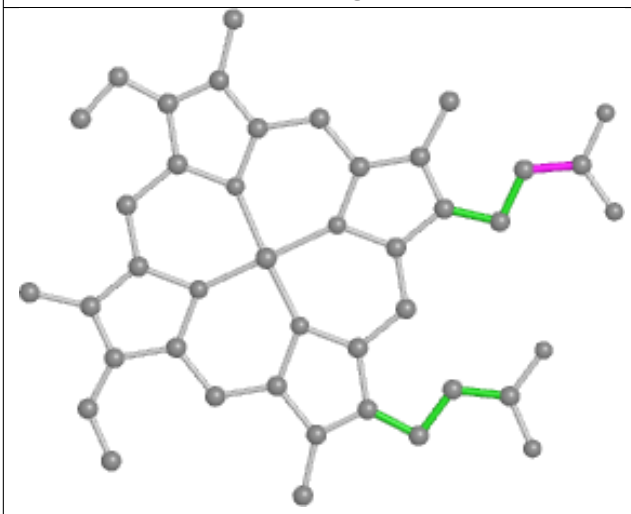
Ligand HEC D 804



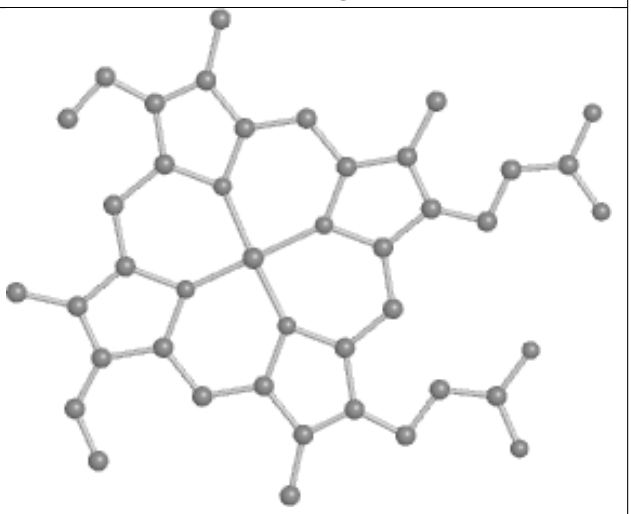
Bond lengths



Bond angles

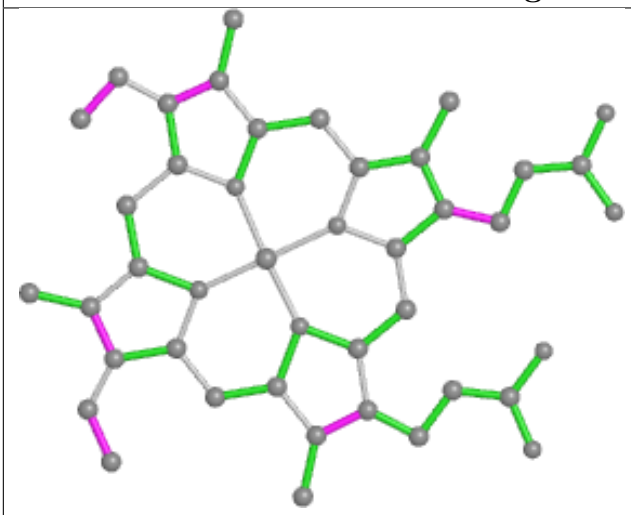


Torsions

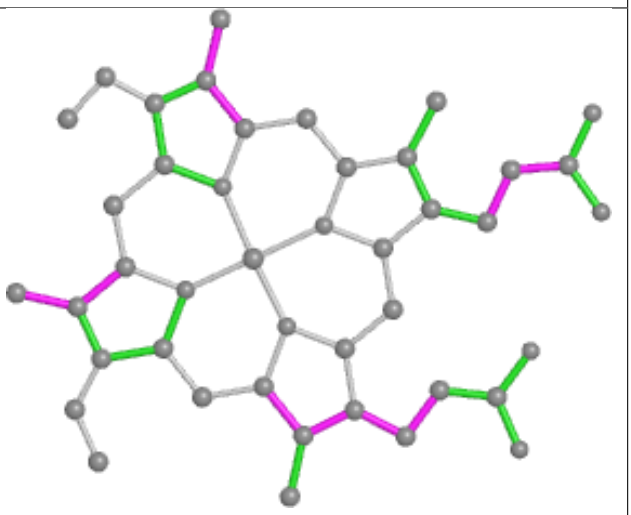


Rings

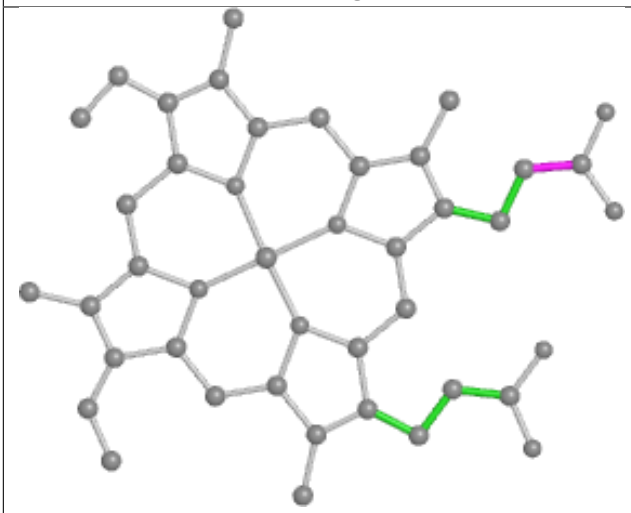
Ligand HEC F 802



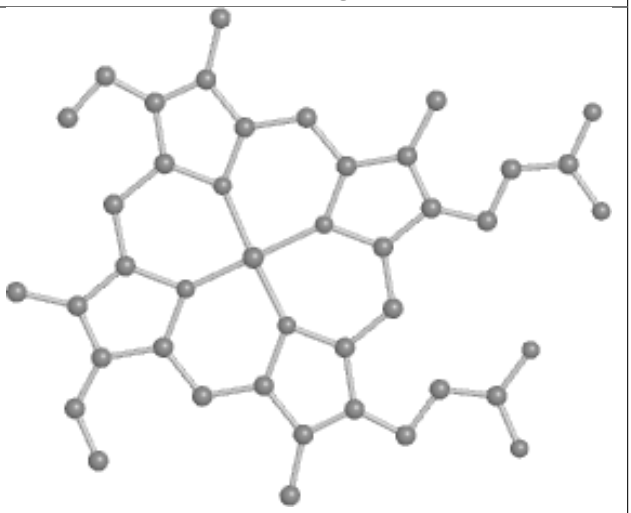
Bond lengths



Bond angles

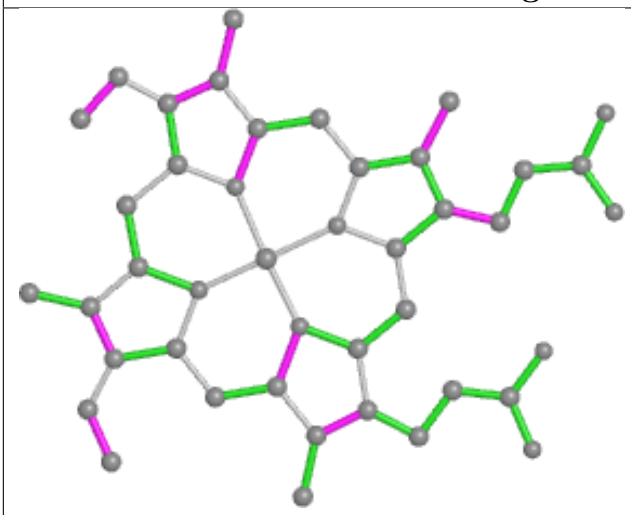


Torsions

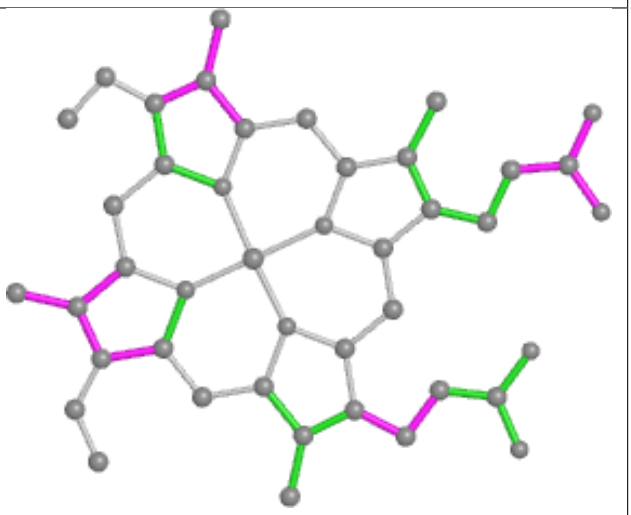


Rings

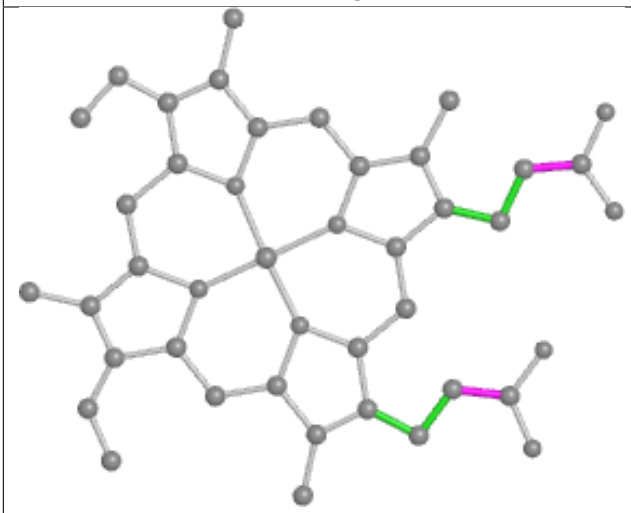
Ligand HEC D 803



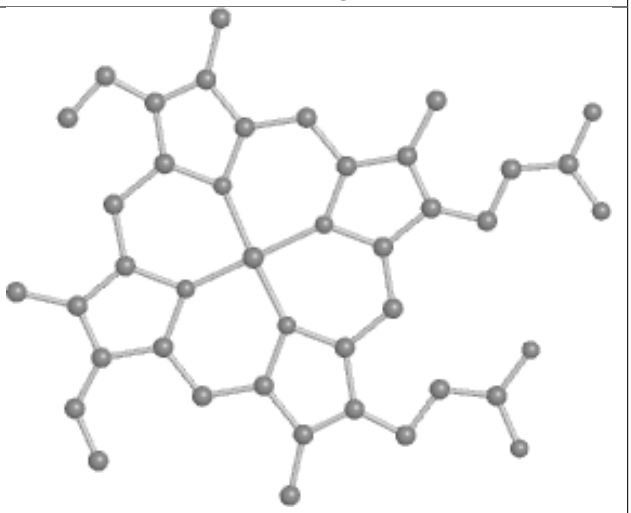
Bond lengths



Bond angles



Torsions



Rings

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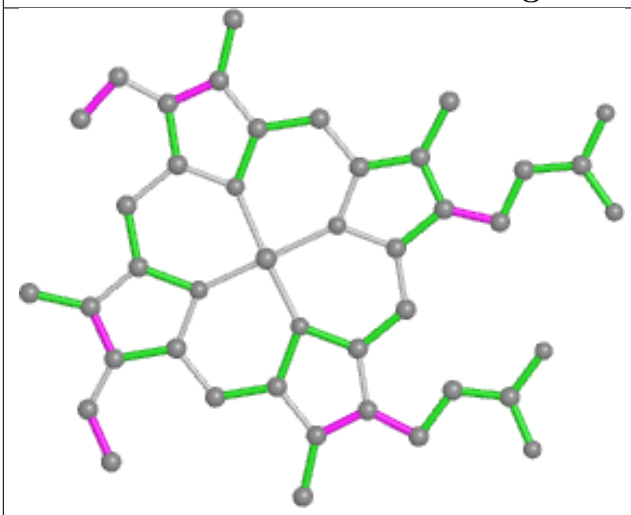

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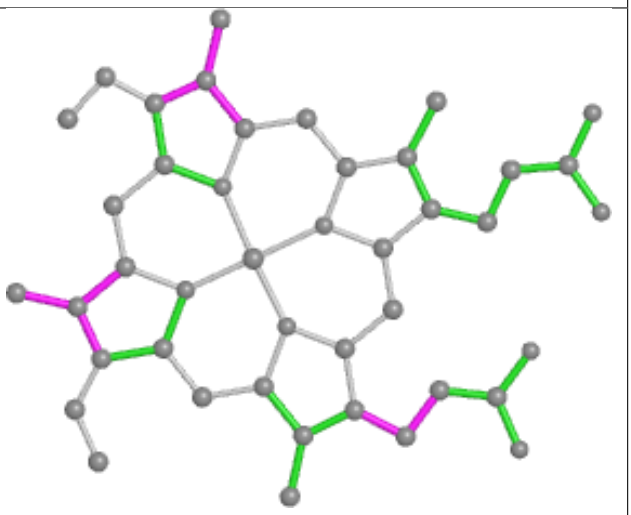
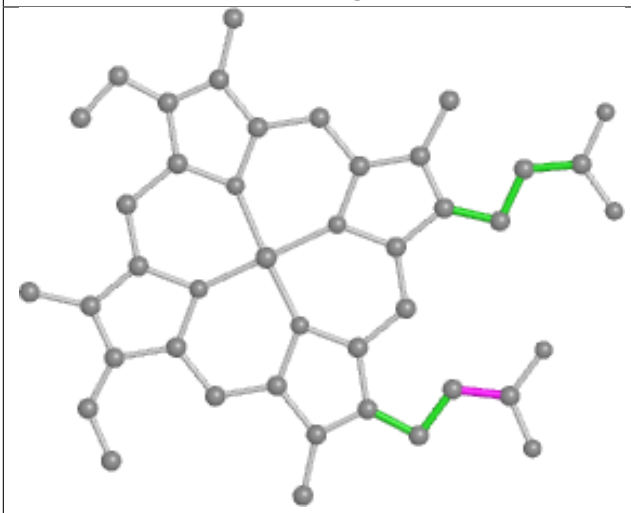
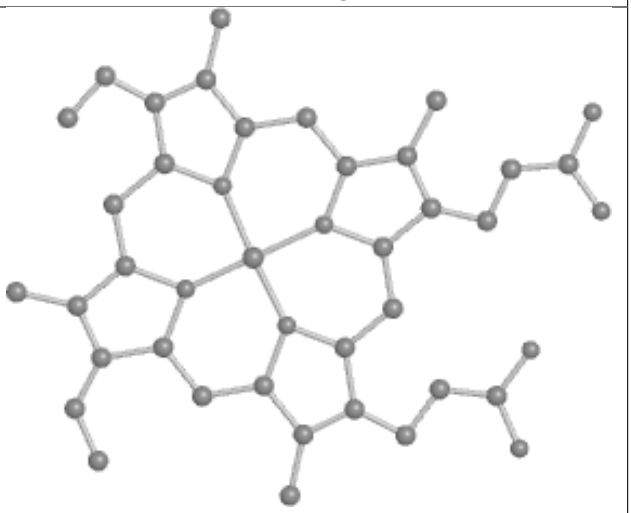


Bond angles

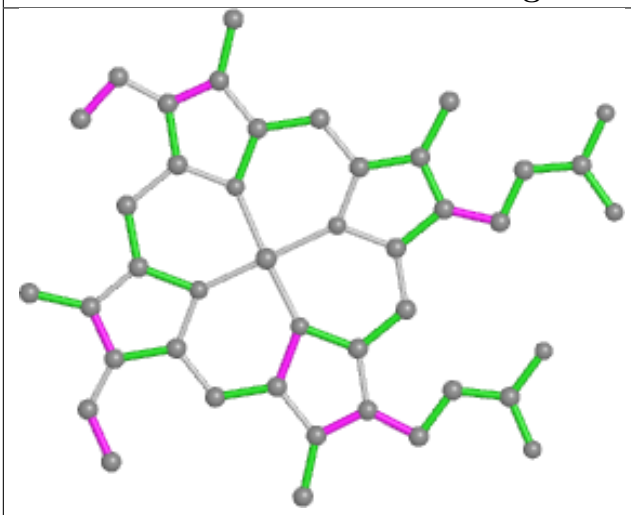


Torsions



Rings

Ligand HEC B 801



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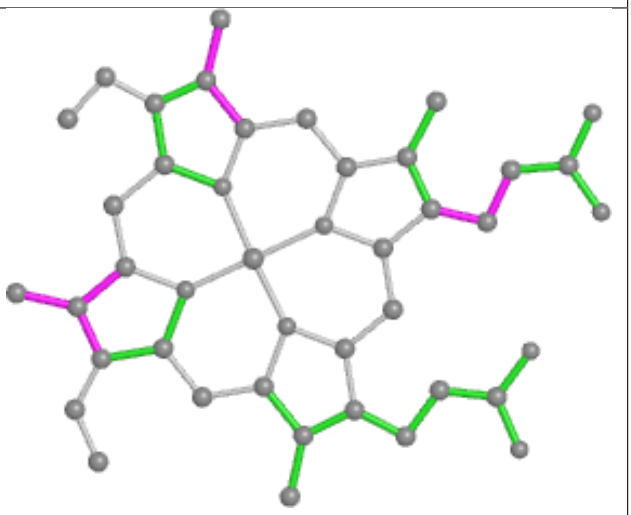
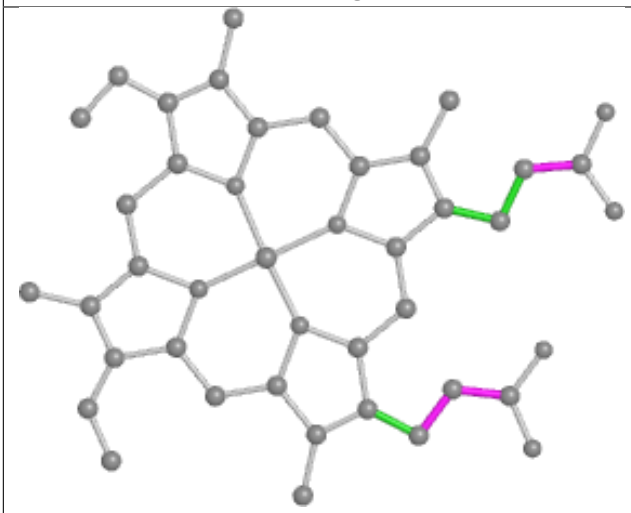
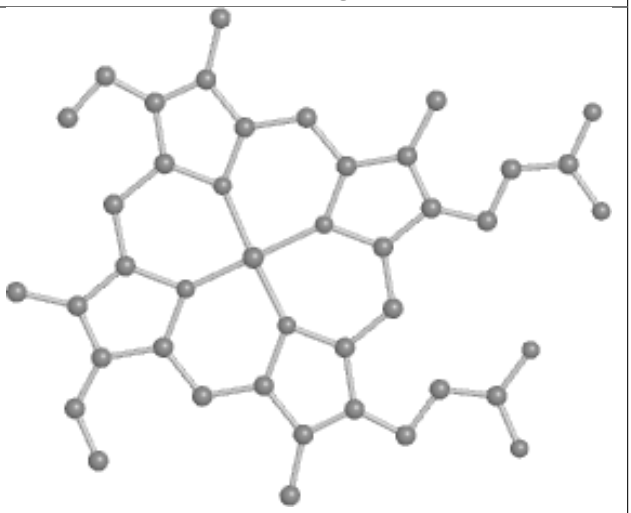


