Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 12:55 PM EDT

PDB ID	:	2CVC
Title	:	Crystal structure of High-Molecular Weight Cytochrome c from Desulfovibrio vulgaris (Hildenborough)
Authors	:	Suto, K.; Sato, M.; Shibata, N.; Kitamura, M.; Morimoto, Y.; Takayama, Y.; Ozawa, K.; Akutsu, H.; Higuchi, Y.; Yasuoka, N.
Deposited on	:	2005-06-02
Resolution	:	2.00 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:

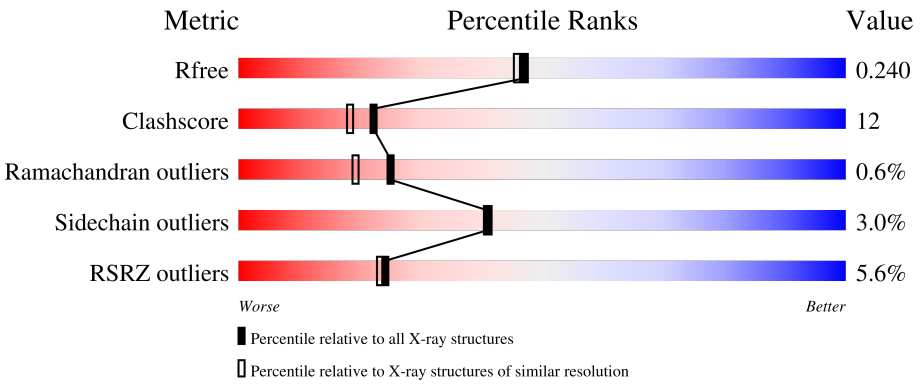
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	545	5% 77% 14% • 8%

2 Entry composition (i)

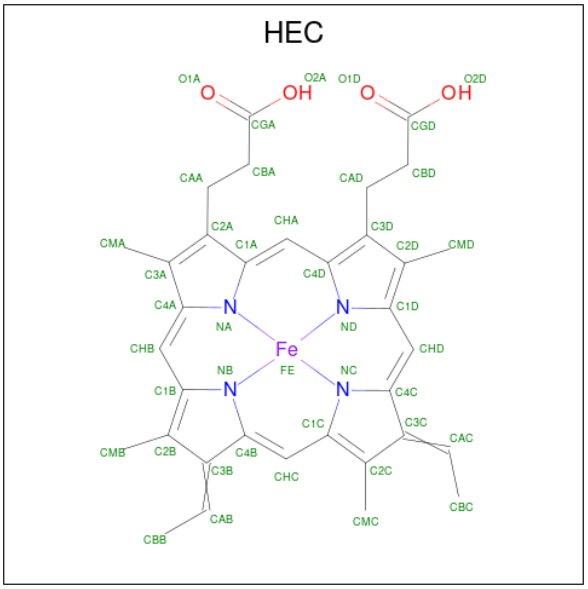
There are 3 unique types of molecules in this entry. The entry contains 4940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 High-molecular-weight cytochrome c precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	500	3779	2322	714	699	44	0	0	0

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



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

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

- Molecule 3 is water.

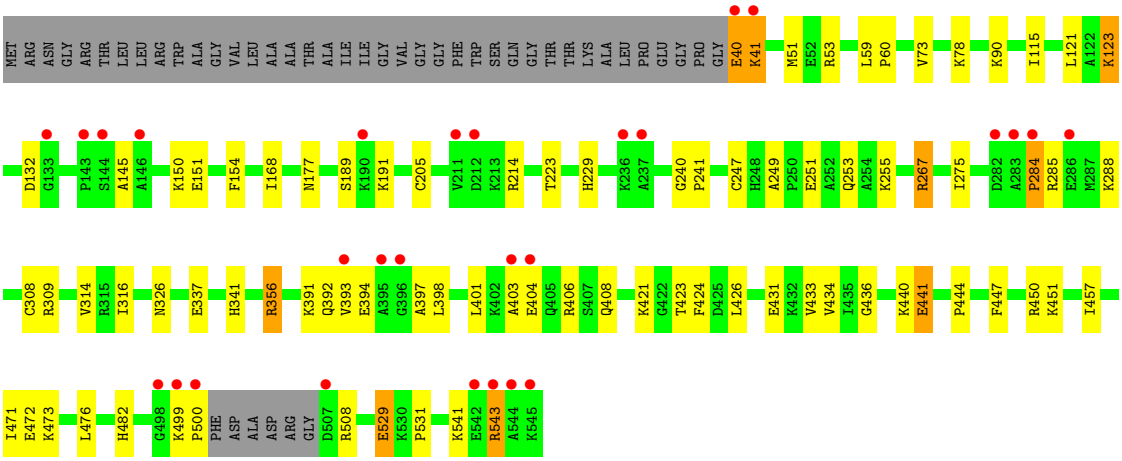
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	473	473	473	0	0

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: High-molecular-weight cytochrome c precursor

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	108.67Å 108.67Å 103.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.35 – 2.00 29.35 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.35-2.00) 99.3 (29.35-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.243 0.197 , 0.240	Depositor DCC
R_{free} test set	4713 reflections (7.37%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4940	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

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	0.27	0/3860	0.46	0/5196

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 (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	3779	0	3714	80	0
2	A	688	0	480	41	0
3	A	473	0	0	10	0
All	All	4940	0	4194	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (101) 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:356:ARG:HH21	1:A:356:ARG:HG3	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.65	0.79
1:A:151:GLU:HG3	2:A:1007:HEC:O1D	1.83	0.78
2:A:1010:HEC:HMC1	2:A:1010:HEC:HBC3	1.66	0.77
2:A:1006:HEC:HMC1	2:A:1006:HEC:HBC3	1.68	0.75
1:A:309:ARG:HG3	2:A:1004:HEC:O1A	1.90	0.72
2:A:1006:HEC:HMB1	2:A:1006:HEC:HBB3	1.72	0.71
1:A:41:LYS:O	1:A:41:LYS:HD2	1.90	0.71
1:A:90:LYS:HE3	1:A:223:THR:HG21	1.78	0.66
1:A:356:ARG:HG3	1:A:356:ARG:NH2	2.12	0.65
1:A:177:ASN:HB2	3:A:1099:HOH:O	1.96	0.64
1:A:508:ARG:HD3	2:A:1014:HEC:HMD3	1.79	0.64
1:A:151:GLU:HG3	2:A:1007:HEC:CGD	2.28	0.64
1:A:316:ILE:HD13	2:A:1008:HEC:HMB3	1.79	0.64
1:A:499:LYS:H	1:A:500:PRO:HA	1.62	0.64
2:A:1016:HEC:HMC1	2:A:1016:HEC:HBC3	1.81	0.62
1:A:403:ALA:HA	1:A:406:ARG:HD3	1.81	0.62
1:A:309:ARG:HG3	2:A:1004:HEC:CGA	2.31	0.61
2:A:1015:HEC:HHA	2:A:1015:HEC:HBA1	1.82	0.61
2:A:1015:HEC:HMB1	2:A:1015:HEC:HBB3	1.82	0.61
1:A:431:GLU:HA	1:A:450:ARG:HB2	1.82	0.61
1:A:73:VAL:HG13	1:A:78:LYS:HB2	1.81	0.60
1:A:314:VAL:HG11	2:A:1009:HEC:HBC2	1.81	0.60
1:A:499:LYS:N	1:A:500:PRO:HA	2.17	0.60
1:A:531:PRO:HD3	2:A:1015:HEC:HAA1	1.84	0.60
1:A:267:ARG:NH2	3:A:1093:HOH:O	2.35	0.59
1:A:341:HIS:HE1	2:A:1012:HEC:NA	1.99	0.59
2:A:1006:HEC:HMC1	2:A:1006:HEC:CBC	2.32	0.59
1:A:151:GLU:HG2	3:A:1188:HOH:O	2.04	0.58
2:A:1011:HEC:HMC1	2:A:1011:HEC:HBC3	1.84	0.58
1:A:154:PHE:HB2	2:A:1004:HEC:HBD1	1.86	0.57
1:A:241:PRO:HG2	1:A:247:CYS:SG	2.44	0.56
1:A:436:GLY:HA3	1:A:444:PRO:HB3	1.86	0.56
1:A:441:GLU:HG2	3:A:1344:HOH:O	2.05	0.56
1:A:40:GLU:O	1:A:145:ALA:HB1	2.05	0.56
1:A:73:VAL:CG1	1:A:78:LYS:HB2	2.36	0.55
1:A:499:LYS:HE2	3:A:1339:HOH:O	2.06	0.55
1:A:398:LEU:HD22	1:A:398:LEU:N	2.22	0.55
2:A:1008:HEC:HBC3	2:A:1008:HEC:HMC1	1.89	0.54
1:A:121:LEU:HD13	2:A:1002:HEC:HMD3	1.90	0.53
1:A:189:SER:HB2	1:A:191:LYS:HE3	1.89	0.53
1:A:316:ILE:CD1	2:A:1004:HEC:HMA3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:O	1:A:267:ARG:HD3	2.10	0.52
1:A:249:ALA:HB1	1:A:251:GLU:OE2	2.10	0.52
1:A:404:GLU:O	1:A:408:GLN:HG3	2.09	0.52
1:A:426:LEU:HD21	1:A:457:ILE:HD12	1.91	0.52
1:A:337:GLU:HG2	3:A:1317:HOH:O	2.10	0.51
1:A:121:LEU:CD1	2:A:1002:HEC:HMD3	2.40	0.51
1:A:398:LEU:HA	1:A:401:LEU:HD13	1.91	0.51
1:A:541:LYS:HE2	3:A:1461:HOH:O	2.10	0.51
1:A:391:LYS:HG3	1:A:392:GLN:HG3	1.93	0.51
1:A:205:CYS:O	1:A:214:ARG:HD2	2.11	0.50
1:A:275:ILE:HG22	2:A:1012:HEC:HBD1	1.94	0.50
1:A:59:LEU:HB3	1:A:60:PRO:HD2	1.93	0.50
1:A:531:PRO:HD3	2:A:1015:HEC:CAA	2.41	0.50
2:A:1005:HEC:HMA2	2:A:1005:HEC:O1A	2.12	0.50
2:A:1011:HEC:HMB1	2:A:1011:HEC:HBB3	1.94	0.49
1:A:499:LYS:HB3	1:A:500:PRO:C	2.33	0.49
2:A:1002:HEC:HMC1	2:A:1002:HEC:CBC	2.39	0.49
1:A:398:LEU:C	1:A:401:LEU:HD13	2.34	0.48
2:A:1010:HEC:HBD2	3:A:1046:HOH:O	2.13	0.48
2:A:1015:HEC:HMC1	2:A:1015:HEC:HBC3	1.94	0.48
1:A:341:HIS:HE1	2:A:1012:HEC:C1A	2.27	0.48
1:A:326:ASN:HB2	3:A:1228:HOH:O	2.13	0.48
1:A:431:GLU:HA	1:A:450:ARG:CB	2.43	0.48
1:A:168:ILE:HG22	1:A:177:ASN:OD1	2.14	0.47
1:A:308:CYS:SG	2:A:1004:HEC:HBA1	2.55	0.47
1:A:90:LYS:HE3	1:A:223:THR:CG2	2.43	0.47
1:A:337:GLU:HG3	1:A:341:HIS:HD1	1.79	0.46
1:A:451:LYS:HE3	2:A:1015:HEC:O2D	2.15	0.46
1:A:433:VAL:HG13	1:A:447:PHE:HB3	1.96	0.46
2:A:1005:HEC:HMC1	2:A:1005:HEC:HBC3	1.97	0.46
2:A:1010:HEC:HMC1	2:A:1010:HEC:CBC	2.42	0.46
1:A:356:ARG:NH2	1:A:356:ARG:CG	2.79	0.46
1:A:115:ILE:HG21	1:A:132:ASP:HB3	1.98	0.46
1:A:406:ARG:HD3	3:A:1301:HOH:O	2.15	0.46
1:A:543:ARG:HG3	1:A:543:ARG:HH11	1.81	0.45
1:A:398:LEU:HA	1:A:401:LEU:CD1	2.47	0.45
1:A:423:THR:HG22	1:A:424:PHE:N	2.31	0.45
2:A:1002:HEC:HMB1	2:A:1002:HEC:HBB3	1.99	0.44
1:A:229:HIS:CE1	1:A:240:GLY:HA3	2.53	0.44
1:A:508:ARG:HG2	2:A:1014:HEC:C3D	2.48	0.44
1:A:255:LYS:HG2	1:A:255:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:H	1:A:123:LYS:HG2	1.59	0.43
1:A:393:VAL:HA	1:A:398:LEU:HD23	1.99	0.43
2:A:1003:HEC:HMC1	2:A:1003:HEC:HBC3	2.01	0.43
1:A:150:LYS:HD2	1:A:253:GLN:OE1	2.19	0.43
1:A:251:GLU:H	1:A:251:GLU:CD	2.21	0.43
2:A:1009:HEC:HBC3	2:A:1009:HEC:HMC1	2.01	0.42
1:A:423:THR:OG1	1:A:476:LEU:HD12	2.20	0.42
1:A:499:LYS:N	1:A:500:PRO:CA	2.83	0.42
1:A:531:PRO:HD3	2:A:1015:HEC:C2A	2.50	0.42
1:A:284:PRO:HA	1:A:285:ARG:HA	1.92	0.41
1:A:397:ALA:HB3	1:A:398:LEU:HD22	2.03	0.41
1:A:434:VAL:HG13	1:A:434:VAL:O	2.21	0.41
1:A:421:LYS:O	1:A:473:LYS:HD3	2.21	0.40
1:A:356:ARG:HD2	1:A:356:ARG:HA	1.92	0.40
1:A:529:GLU:HA	1:A:529:GLU:OE1	2.21	0.40
1:A:436:GLY:CA	1:A:444:PRO:HB3	2.52	0.40
2:A:1012:HEC:HBC3	2:A:1012:HEC:HMC1	2.03	0.40
1:A:471:ILE:HG13	1:A:472:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	496/545 (91%)	470 (95%)	23 (5%)	3 (1%)	25 19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	440	LYS
1	A	284	PRO
1	A	543	ARG

