wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2020 – 07:12 pm BST

PDB ID	:	6I5B
Title	:	Crystal Structure of Outer Cell Wall Cytochrome OcwA
Authors	:	Hermann, B.; Einsle, O.
Deposited on	:	2018-11-13
Resolution	:	2.20 Å(reported)

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

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

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

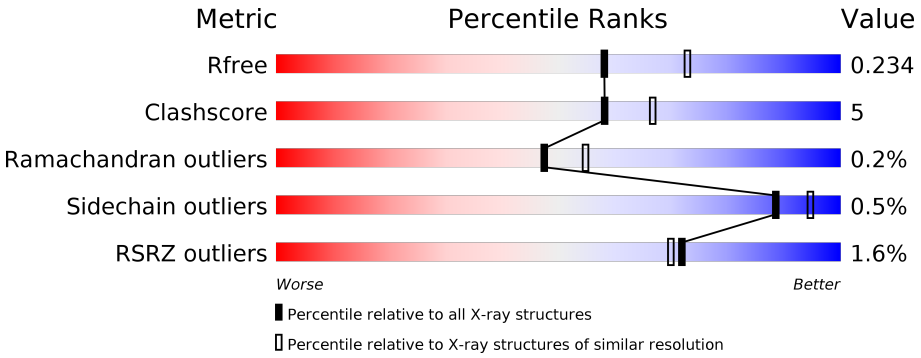
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

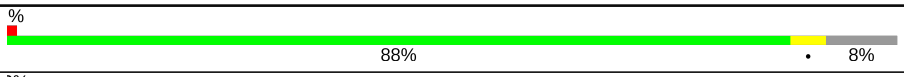
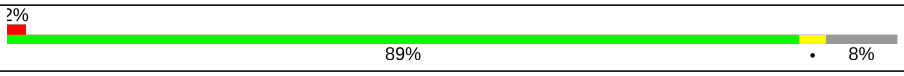
The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	526	
1	B	526	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8278 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3667	2298	636	704	29			
1	B	483	Total	C	N	O	S	0	0	0
			3659	2294	634	702	29			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	LYS	-	expression tag	UNP D5XBK3
A	527	GLY	-	expression tag	UNP D5XBK3
A	528	GLU	-	expression tag	UNP D5XBK3
A	529	LEU	-	expression tag	UNP D5XBK3
A	530	LYS	-	expression tag	UNP D5XBK3
A	531	LEU	-	expression tag	UNP D5XBK3
A	532	GLU	-	expression tag	UNP D5XBK3
A	533	GLY	-	expression tag	UNP D5XBK3
A	534	LYS	-	expression tag	UNP D5XBK3
A	535	PRO	-	expression tag	UNP D5XBK3
A	536	ILE	-	expression tag	UNP D5XBK3
A	537	PRO	-	expression tag	UNP D5XBK3
A	538	ASP	-	expression tag	UNP D5XBK3
A	539	PRO	-	expression tag	UNP D5XBK3
A	540	LEU	-	expression tag	UNP D5XBK3
A	541	LEU	-	expression tag	UNP D5XBK3
A	542	GLY	-	expression tag	UNP D5XBK3
A	543	LEU	-	expression tag	UNP D5XBK3
A	544	ASP	-	expression tag	UNP D5XBK3
A	545	SER	-	expression tag	UNP D5XBK3
A	546	THR	-	expression tag	UNP D5XBK3
A	547	ARG	-	expression tag	UNP D5XBK3
A	548	THR	-	expression tag	UNP D5XBK3
A	549	GLY	-	expression tag	UNP D5XBK3
A	550	HIS	-	expression tag	UNP D5XBK3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	551	HIS	-	expression tag	UNP D5XBK3
A	552	HIS	-	expression tag	UNP D5XBK3
A	553	HIS	-	expression tag	UNP D5XBK3
A	554	HIS	-	expression tag	UNP D5XBK3
A	555	HIS	-	expression tag	UNP D5XBK3
B	526	LYS	-	expression tag	UNP D5XBK3
B	527	GLY	-	expression tag	UNP D5XBK3
B	528	GLU	-	expression tag	UNP D5XBK3
B	529	LEU	-	expression tag	UNP D5XBK3
B	530	LYS	-	expression tag	UNP D5XBK3
B	531	LEU	-	expression tag	UNP D5XBK3
B	532	GLU	-	expression tag	UNP D5XBK3
B	533	GLY	-	expression tag	UNP D5XBK3
B	534	LYS	-	expression tag	UNP D5XBK3
B	535	PRO	-	expression tag	UNP D5XBK3
B	536	ILE	-	expression tag	UNP D5XBK3
B	537	PRO	-	expression tag	UNP D5XBK3
B	538	ASP	-	expression tag	UNP D5XBK3
B	539	PRO	-	expression tag	UNP D5XBK3
B	540	LEU	-	expression tag	UNP D5XBK3
B	541	LEU	-	expression tag	UNP D5XBK3
B	542	GLY	-	expression tag	UNP D5XBK3
B	543	LEU	-	expression tag	UNP D5XBK3
B	544	ASP	-	expression tag	UNP D5XBK3
B	545	SER	-	expression tag	UNP D5XBK3
B	546	THR	-	expression tag	UNP D5XBK3
B	547	ARG	-	expression tag	UNP D5XBK3
B	548	THR	-	expression tag	UNP D5XBK3
B	549	GLY	-	expression tag	UNP D5XBK3
B	550	HIS	-	expression tag	UNP D5XBK3
B	551	HIS	-	expression tag	UNP D5XBK3
B	552	HIS	-	expression tag	UNP D5XBK3
B	553	HIS	-	expression tag	UNP D5XBK3
B	554	HIS	-	expression tag	UNP D5XBK3
B	555	HIS	-	expression tag	UNP D5XBK3

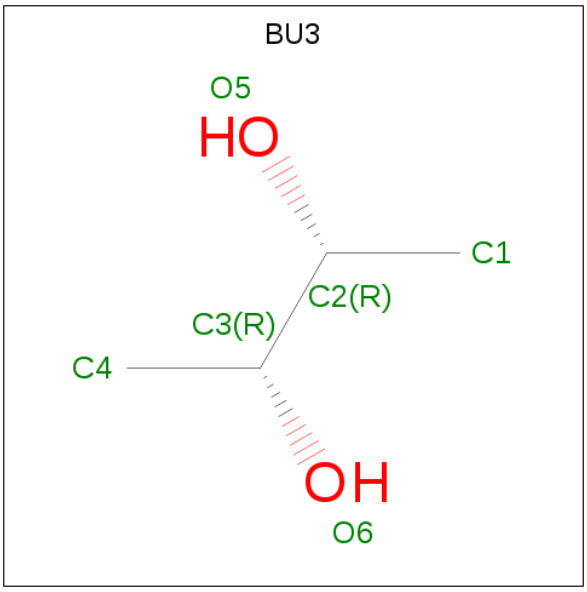
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

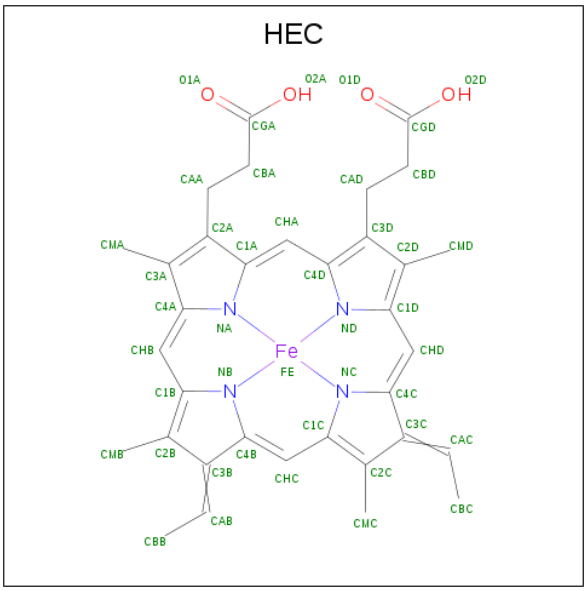
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is (R,R)-2,3-BUTANEDIOL (three-letter code: BU3) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 4 2	0	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 6 is water.

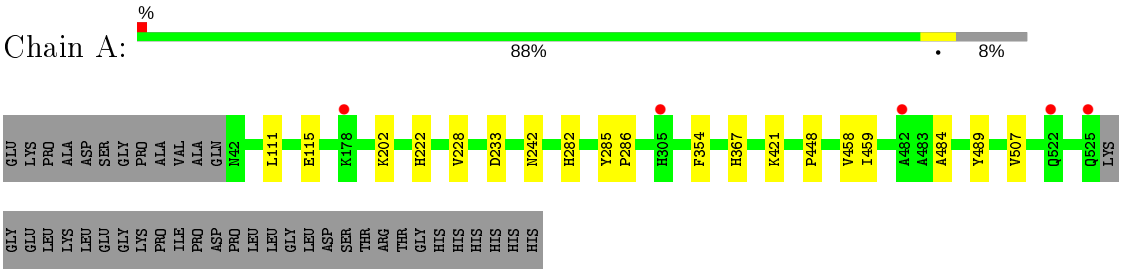
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	78	Total 78	O 78	0	0
6	B	92	Total 92	O 92	0	0

3 Residue-property plots (i)

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

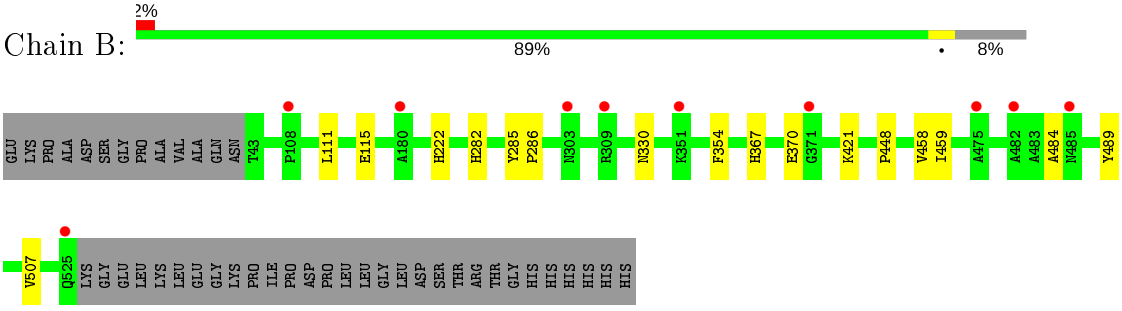
- Molecule 1: Uncharacterized protein

Chain A:



- Molecule 1: Uncharacterized protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.85Å 62.97Å 84.21Å 101.54° 99.13° 98.41°	Depositor
Resolution (Å)	80.94 – 2.20 49.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (80.94-2.20) 98.1 (49.06-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.203 , 0.233 0.208 , 0.234	Depositor DCC
R_{free} test set	2643 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.1	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	8278	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BU3, MG, CL, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/3760	0.58	0/5092
1	B	0.41	0/3752	0.59	0/5081
All	All	0.41	0/7512	0.58	0/10173

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3667	0	3536	13	1
1	B	3659	0	3530	11	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	10	0	0
5	A	387	0	271	38	0
5	B	387	0	270	28	0
6	A	78	0	0	0	0
6	B	92	0	0	0	0
All	All	8278	0	7617	75	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 5.

The worst 5 of 75 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:A:459:ILE:HD11	5:A:612:HEC:HBB3	1.66	0.76
1:A:458:VAL:HG11	5:A:612:HEC:HMA1	1.72	0.70
1:B:459:ILE:HD11	5:B:1009:HEC:HBB3	1.73	0.68
5:A:604:HEC:HBD2	5:A:604:HEC:HMD1	1.76	0.68
5:A:612:HEC:HBB3	5:A:612:HEC:HMB1	1.76	0.67

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)
1:A:202:LYS:O	1:B:370:GLU:O[1_544]	2.05	0.15

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	482/526 (92%)	468 (97%)	13 (3%)	1 (0%)	47	55
1	B	481/526 (91%)	469 (98%)	11 (2%)	1 (0%)	47	55
All	All	963/1052 (92%)	937 (97%)	24 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	HIS
1	B	282	HIS

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	387/421 (92%)	385 (100%)	2 (0%)	88 94
1	B	386/421 (92%)	384 (100%)	2 (0%)	88 94
All	All	773/842 (92%)	769 (100%)	4 (0%)	88 94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	ASP
1	A	354	PHE
1	B	330	ASN
1	B	354	PHE

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

Mol	Chain	Res	Type
1	B	525	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	HEC	B	1004	1	26,50,50	1.02	2 (7%)	18,82,82	1.26	2 (11%)
5	HEC	A	607	1	26,50,50	1.07	2 (7%)	18,82,82	1.44	3 (16%)
5	HEC	B	1008	1	26,50,50	1.00	2 (7%)	18,82,82	1.38	3 (16%)
5	HEC	B	1003	1	26,50,50	1.27	3 (11%)	18,82,82	1.25	1 (5%)
5	HEC	A	612	1,2	26,50,50	1.12	2 (7%)	18,82,82	1.72	5 (27%)
5	HEC	A	604	1	26,50,50	1.02	2 (7%)	18,82,82	1.46	2 (11%)
5	HEC	B	1007	1	26,50,50	1.31	3 (11%)	18,82,82	1.37	2 (11%)
5	HEC	B	1009	1,2	26,50,50	1.17	2 (7%)	18,82,82	2.03	3 (16%)
5	HEC	B	1002	1	26,50,50	1.01	1 (3%)	18,82,82	1.29	2 (11%)
5	HEC	A	605	1	26,50,50	0.92	1 (3%)	18,82,82	1.34	3 (16%)
5	HEC	B	1006	1	26,50,50	1.52	4 (15%)	18,82,82	1.30	0
5	HEC	A	611	1	26,50,50	0.92	2 (7%)	18,82,82	1.59	2 (11%)
5	HEC	A	609	1	26,50,50	1.04	2 (7%)	18,82,82	1.43	3 (16%)
5	HEC	B	1001	1	26,50,50	1.02	2 (7%)	18,82,82	1.32	3 (16%)
5	HEC	B	1005	1	26,50,50	1.56	2 (7%)	18,82,82	1.79	7 (38%)
5	HEC	A	610	1	26,50,50	1.03	2 (7%)	18,82,82	1.16	2 (11%)
5	HEC	A	606	1	26,50,50	1.00	2 (7%)	18,82,82	1.34	2 (11%)
4	BU3	A	603	-	4,5,5	0.40	0	6,6,6	0.33	0
5	HEC	A	608	1,6	26,50,50	0.99	2 (7%)	18,82,82	1.28	2 (11%)

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
5	HEC	B	1004	1	-	1/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	607	1	-	1/6/54/54	-
5	HEC	B	1008	1	-	0/6/54/54	-
5	HEC	B	1003	1	-	2/6/54/54	-
5	HEC	A	612	1,2	-	1/6/54/54	-
5	HEC	A	604	1	-	2/6/54/54	-
5	HEC	B	1007	1	-	0/6/54/54	-
5	HEC	B	1009	1,2	-	0/6/54/54	-
5	HEC	B	1002	1	-	1/6/54/54	-
5	HEC	A	605	1	-	1/6/54/54	-
5	HEC	B	1006	1	-	1/6/54/54	-
5	HEC	A	611	1	-	0/6/54/54	-
5	HEC	A	609	1	-	1/6/54/54	-
5	HEC	B	1001	1	-	0/6/54/54	-
5	HEC	B	1005	1	-	3/6/54/54	-
5	HEC	A	610	1	-	0/6/54/54	-
5	HEC	A	606	1	-	2/6/54/54	-
4	BU3	A	603	-	-	4/4/4/4	-
5	HEC	A	608	1,6	-	1/6/54/54	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1005	HEC	CBB-CAB	-6.22	1.26	1.49
5	B	1006	HEC	CBB-CAB	4.36	1.66	1.49
5	B	1003	HEC	CBC-CAC	-4.17	1.33	1.49
5	B	1007	HEC	C3B-C4B	4.02	1.50	1.43
5	B	1006	HEC	C3B-C2B	-3.96	1.36	1.40

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1009	HEC	CBA-CAA-C2A	-6.21	101.03	112.48
5	A	611	HEC	CBA-CAA-C2A	-4.78	103.67	112.48
5	B	1005	HEC	CBD-CAD-C3D	-3.73	105.60	112.49
5	B	1007	HEC	CBD-CAD-C3D	-3.36	106.29	112.49
5	A	604	HEC	CBD-CAD-C3D	3.32	118.60	112.49

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1003	HEC	C1A-C2A-CAA-CBA
5	B	1003	HEC	C3A-C2A-CAA-CBA
5	A	604	HEC	C2D-C3D-CAD-CBD
5	A	604	HEC	C4D-C3D-CAD-CBD
5	B	1002	HEC	C2A-CAA-CBA-CGA

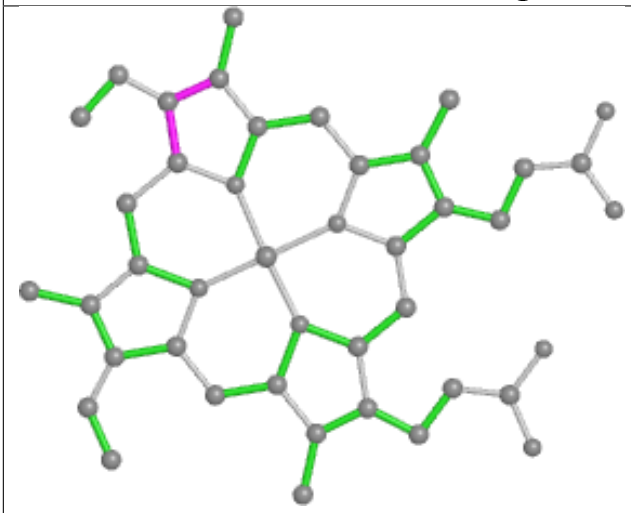
There are no ring outliers.