Bond angles



Torsions



Rings

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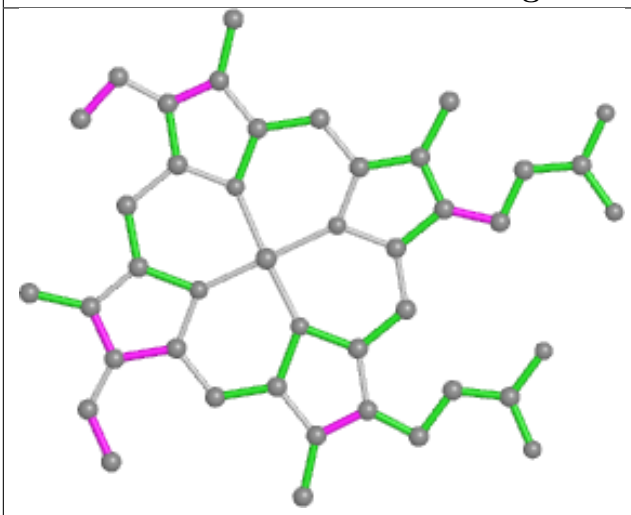

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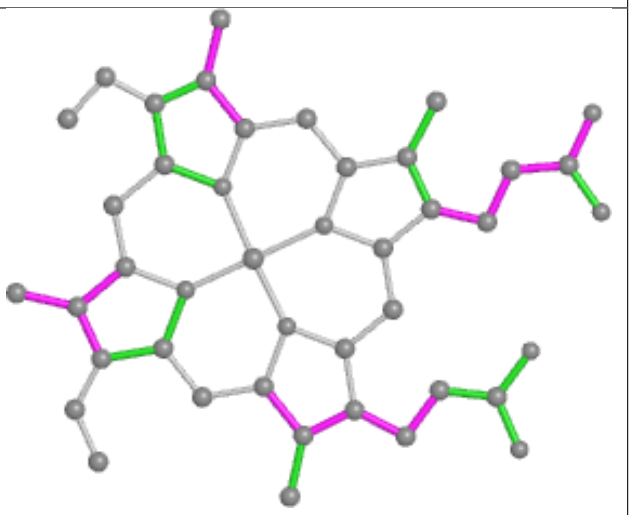
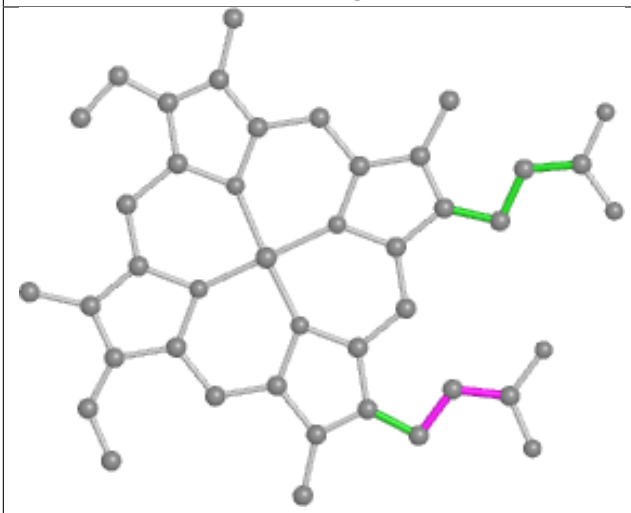


Bond angles



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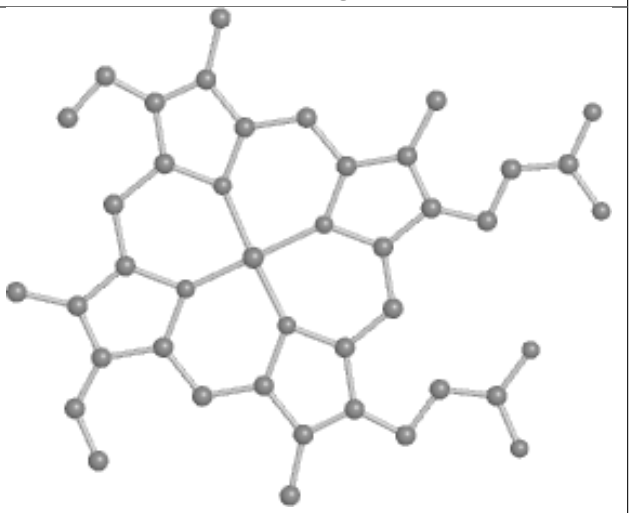
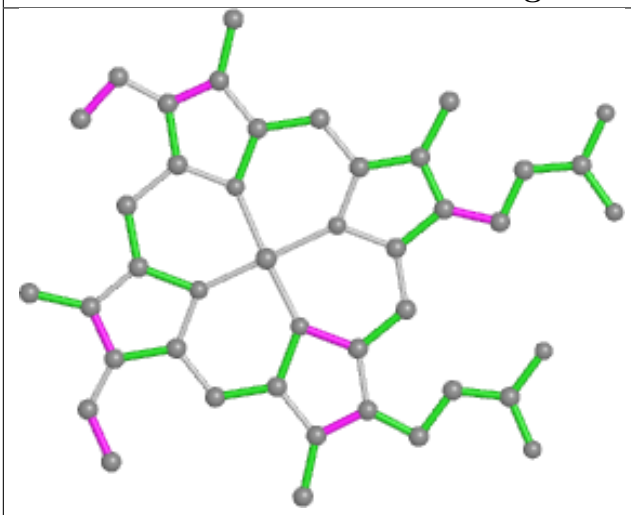


Rings

Ligand HEC E 803



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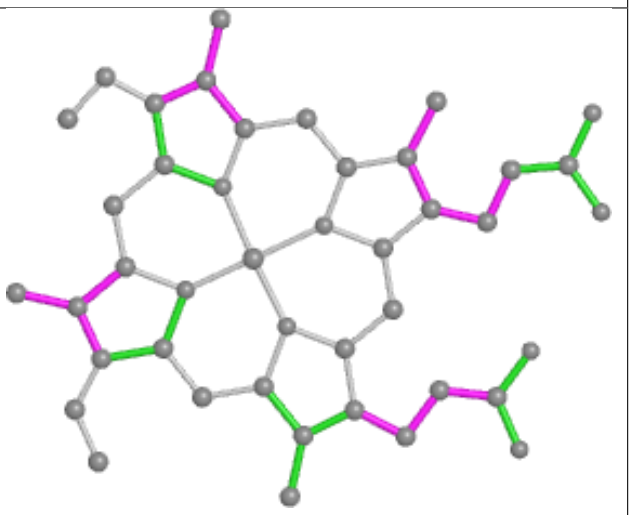

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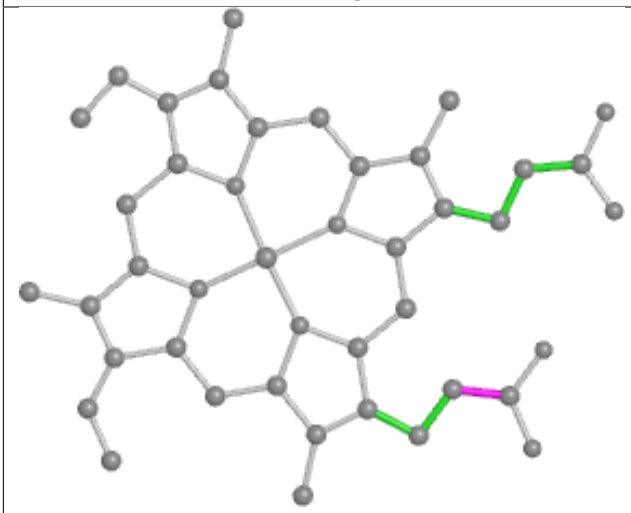

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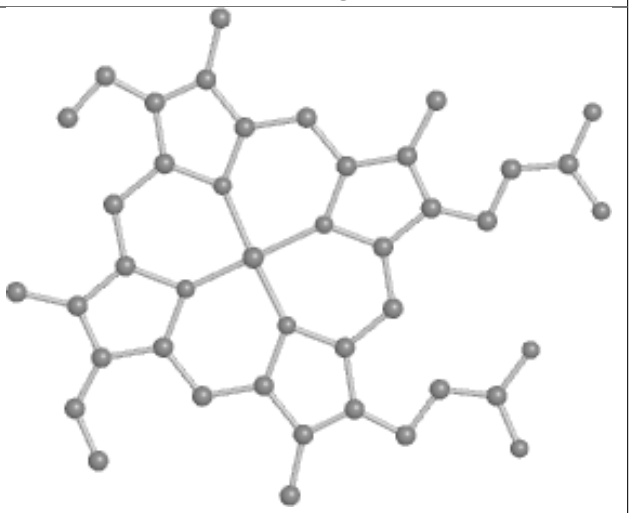
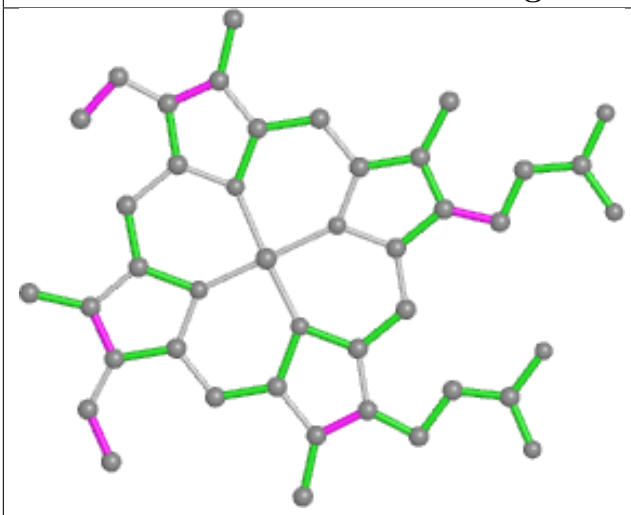
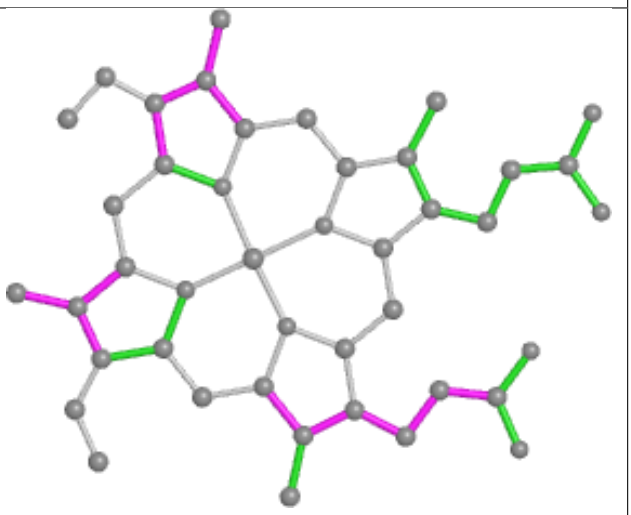


Rings

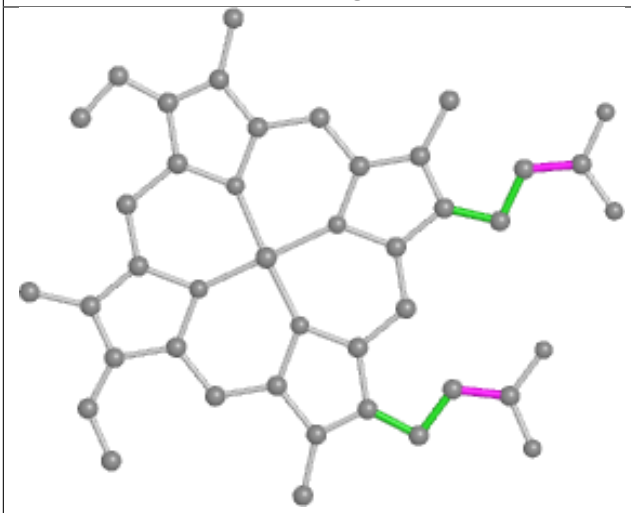
Ligand HEC F 803



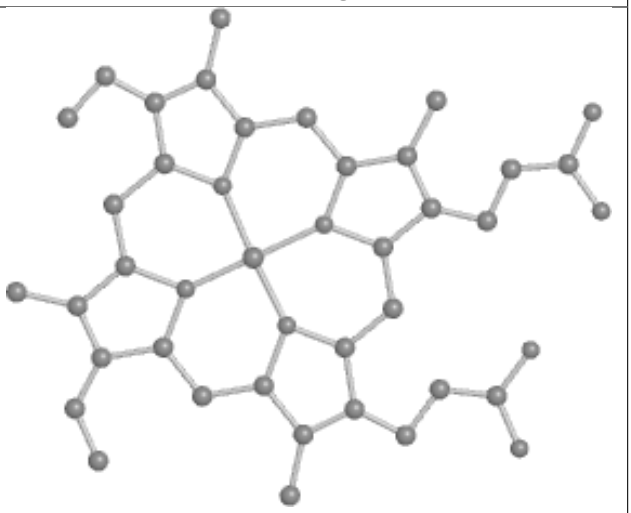
Bond lengths



Bond angles

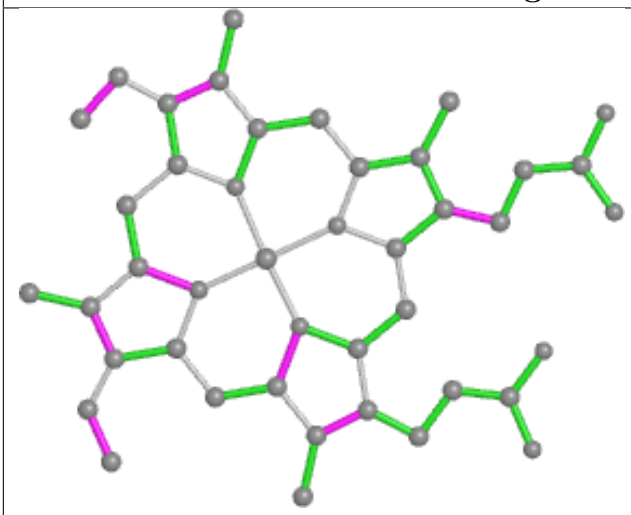


Torsions

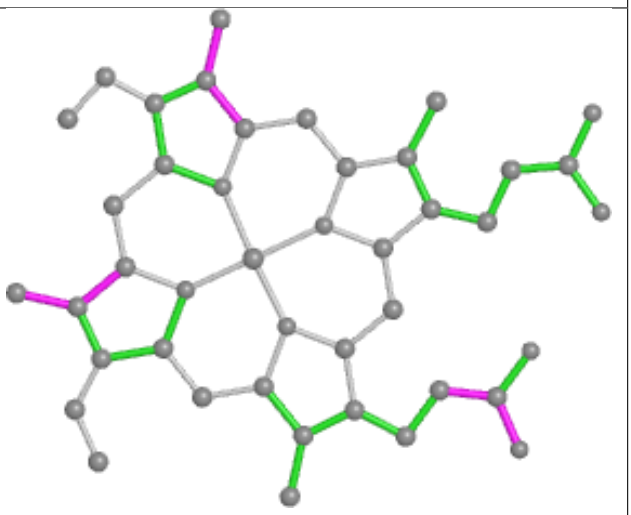


Rings

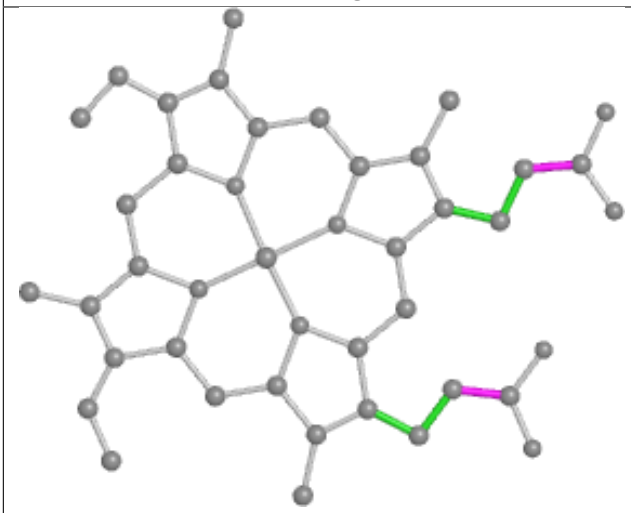
Ligand HEC E 804



Bond lengths



Bond angles



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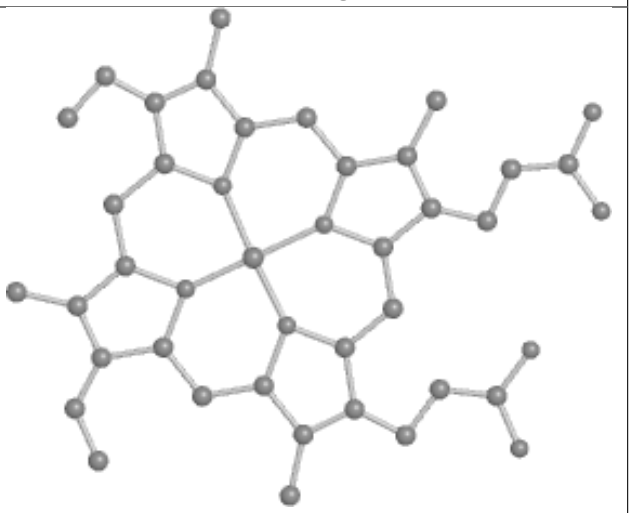
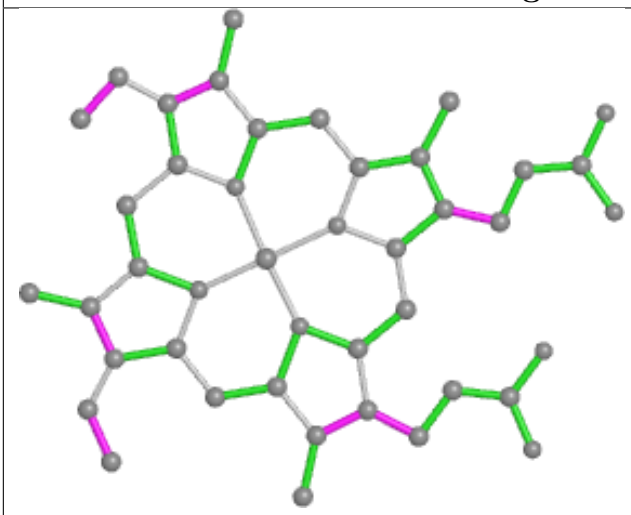
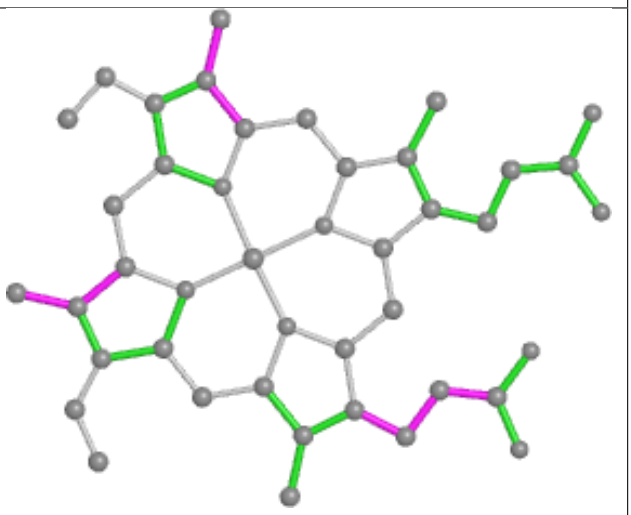