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	405/435 (93%)	393 (97%)	12 (3%)	41 41

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	41	LYS
1	A	51	MET
1	A	53	ARG
1	A	123	LYS
1	A	267	ARG
1	A	288	LYS
1	A	356	ARG
1	A	394	GLU
1	A	441	GLU
1	A	482	HIS
1	A	529	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	326	ASN
1	A	400	ASN
1	A	405	GLN
1	A	443	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)

16 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	$\#\|Z\| > 2$
2	HEC	A	1008	1	32,50,50	1.15	4 (12%)	30,82,82	2.27	6 (20%)
2	HEC	A	1006	1	32,50,50	1.07	2 (6%)	30,82,82	2.37	8 (26%)
2	HEC	A	1011	1	32,50,50	1.14	2 (6%)	30,82,82	2.45	7 (23%)
2	HEC	A	1015	1	32,50,50	0.94	1 (3%)	30,82,82	1.39	5 (16%)
2	HEC	A	1005	1	32,50,50	1.14	1 (3%)	30,82,82	2.26	5 (16%)
2	HEC	A	1009	1	32,50,50	1.08	1 (3%)	30,82,82	2.48	7 (23%)
2	HEC	A	1012	1	32,50,50	1.07	1 (3%)	30,82,82	2.27	5 (16%)
2	HEC	A	1013	1	32,50,50	1.09	1 (3%)	30,82,82	2.33	6 (20%)
2	HEC	A	1007	1	32,50,50	1.05	2 (6%)	30,82,82	2.38	8 (26%)
2	HEC	A	1014	1	32,50,50	1.12	2 (6%)	30,82,82	2.40	8 (26%)
2	HEC	A	1016	1	32,50,50	1.10	2 (6%)	30,82,82	2.37	8 (26%)
2	HEC	A	1002	1	32,50,50	1.10	2 (6%)	30,82,82	2.40	8 (26%)
2	HEC	A	1003	1	32,50,50	1.03	1 (3%)	30,82,82	2.51	9 (30%)
2	HEC	A	1004	1	32,50,50	1.12	3 (9%)	30,82,82	2.37	7 (23%)
2	HEC	A	1001	1	32,50,50	1.09	2 (6%)	30,82,82	2.25	6 (20%)
2	HEC	A	1010	1	32,50,50	1.00	1 (3%)	30,82,82	2.58	9 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	1008	1	-	2/10/54/54	-
2	HEC	A	1006	1	-	2/10/54/54	-
2	HEC	A	1011	1	-	2/10/54/54	-
2	HEC	A	1015	1	-	4/10/54/54	-
2	HEC	A	1005	1	-	4/10/54/54	-
2	HEC	A	1009	1	-	2/10/54/54	-
2	HEC	A	1012	1	-	2/10/54/54	-
2	HEC	A	1013	1	-	2/10/54/54	-
2	HEC	A	1007	1	-	5/10/54/54	-
2	HEC	A	1014	1	-	3/10/54/54	-
2	HEC	A	1016	1	-	4/10/54/54	-
2	HEC	A	1002	1	-	2/10/54/54	-
2	HEC	A	1003	1	-	2/10/54/54	-
2	HEC	A	1004	1	-	3/10/54/54	-
2	HEC	A	1001	1	-	3/10/54/54	-
2	HEC	A	1010	1	-	5/10/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1005	HEC	C3C-C4C	-3.01	1.37	1.43
2	A	1010	HEC	C4B-C3B	-2.91	1.37	1.43
2	A	1012	HEC	C4B-C3B	-2.66	1.38	1.43
2	A	1013	HEC	C4B-C3B	-2.51	1.38	1.43
2	A	1009	HEC	C3C-C4C	-2.50	1.38	1.43
2	A	1004	HEC	C3C-C4C	-2.38	1.38	1.43
2	A	1008	HEC	C1B-NB	-2.27	1.31	1.36
2	A	1008	HEC	C4B-C3B	-2.24	1.39	1.43
2	A	1014	HEC	C1B-NB	-2.17	1.31	1.36
2	A	1002	HEC	C1C-NC	-2.17	1.31	1.36
2	A	1001	HEC	C4B-C3B	-2.16	1.39	1.43
2	A	1004	HEC	C4D-ND	-2.14	1.32	1.36
2	A	1001	HEC	C2A-C1A	-2.14	1.37	1.42
2	A	1011	HEC	C3C-C4C	-2.12	1.39	1.43
2	A	1006	HEC	C1B-NB	-2.12	1.32	1.36
2	A	1016	HEC	C3C-C4C	-2.09	1.39	1.43
2	A	1008	HEC	C3C-C4C	-2.08	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	HEC	C1C-NC	-2.07	1.32	1.36
2	A	1003	HEC	C3A-C4A	-2.06	1.37	1.42
2	A	1016	HEC	C3A-C4A	-2.05	1.37	1.42
2	A	1007	HEC	C3C-C4C	-2.05	1.39	1.43
2	A	1011	HEC	C3A-C4A	-2.05	1.37	1.42
2	A	1007	HEC	C3A-C4A	-2.04	1.37	1.42
2	A	1015	HEC	C4B-C3B	-2.04	1.39	1.43
2	A	1014	HEC	C4B-C3B	-2.03	1.39	1.43
2	A	1002	HEC	C4B-C3B	-2.03	1.39	1.43
2	A	1008	HEC	C1D-ND	-2.03	1.32	1.36
2	A	1006	HEC	C1C-NC	-2.01	1.32	1.36