18 monomers are involved in 66 short contacts:

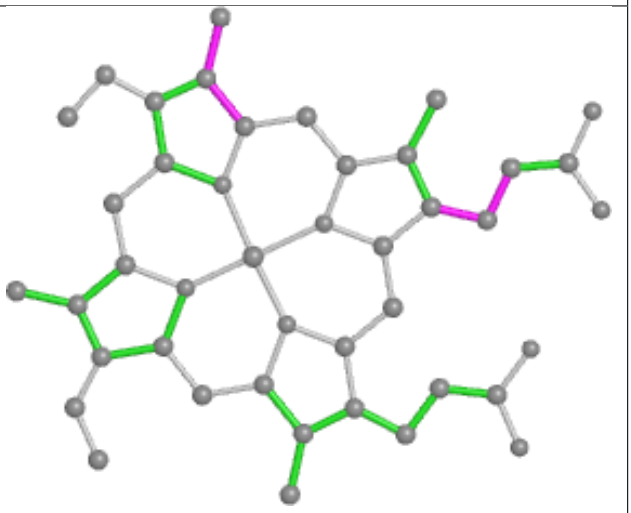
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1004	HEC	3	0
5	A	607	HEC	3	0
5	B	1008	HEC	3	0
5	B	1003	HEC	3	0
5	A	612	HEC	5	0
5	A	604	HEC	4	0
5	B	1007	HEC	1	0
5	B	1009	HEC	5	0
5	B	1002	HEC	4	0
5	A	605	HEC	7	0
5	B	1006	HEC	3	0
5	A	611	HEC	4	0
5	A	609	HEC	3	0
5	B	1001	HEC	3	0
5	B	1005	HEC	3	0
5	A	610	HEC	3	0
5	A	606	HEC	5	0
5	A	608	HEC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

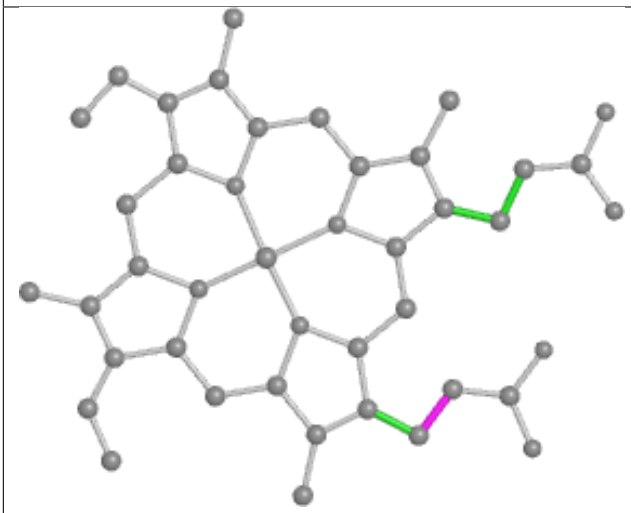
Ligand HEC B 1004



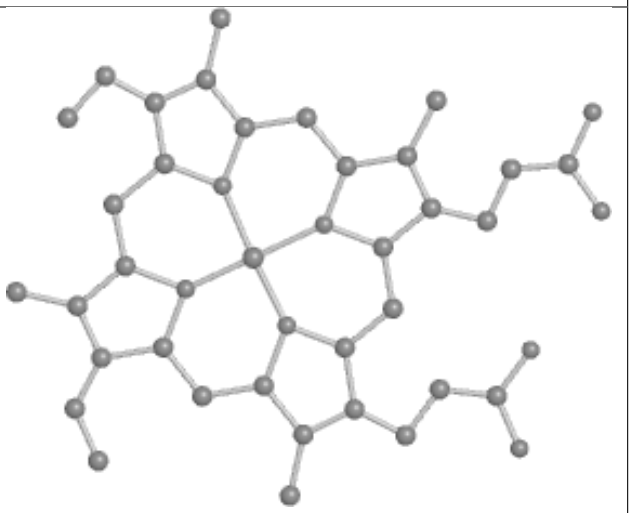
Bond lengths



Bond angles

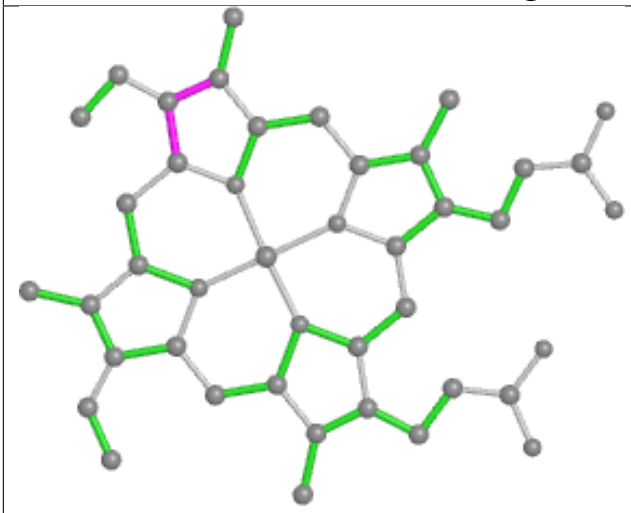


Torsions



Rings

Ligand HEC A 607



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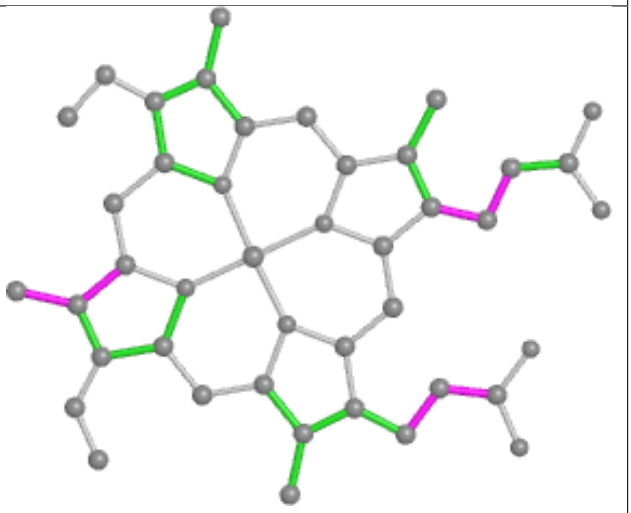
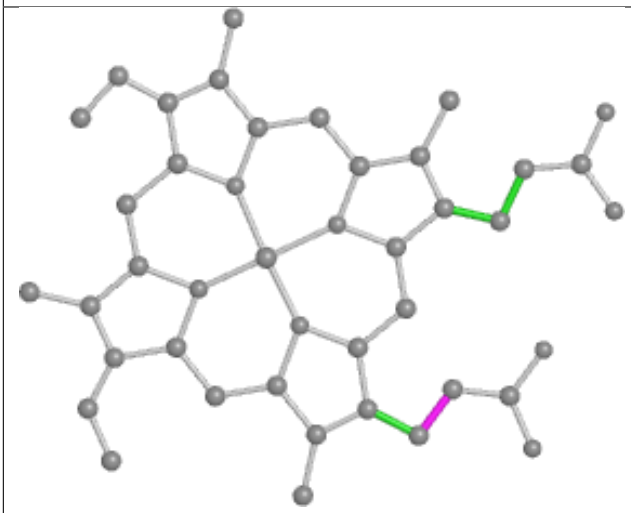


Bond angles



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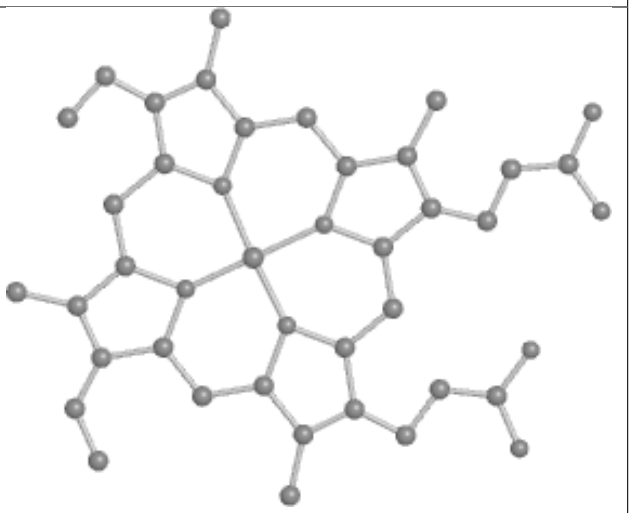
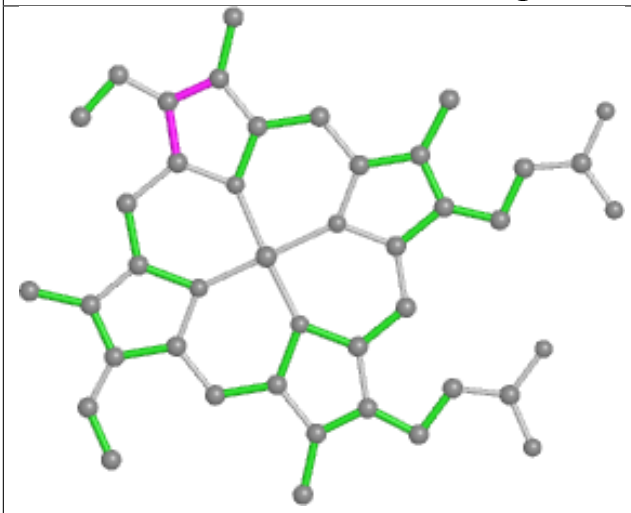
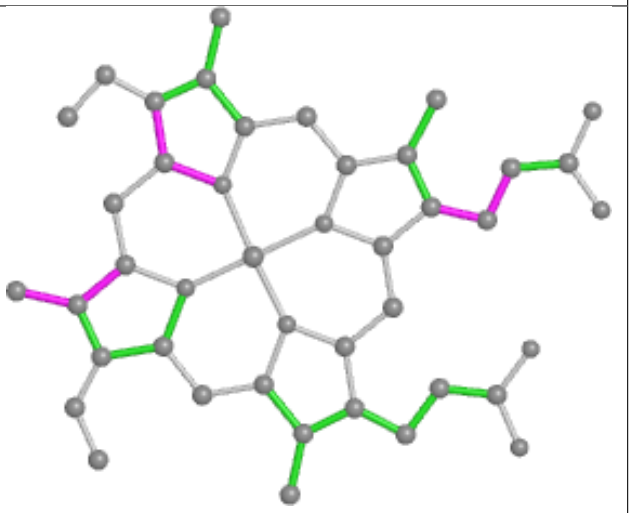


Rings

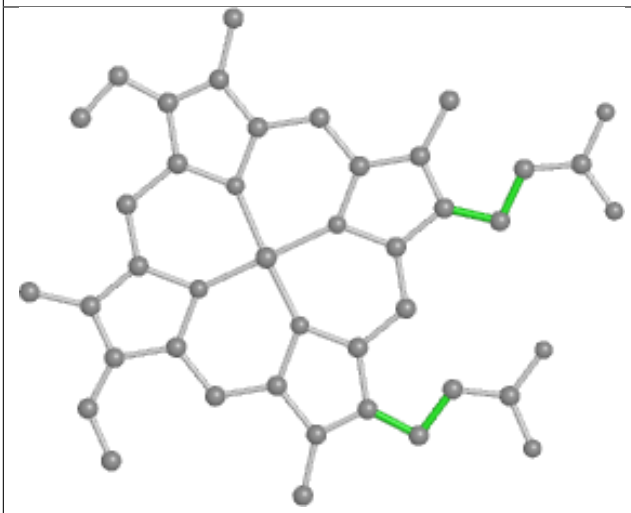
Ligand HEC B 1008



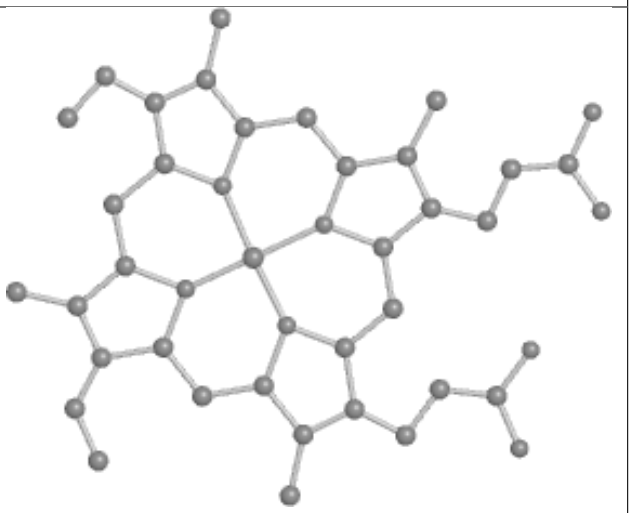
Bond lengths



Bond angles

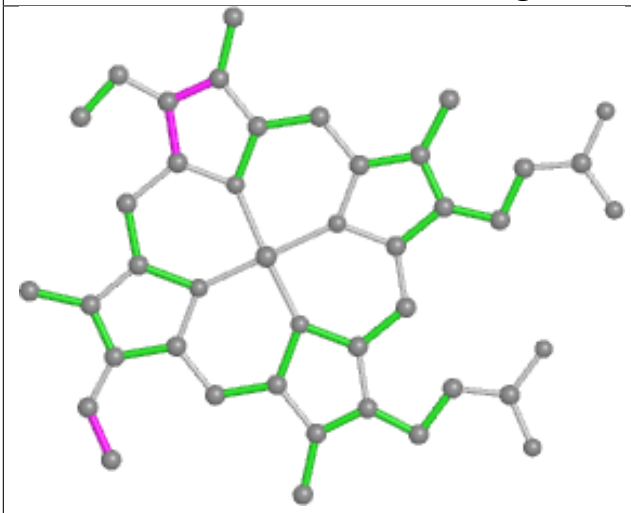


Torsions



Rings

Ligand HEC B 1003



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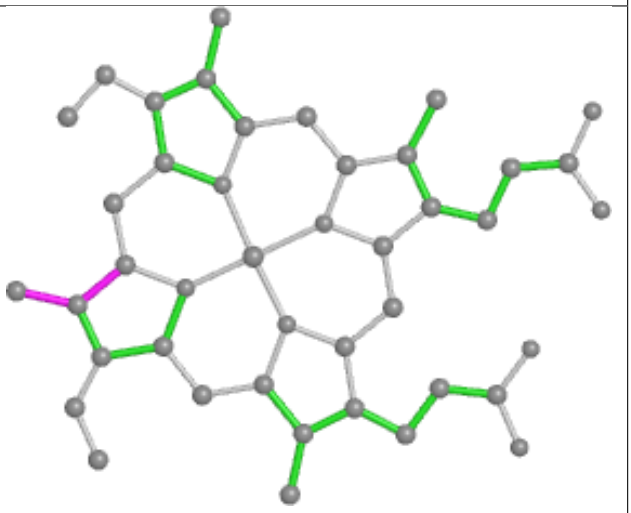
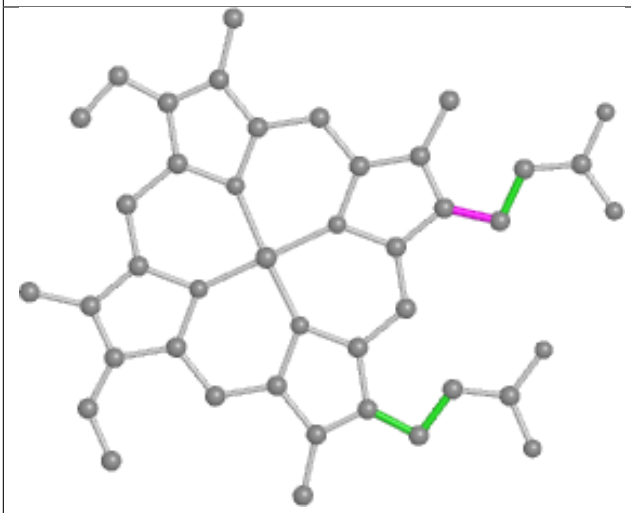