Rings

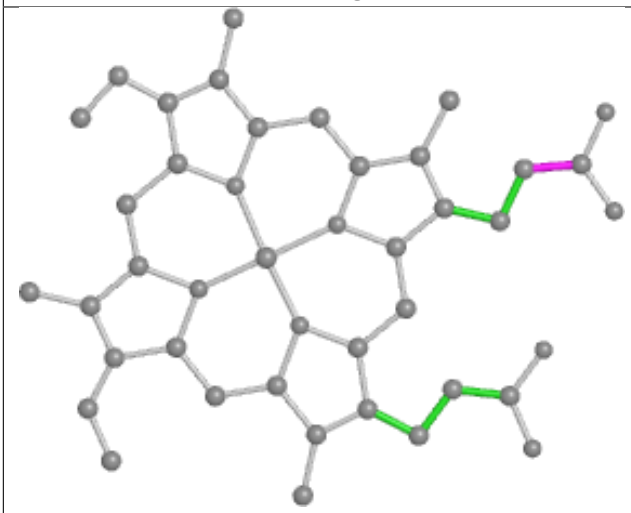
Ligand HEC C 802



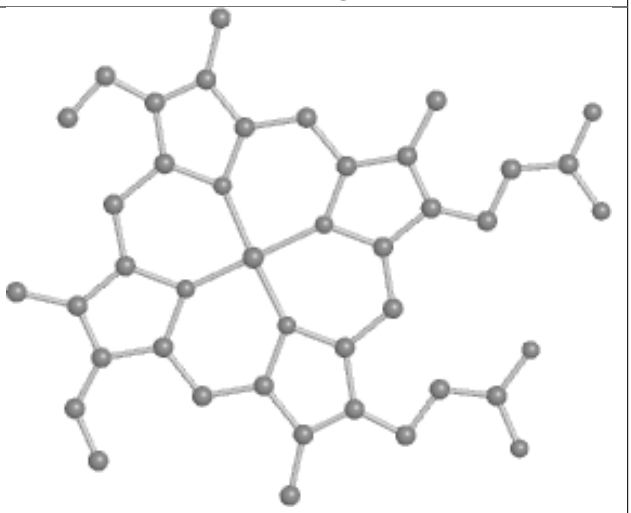
Bond lengths



Bond angles

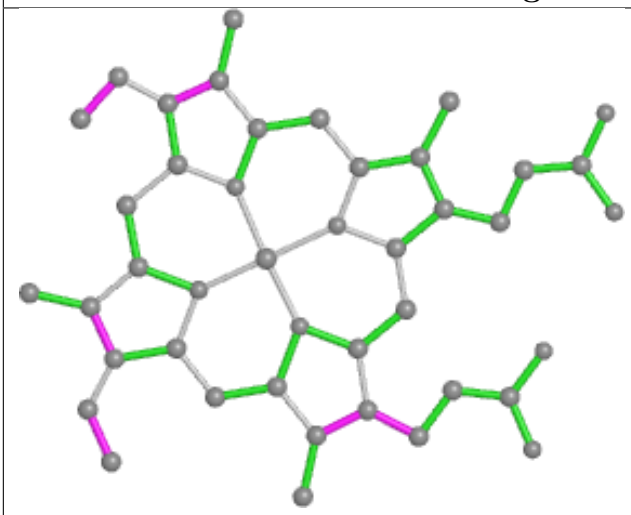


Torsions



Rings

Ligand HEC B 804



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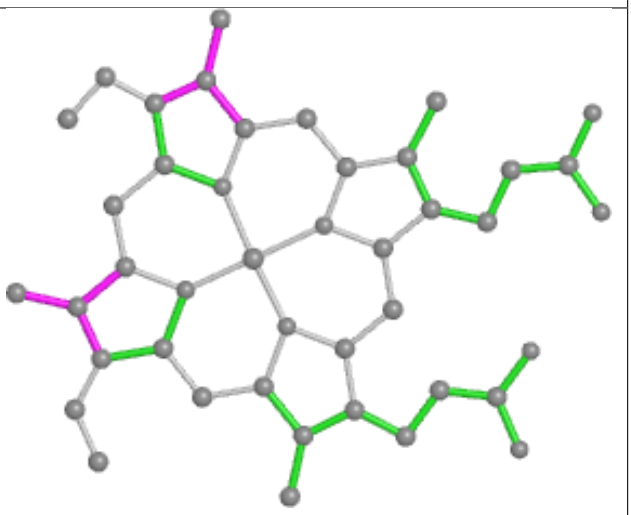

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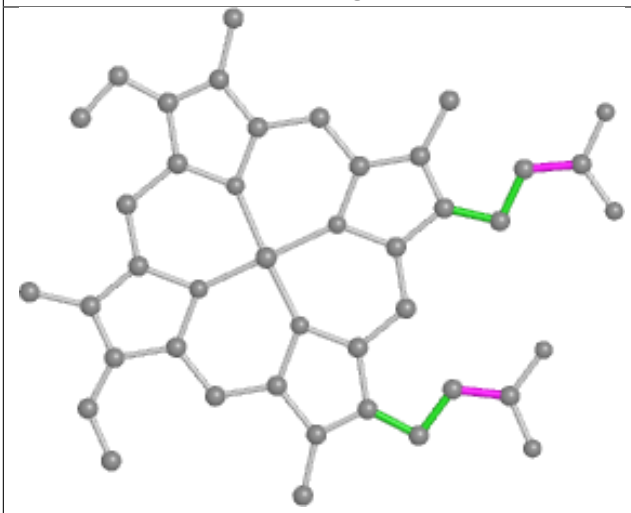

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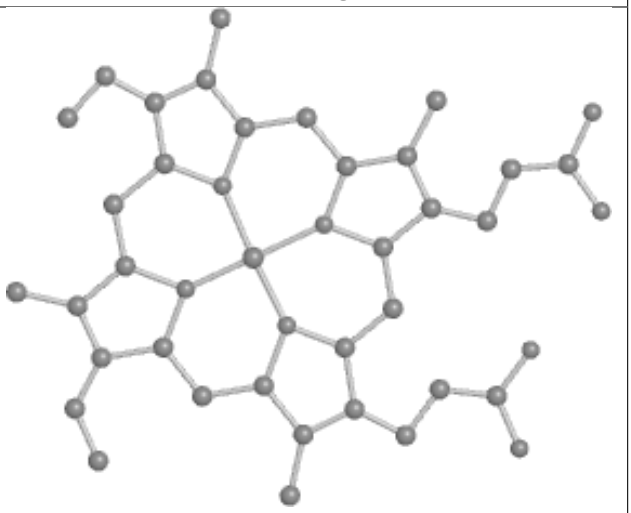
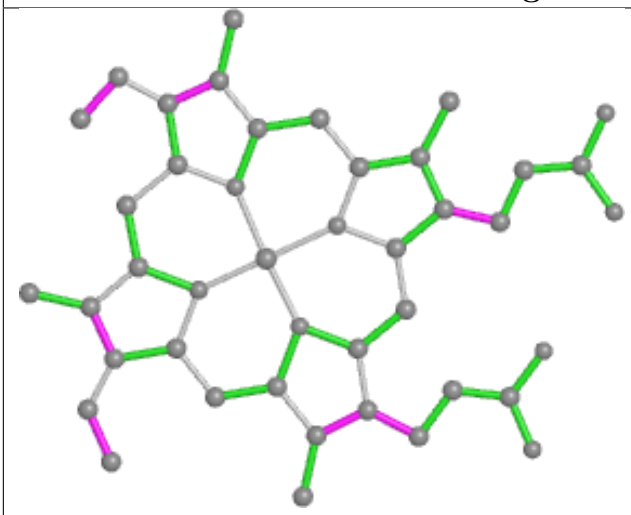


Rings

Ligand HEC C 804



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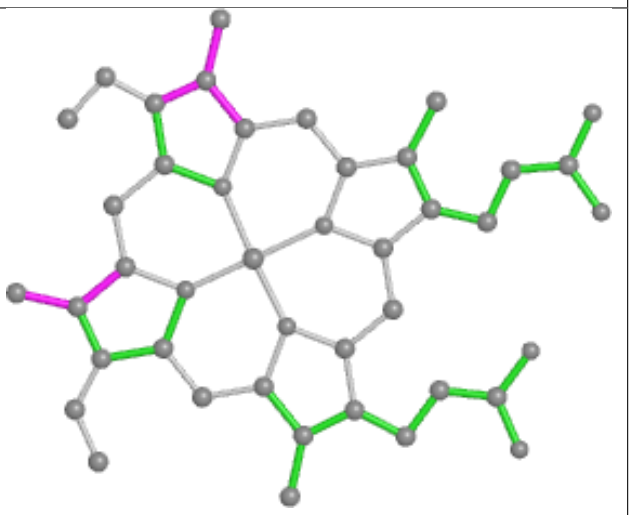

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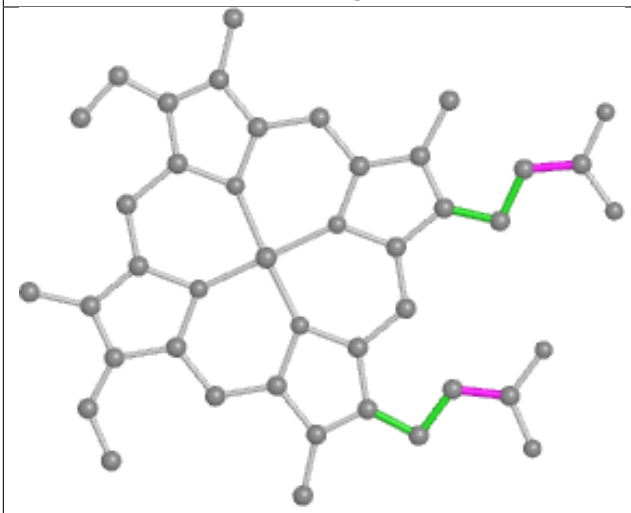

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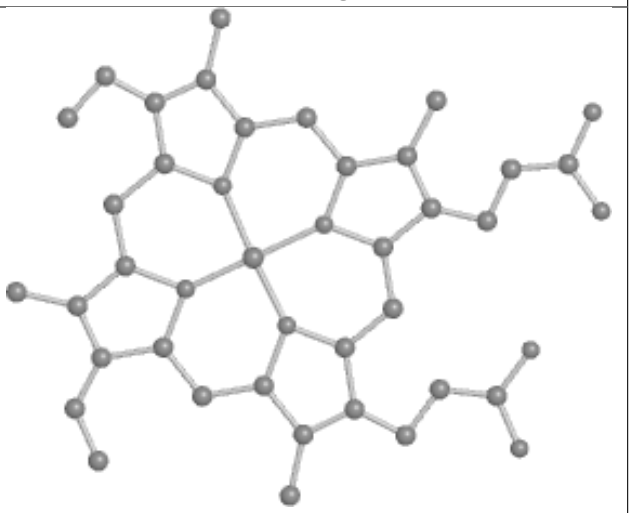
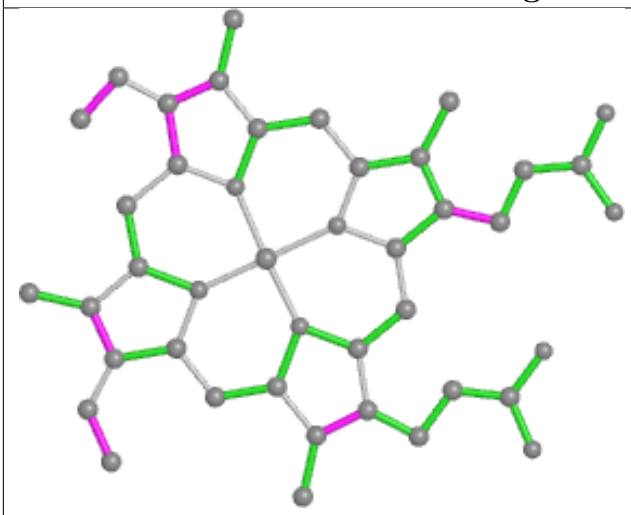


Rings

Ligand HEC B 803



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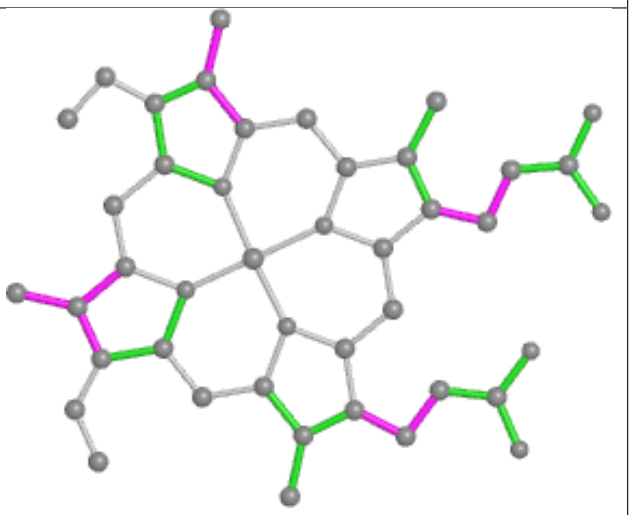

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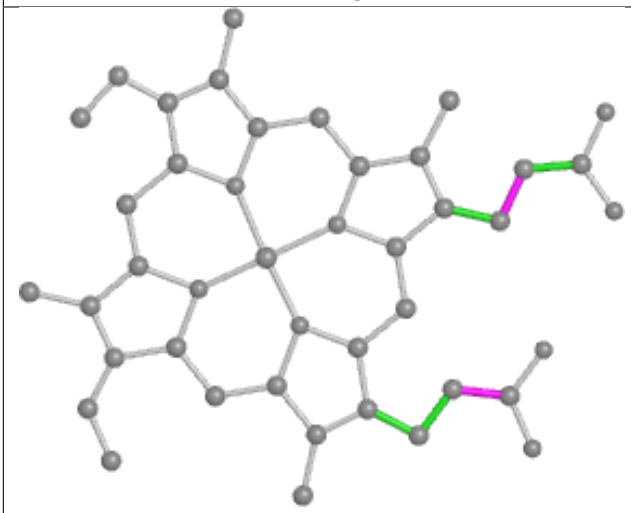

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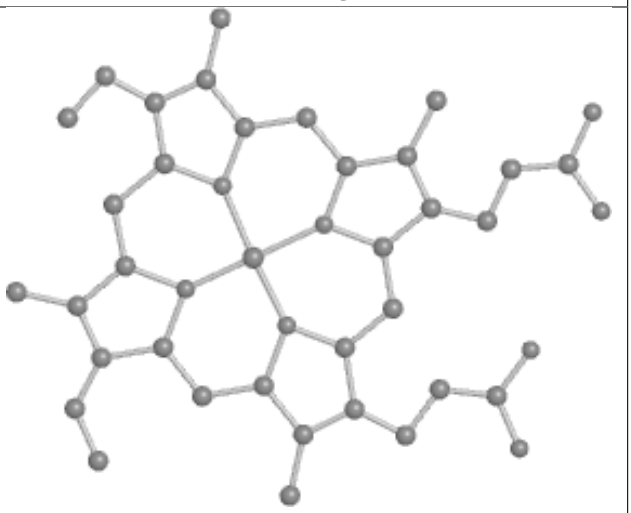
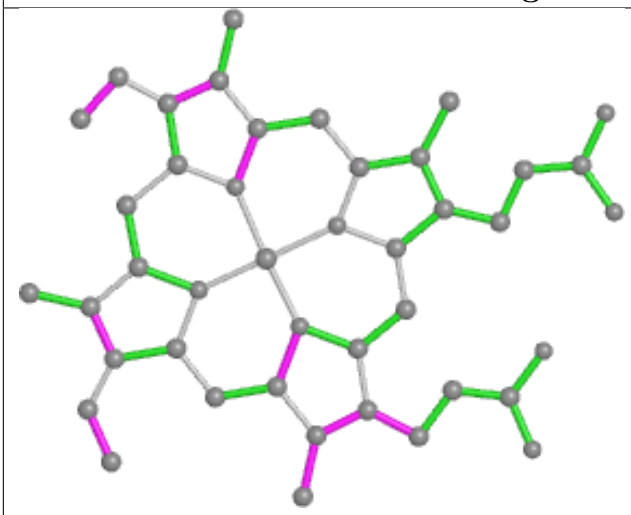


Rings

Ligand HEC D 802



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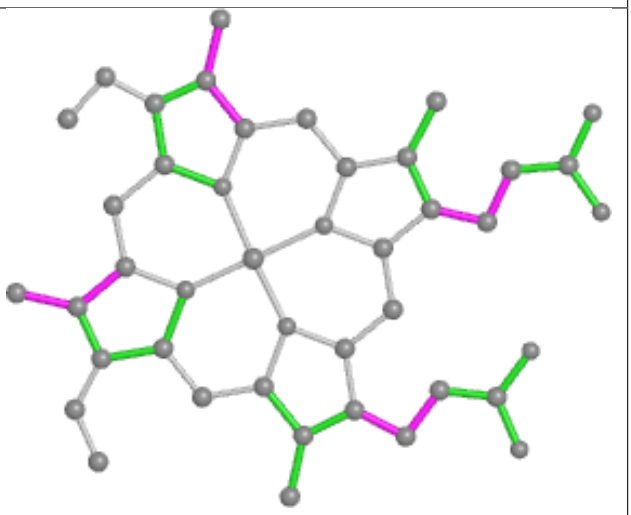

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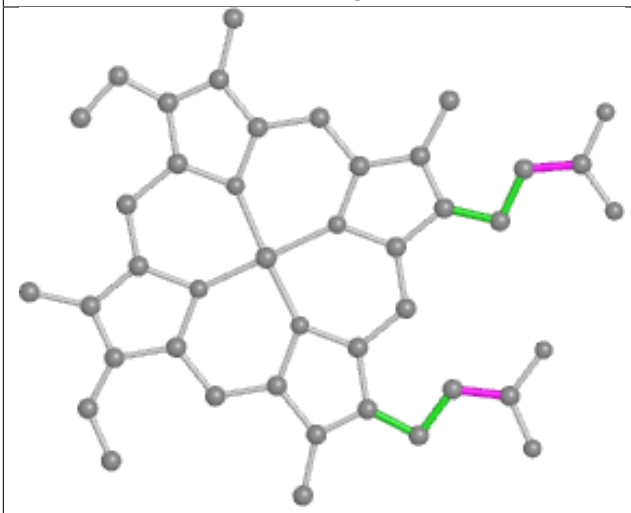

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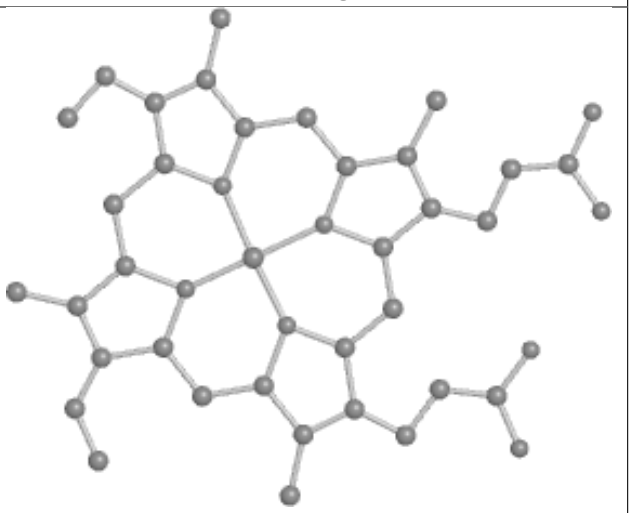