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1007	HEC	CBB-CAB-C3B	-7.59	109.72	127.49
2	A	1002	HEC	CBB-CAB-C3B	-7.56	109.79	127.49
2	A	1016	HEC	CBB-CAB-C3B	-7.53	109.87	127.49
2	A	1014	HEC	CBB-CAB-C3B	-7.52	109.88	127.49
2	A	1009	HEC	CBC-CAC-C3C	-7.52	109.89	127.49
2	A	1004	HEC	CBB-CAB-C3B	-7.50	109.94	127.49
2	A	1013	HEC	CBC-CAC-C3C	-7.47	110.01	127.49
2	A	1003	HEC	CBB-CAB-C3B	-7.47	110.02	127.49
2	A	1005	HEC	CBB-CAB-C3B	-7.46	110.03	127.49
2	A	1010	HEC	CBB-CAB-C3B	-7.44	110.07	127.49
2	A	1003	HEC	CBC-CAC-C3C	-7.40	110.18	127.49
2	A	1001	HEC	CBB-CAB-C3B	-7.39	110.20	127.49
2	A	1009	HEC	CBB-CAB-C3B	-7.39	110.20	127.49
2	A	1007	HEC	CBC-CAC-C3C	-7.36	110.27	127.49
2	A	1011	HEC	CBC-CAC-C3C	-7.35	110.28	127.49
2	A	1005	HEC	CBC-CAC-C3C	-7.35	110.28	127.49
2	A	1011	HEC	CBB-CAB-C3B	-7.35	110.30	127.49
2	A	1012	HEC	CBB-CAB-C3B	-7.32	110.36	127.49
2	A	1014	HEC	CBC-CAC-C3C	-7.29	110.42	127.49
2	A	1008	HEC	CBB-CAB-C3B	-7.29	110.42	127.49
2	A	1004	HEC	CBC-CAC-C3C	-7.26	110.49	127.49
2	A	1006	HEC	CBB-CAB-C3B	-7.25	110.53	127.49
2	A	1001	HEC	CBC-CAC-C3C	-7.23	110.58	127.49
2	A	1013	HEC	CBB-CAB-C3B	-7.20	110.65	127.49
2	A	1012	HEC	CBC-CAC-C3C	-7.19	110.67	127.49
2	A	1010	HEC	CBC-CAC-C3C	-7.12	110.83	127.49
2	A	1016	HEC	CBC-CAC-C3C	-7.12	110.84	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1008	HEC	CBC-CAC-C3C	-7.06	110.96	127.49
2	A	1002	HEC	CBC-CAC-C3C	-6.94	111.24	127.49
2	A	1006	HEC	CBC-CAC-C3C	-6.84	111.48	127.49
2	A	1003	HEC	CMB-C2B-C3B	4.53	131.14	125.82
2	A	1010	HEC	CMC-C2C-C3C	4.39	130.99	125.82
2	A	1011	HEC	CMB-C2B-C3B	4.26	130.83	125.82
2	A	1009	HEC	CMB-C2B-C3B	3.77	130.25	125.82
2	A	1011	HEC	CMB-C2B-C1B	-3.71	123.03	128.46
2	A	1010	HEC	CMC-C2C-C1C	-3.56	123.25	128.46
2	A	1013	HEC	C4C-CHD-C1D	3.54	134.04	123.67
2	A	1010	HEC	C1D-C2D-C3D	-3.44	104.60	107.00
2	A	1014	HEC	C1D-C2D-C3D	-3.42	104.61	107.00
2	A	1009	HEC	CMB-C2B-C1B	-3.38	123.50	128.46
2	A	1002	HEC	CMC-C2C-C3C	3.37	129.78	125.82
2	A	1002	HEC	CMC-C2C-C1C	-3.22	123.73	128.46
2	A	1003	HEC	CMB-C2B-C1B	-3.17	123.81	128.46
2	A	1013	HEC	C4A-CHB-C1B	3.14	132.86	123.67
2	A	1015	HEC	CMC-C2C-C3C	3.04	129.39	125.82
2	A	1013	HEC	CMC-C2C-C3C	3.01	129.36	125.82
2	A	1006	HEC	CMC-C2C-C1C	-2.99	124.07	128.46
2	A	1012	HEC	C4C-CHD-C1D	2.94	132.29	123.67
2	A	1009	HEC	C1C-CHC-C4B	2.94	132.28	123.67
2	A	1008	HEC	C4A-CHB-C1B	2.86	132.06	123.67
2	A	1001	HEC	C4C-CHD-C1D	2.82	131.92	123.67
2	A	1006	HEC	C4A-CHB-C1B	2.81	131.89	123.67
2	A	1006	HEC	CMC-C2C-C3C	2.76	129.07	125.82
2	A	1003	HEC	C4A-CHB-C1B	2.68	131.53	123.67
2	A	1004	HEC	C4D-CHA-C1A	2.68	131.53	123.67
2	A	1014	HEC	C4A-CHB-C1B	2.68	131.51	123.67
2	A	1006	HEC	C4C-CHD-C1D	2.67	131.50	123.67
2	A	1010	HEC	CMB-C2B-C3B	2.63	128.91	125.82
2	A	1009	HEC	C4D-CHA-C1A	2.61	131.31	123.67
2	A	1011	HEC	C4D-CHA-C1A	2.58	131.21	123.67
2	A	1012	HEC	CMD-C2D-C1D	-2.57	124.69	128.46
2	A	1007	HEC	CMB-C2B-C3B	2.56	128.84	125.82
2	A	1004	HEC	C1C-CHC-C4B	2.55	131.13	123.67
2	A	1010	HEC	CMB-C2B-C1B	-2.54	124.73	128.46
2	A	1003	HEC	C1C-CHC-C4B	2.53	131.08	123.67
2	A	1016	HEC	CMB-C2B-C3B	2.50	128.76	125.82
2	A	1005	HEC	C4D-CHA-C1A	2.50	130.99	123.67
2	A	1001	HEC	C4D-CHA-C1A	2.49	130.96	123.67
2	A	1014	HEC	C4C-CHD-C1D	2.46	130.88	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1006	HEC	C4C-C3C-C2C	-2.44	103.71	106.35
2	A	1016	HEC	C1C-CHC-C4B	2.44	130.81	123.67
2	A	1015	HEC	C1C-CHC-C4B	2.44	130.80	123.67
2	A	1010	HEC	C4C-CHD-C1D	2.40	130.69	123.67
2	A	1011	HEC	C1C-CHC-C4B	2.38	130.65	123.67
2	A	1012	HEC	C4A-CHB-C1B	2.36	130.60	123.67
2	A	1002	HEC	C4A-CHB-C1B	2.36	130.59	123.67
2	A	1002	HEC	C4D-CHA-C1A	2.36	130.58	123.67
2	A	1004	HEC	C4C-CHD-C1D	2.35	130.56	123.67
2	A	1002	HEC	C4C-CHD-C1D	2.35	130.56	123.67
2	A	1003	HEC	C4C-CHD-C1D	2.34	130.52	123.67
2	A	1008	HEC	CMB-C2B-C3B	2.33	128.56	125.82
2	A	1008	HEC	C4C-CHD-C1D	2.32	130.48	123.67
2	A	1002	HEC	C1C-CHC-C4B	2.30	130.40	123.67
2	A	1016	HEC	CMC-C2C-C3C	2.29	128.51	125.82
2	A	1014	HEC	C1C-CHC-C4B	2.28	130.36	123.67
2	A	1015	HEC	CMB-C2B-C3B	2.28	128.50	125.82
2	A	1015	HEC	CBB-CAB-C3B	-2.28	122.17	127.49
2	A	1001	HEC	CMB-C2B-C3B	2.27	128.49	125.82
2	A	1004	HEC	CMC-C2C-C3C	2.27	128.49	125.82
2	A	1015	HEC	C4D-CHA-C1A	2.27	130.32	123.67
2	A	1005	HEC	C1C-CHC-C4B	2.25	130.27	123.67
2	A	1007	HEC	C4C-CHD-C1D	2.24	130.24	123.67
2	A	1004	HEC	CMC-C2C-C1C	-2.24	125.17	128.46
2	A	1007	HEC	C4A-CHB-C1B	2.24	130.24	123.67
2	A	1016	HEC	CMC-C2C-C1C	-2.23	125.19	128.46
2	A	1006	HEC	C1C-CHC-C4B	2.20	130.12	123.67
2	A	1010	HEC	C4A-CHB-C1B	2.20	130.10	123.67
2	A	1007	HEC	C1C-CHC-C4B	2.18	130.06	123.67
2	A	1014	HEC	C4D-CHA-C1A	2.18	130.05	123.67
2	A	1013	HEC	CMC-C2C-C1C	-2.18	125.27	128.46
2	A	1001	HEC	C4A-CHB-C1B	2.17	130.01	123.67
2	A	1016	HEC	C1D-C2D-C3D	-2.15	105.50	107.00
2	A	1008	HEC	CMB-C2B-C1B	-2.14	125.32	128.46
2	A	1003	HEC	C4D-CHA-C1A	2.12	129.87	123.67
2	A	1016	HEC	C4A-CHB-C1B	2.11	129.85	123.67
2	A	1011	HEC	CMD-C2D-C1D	-2.09	125.40	128.46
2	A	1003	HEC	CMA-C3A-C2A	2.06	128.82	124.94
2	A	1014	HEC	CMC-C2C-C3C	2.05	128.23	125.82
2	A	1009	HEC	C4A-CHB-C1B	2.04	129.65	123.67
2	A	1005	HEC	C4C-CHD-C1D	2.03	129.62	123.67
2	A	1007	HEC	CMD-C2D-C1D	-2.03	125.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1007	HEC	CMC-C2C-C3C	2.03	128.20	125.82

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1015	HEC	C1A-C2A-CAA-CBA
2	A	1015	HEC	C3A-C2A-CAA-CBA
2	A	1001	HEC	C3D-CAD-CBD-CGD
2	A	1010	HEC	C2A-CAA-CBA-CGA
2	A	1007	HEC	C3D-CAD-CBD-CGD
2	A	1004	HEC	C2A-CAA-CBA-CGA
2	A	1009	HEC	CAD-CBD-CGD-O2D
2	A	1006	HEC	CAD-CBD-CGD-O1D
2	A	1009	HEC	CAD-CBD-CGD-O1D
2	A	1014	HEC	CAD-CBD-CGD-O1D
2	A	1004	HEC	CAA-CBA-CGA-O1A
2	A	1010	HEC	CAD-CBD-CGD-O1D
2	A	1012	HEC	CAD-CBD-CGD-O1D
2	A	1005	HEC	CAD-CBD-CGD-O1D
2	A	1006	HEC	CAD-CBD-CGD-O2D
2	A	1015	HEC	CAD-CBD-CGD-O2D
2	A	1007	HEC	CAD-CBD-CGD-O2D
2	A	1010	HEC	CAA-CBA-CGA-O1A
2	A	1010	HEC	CAD-CBD-CGD-O2D
2	A	1014	HEC	CAD-CBD-CGD-O2D
2	A	1011	HEC	CAA-CBA-CGA-O2A
2	A	1007	HEC	CAA-CBA-CGA-O1A
2	A	1011	HEC	CAA-CBA-CGA-O1A
2	A	1003	HEC	CAA-CBA-CGA-O1A
2	A	1015	HEC	CAD-CBD-CGD-O1D
2	A	1007	HEC	CAD-CBD-CGD-O1D
2	A	1012	HEC	CAD-CBD-CGD-O2D
2	A	1003	HEC	CAA-CBA-CGA-O2A
2	A	1010	HEC	CAA-CBA-CGA-O2A
2	A	1005	HEC	CAA-CBA-CGA-O2A
2	A	1005	HEC	CAD-CBD-CGD-O2D
2	A	1004	HEC	CAA-CBA-CGA-O2A
2	A	1002	HEC	CAA-CBA-CGA-O1A
2	A	1005	HEC	CAA-CBA-CGA-O1A
2	A	1007	HEC	CAA-CBA-CGA-O2A
2	A	1002	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
2	A	1016	HEC	CAA-CBA-CGA-O2A
2	A	1014	HEC	C3D-CAD-CBD-CGD
2	A	1016	HEC	CAD-CBD-CGD-O1D
2	A	1013	HEC	CAA-CBA-CGA-O2A
2	A	1001	HEC	CAA-CBA-CGA-O2A
2	A	1013	HEC	CAA-CBA-CGA-O1A
2	A	1008	HEC	CAD-CBD-CGD-O1D
2	A	1016	HEC	CAA-CBA-CGA-O1A
2	A	1016	HEC	CAD-CBD-CGD-O2D
2	A	1008	HEC	CAD-CBD-CGD-O2D
2	A	1001	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