Bond angles



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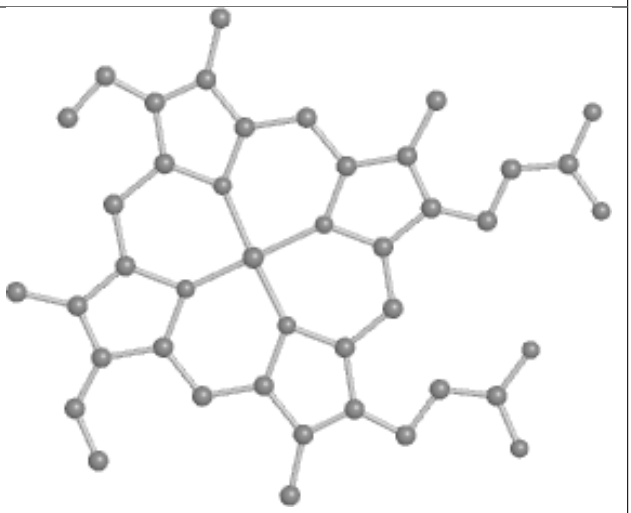
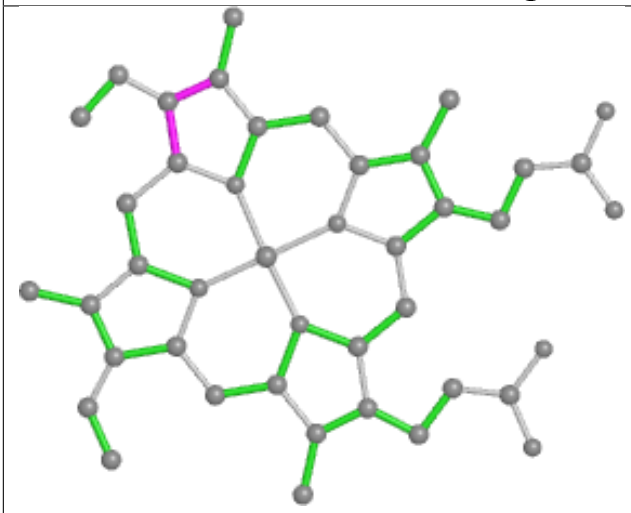


Rings

Ligand HEC A 612



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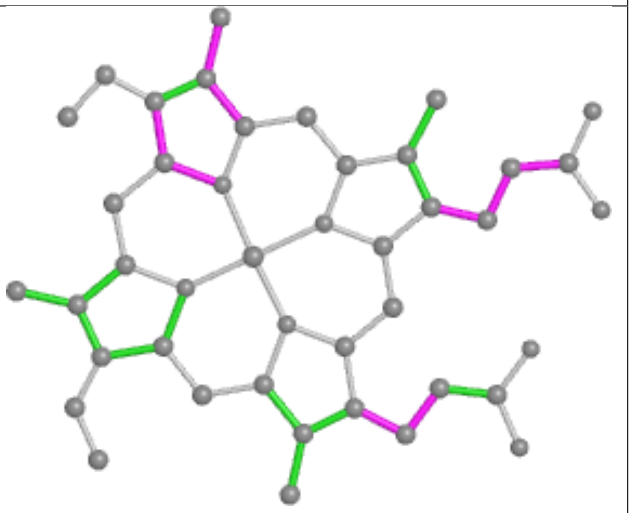
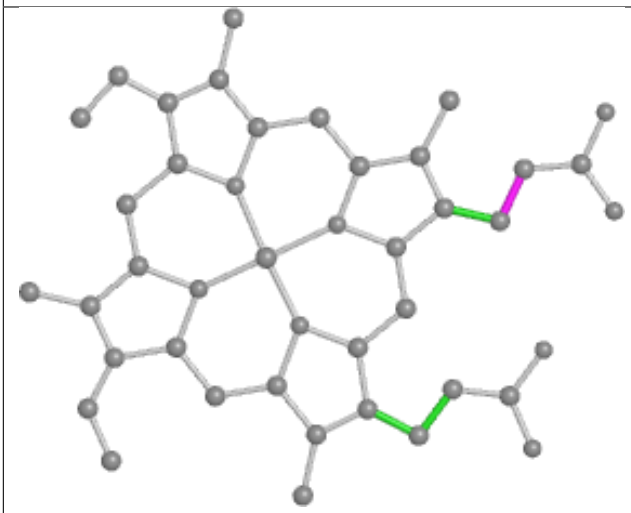


Bond angles



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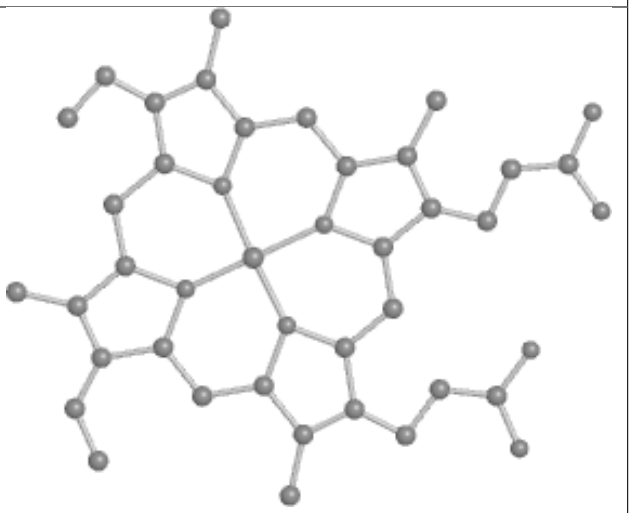
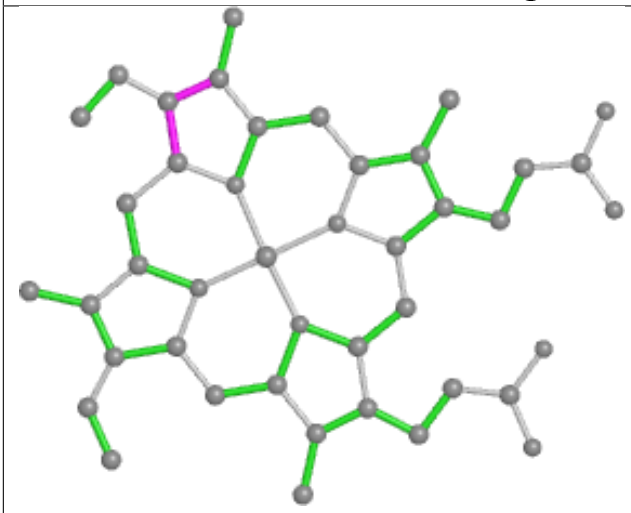


Rings

Ligand HEC A 604



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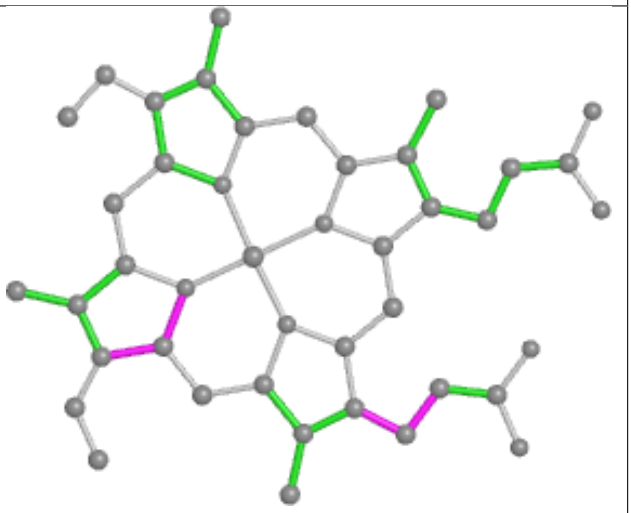
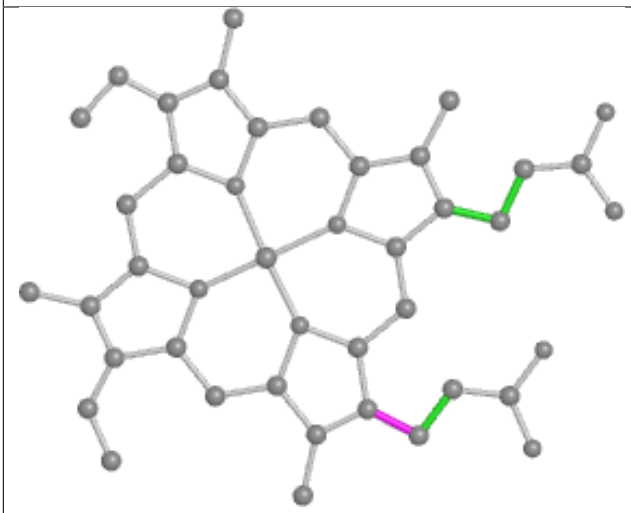


Bond angles



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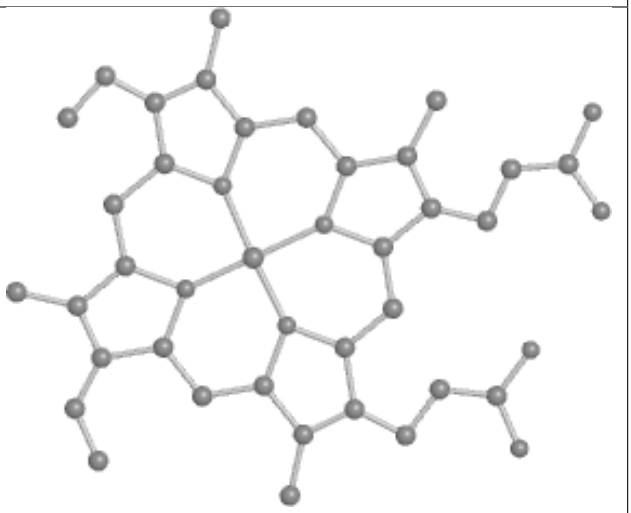
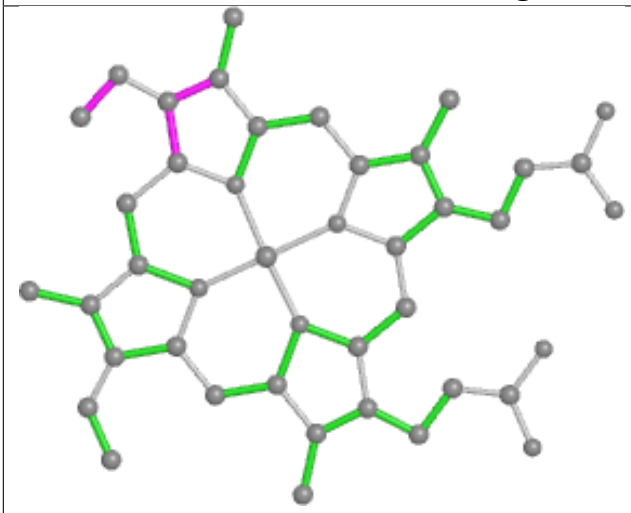


Rings

Ligand HEC B 1007



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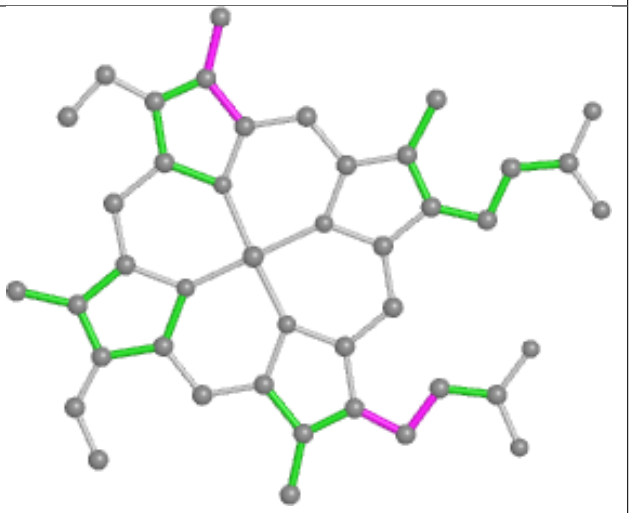

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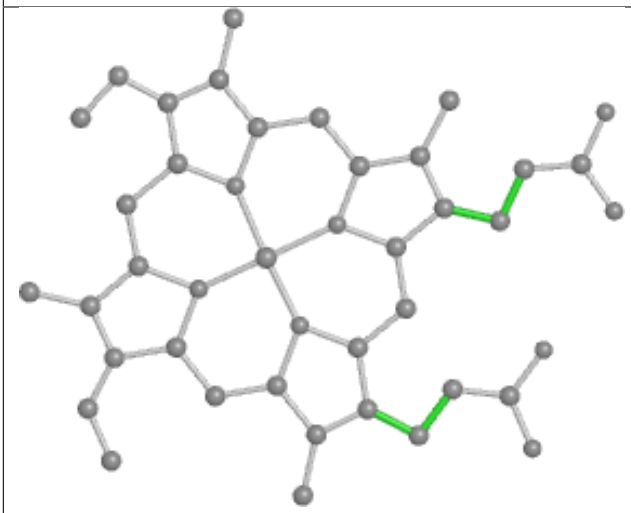

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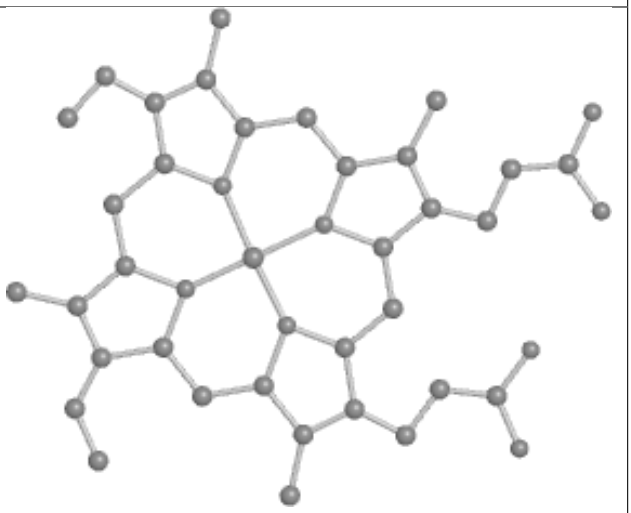
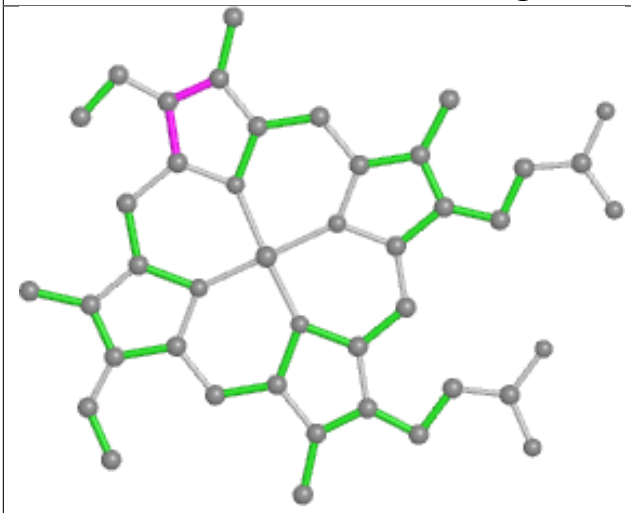


Rings

Ligand HEC B 1009



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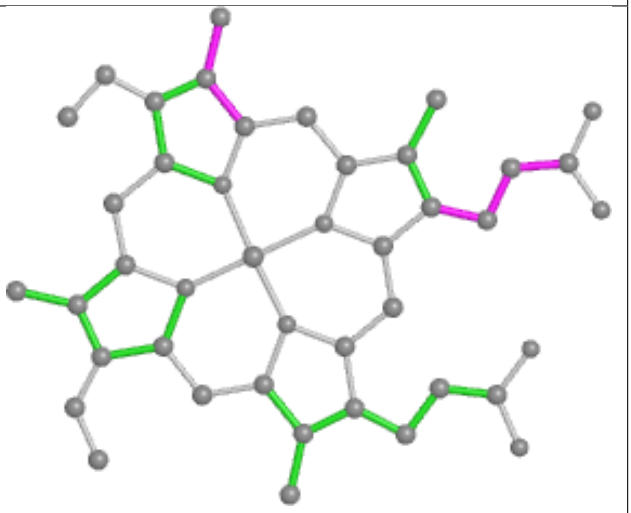

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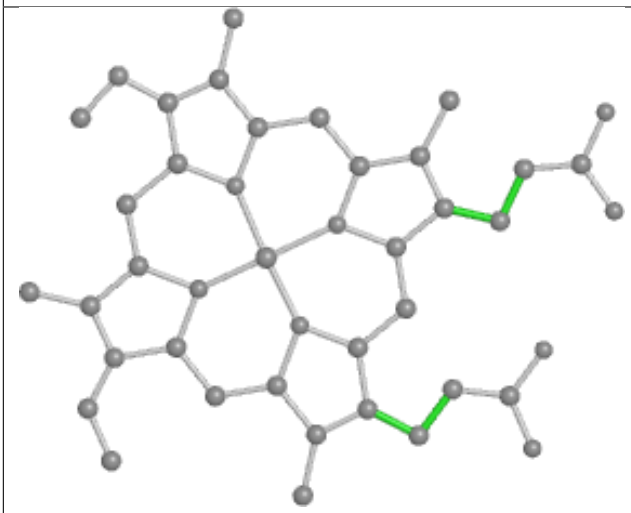
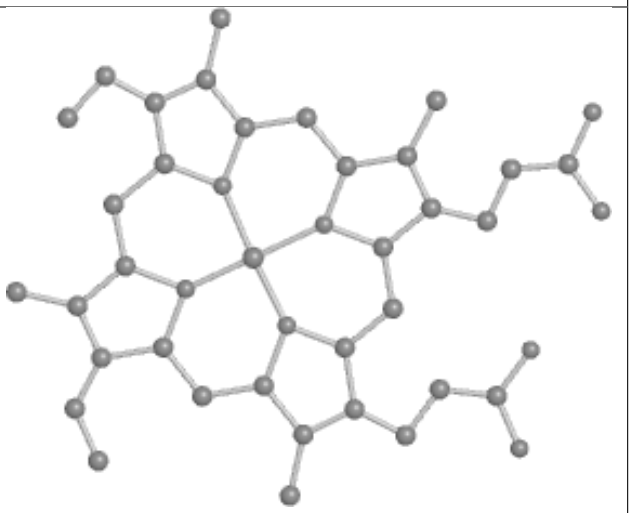
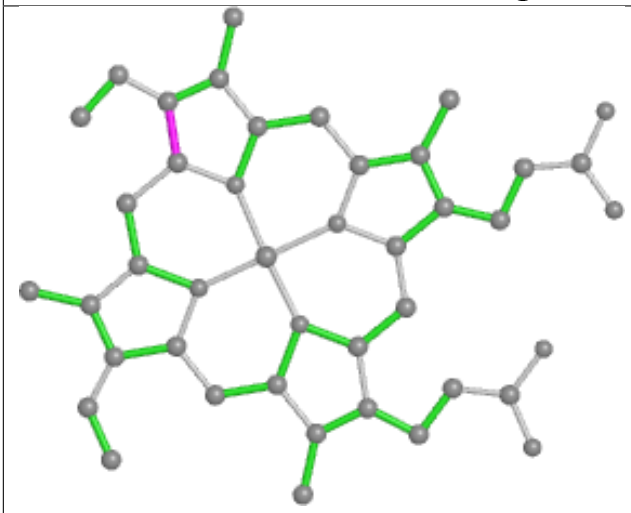