Rings

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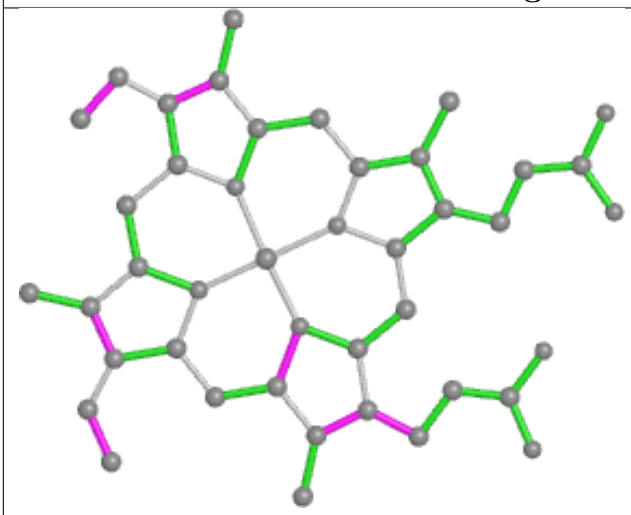

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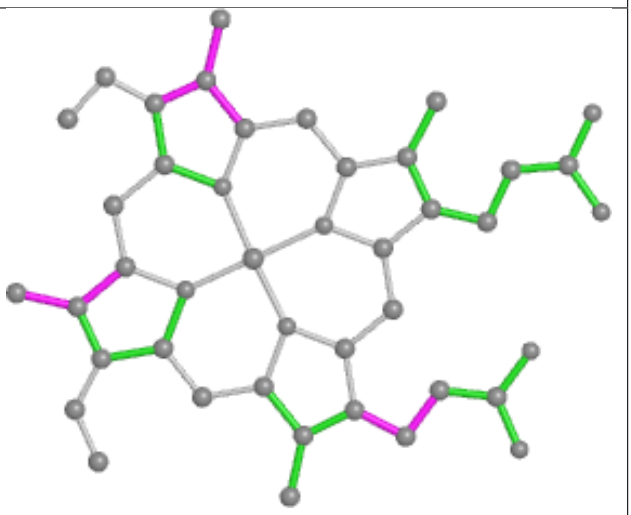

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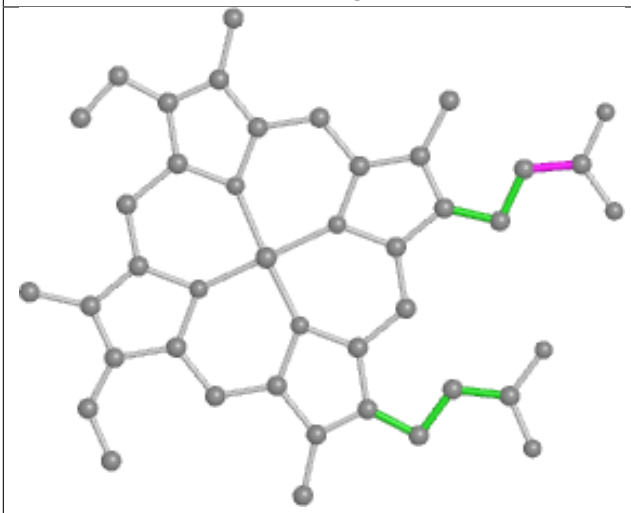

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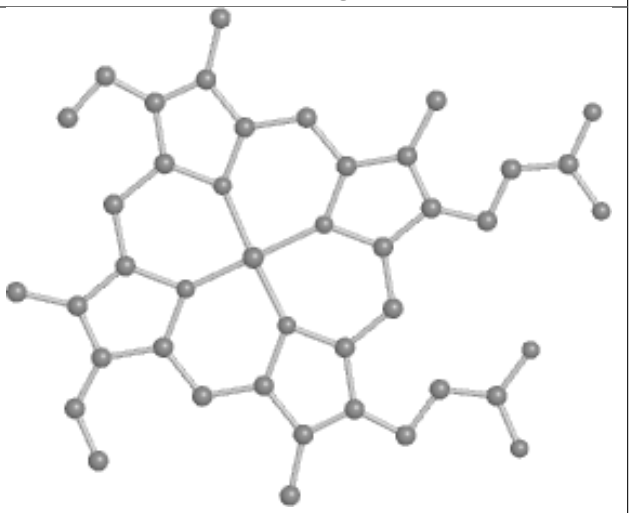

Rings

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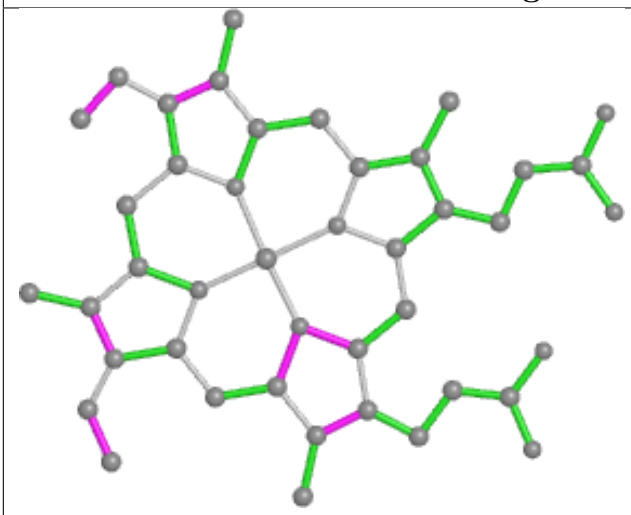

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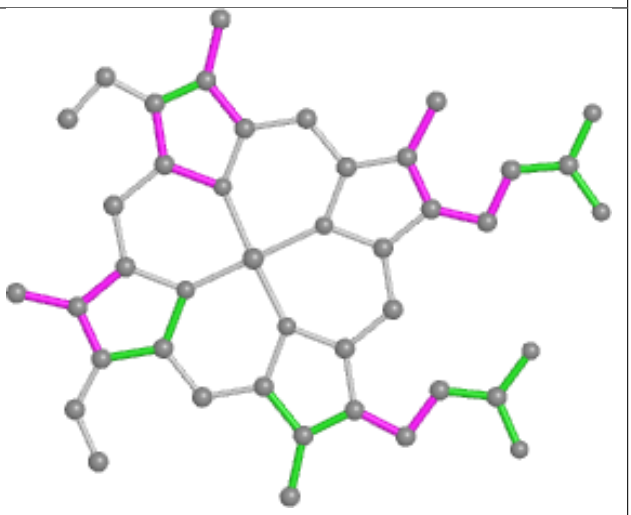

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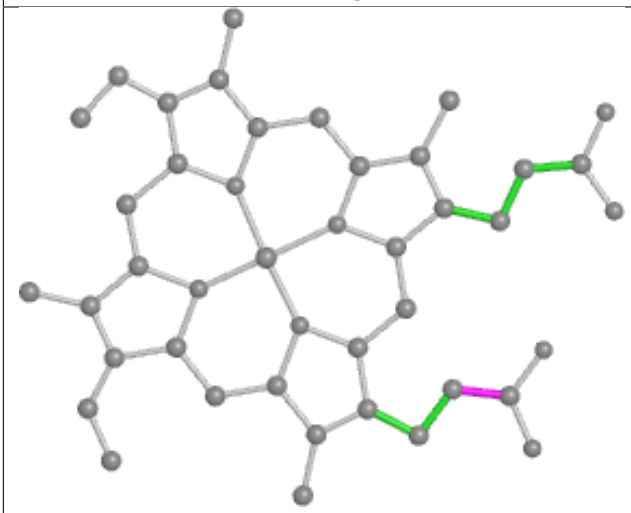

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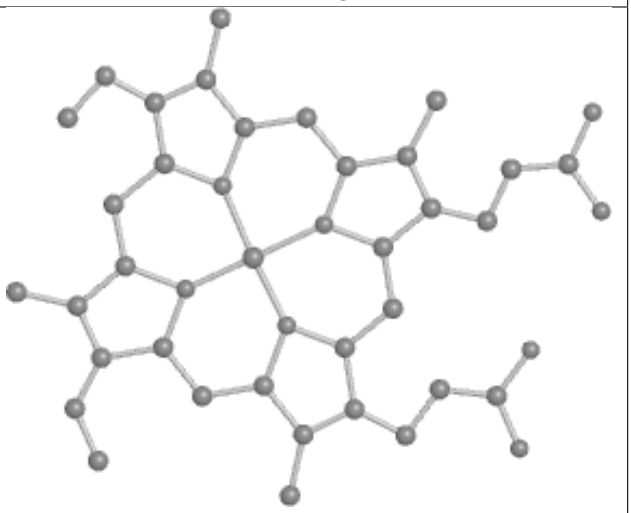

Rings

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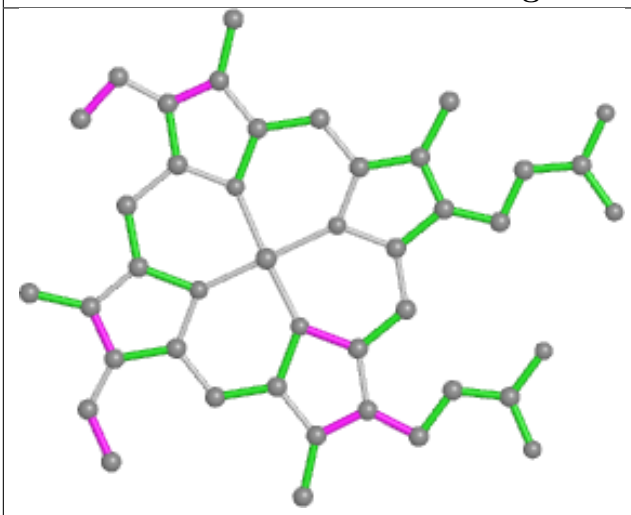

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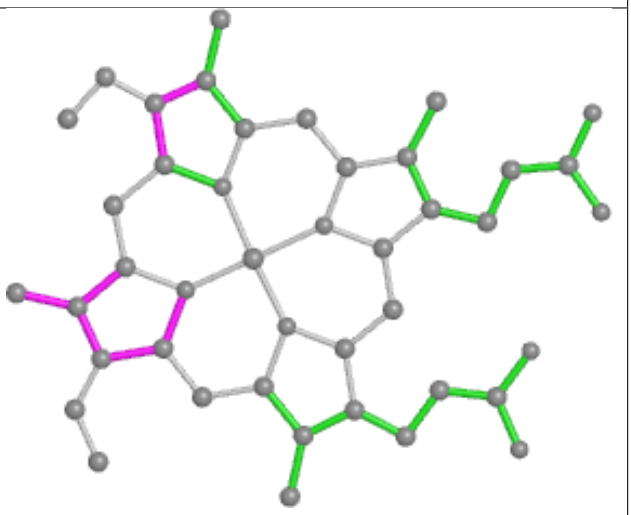

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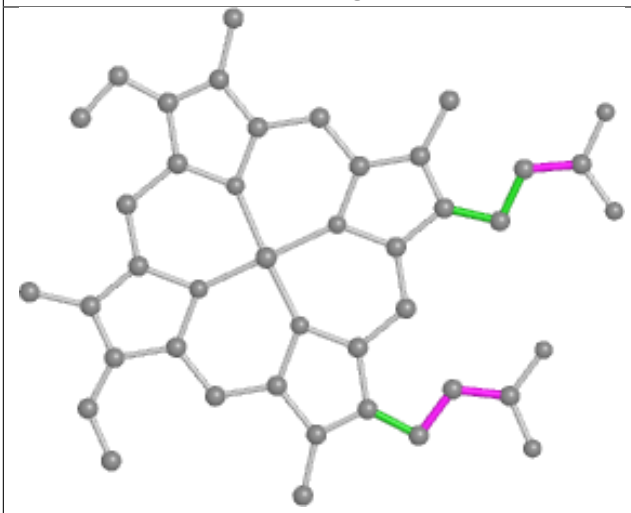

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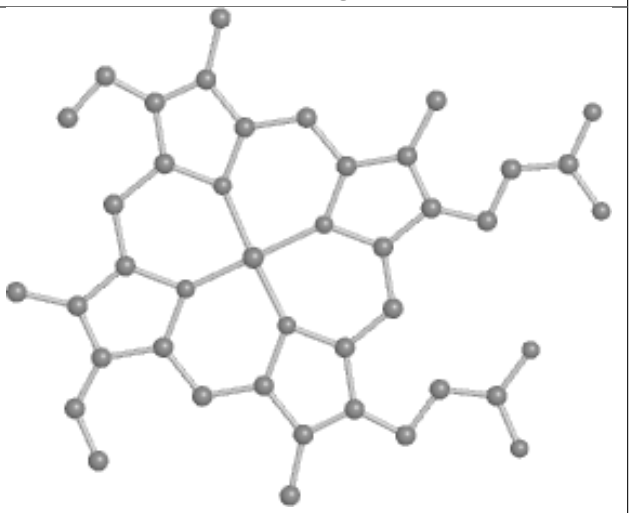

Rings

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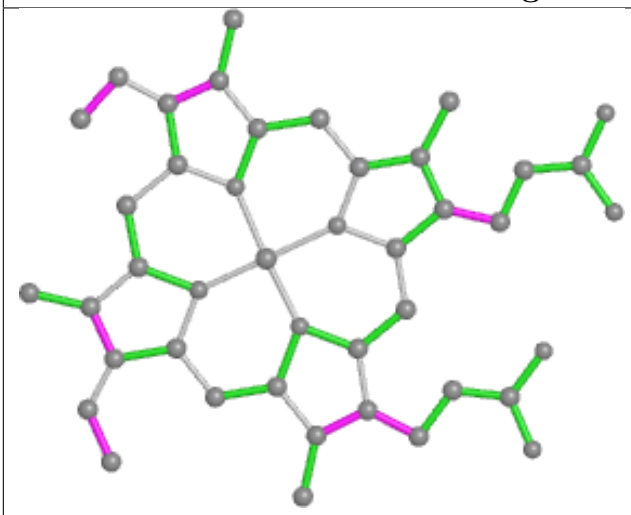

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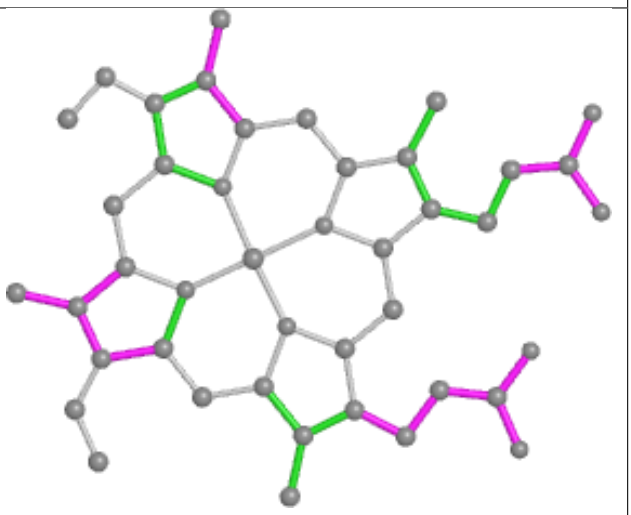

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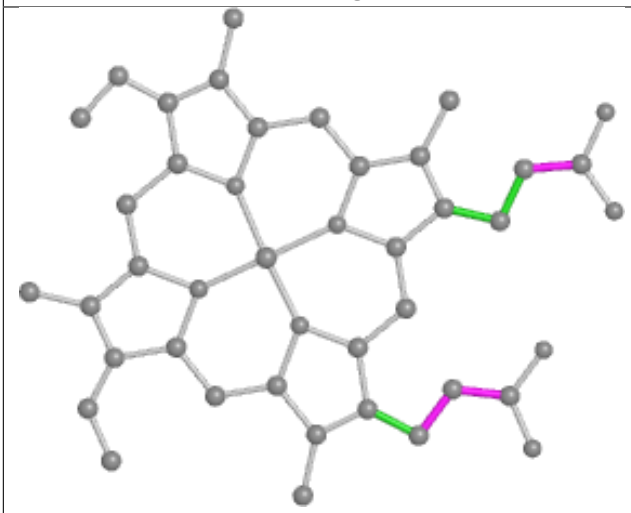

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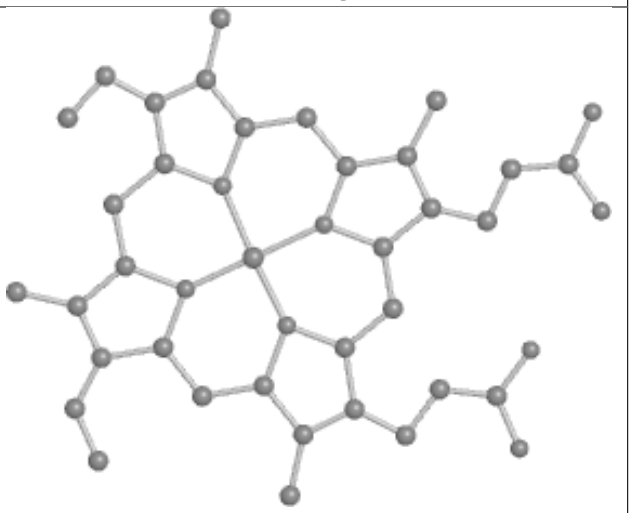

Rings

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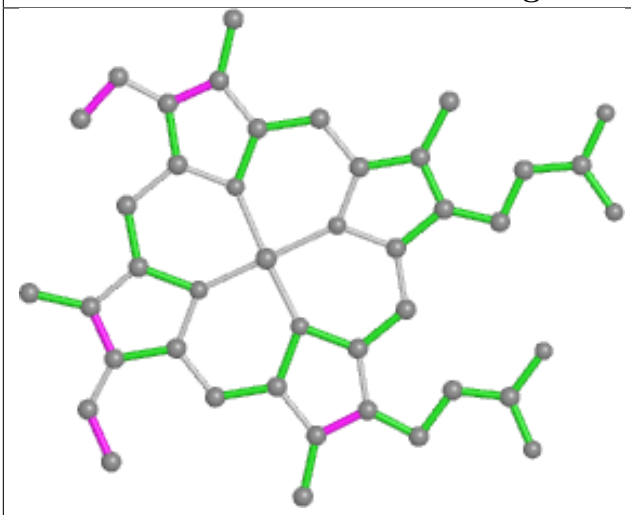

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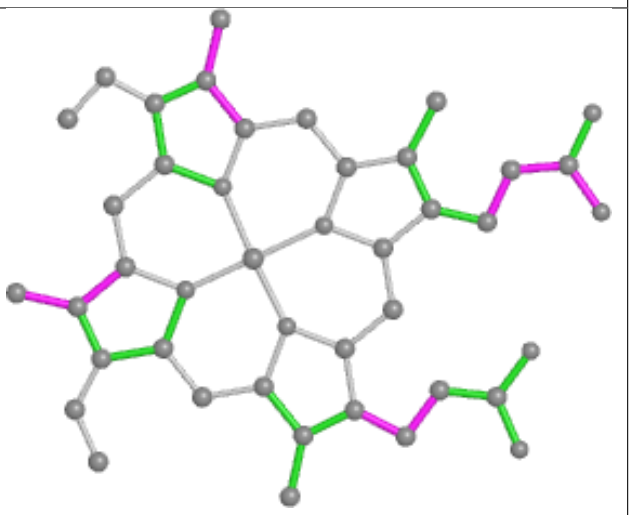