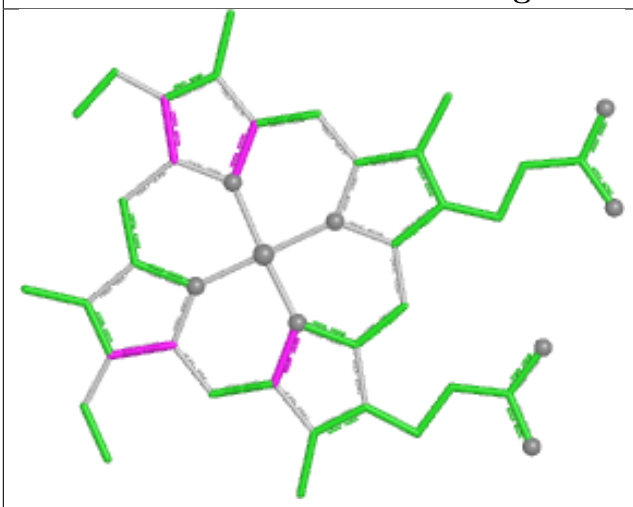
14 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1008	HEC	2	0
2	A	1006	HEC	3	0
2	A	1011	HEC	2	0
2	A	1015	HEC	7	0
2	A	1005	HEC	2	0
2	A	1009	HEC	2	0
2	A	1012	HEC	4	0
2	A	1007	HEC	2	0
2	A	1014	HEC	2	0
2	A	1016	HEC	1	0
2	A	1002	HEC	5	0
2	A	1003	HEC	1	0
2	A	1004	HEC	5	0
2	A	1010	HEC	3	0

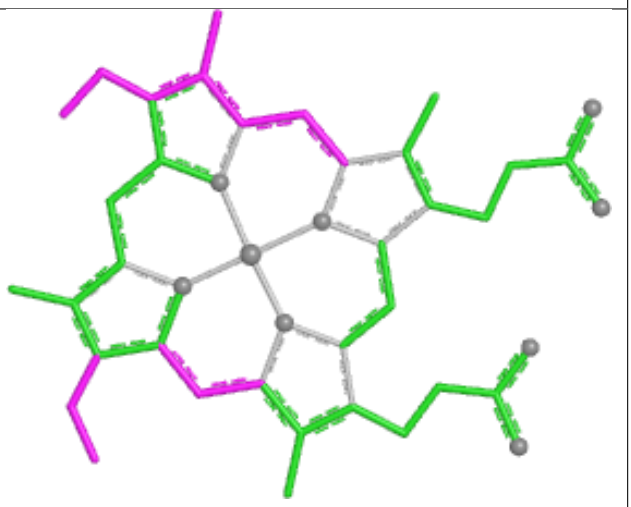
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

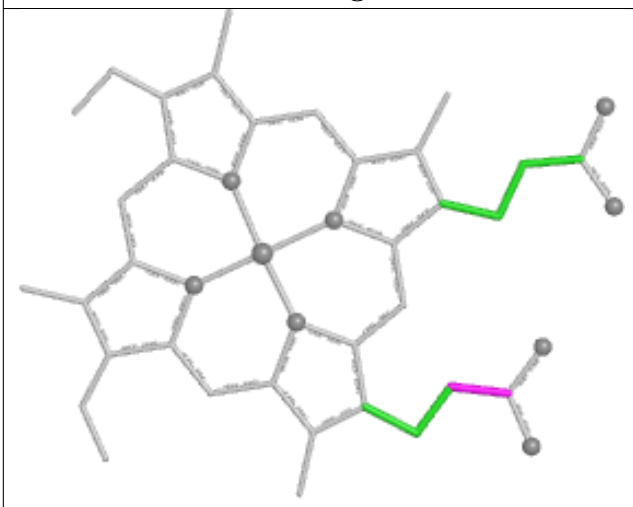
Ligand HEC A 1008



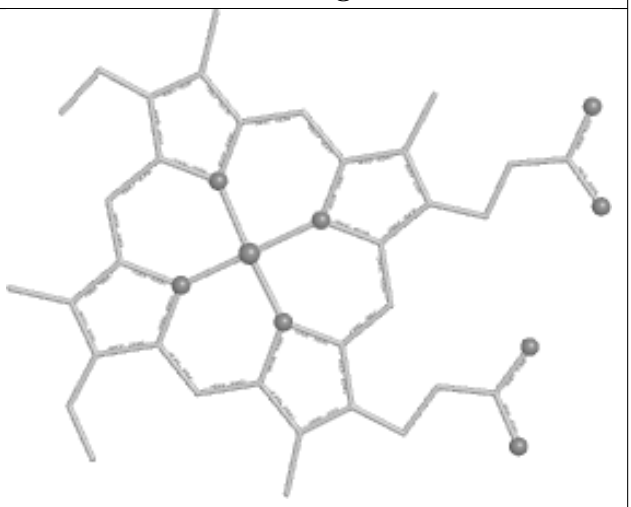
Bond lengths



Bond angles

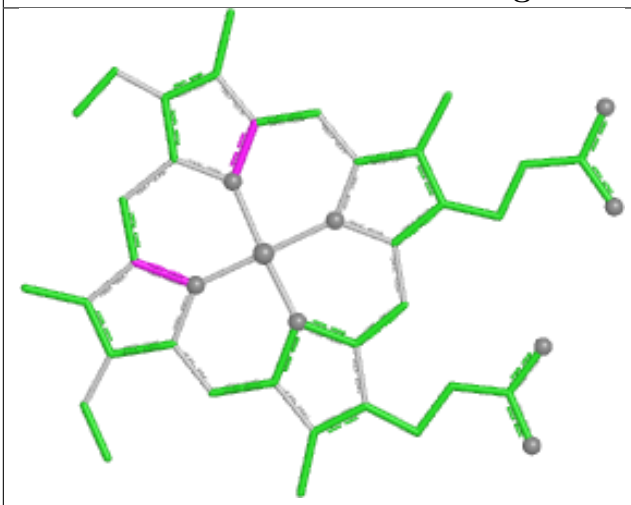


Torsions

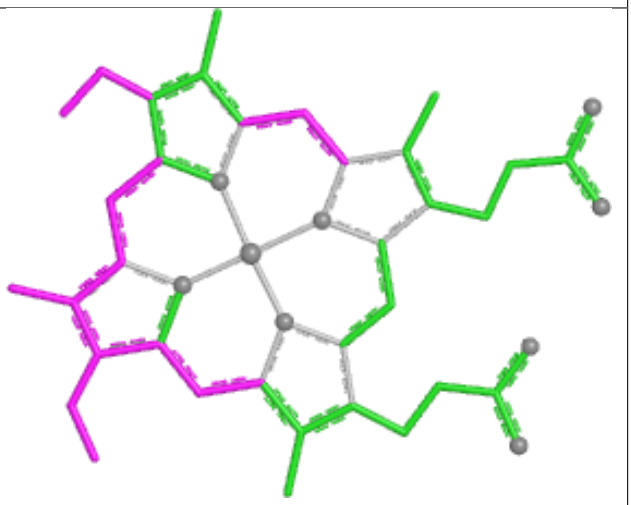


Rings

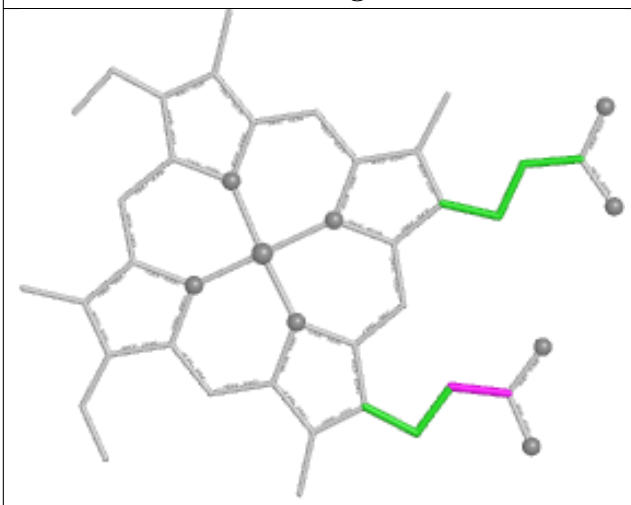
Ligand HEC A 1006



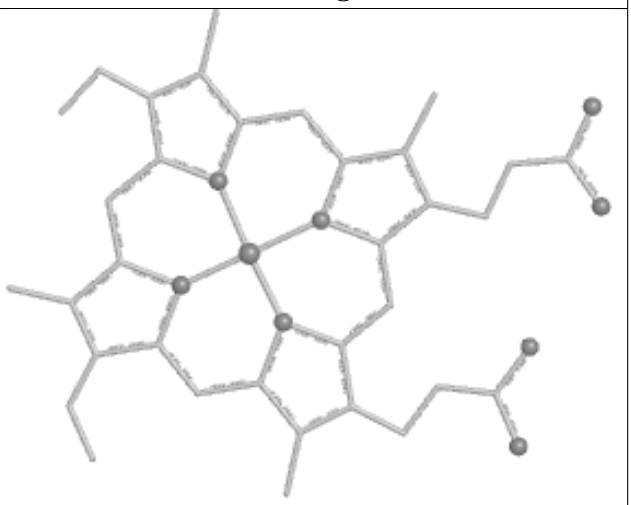
Bond lengths



Bond angles

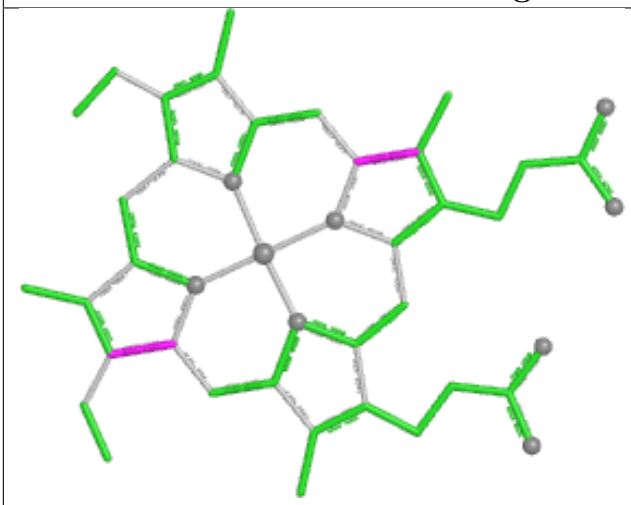


Torsions



Rings

Ligand HEC A 1011



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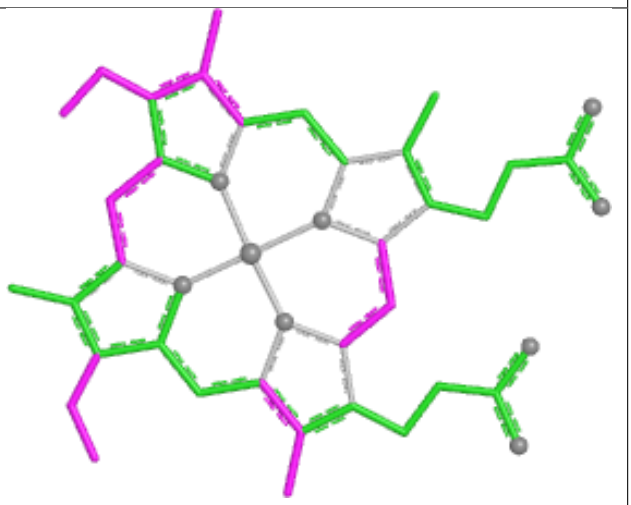