Torsions



Rings

Ligand HEC B 1002



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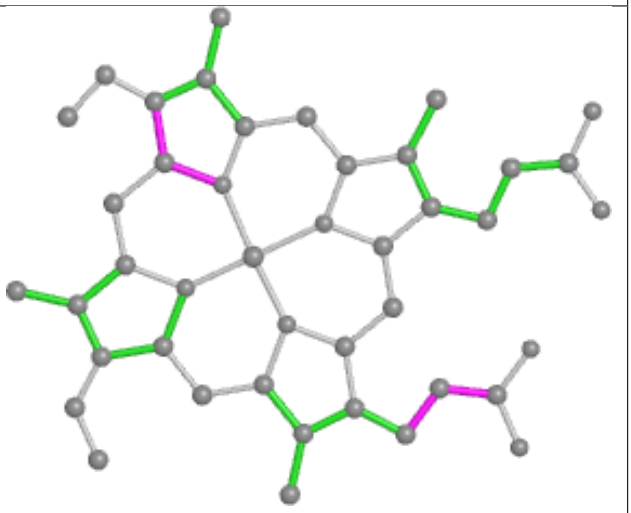
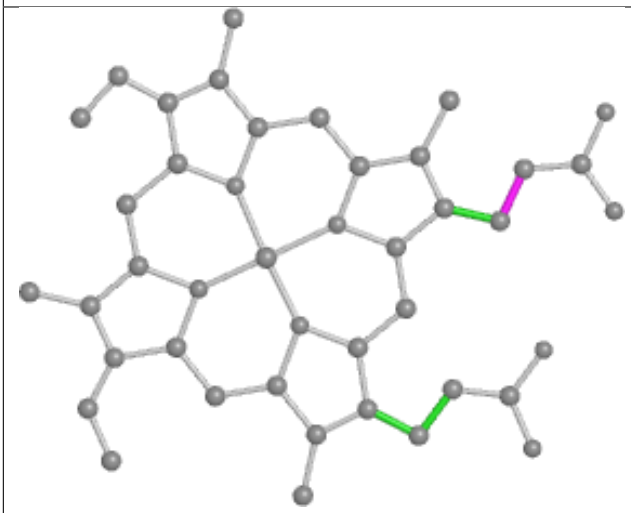


Bond angles



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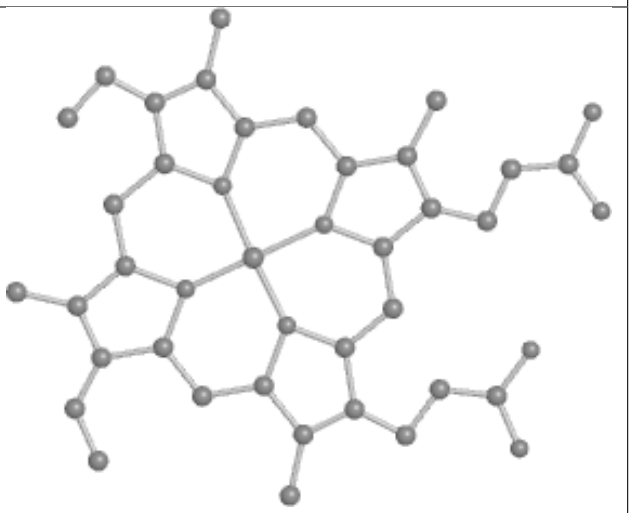
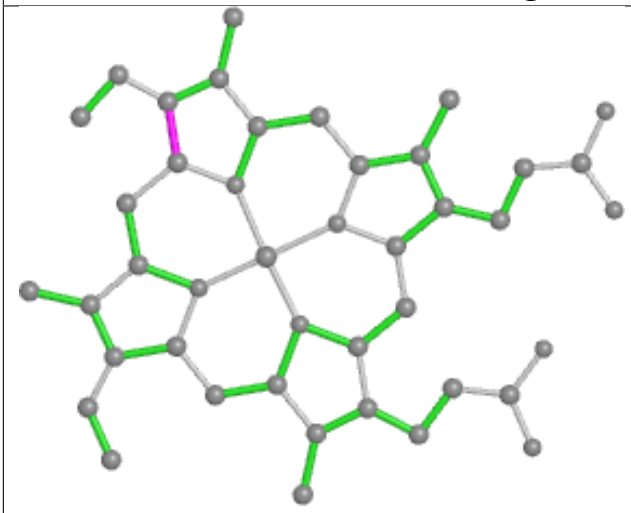


Rings

Ligand HEC A 605



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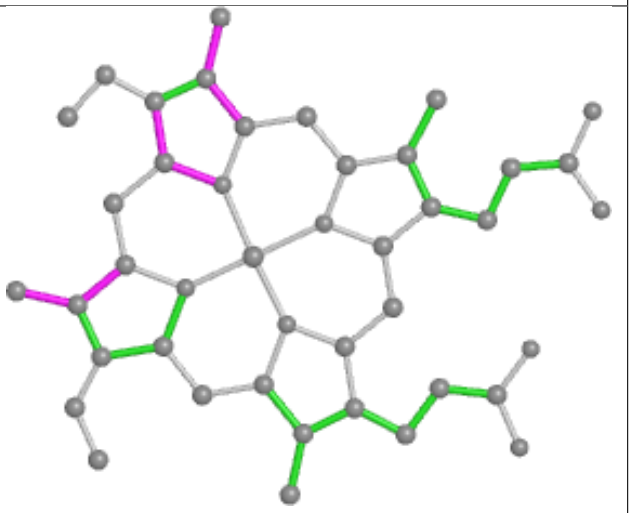

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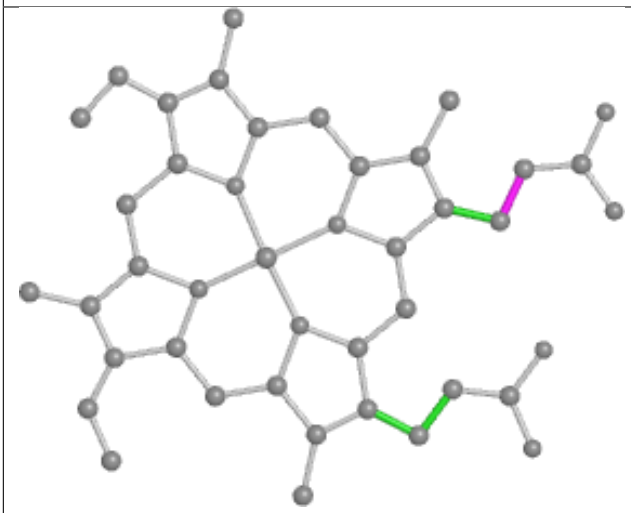

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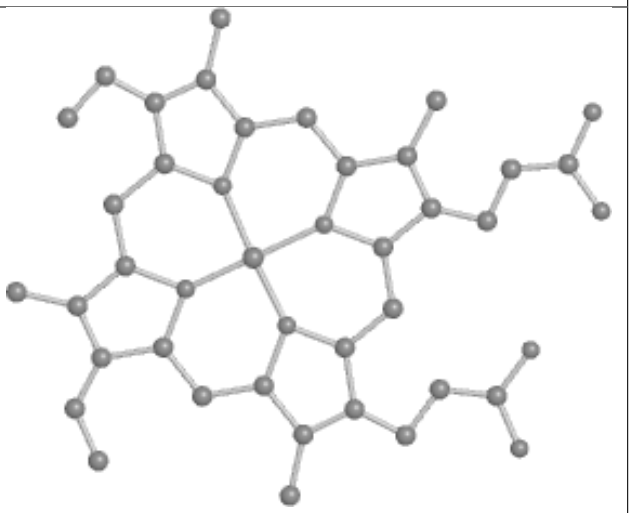
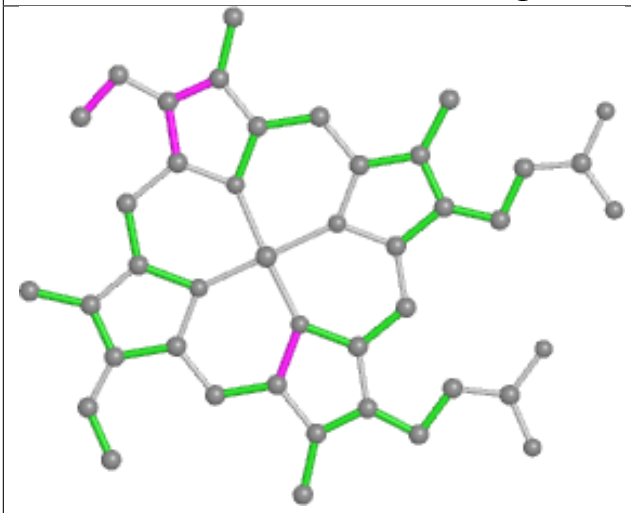


Rings

Ligand HEC B 1006



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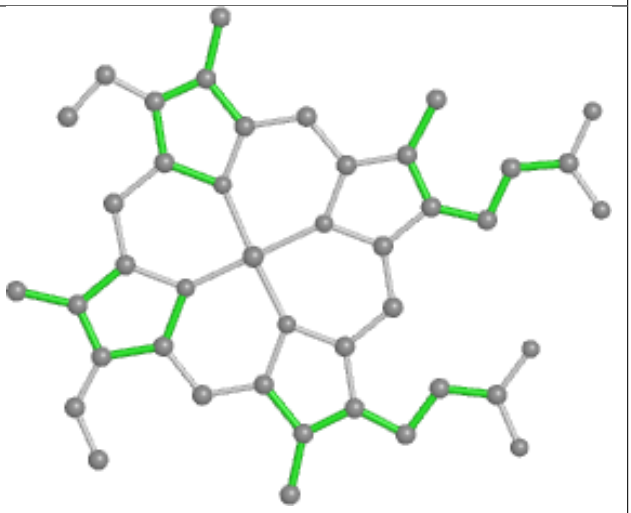
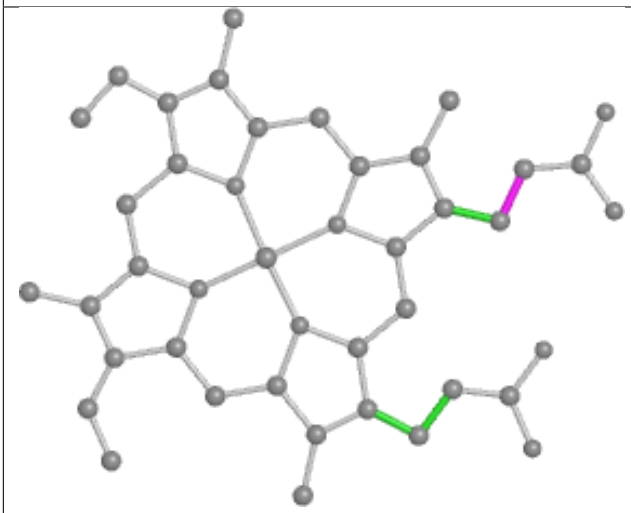


Bond angles



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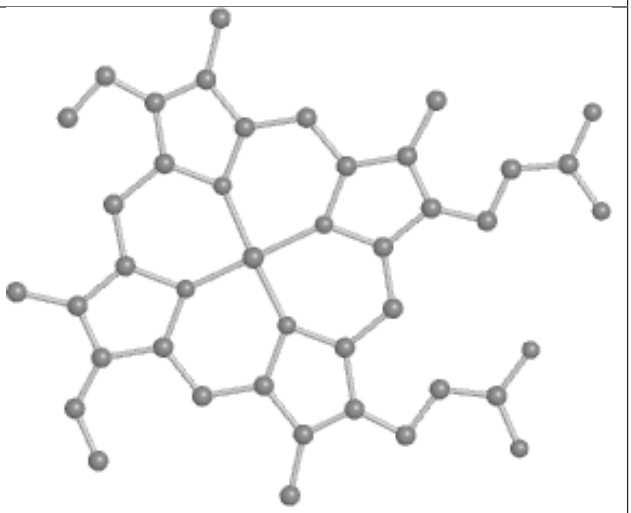
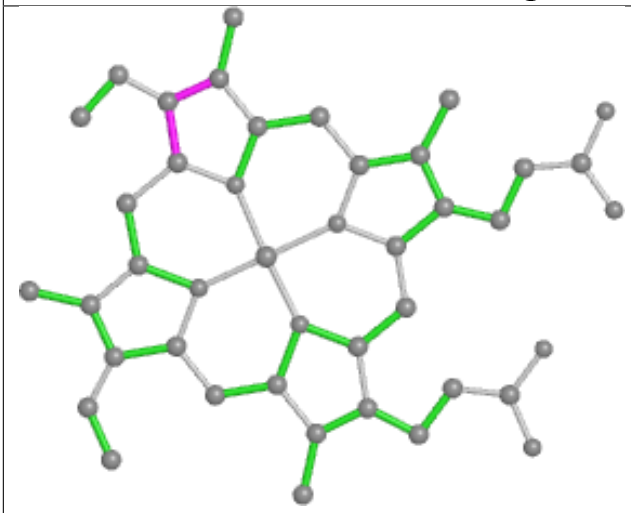
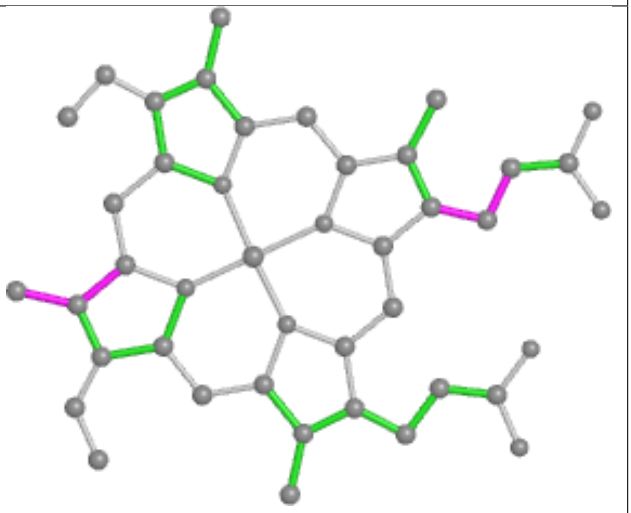