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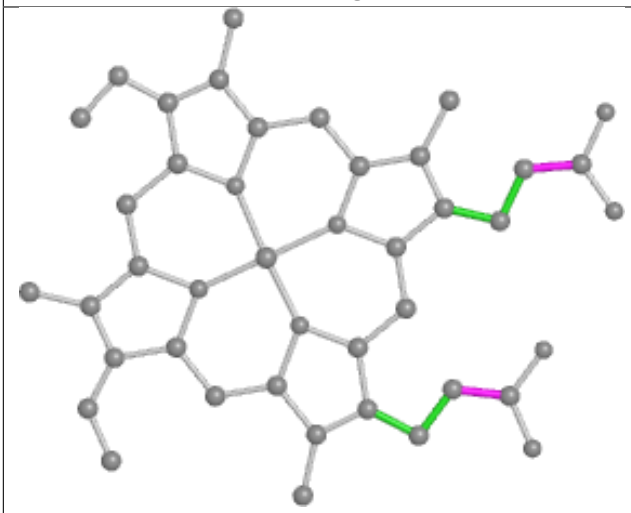

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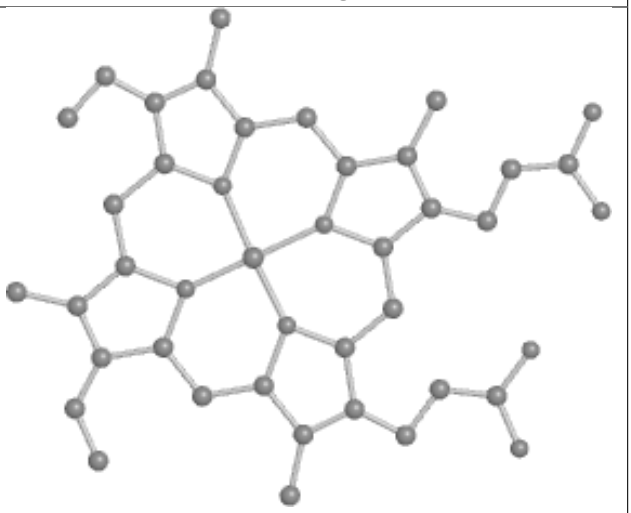

Rings

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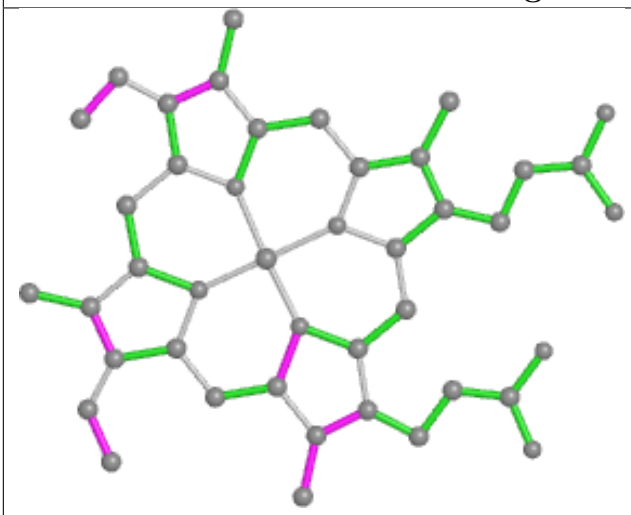

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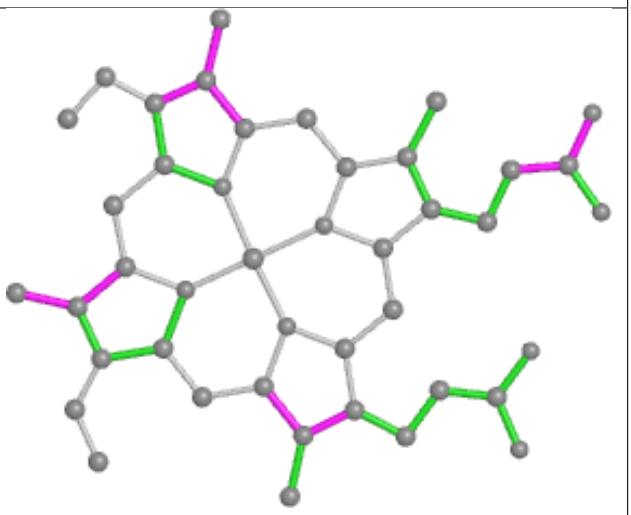

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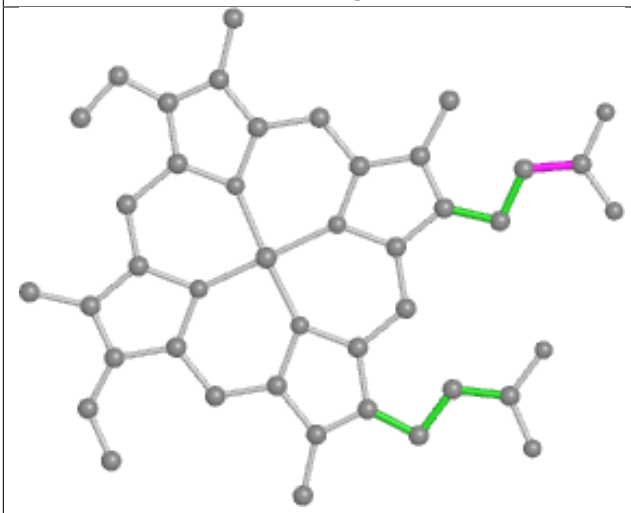

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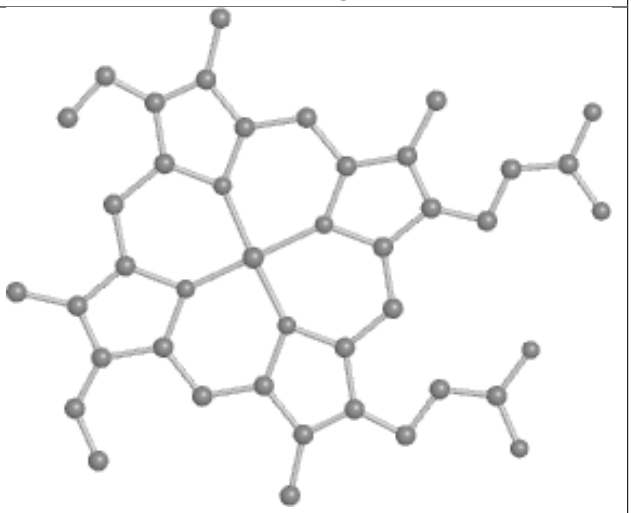

Rings

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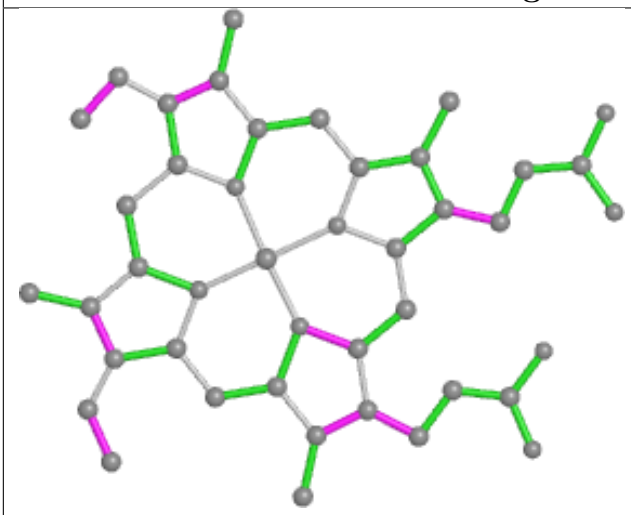

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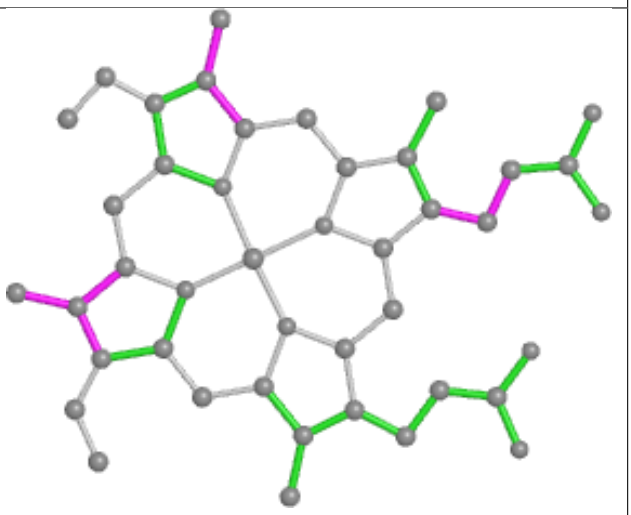

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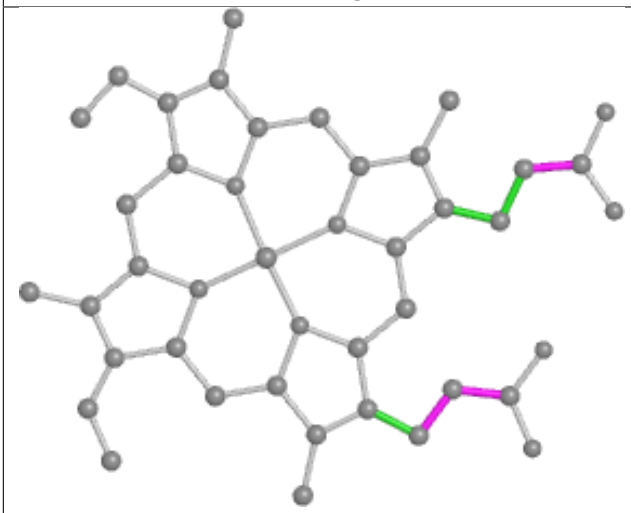

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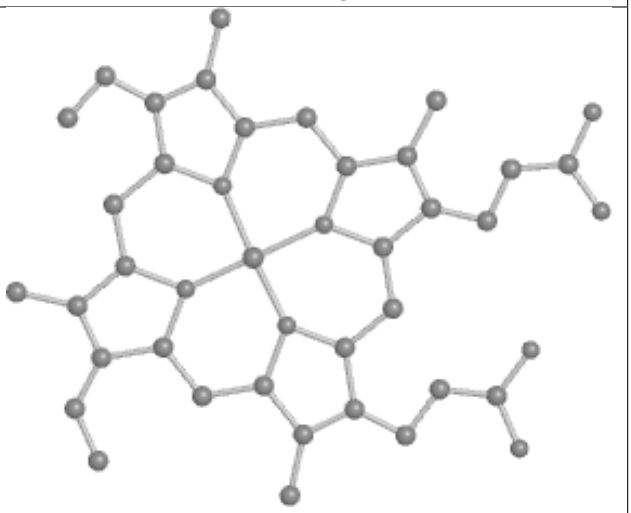

Rings

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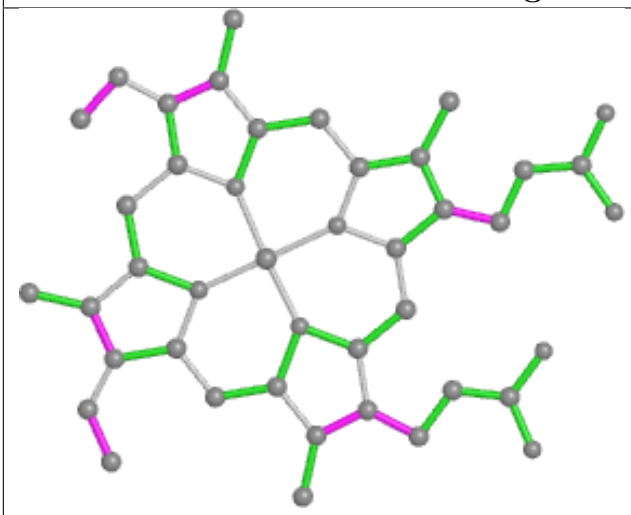

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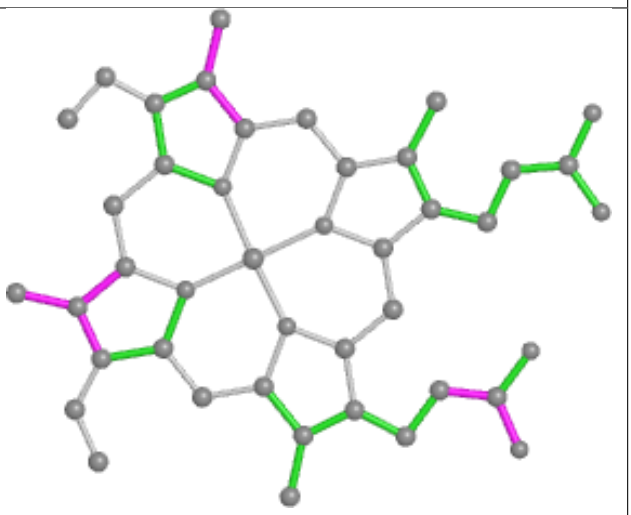

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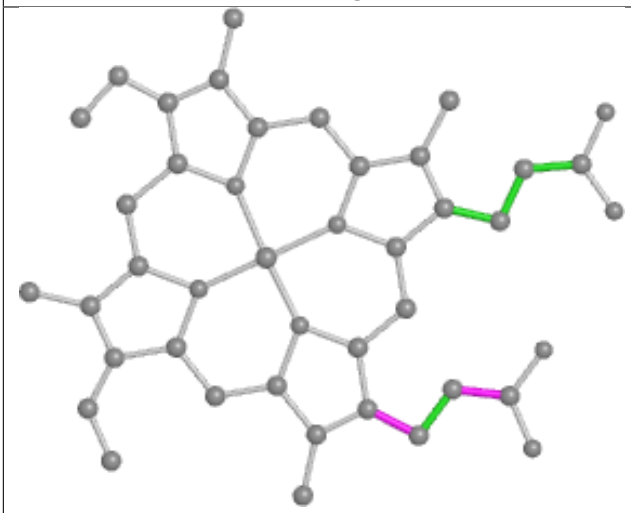

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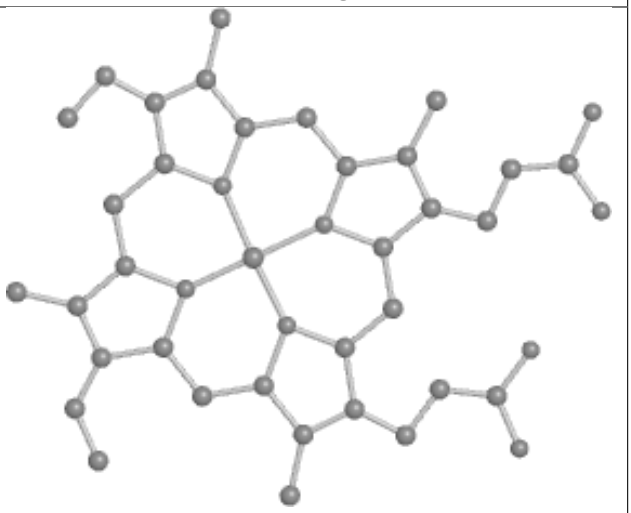
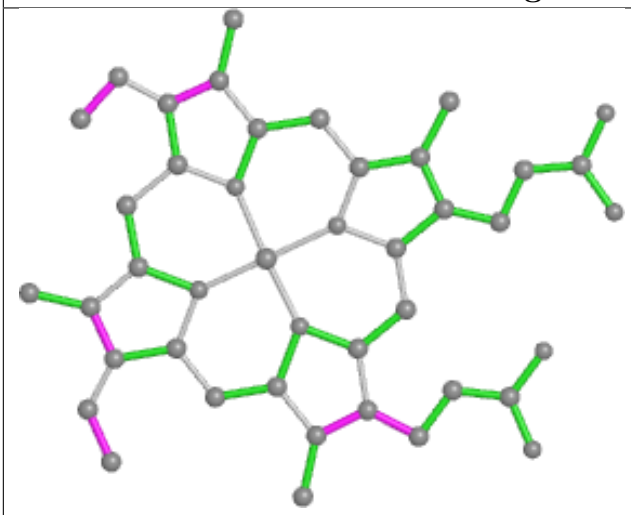


Rings

Ligand HEC F 804



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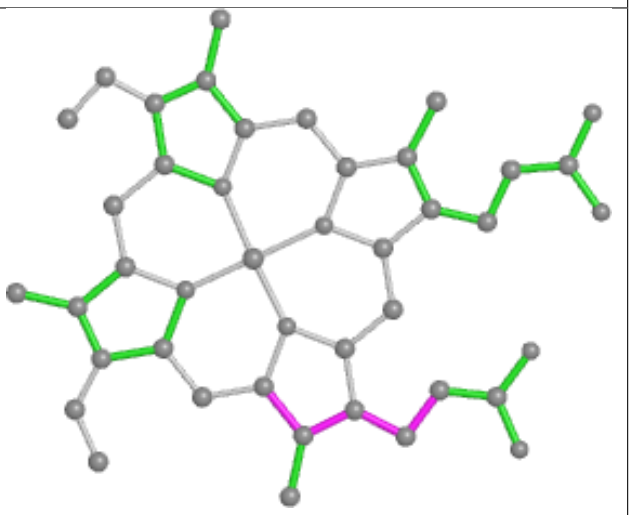

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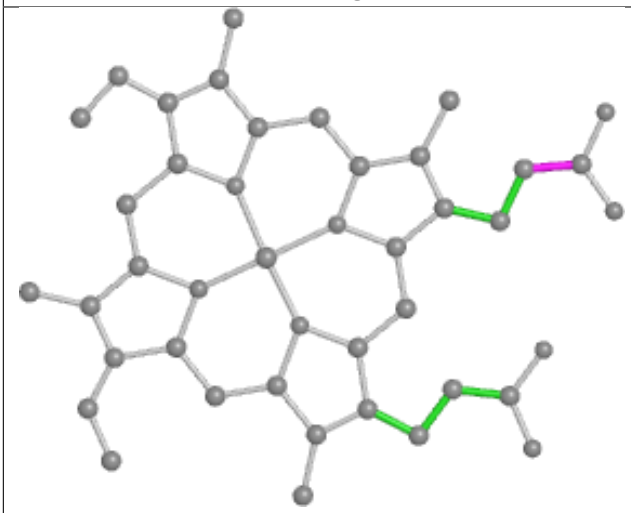