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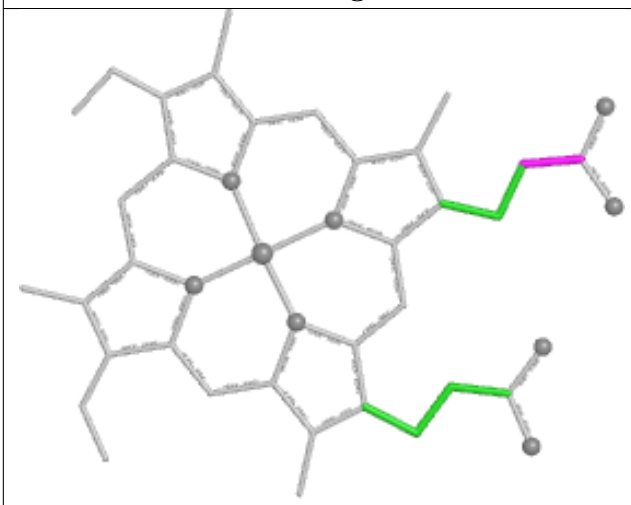

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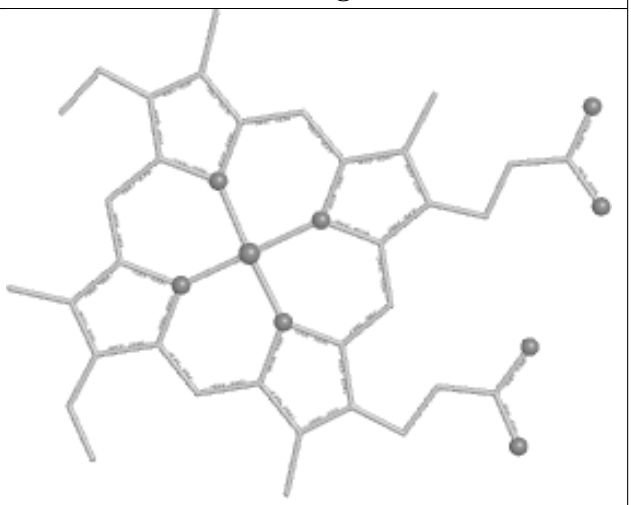
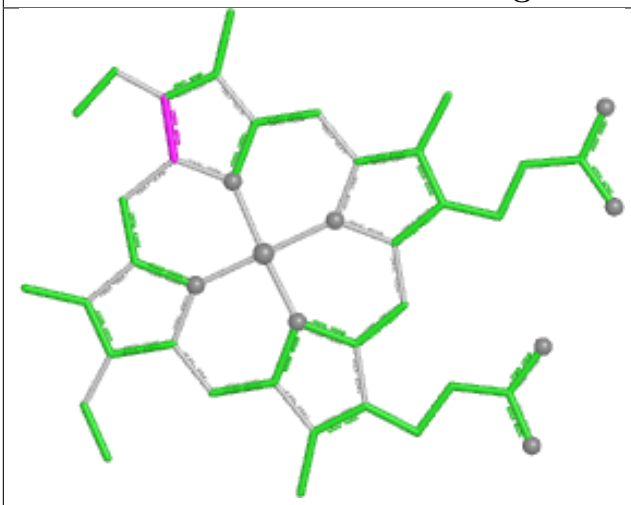


Rings

Ligand HEC A 1015



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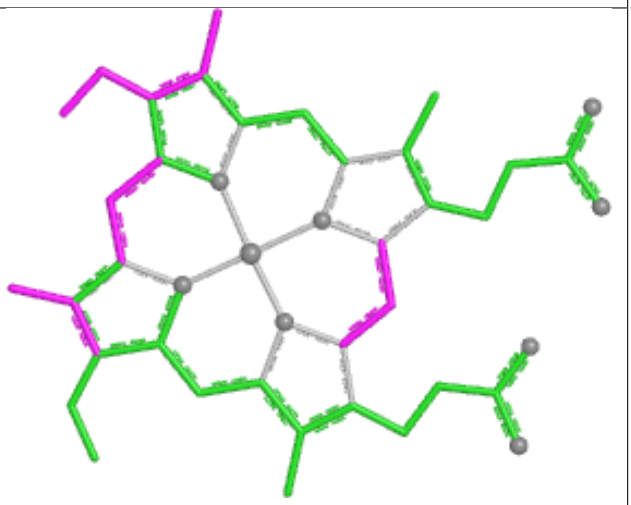

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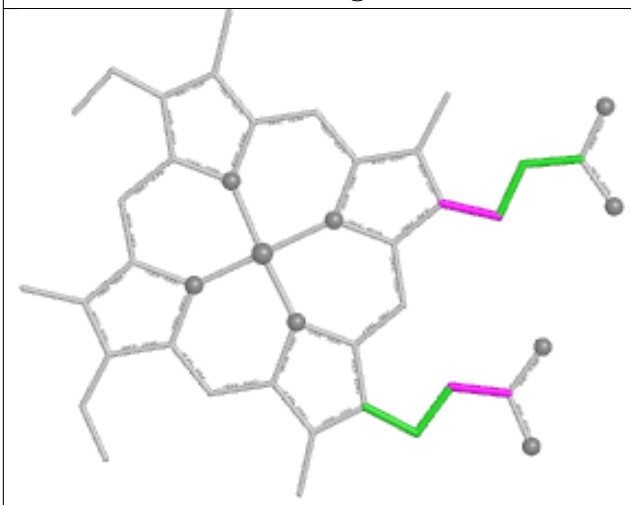

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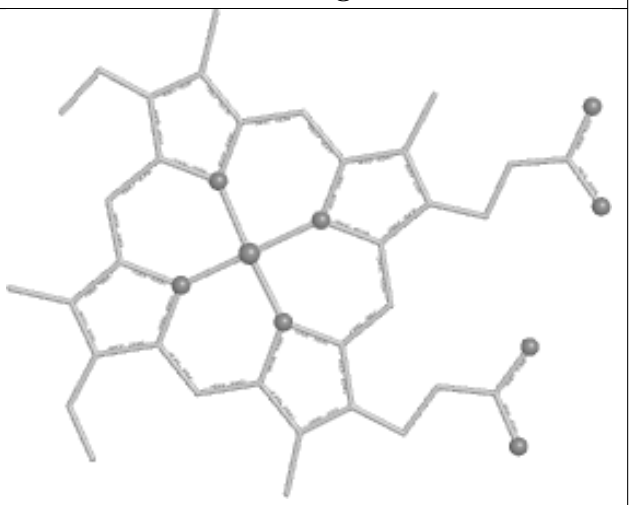

Rings

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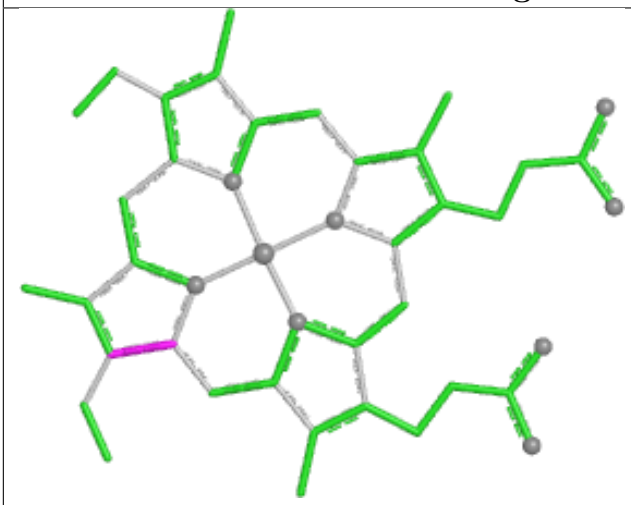

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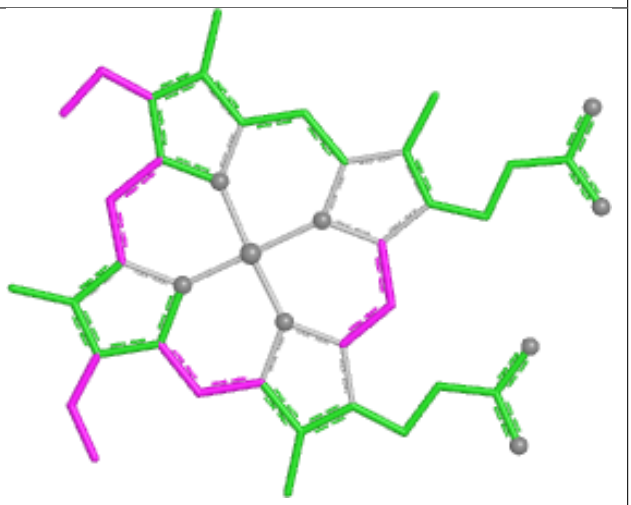

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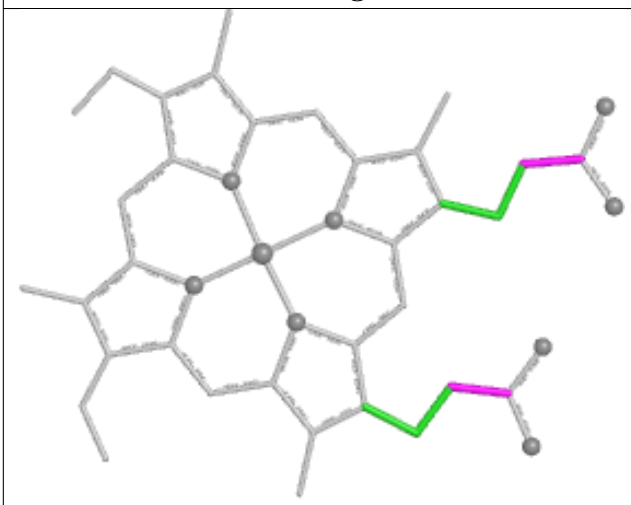