Rings

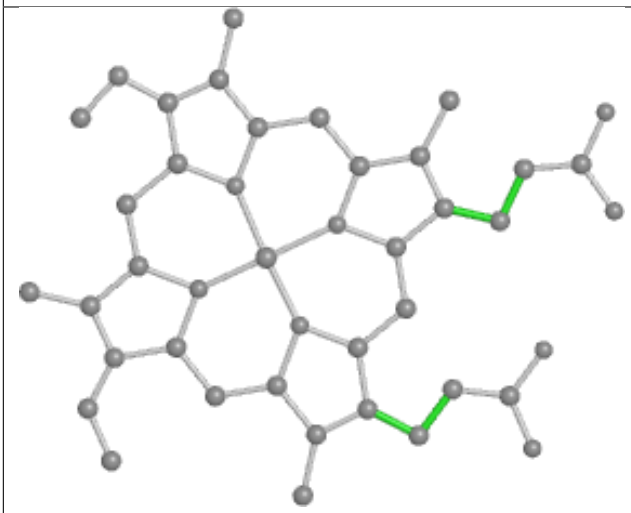
Ligand HEC A 611



Bond lengths



Bond angles



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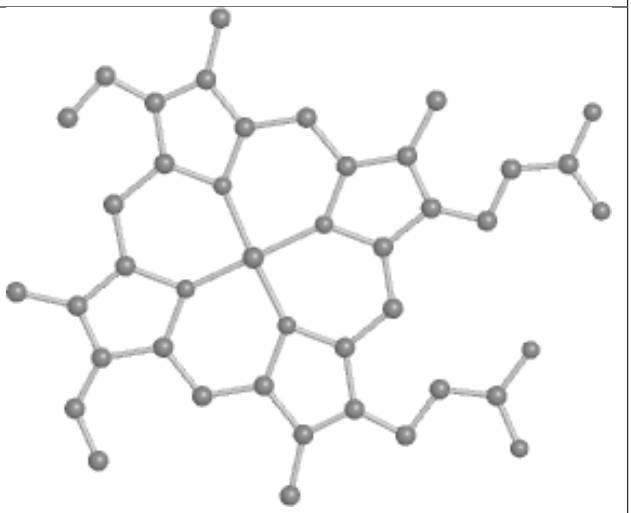
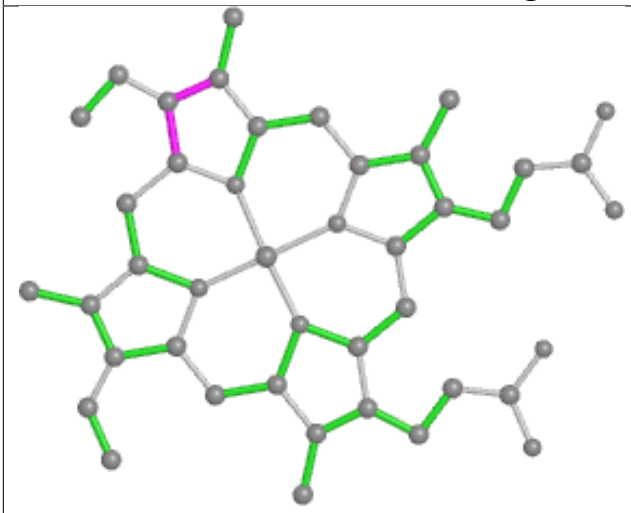
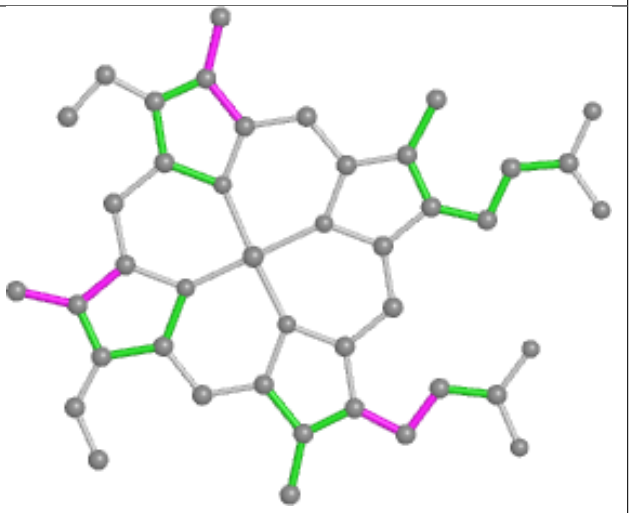


Rings

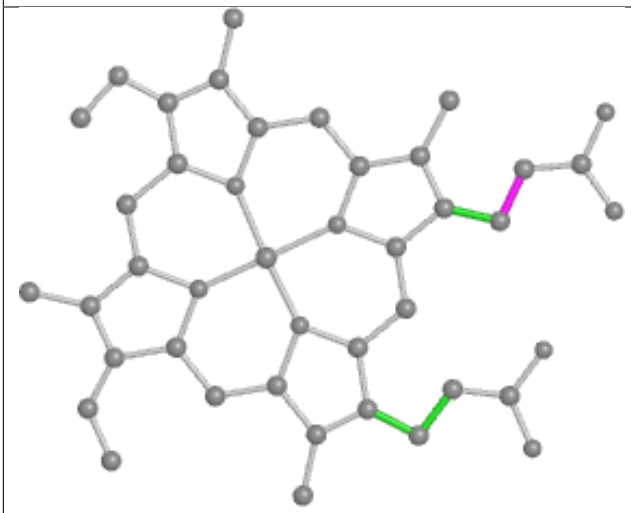
Ligand HEC A 609



Bond lengths



Bond angles



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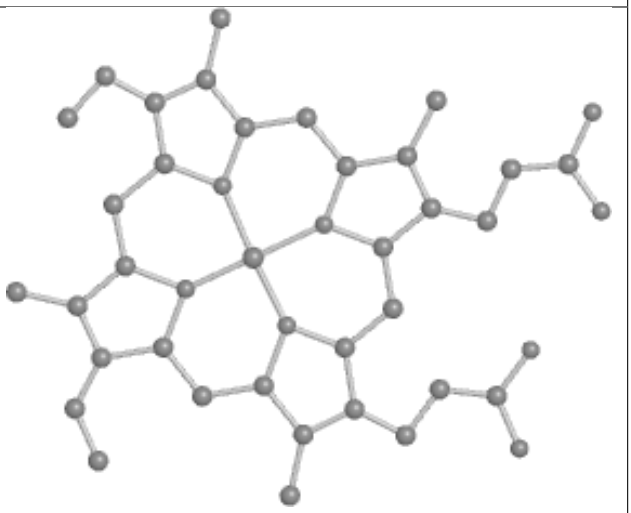
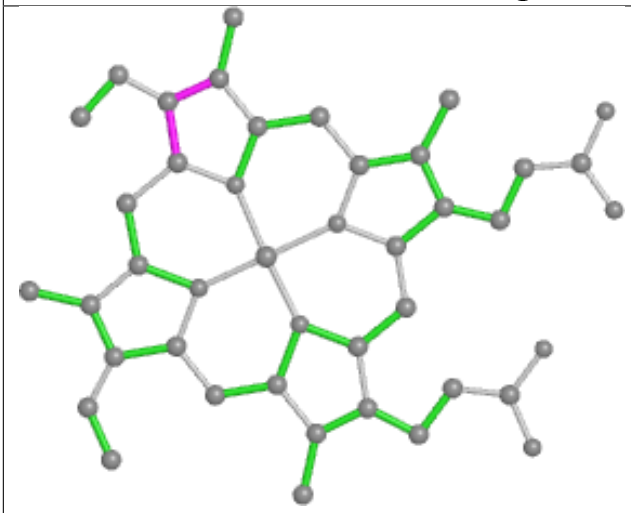
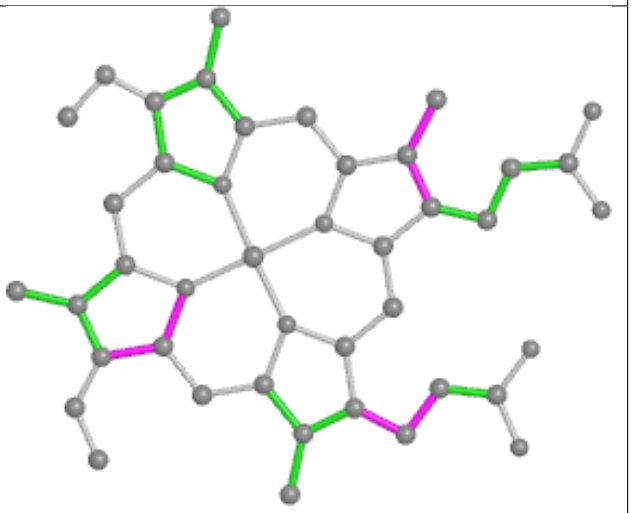