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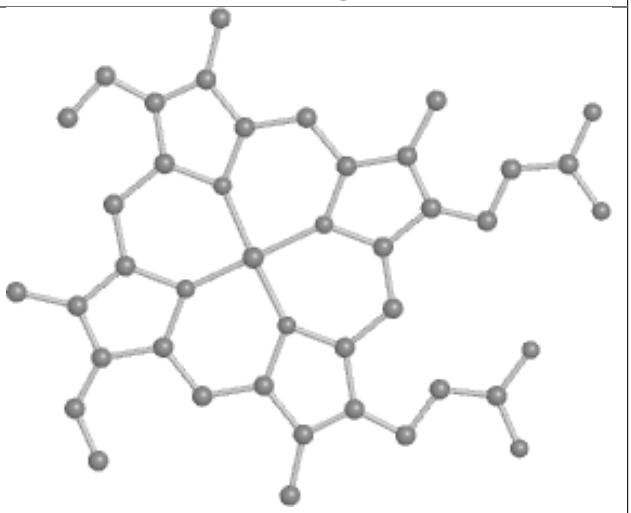
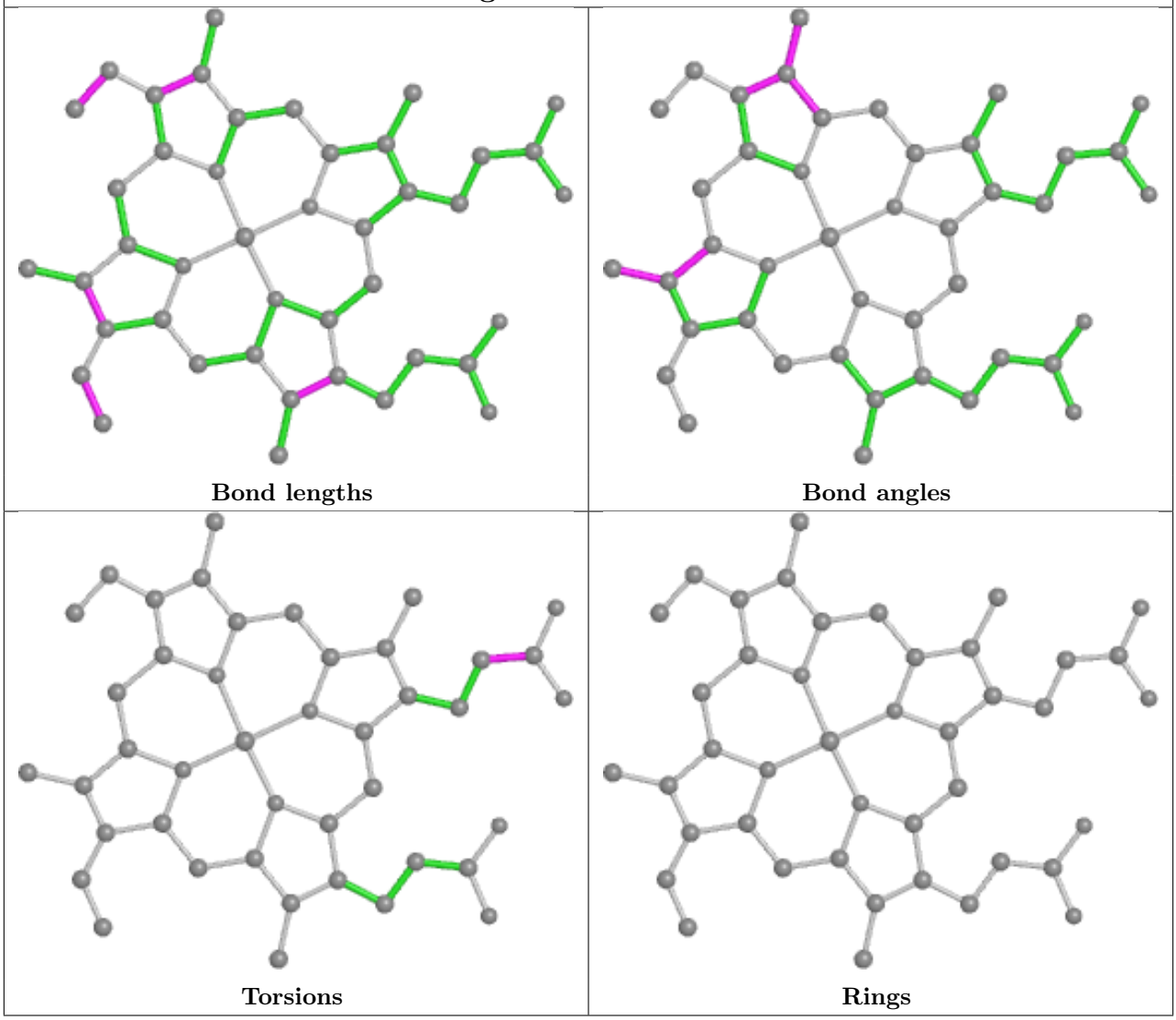


Rings

Ligand HEC A 802



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	88/91 (96%)	-0.15	0	100	100	8, 14, 24, 32	0
1	B	89/91 (97%)	0.06	1 (1%)	80	84	10, 17, 25, 32	0
1	C	86/91 (94%)	0.36	3 (3%)	44	52	12, 19, 26, 30	0
1	D	86/91 (94%)	0.06	1 (1%)	79	83	10, 15, 22, 28	0
1	E	88/91 (96%)	0.07	2 (2%)	60	66	11, 14, 21, 28	0
1	F	88/91 (96%)	0.18	4 (4%)	33	38	10, 16, 32, 38	0
All	All	525/546 (96%)	0.10	11 (2%)	63	69	8, 16, 26, 38	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	ASP	4.4
1	F	2	ASP	3.7
1	C	89	LEU	3.2
1	E	26	ALA	2.8
1	B	2	ASP	2.7
1	F	86	ALA	2.5
1	F	81	ASP	2.4
1	D	37	SER	2.1
1	C	26	ALA	2.1
1	F	87	SER	2.0
1	C	41	LYS	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.

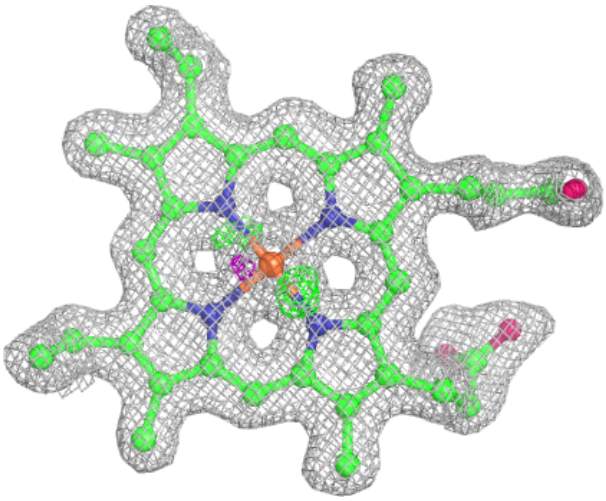
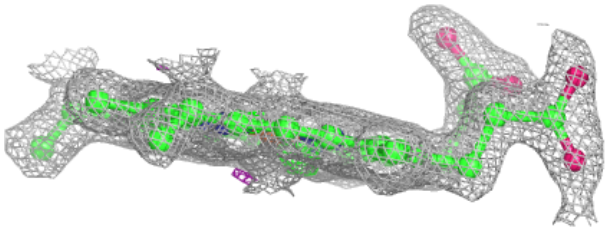
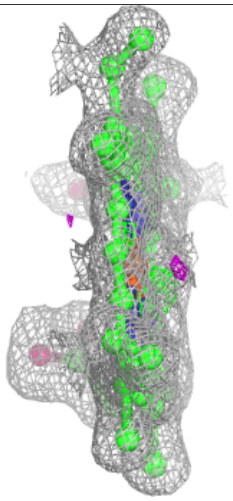
6.4 Ligands (i)

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
2	SO4	F	1163	5/5	0.93	0.16	32,33,34,35	0
3	HEC	F	804	43/43	0.94	0.14	14,18,29,32	0
3	HEC	B	802	43/43	0.95	0.12	11,16,35,36	0
3	HEC	B	803	43/43	0.95	0.12	11,14,30,40	0
3	HEC	C	804	43/43	0.95	0.13	14,17,30,36	0
3	HEC	C	802	43/43	0.95	0.12	12,15,25,31	0
3	HEC	C	803	43/43	0.95	0.13	9,13,25,33	0
2	SO4	C	1162	5/5	0.95	0.17	24,25,27,28	0
3	HEC	B	804	43/43	0.96	0.11	12,15,32,39	0
3	HEC	D	801	43/43	0.96	0.12	9,12,25,29	0
3	HEC	D	802	43/43	0.96	0.10	9,14,22,24	0
3	HEC	E	801	43/43	0.96	0.12	9,13,32,39	0
3	HEC	E	803	43/43	0.96	0.10	9,11,25,34	0
3	HEC	C	801	43/43	0.96	0.12	10,14,31,32	0
2	SO4	A	1164	5/5	0.97	0.13	24,26,26,28	0
3	HEC	D	803	43/43	0.97	0.10	9,11,23,34	0
3	HEC	A	804	43/43	0.97	0.11	10,13,28,35	0
3	HEC	E	802	43/43	0.97	0.10	8,11,24,26	0
3	HEC	A	803	43/43	0.97	0.09	7,10,23,30	0
3	HEC	B	801	43/43	0.97	0.11	9,12,32,36	0
3	HEC	F	802	43/43	0.97	0.11	8,11,27,35	0
3	HEC	F	803	43/43	0.97	0.10	9,12,29,34	0
3	HEC	D	804	43/43	0.98	0.09	7,10,14,19	0
2	SO4	B	1165	5/5	0.98	0.06	18,21,22,23	0
3	HEC	F	801	43/43	0.98	0.09	8,11,22,24	0
3	HEC	A	802	43/43	0.98	0.09	5,9,20,23	0
3	HEC	A	801	43/43	0.98	0.10	7,10,23,32	0
3	HEC	E	804	43/43	0.98	0.07	8,11,16,22	0

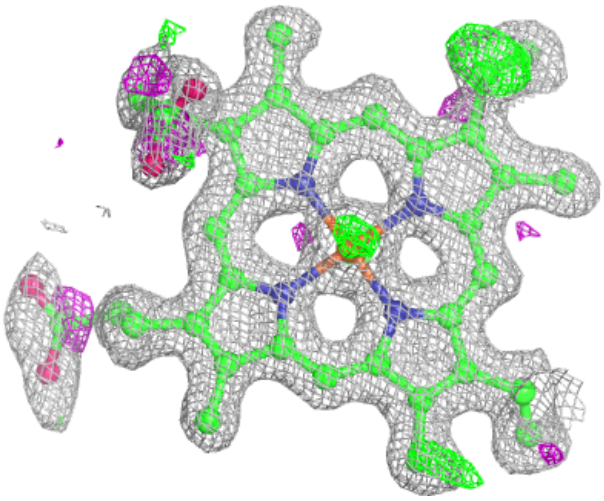
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

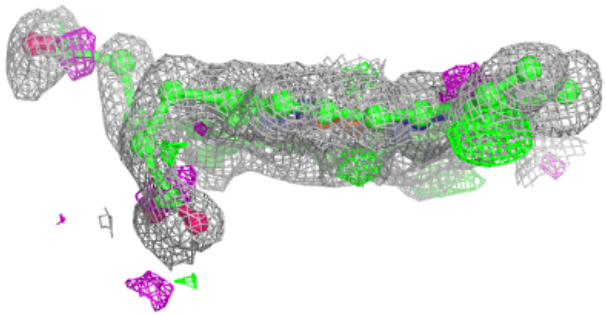
orientation to approximate a three-dimensional view.

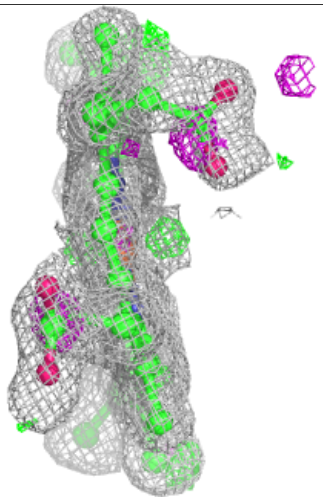
Electron density around HEC F 804: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around HEC B 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 803:

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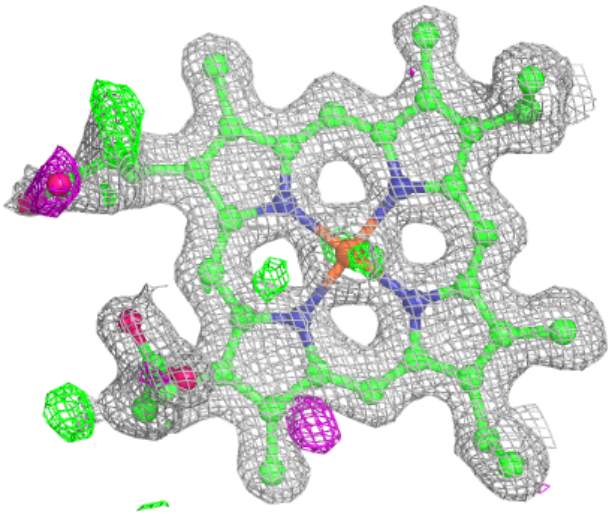
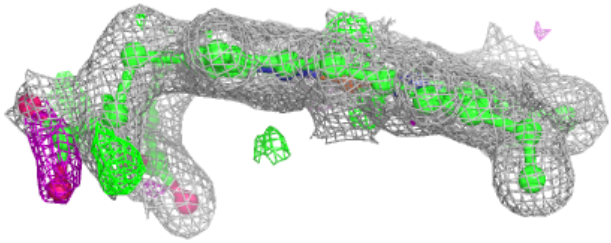
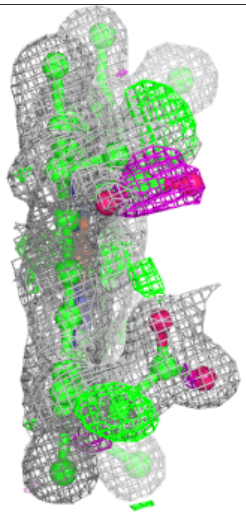
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC C 804:

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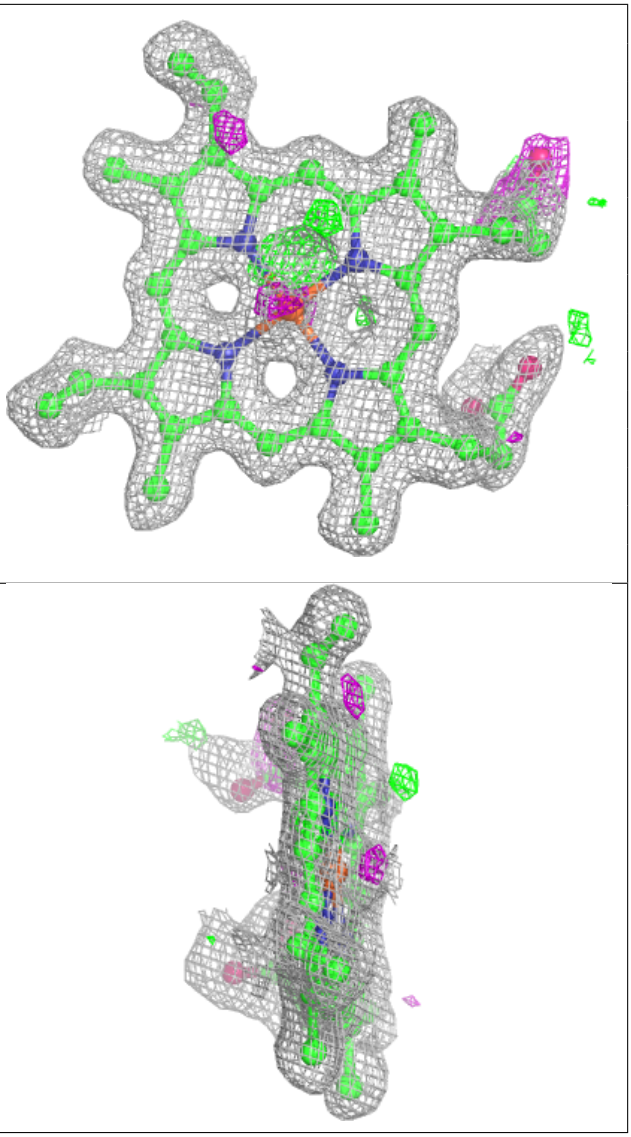
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 802:

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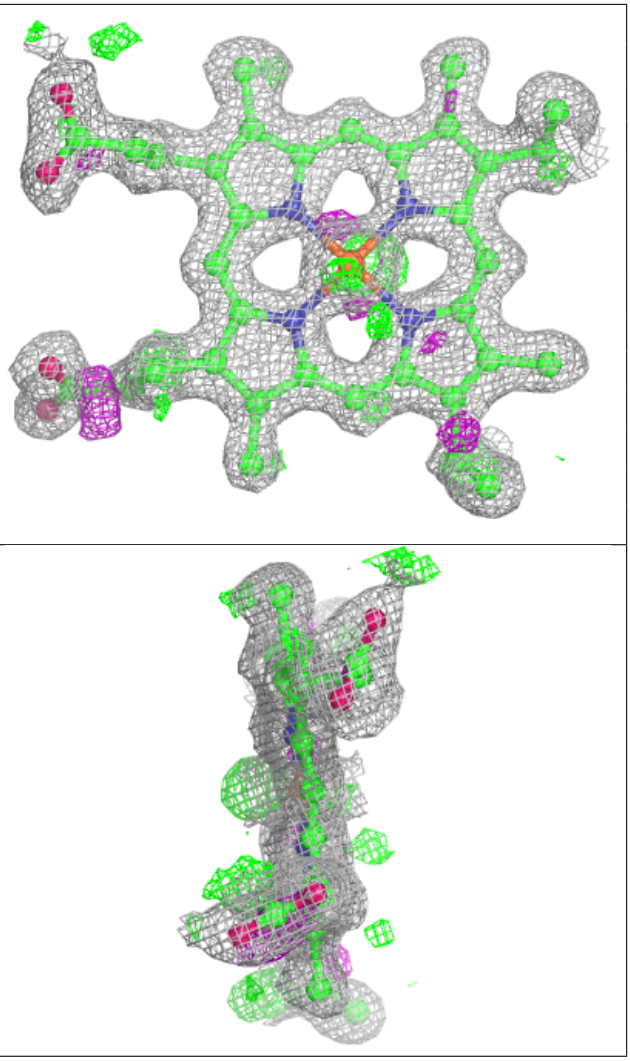
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 803:

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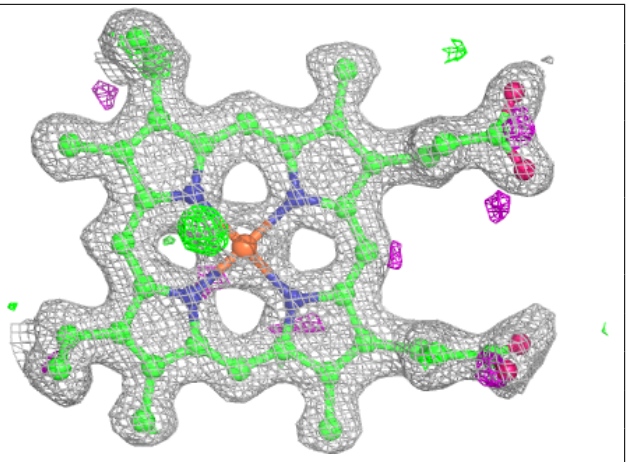
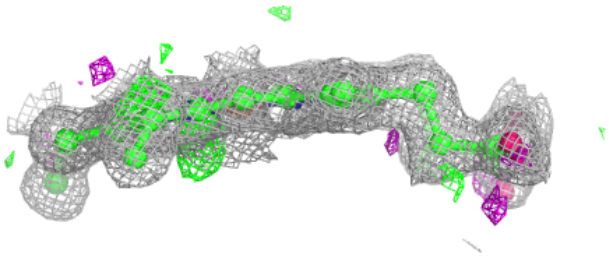
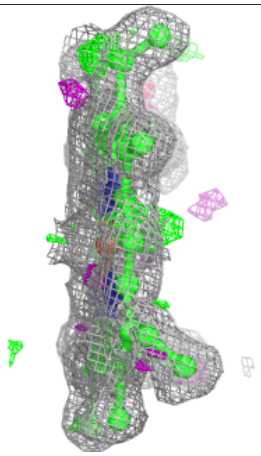
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC B 804:

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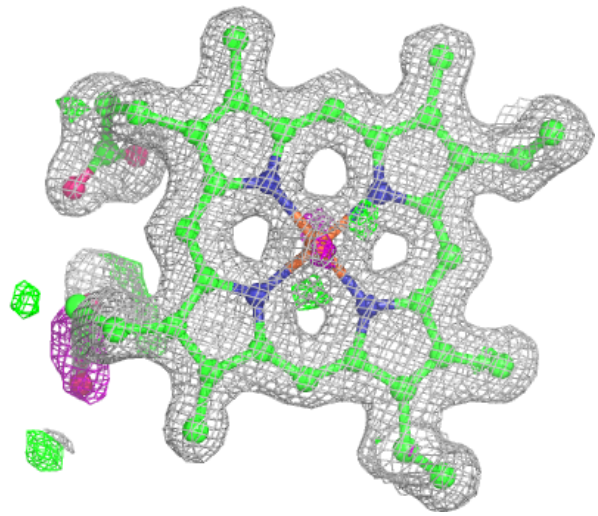
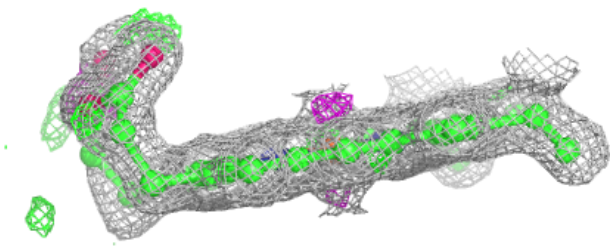
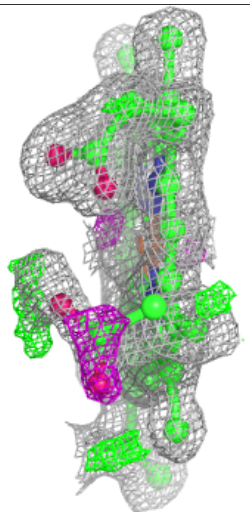
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC D 801:

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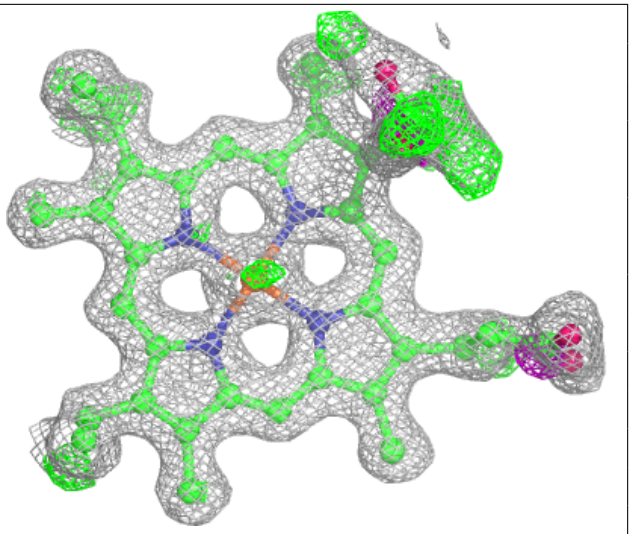
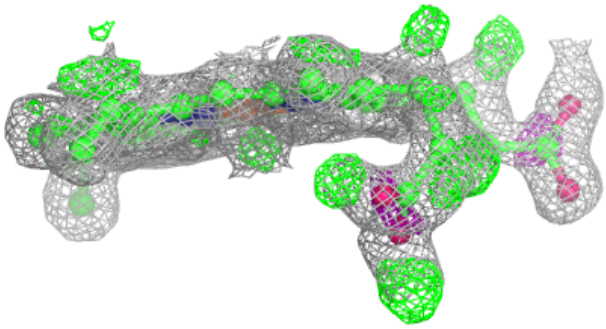
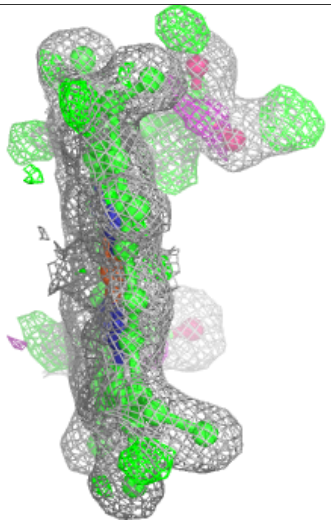
and green (positive)







Electron density around HEC D 802:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
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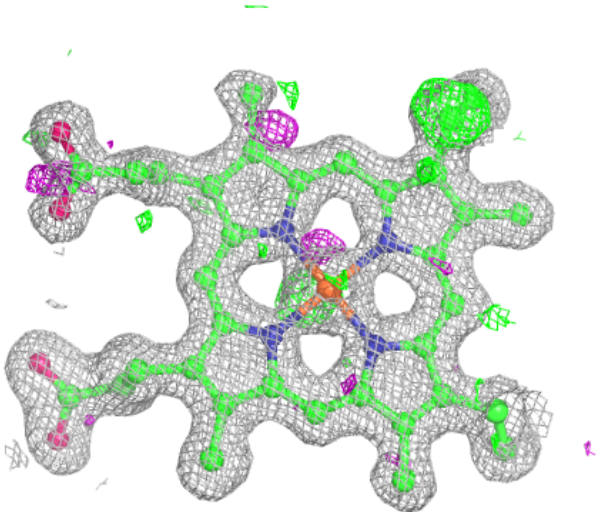

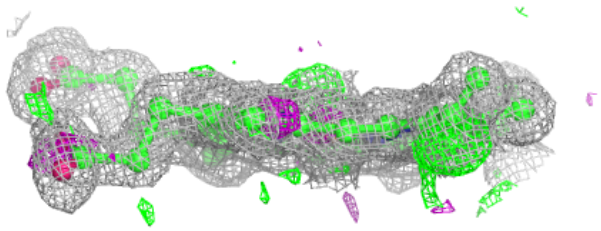

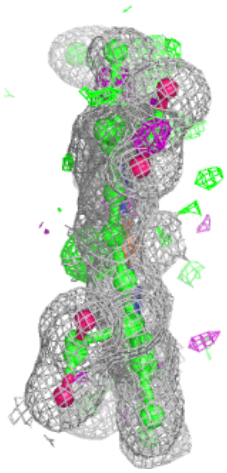

Electron density around HEC E 801:

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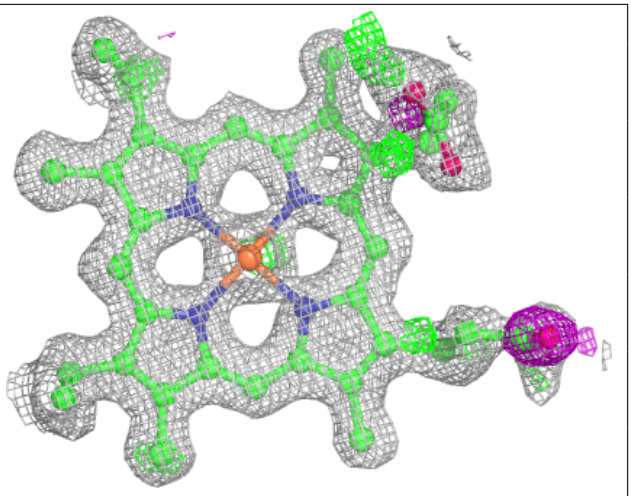
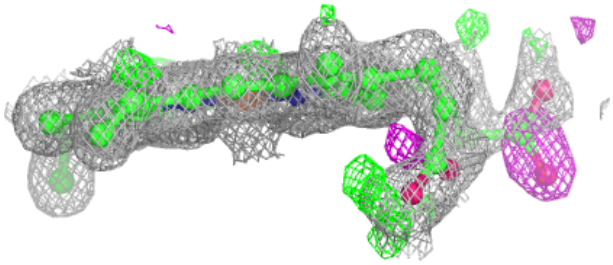
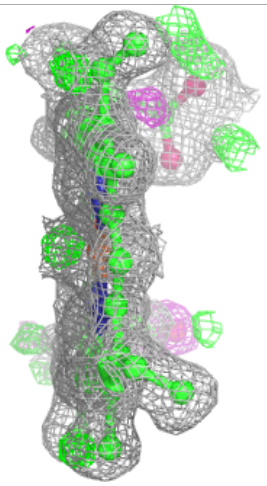
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC E 803:

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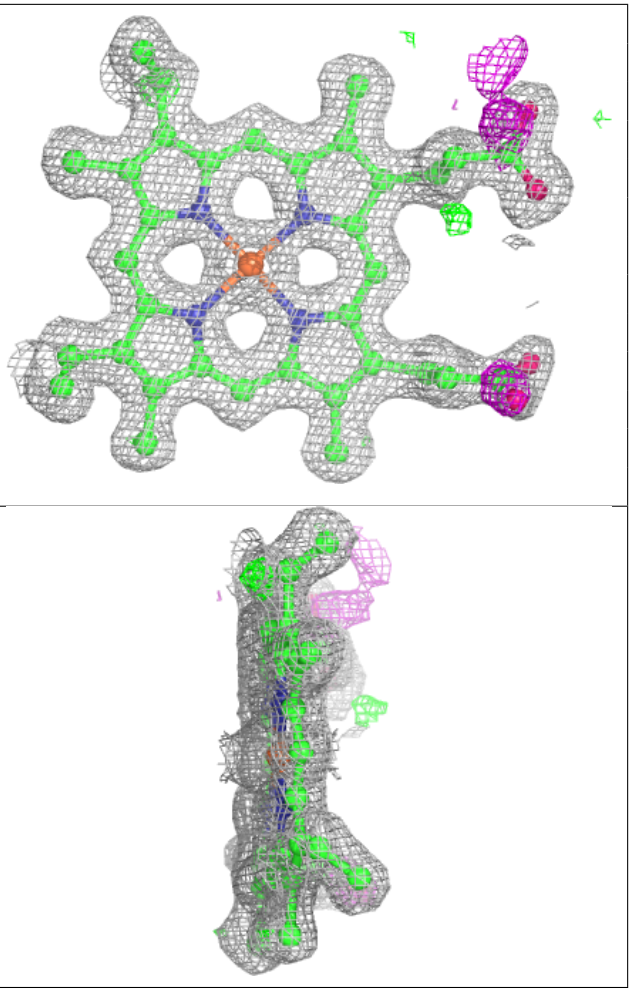
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 801:

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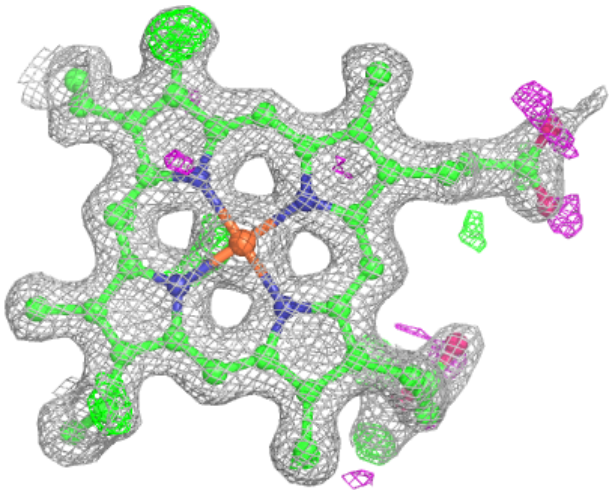
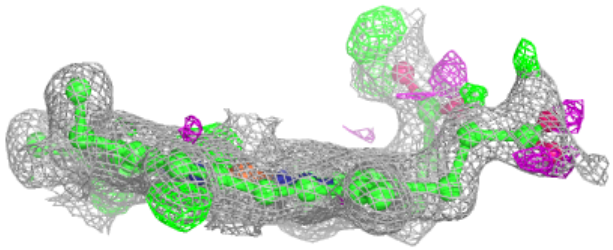
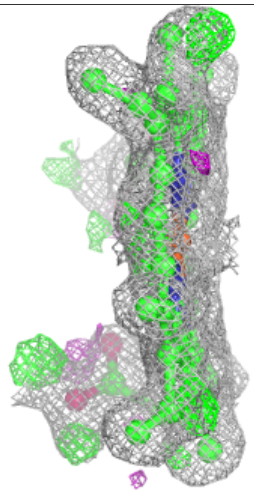
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC D 803:

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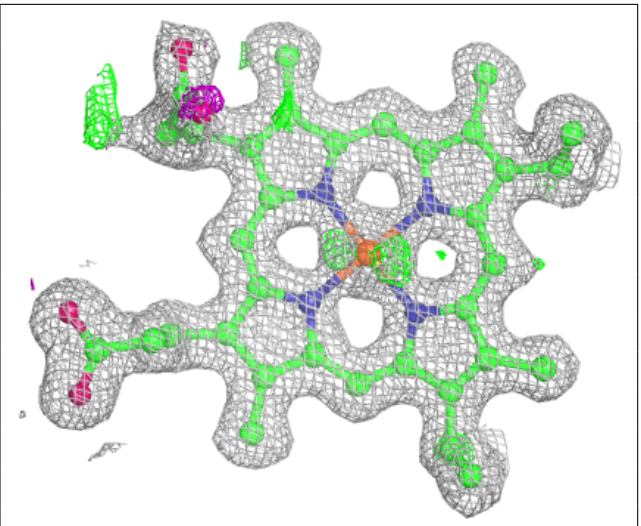
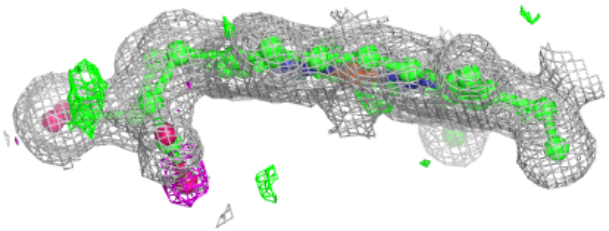
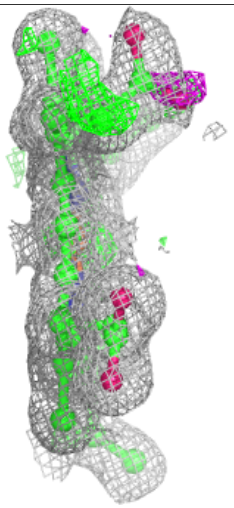
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC A 804:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
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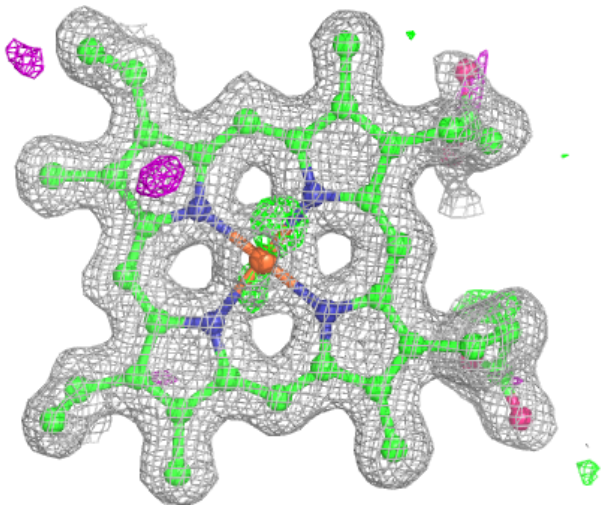
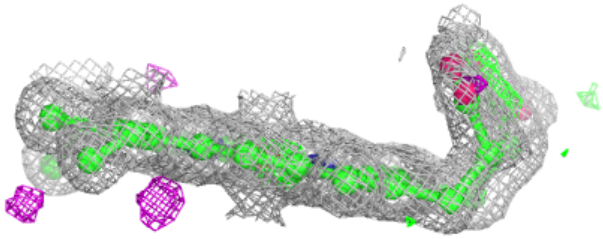
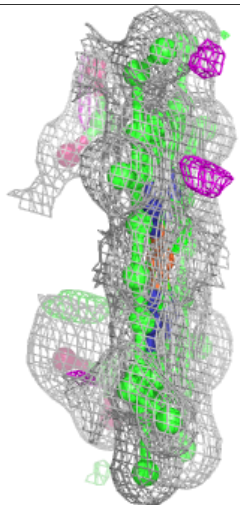
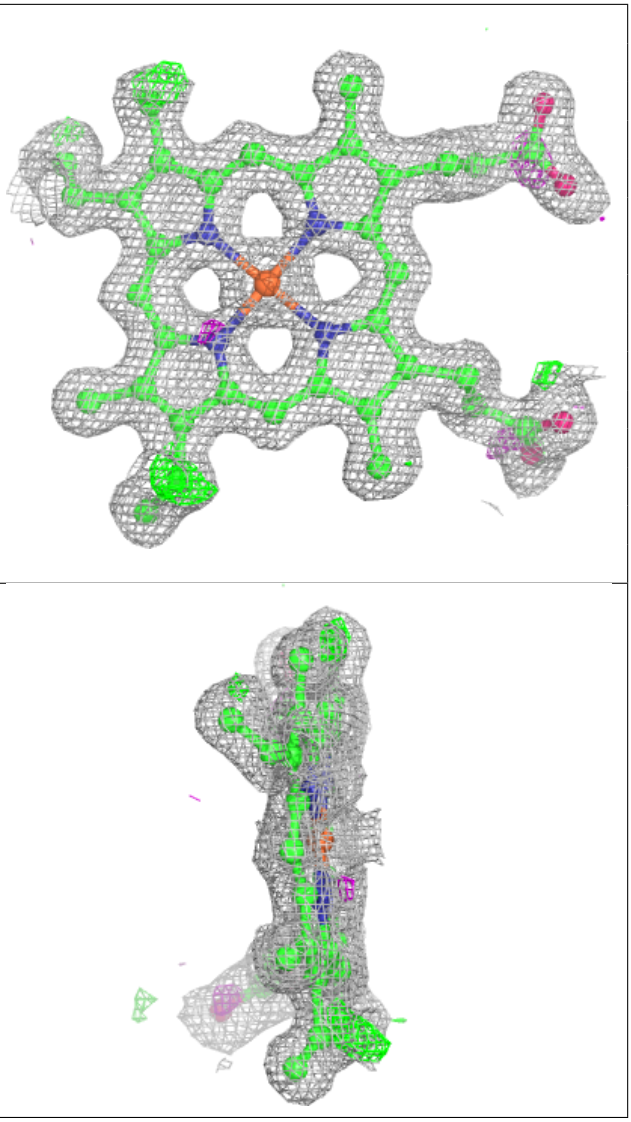