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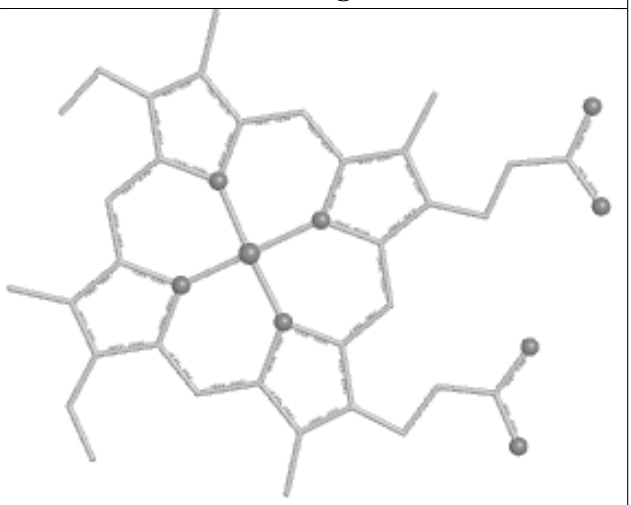
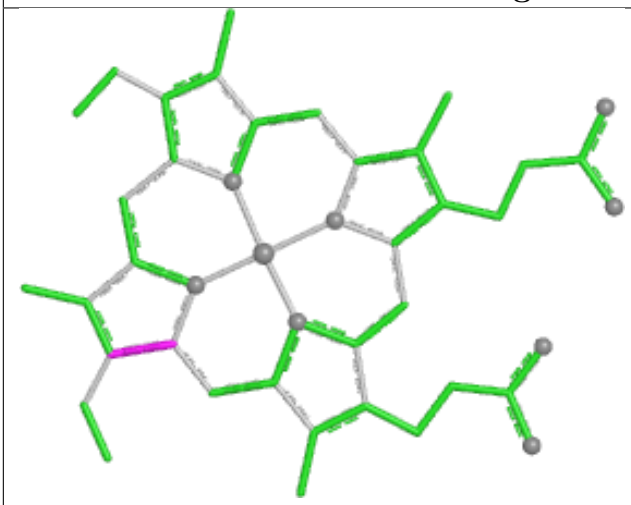


Rings

Ligand HEC A 1009



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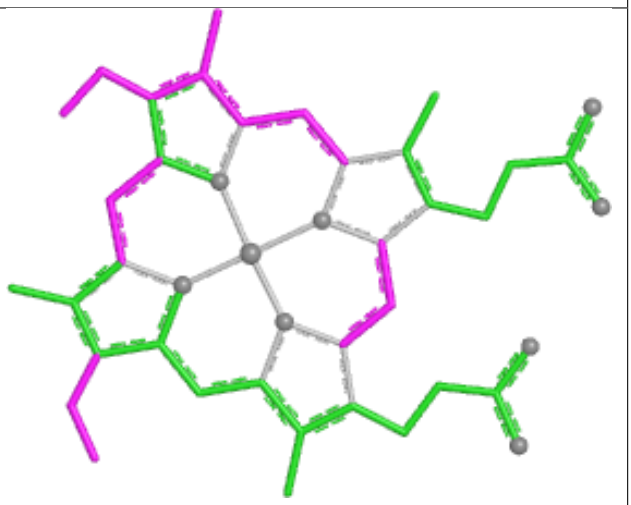

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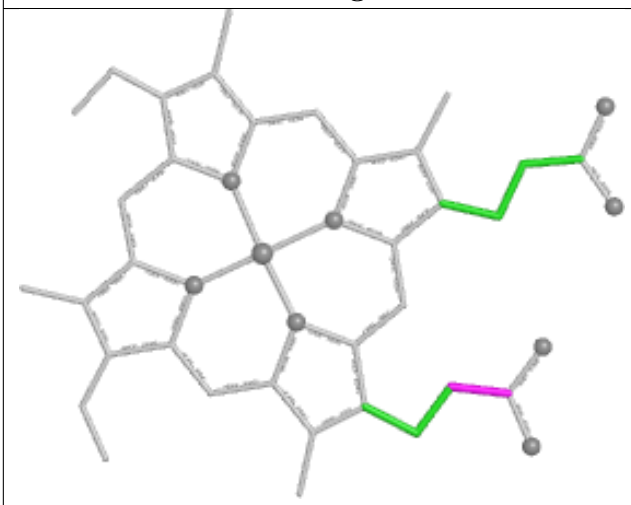

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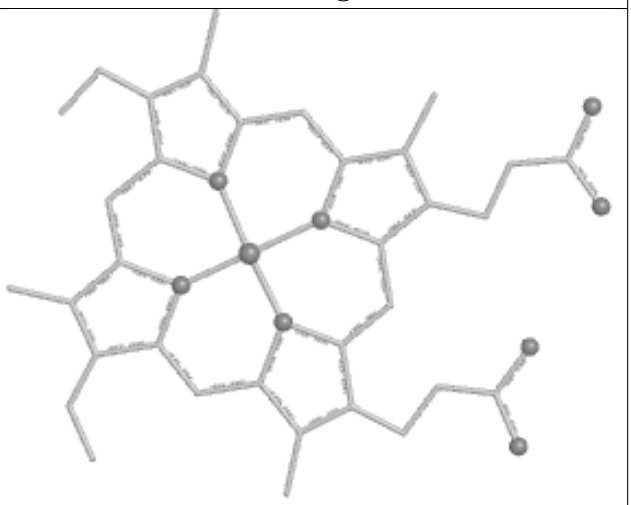
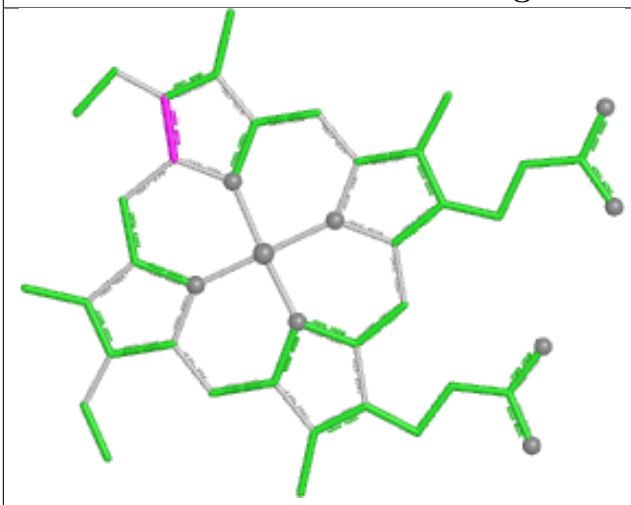


Rings

Ligand HEC A 1012



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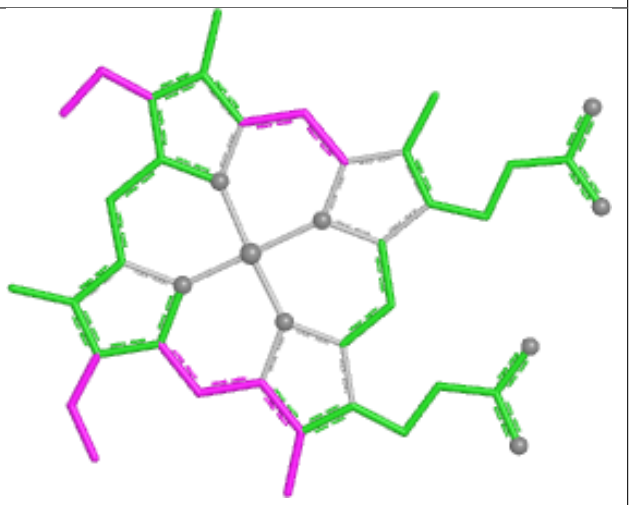

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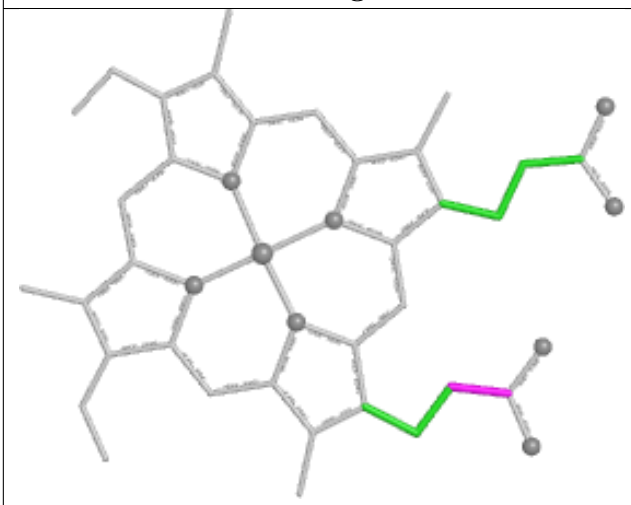

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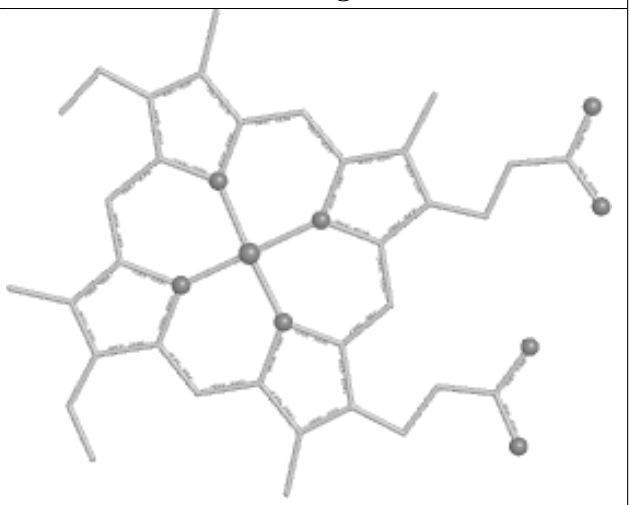
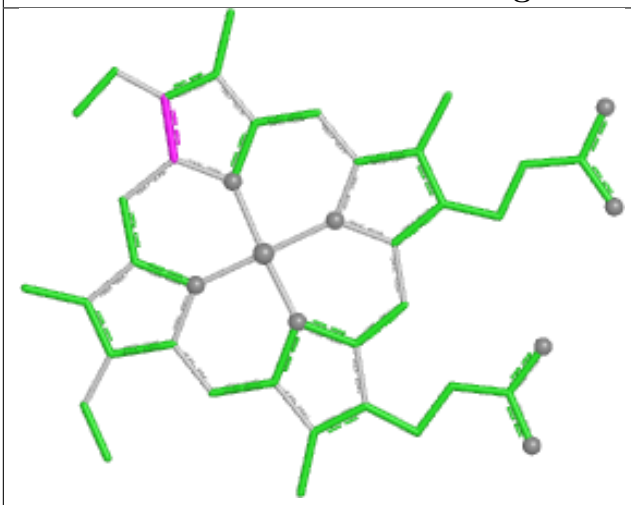


Rings

Ligand HEC A 1013



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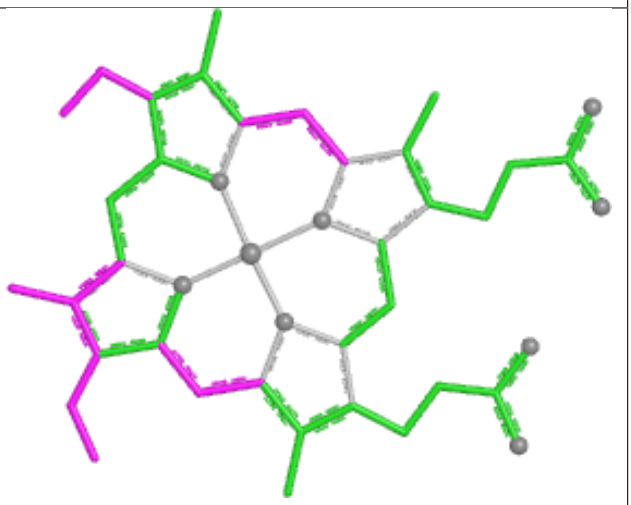