Rings

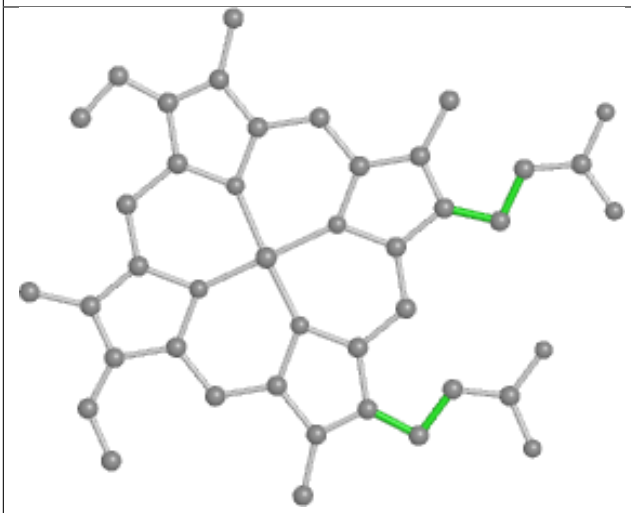
Ligand HEC B 1001



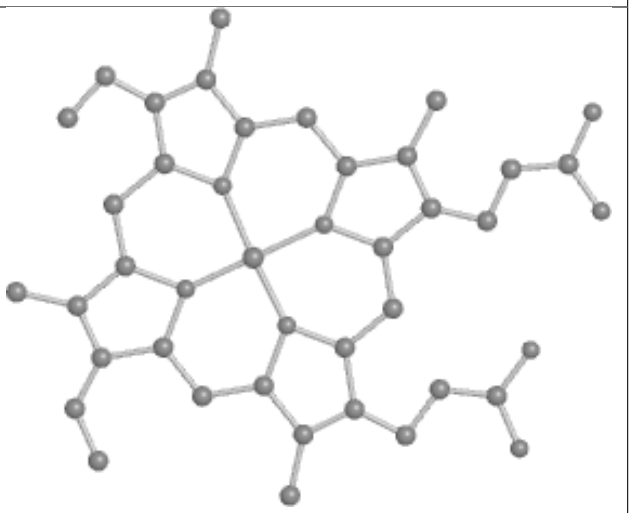
Bond lengths



Bond angles

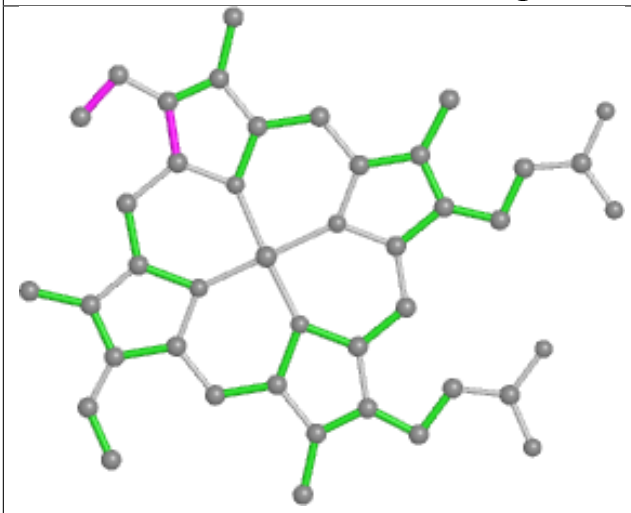


Torsions

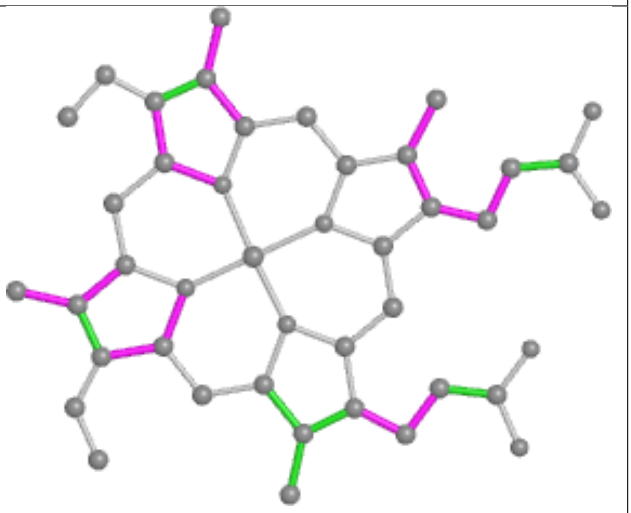


Rings

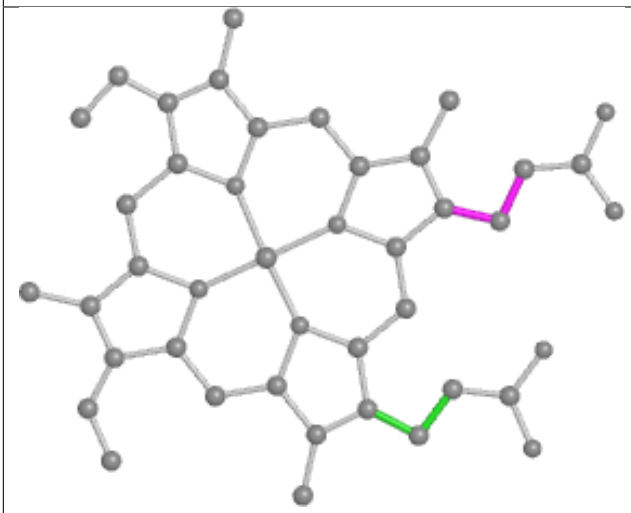
Ligand HEC B 1005



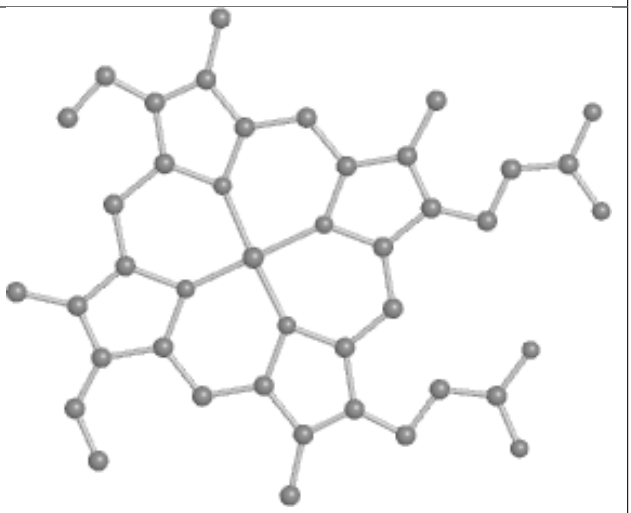
Bond lengths



Bond angles

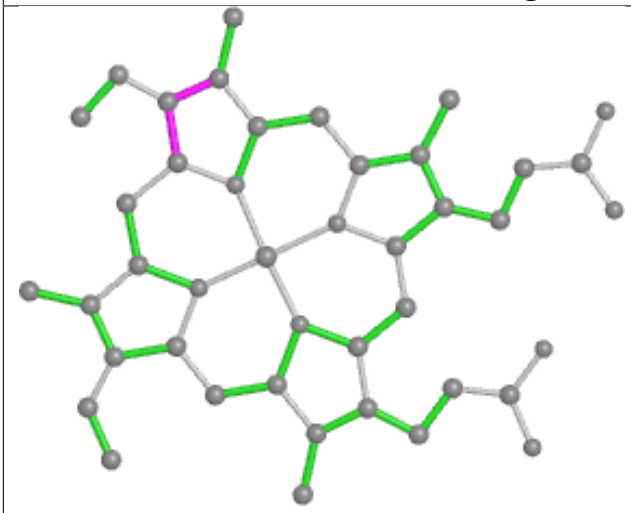


Torsions

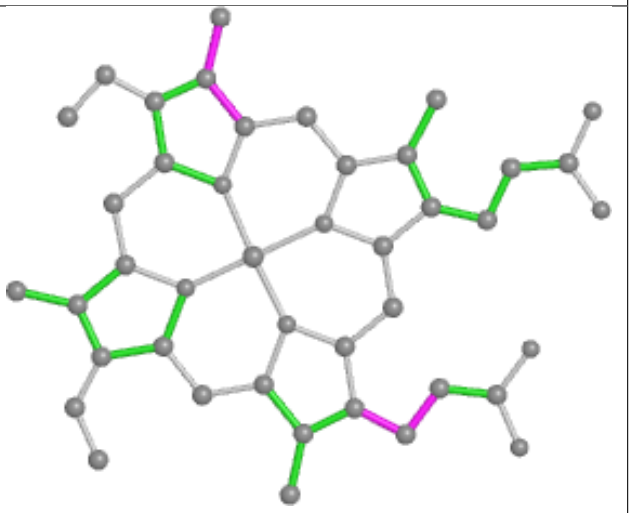


Rings

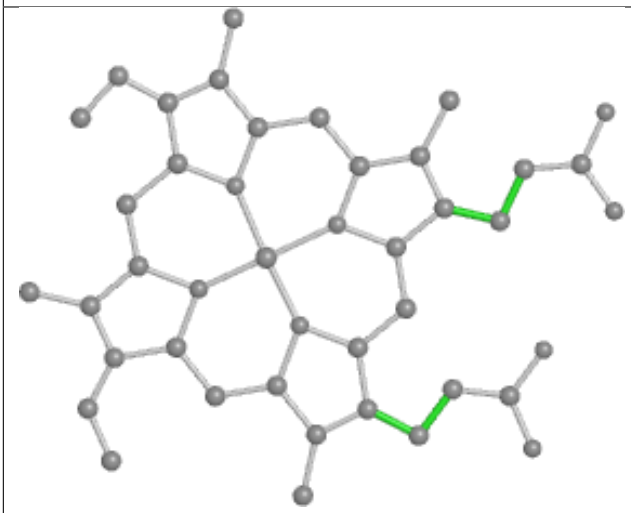
Ligand HEC A 610



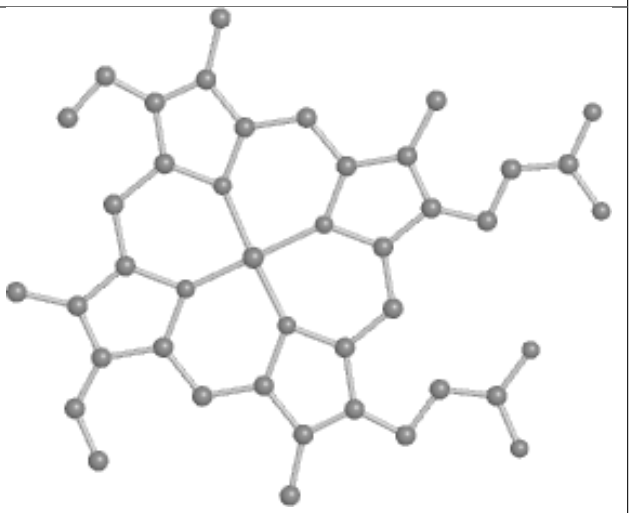
Bond lengths



Bond angles

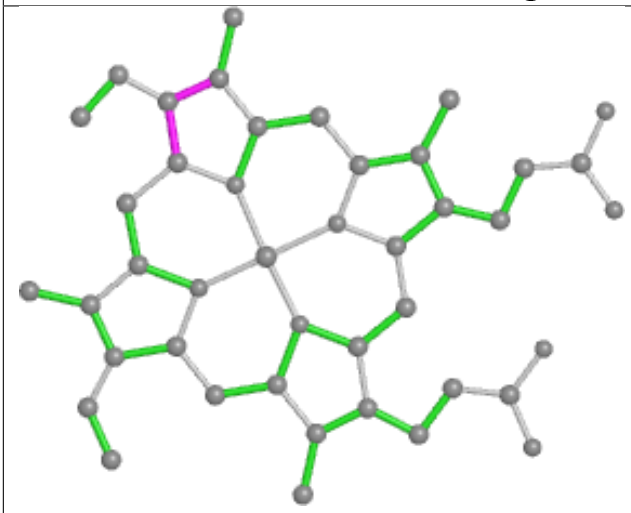


Torsions

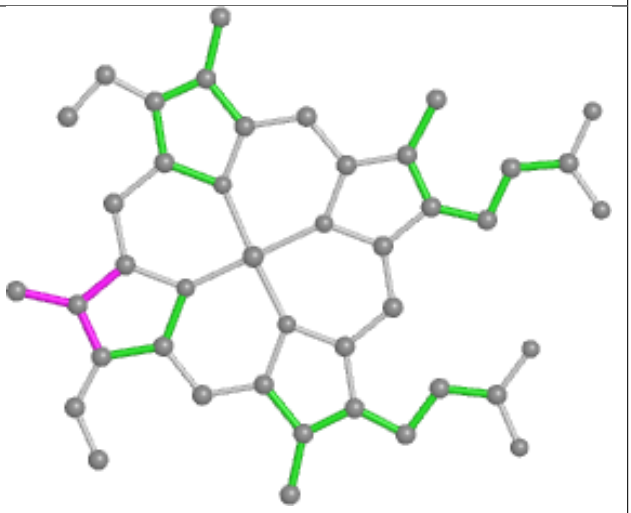


Rings

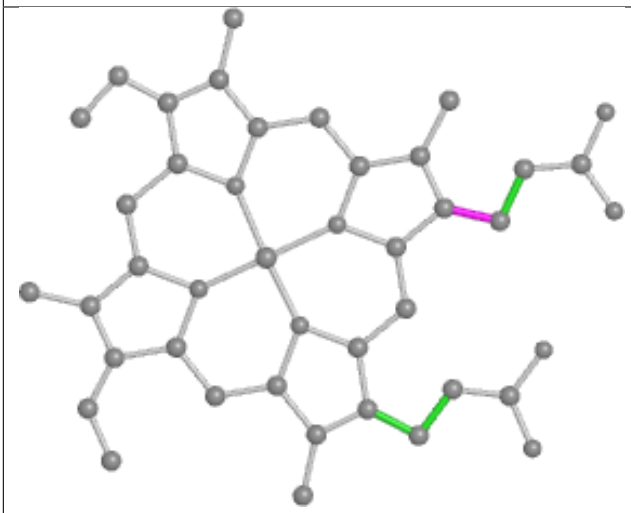
Ligand HEC A 606



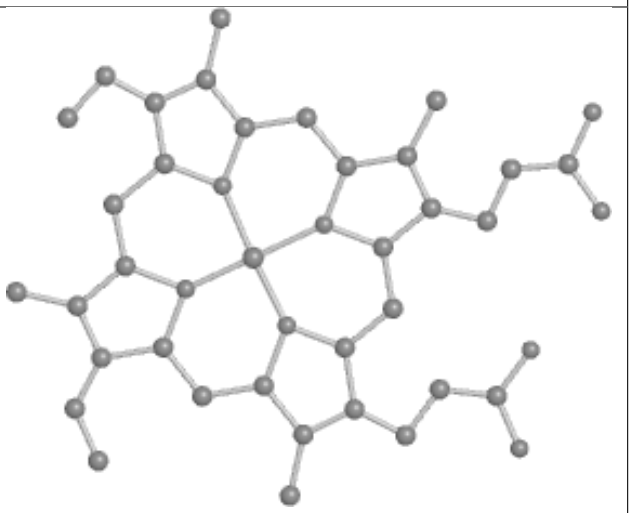
Bond lengths



Bond angles

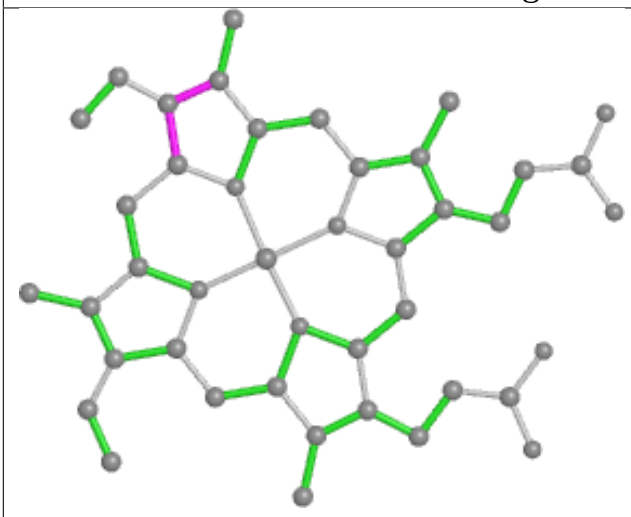


Torsions

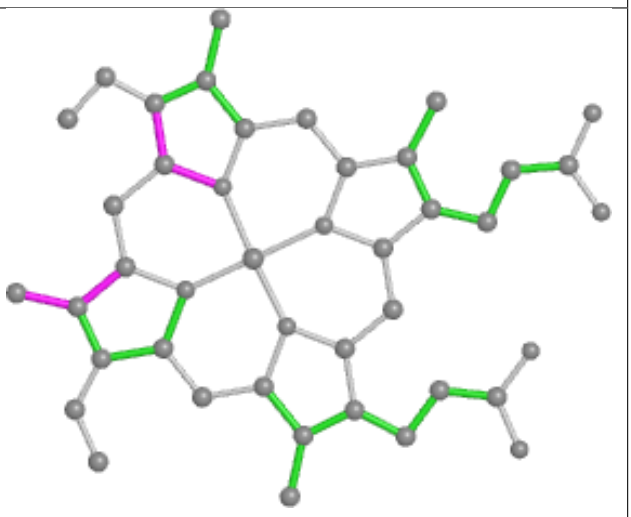


Rings

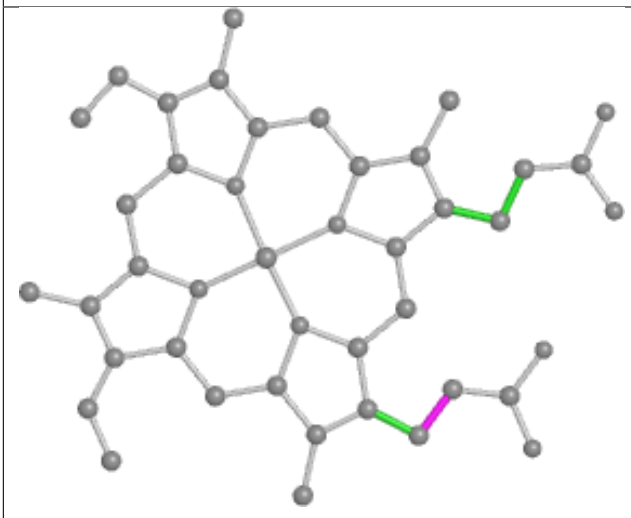
Ligand HEC A 608



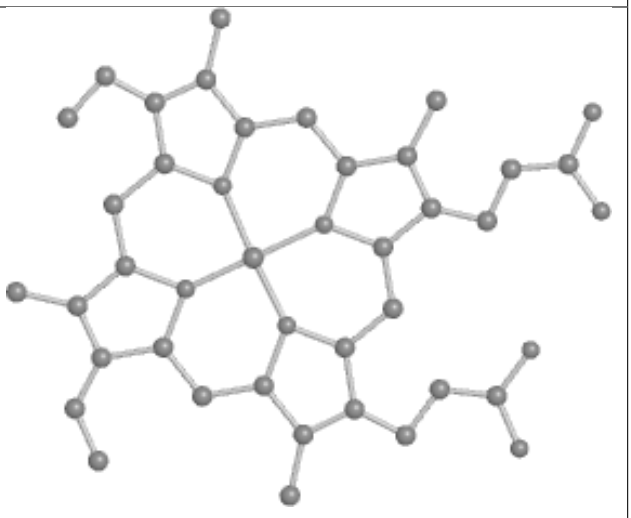
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	484/526 (92%)	-0.20	5 (1%)	82	81	33, 56, 84, 107	0
1	B	483/526 (91%)	-0.14	10 (2%)	63	61	35, 59, 94, 118	0
All	All	967/1052 (91%)	-0.17	15 (1%)	72	70	33, 57, 89, 118	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	HIS	4.7
1	A	482	ALA	4.7
1	B	482	ALA	4.7
1	B	525	GLN	4.3
1	B	371	GLY	4.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

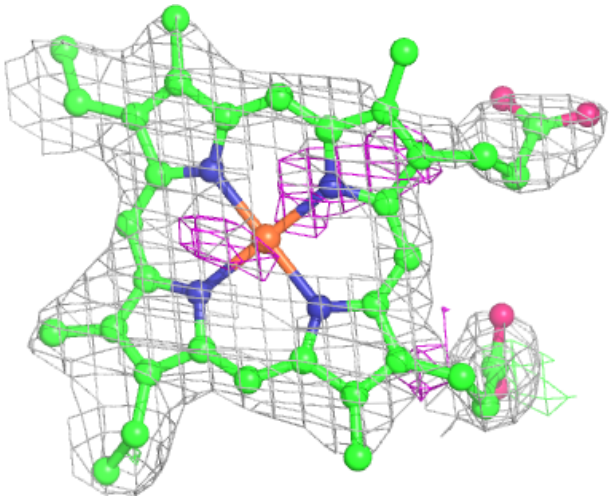
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

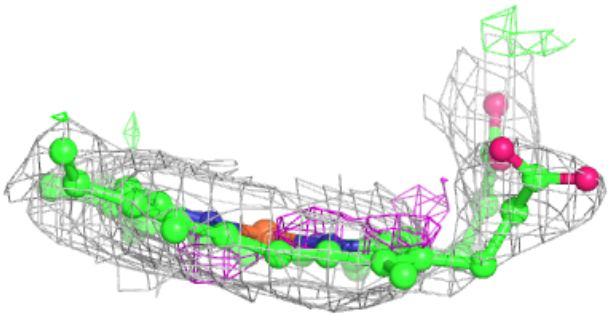
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BU3	A	603	6/6	0.82	0.26	76,79,81,84	0
5	HEC	B	1002	43/43	0.91	0.15	62,81,100,104	0
5	HEC	A	605	43/43	0.92	0.16	51,71,98,101	0
2	MG	A	601	1/1	0.92	0.07	69,69,69,69	0
5	HEC	B	1005	43/43	0.94	0.13	50,58,90,99	0
5	HEC	B	1001	43/43	0.95	0.15	61,70,93,109	0
5	HEC	A	604	43/43	0.96	0.15	58,63,81,89	0
5	HEC	A	608	43/43	0.96	0.12	43,54,90,113	0
5	HEC	B	1008	43/43	0.97	0.12	35,39,52,69	0
5	HEC	B	1006	43/43	0.97	0.14	34,38,57,63	0
5	HEC	A	611	43/43	0.97	0.12	33,35,45,58	0
5	HEC	A	612	43/43	0.97	0.13	37,40,53,59	0
5	HEC	B	1004	43/43	0.97	0.13	40,43,57,71	0
5	HEC	A	606	43/43	0.97	0.13	43,48,68,79	0
5	HEC	B	1009	43/43	0.97	0.14	37,40,50,52	0
5	HEC	A	607	43/43	0.97	0.13	37,42,57,69	0
5	HEC	B	1003	43/43	0.98	0.13	48,52,64,75	0
5	HEC	A	610	43/43	0.98	0.12	29,33,46,52	0
3	CL	A	602	1/1	0.98	0.06	51,51,51,51	0
5	HEC	A	609	43/43	0.98	0.13	30,34,52,64	0
5	HEC	B	1007	43/43	0.98	0.11	36,40,49,52	0

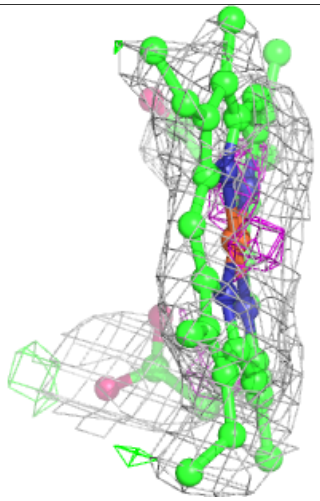
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC B 1002:

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

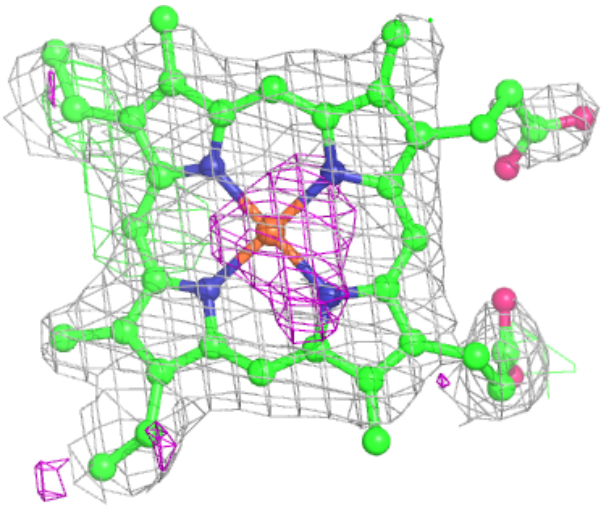


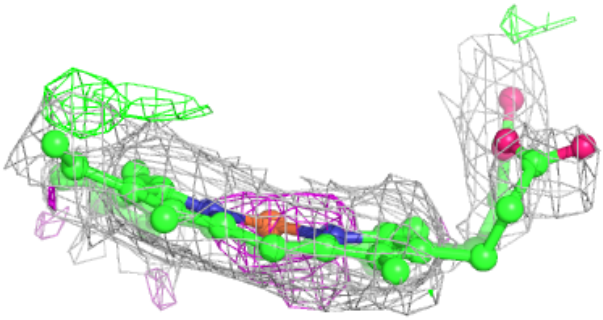


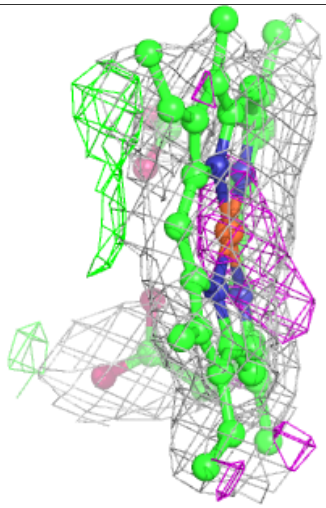


Electron density around HEC A 605:

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

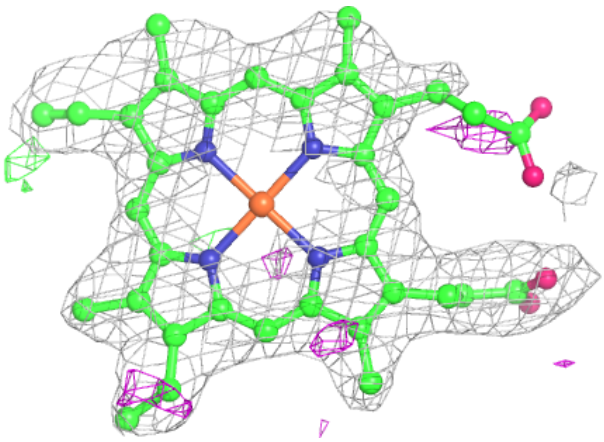


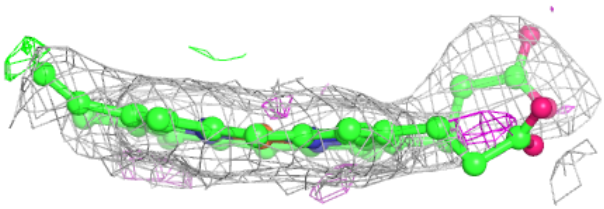


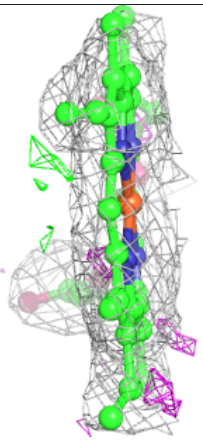


Electron density around HEC B 1005:

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

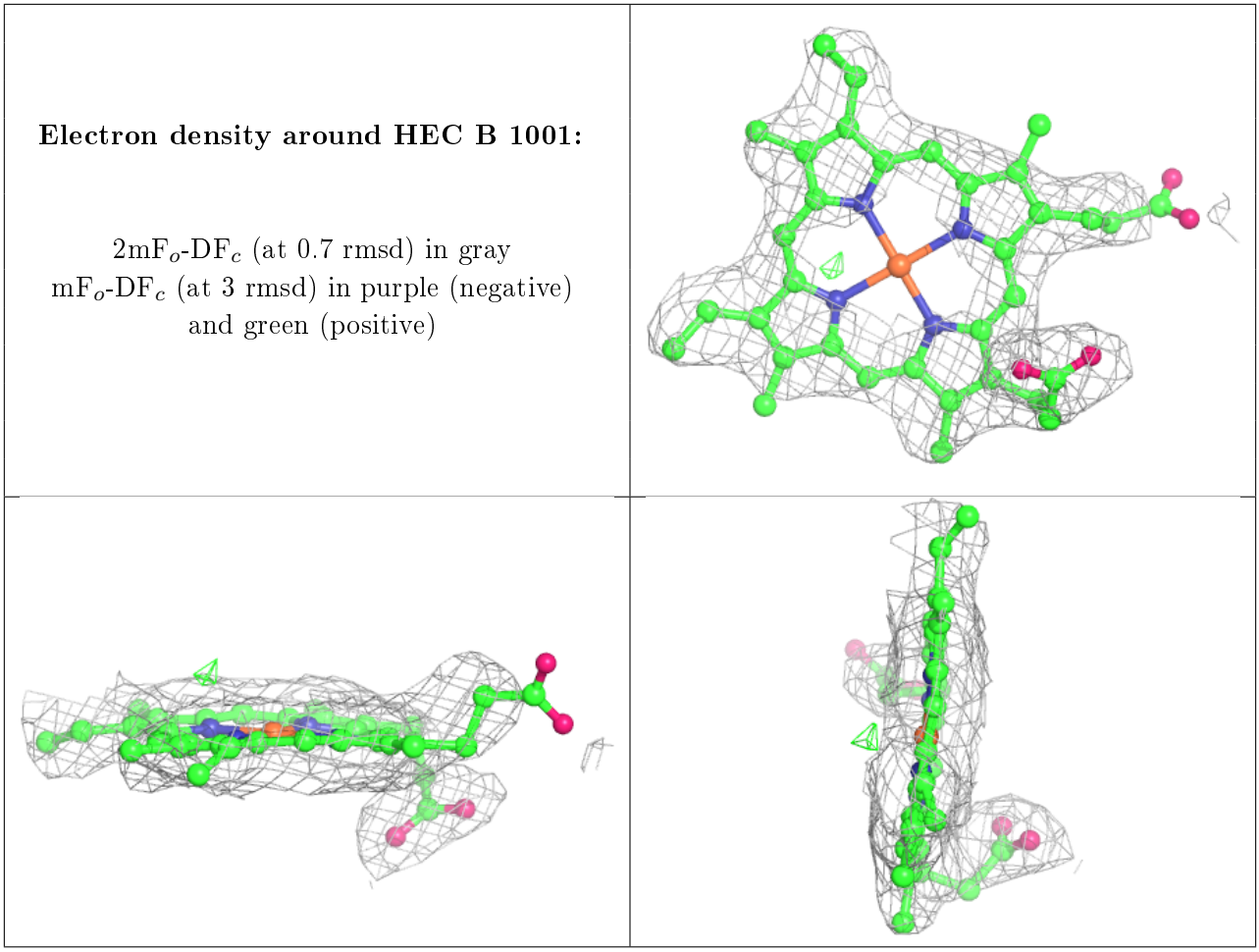






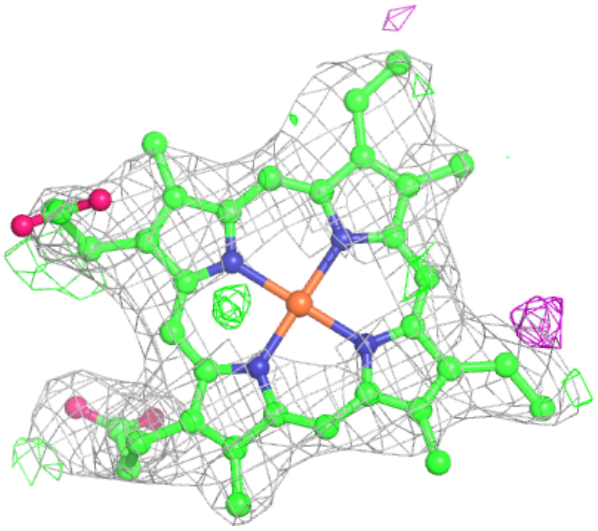
Electron density around HEC B 1001:

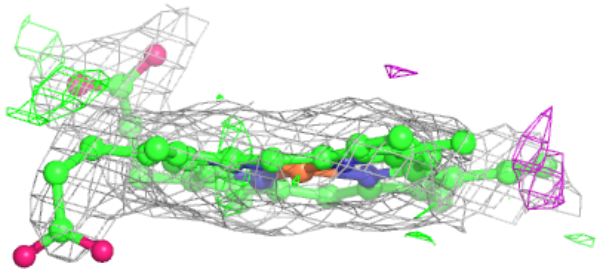
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

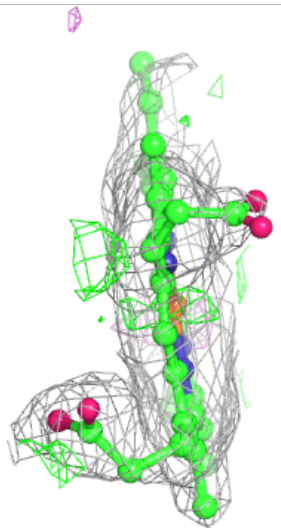


Electron density around HEC A 604:

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

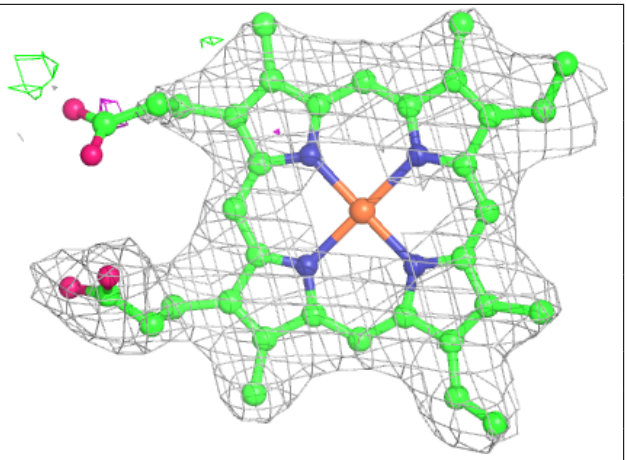


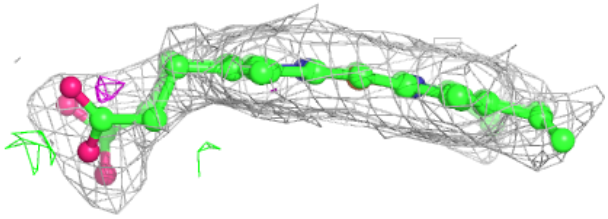


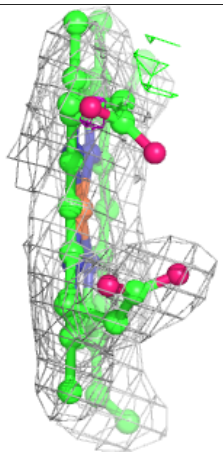


Electron density around HEC A 608:

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

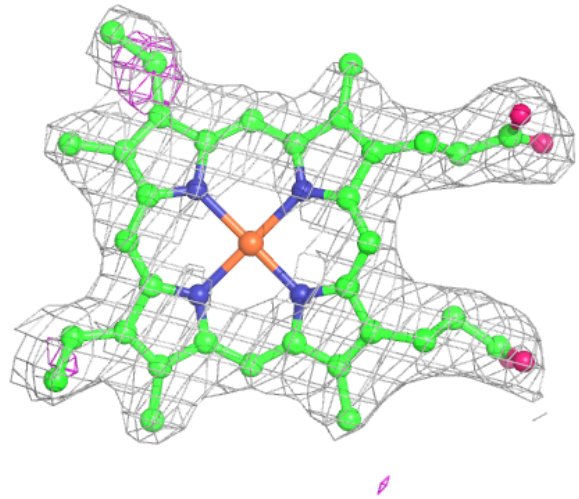


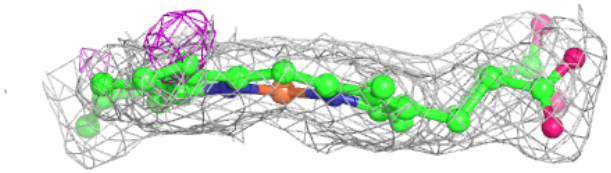


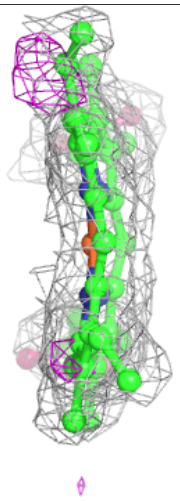


Electron density around HEC B 1008:

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

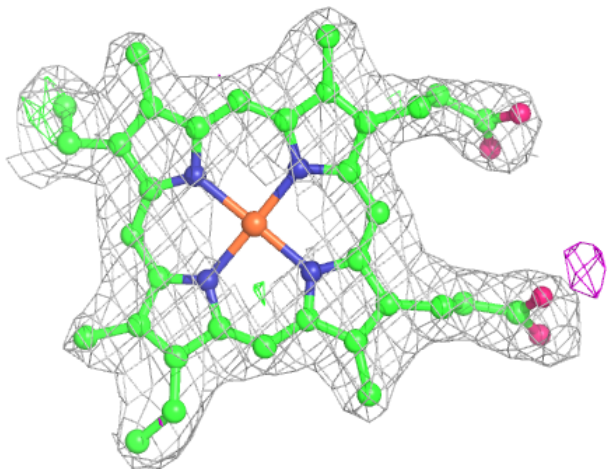


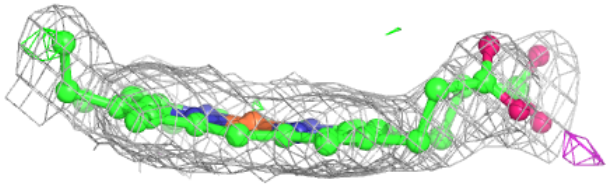


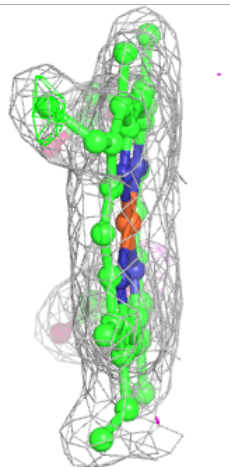


Electron density around HEC B 1006:

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

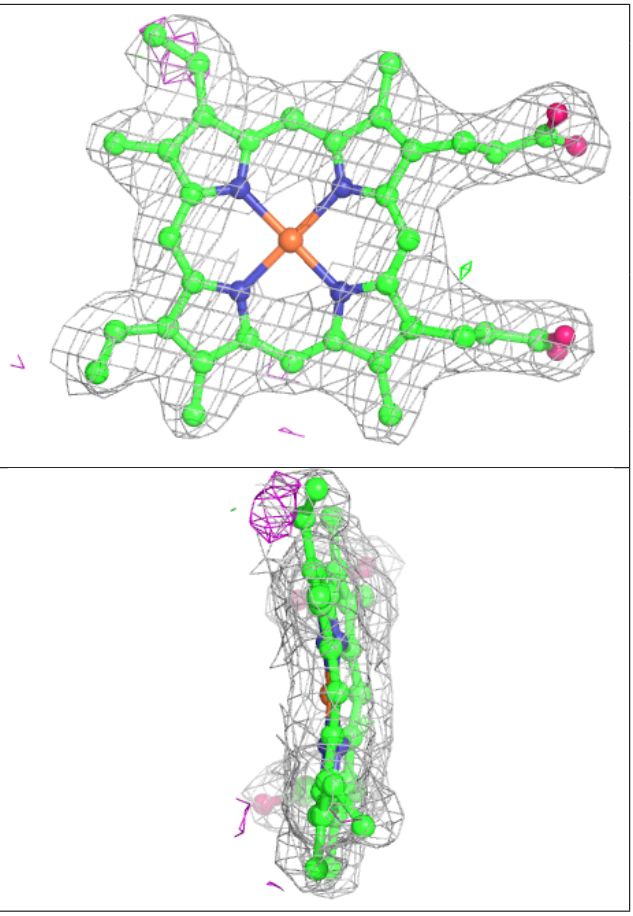






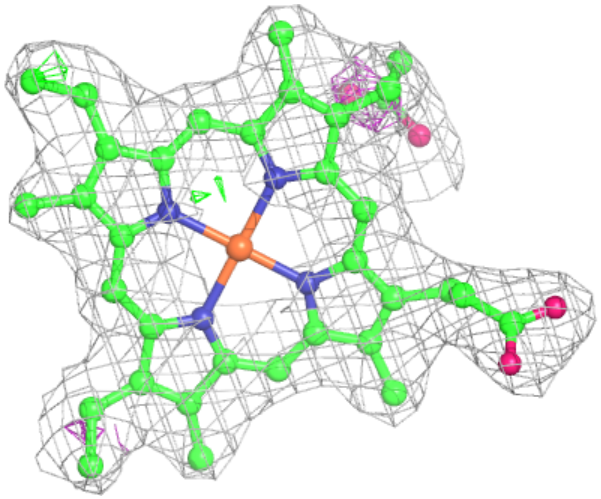
Electron density around HEC A 611:

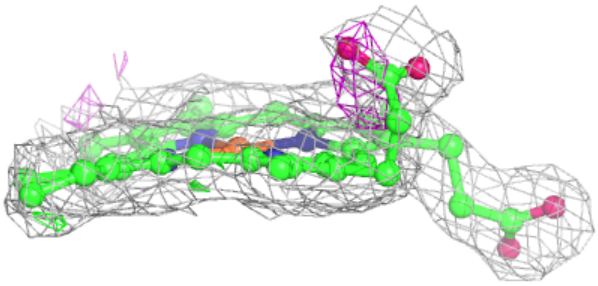
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

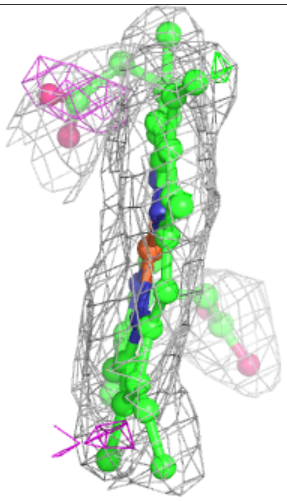


Electron density around HEC A 612:

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

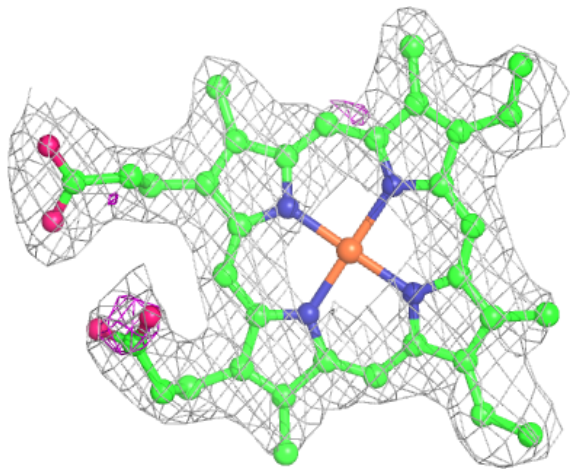


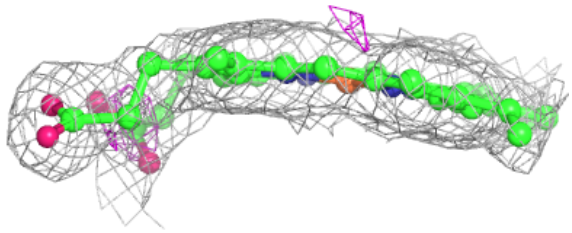


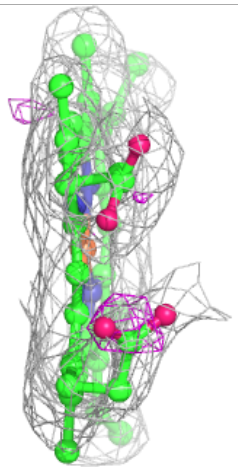


Electron density around HEC B 1004:

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

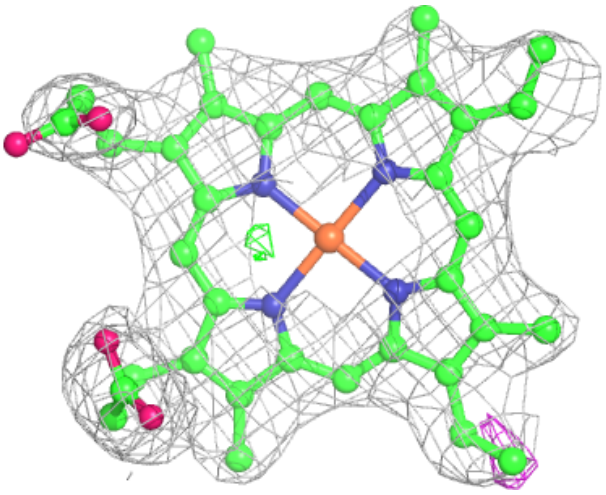


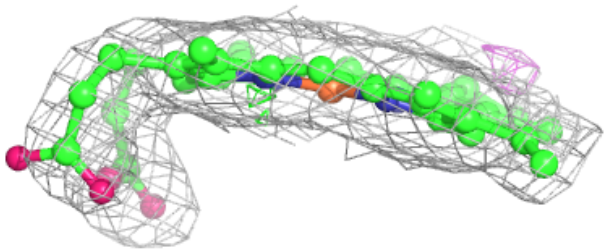


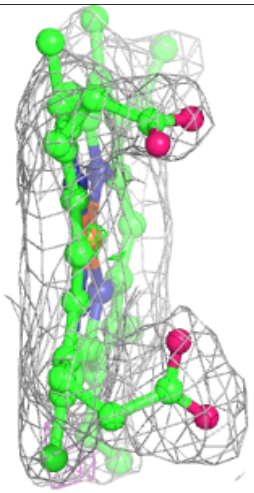


Electron density around HEC A 606:

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

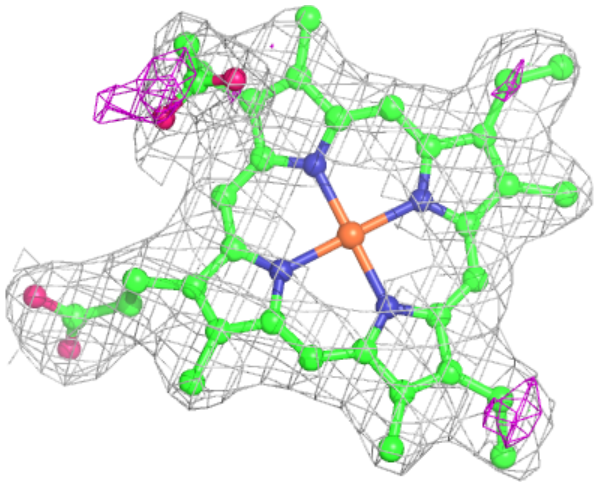


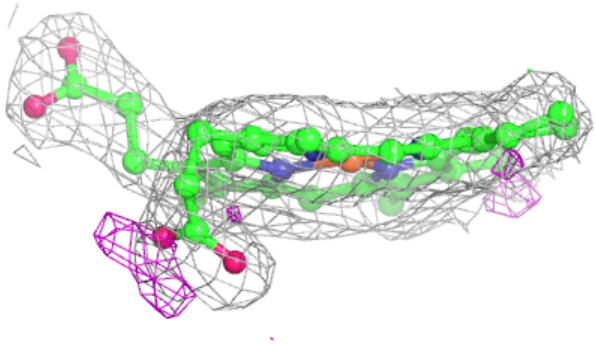


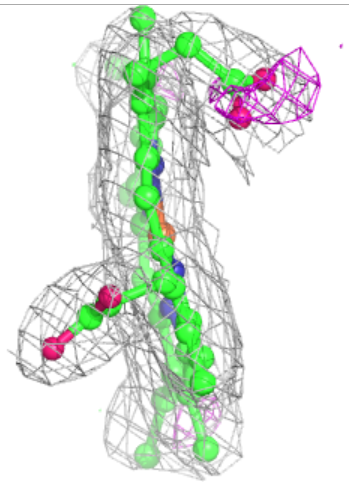


Electron density around HEC B 1009:

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

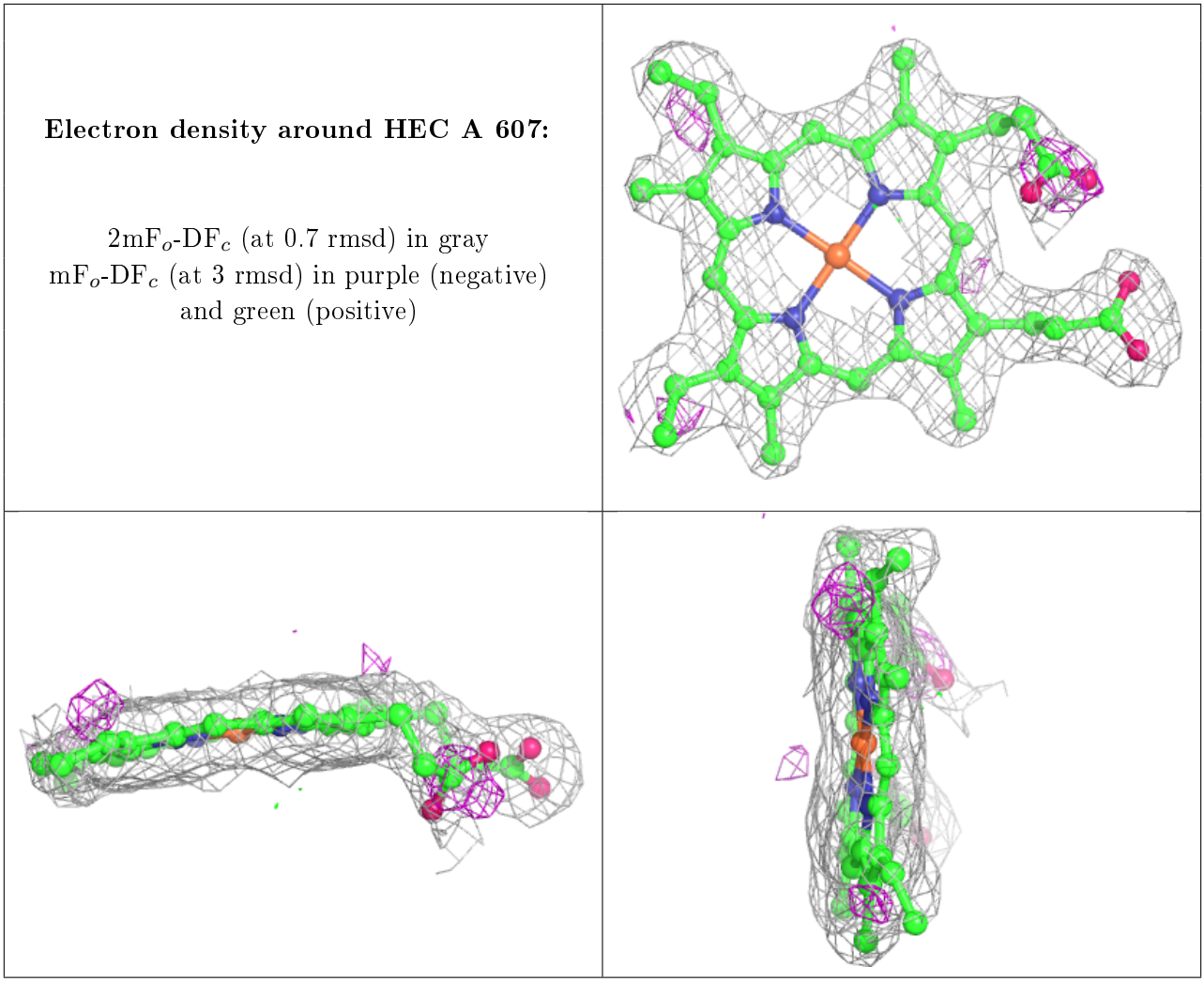






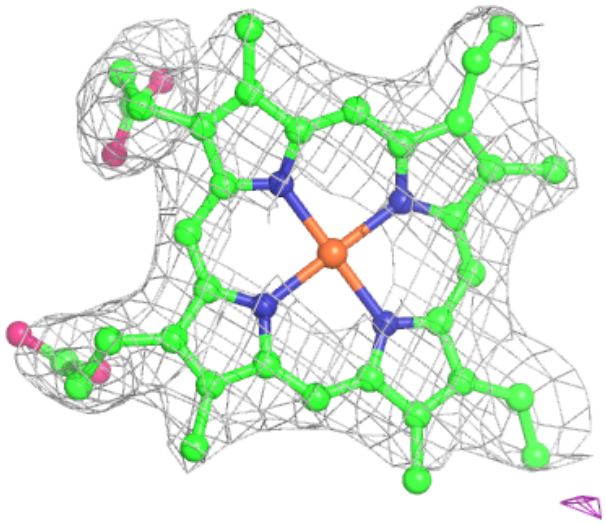
Electron density around HEC A 607:

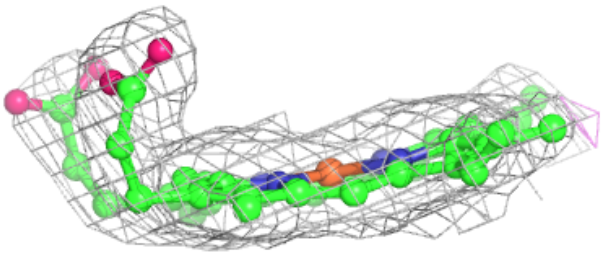
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

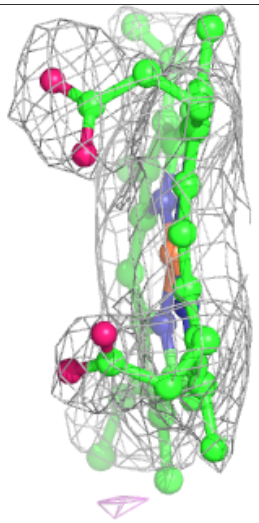


Electron density around HEC B 1003:

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

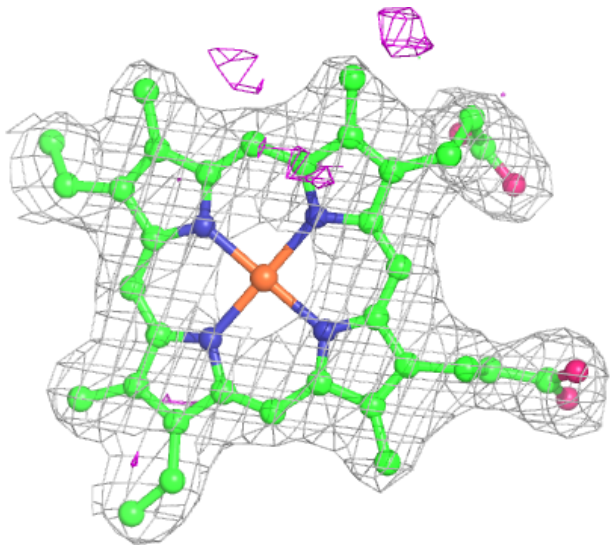


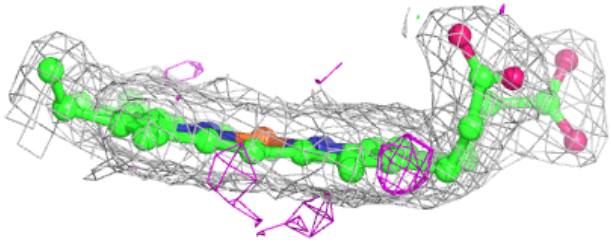


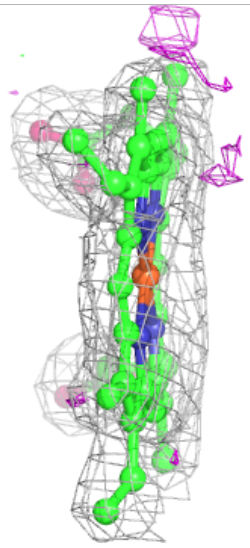


Electron density around HEC A 610:

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

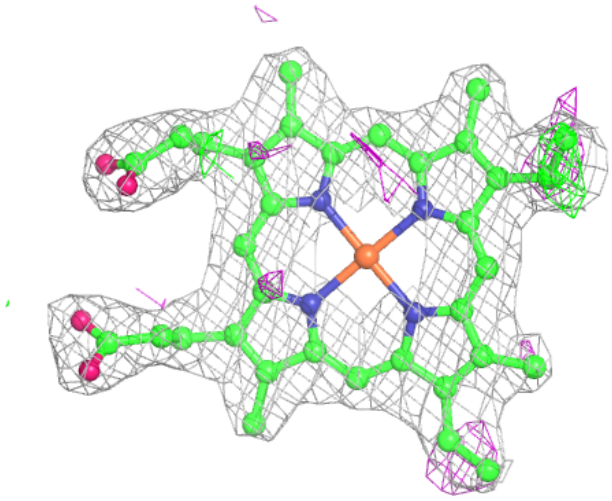


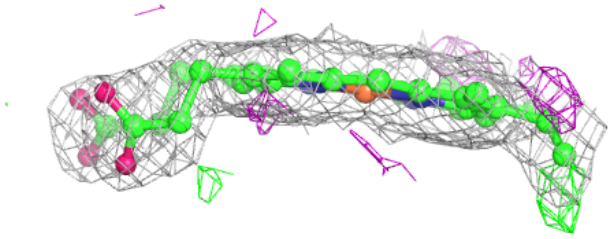


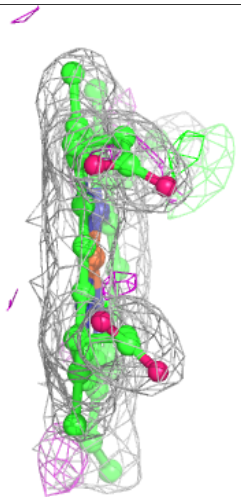


Electron density around HEC A 609:

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

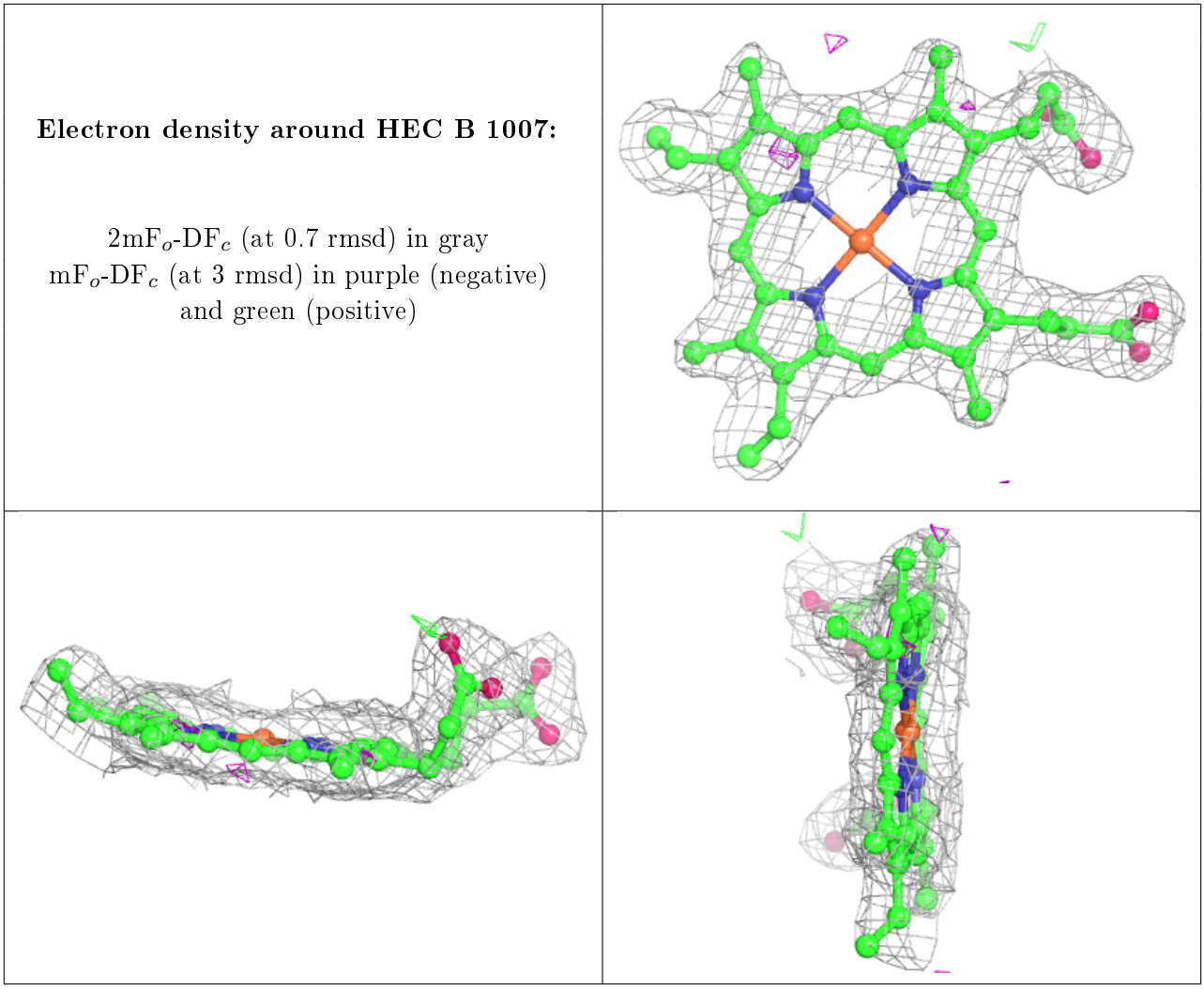






Electron density around HEC B 1007:

$2mF_o$-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.