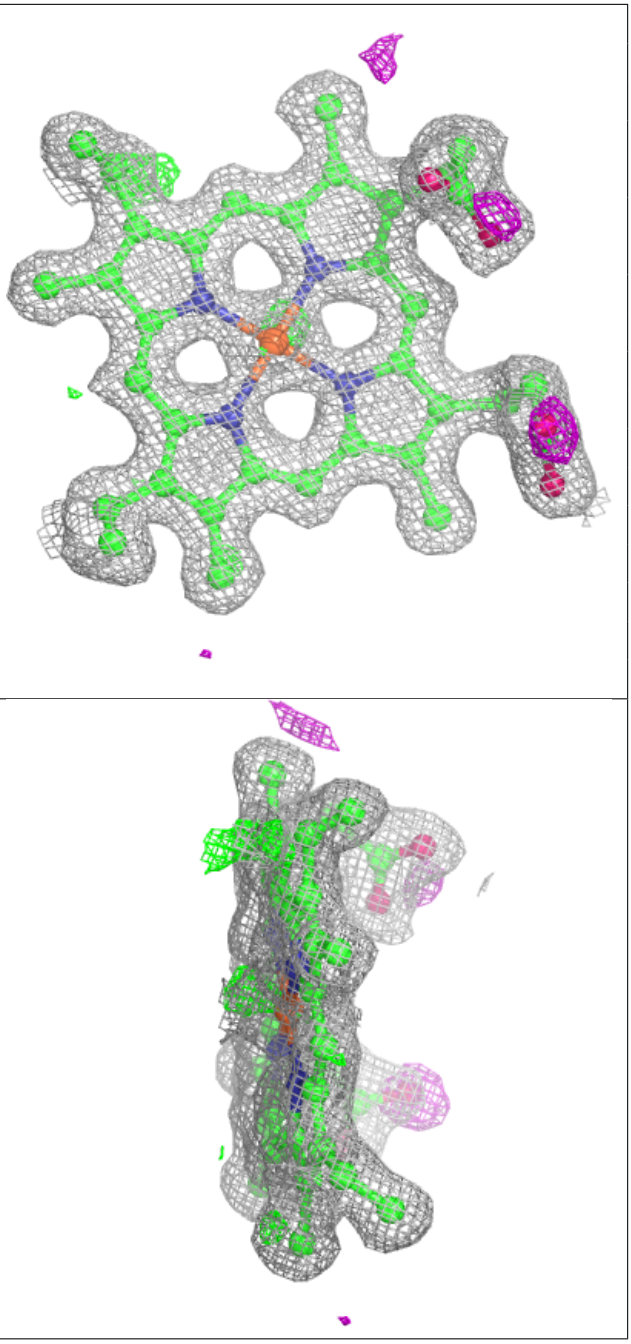
Electron density around HEC E 802:

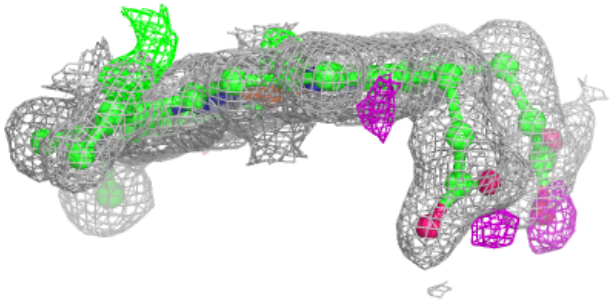
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 803:

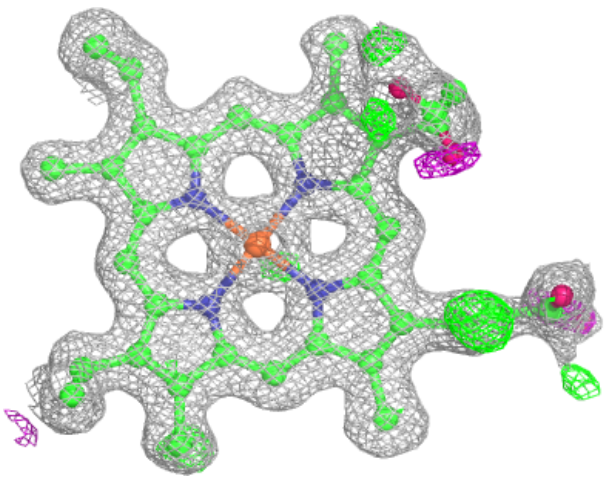
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

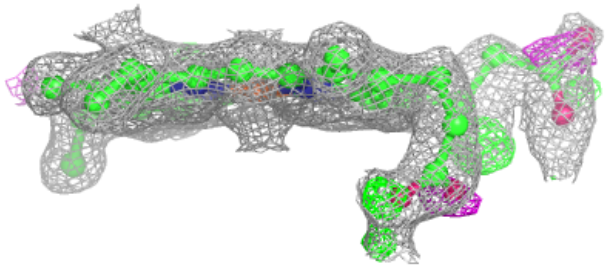


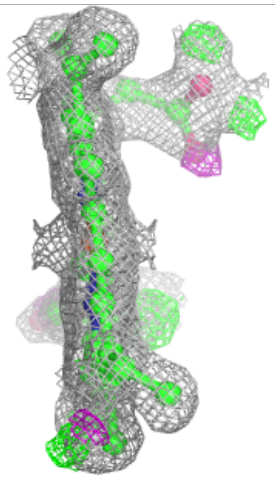


Electron density around HEC B 801:

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

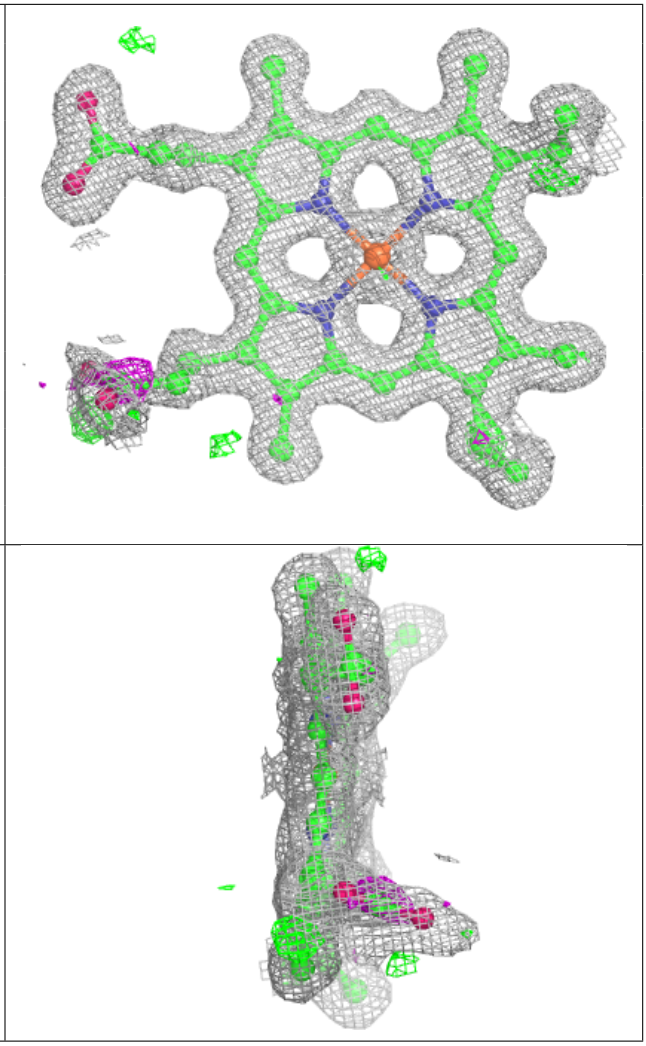






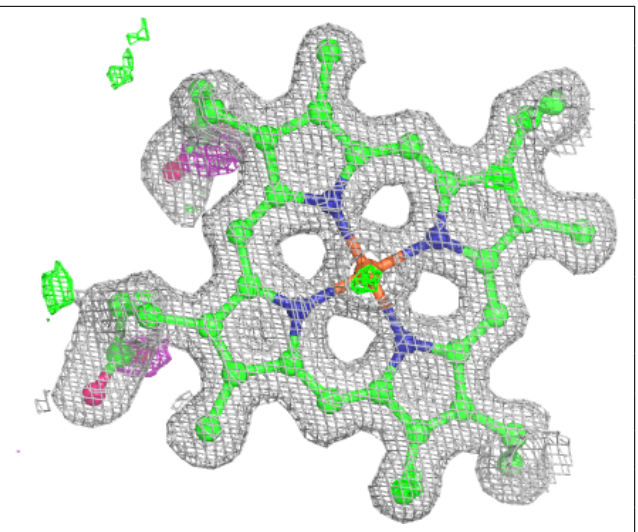
Electron density around HEC F 802:

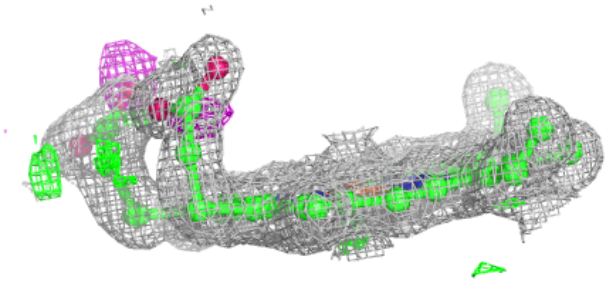
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

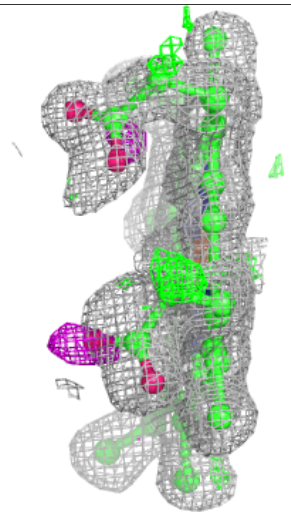


Electron density around HEC F 803:

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

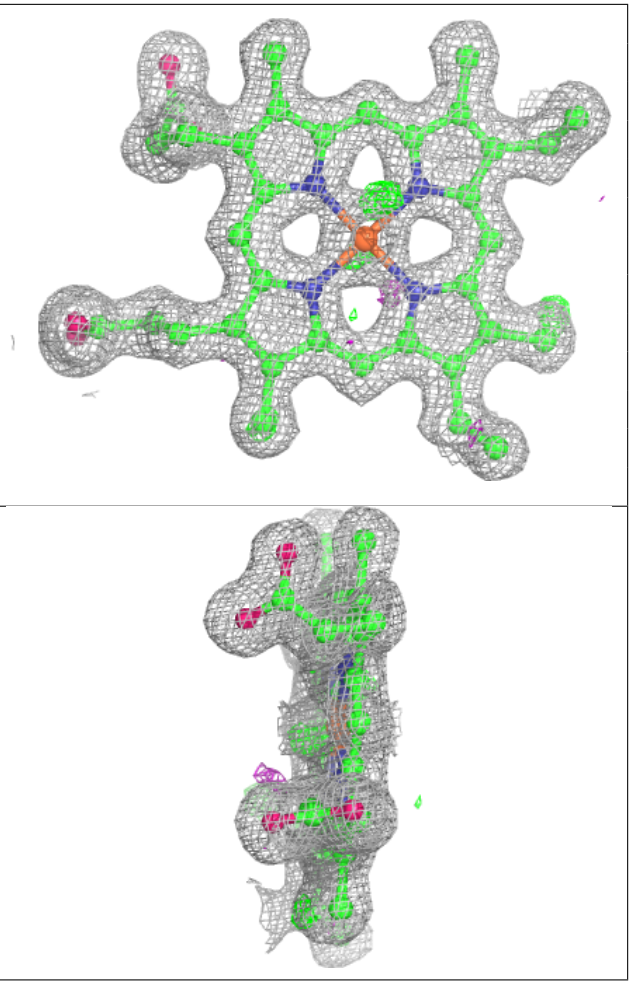






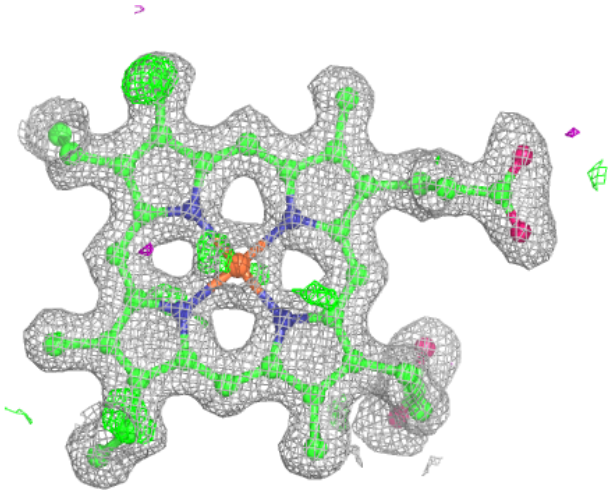
Electron density around HEC D 804:

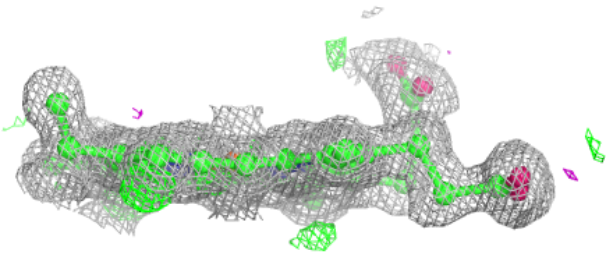
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

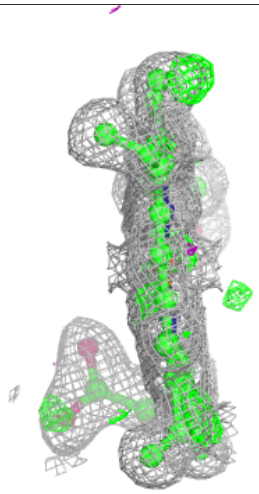


Electron density around HEC F 801:

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

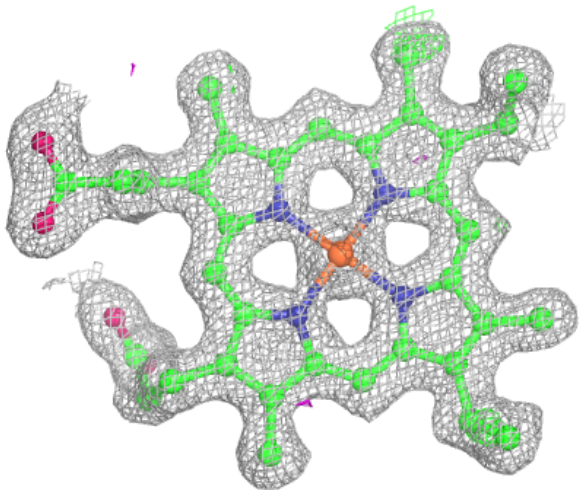


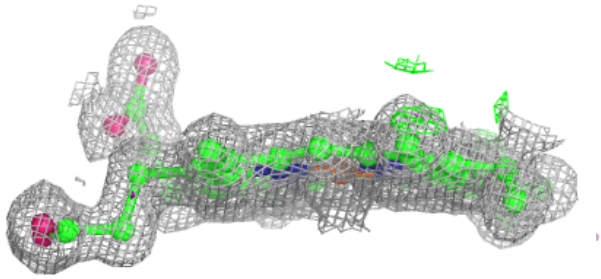


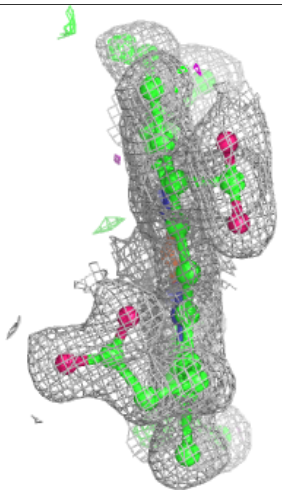


Electron density around HEC A 802:

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

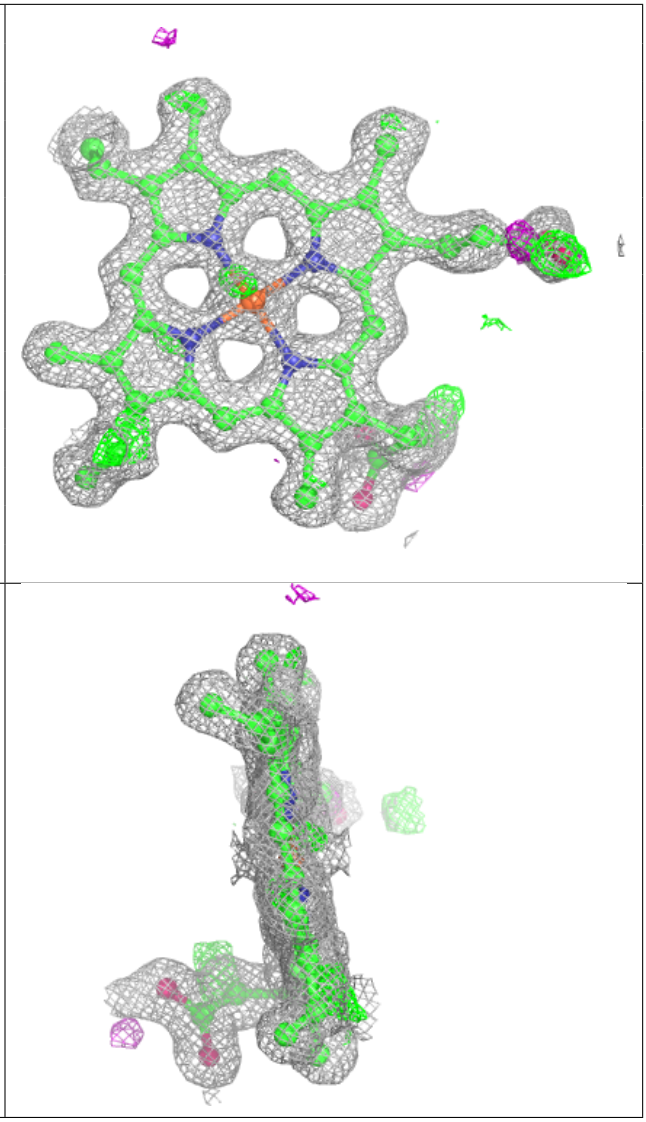






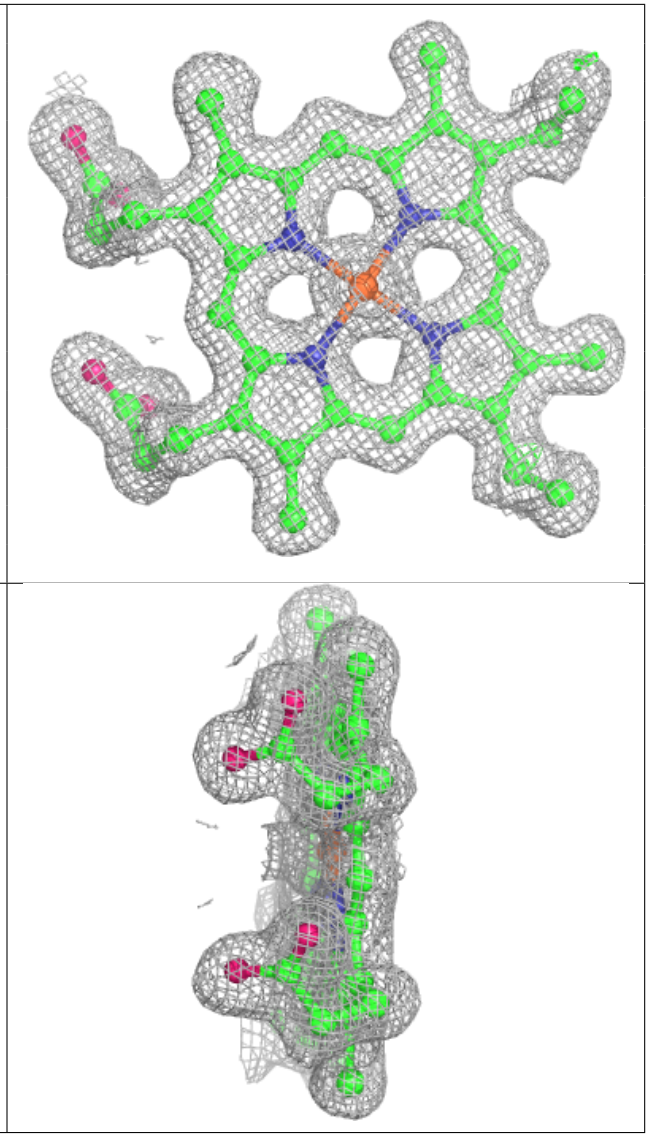
Electron density around HEC A 801:

$2mF_o$-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 E 804:

$2mF_o$-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.