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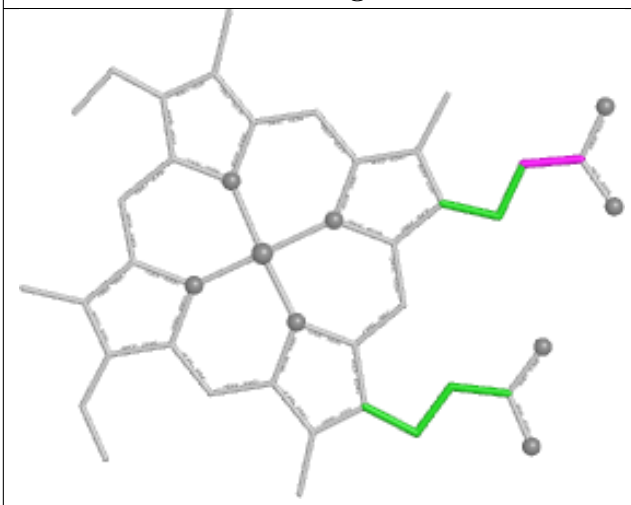

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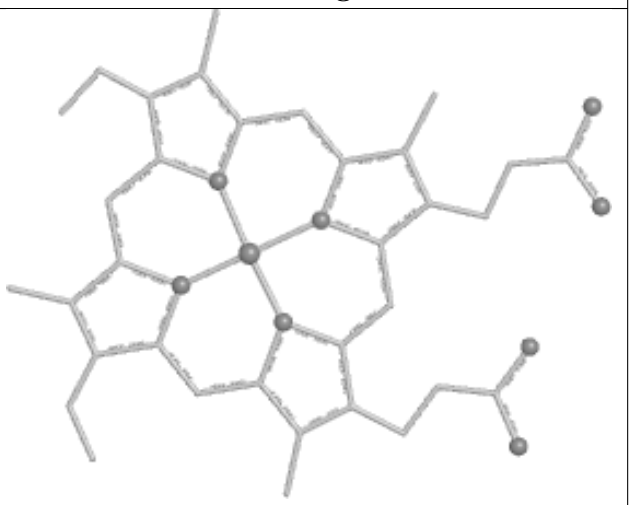
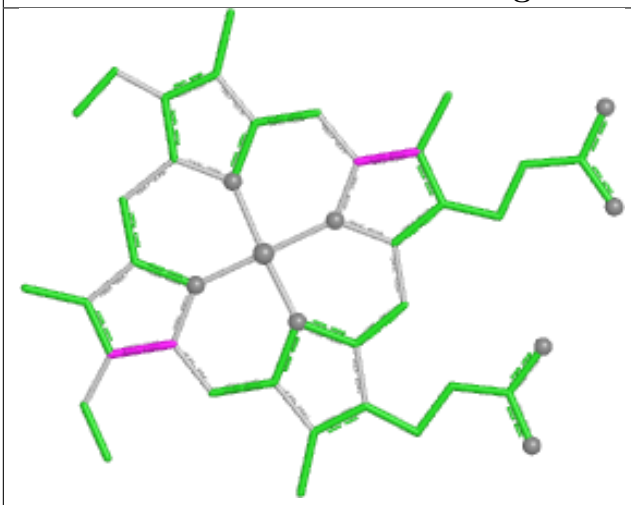


Rings

Ligand HEC A 1007



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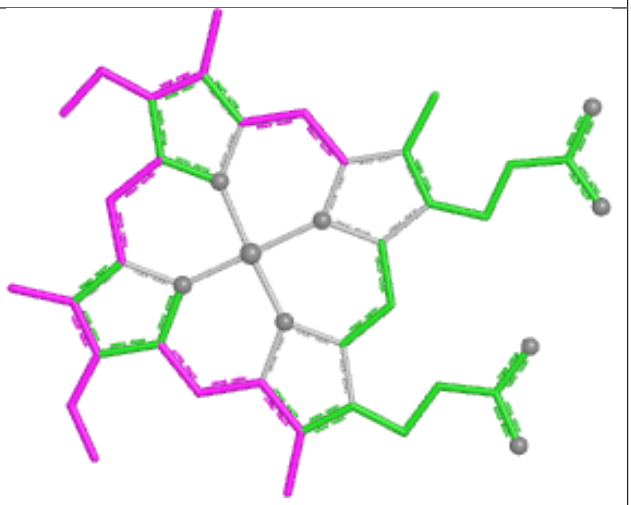

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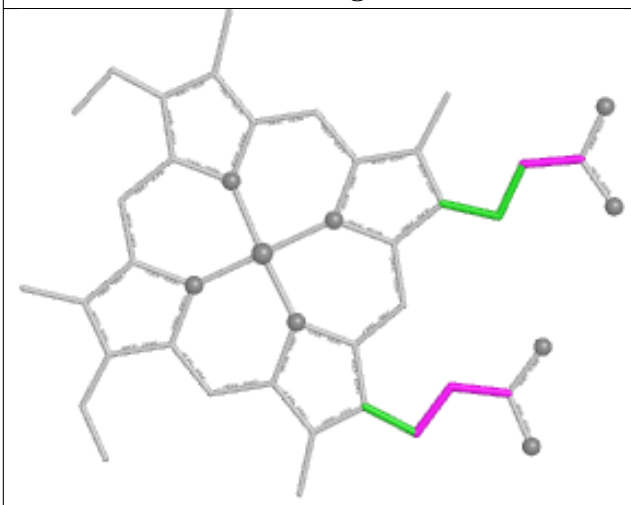

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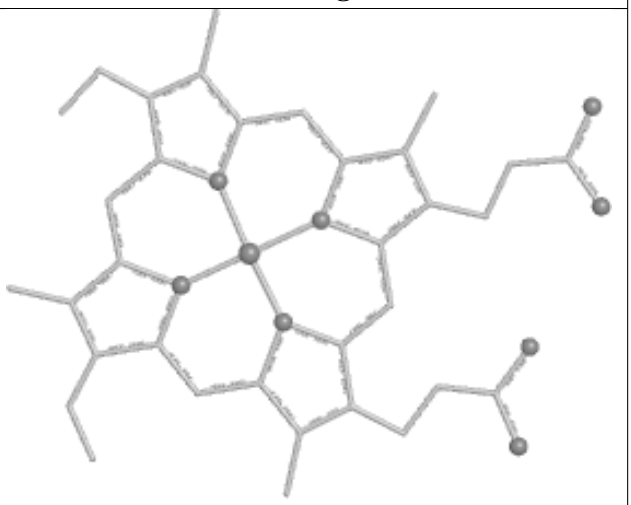
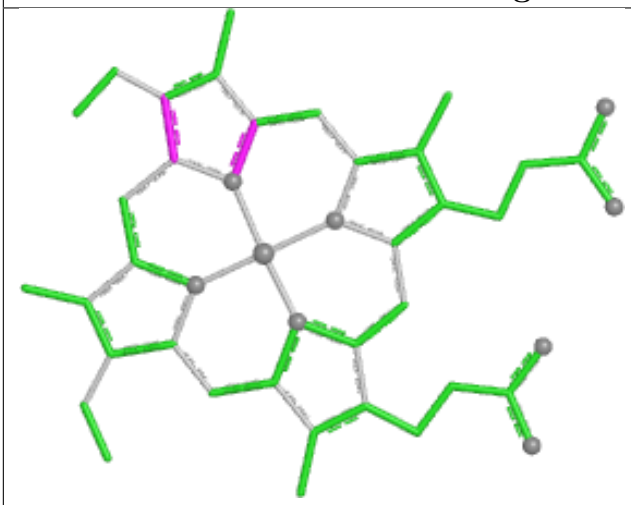


Rings

Ligand HEC A 1014



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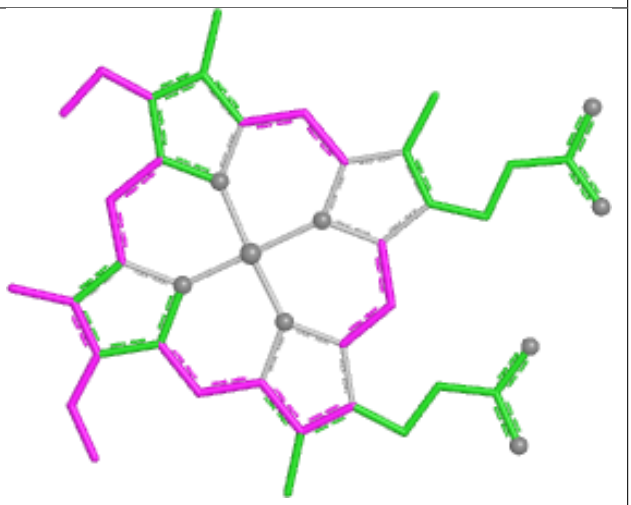

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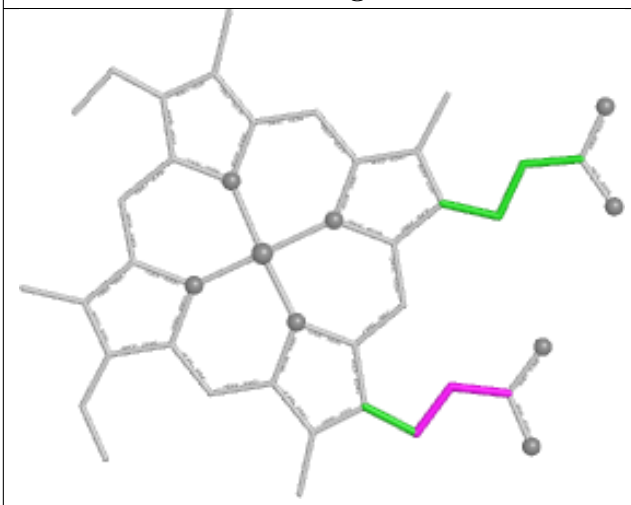

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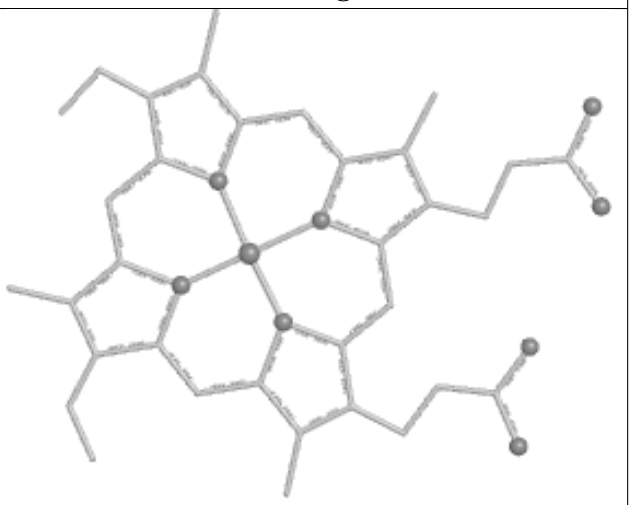
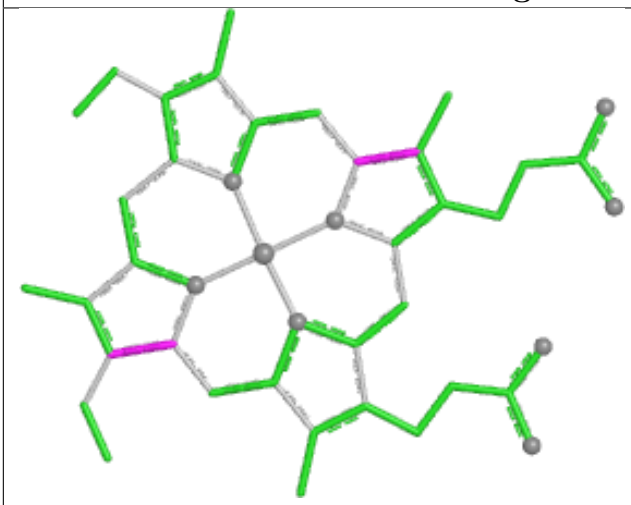


Rings

Ligand HEC A 1016



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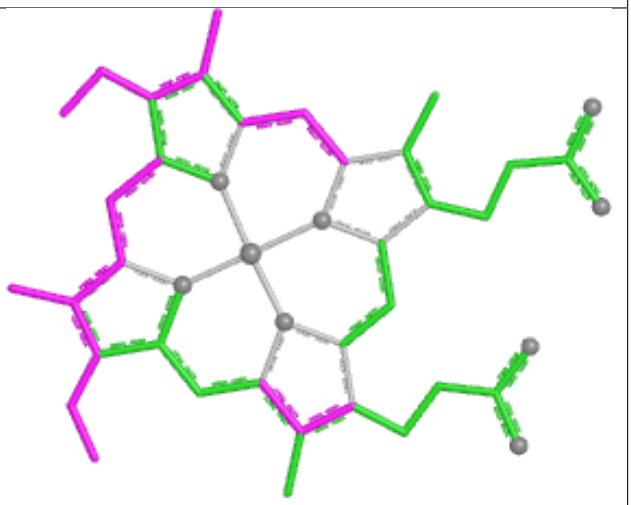

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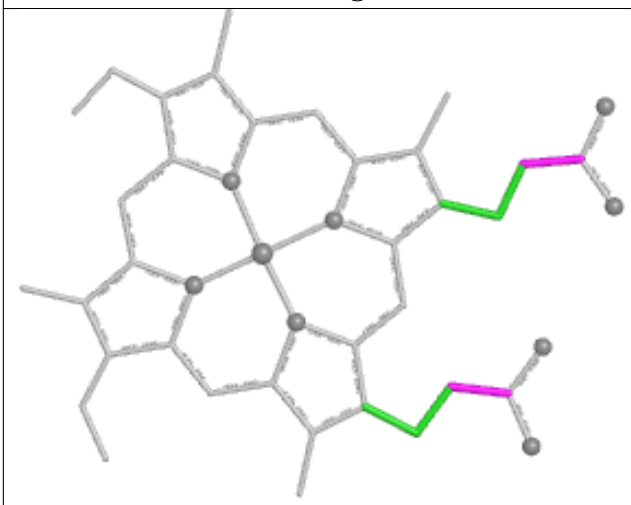

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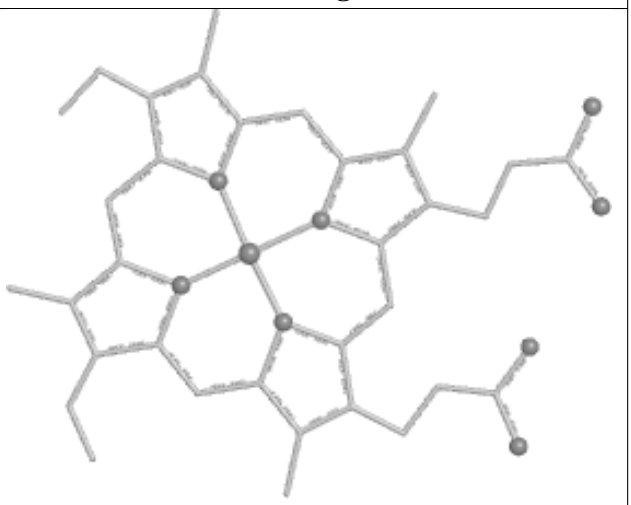
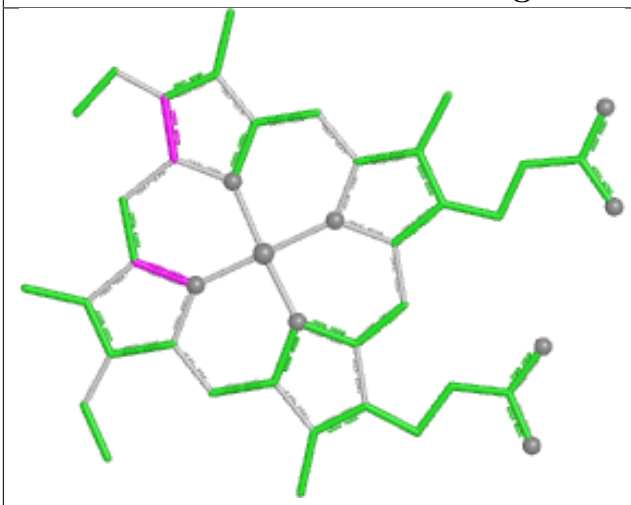


Rings

Ligand HEC A 1002



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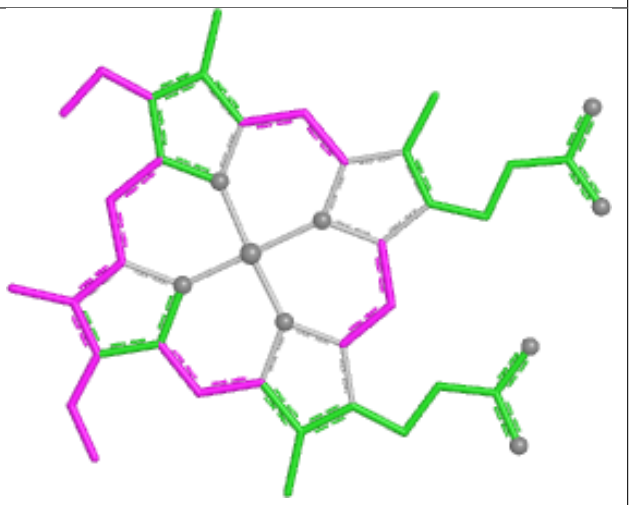

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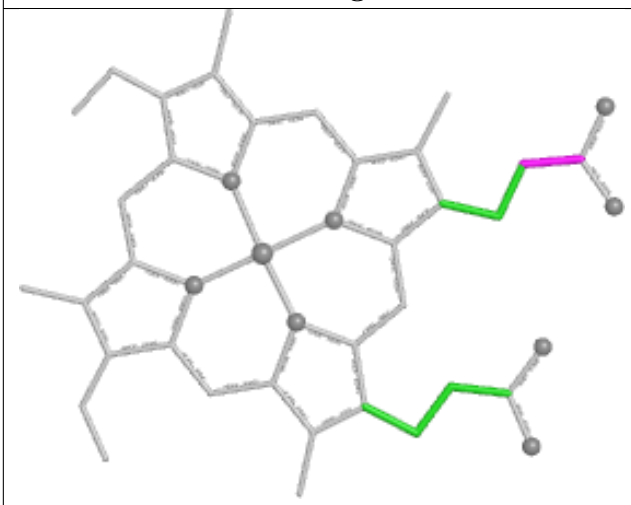

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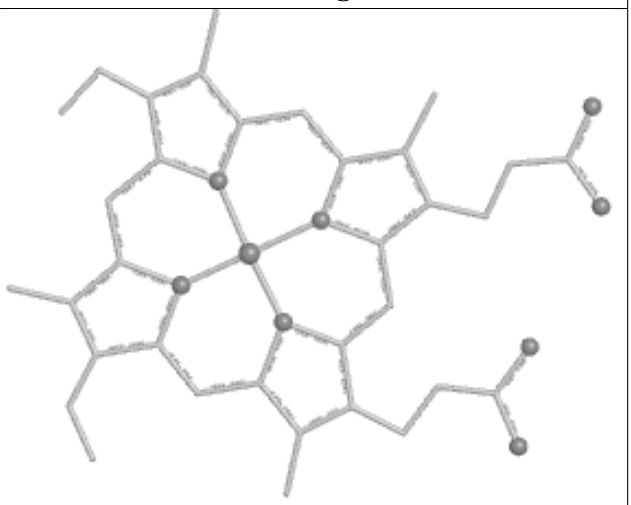
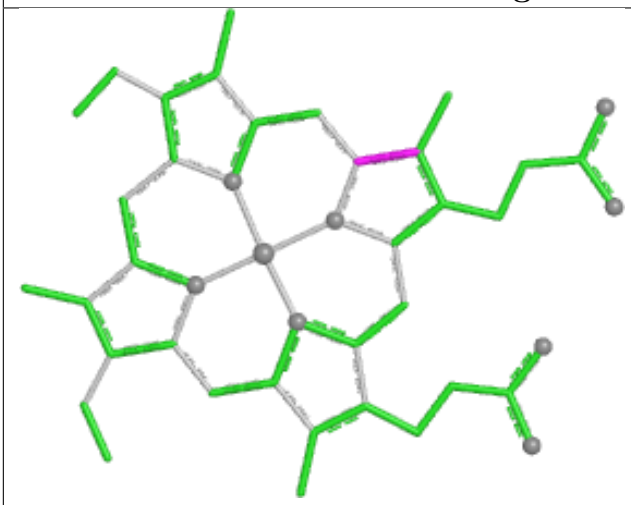


Rings

Ligand HEC A 1003



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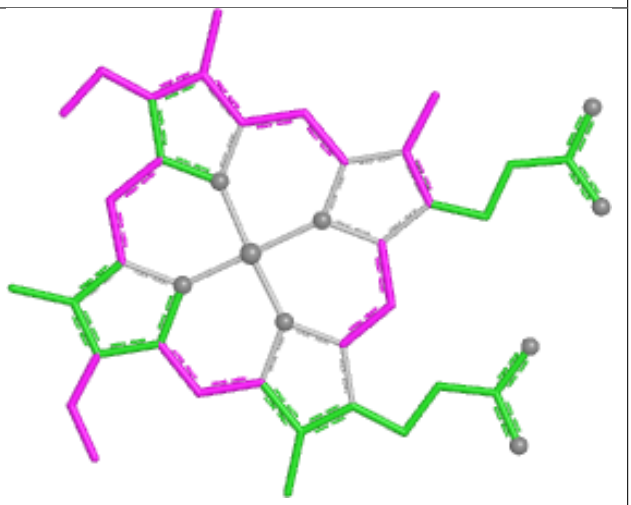

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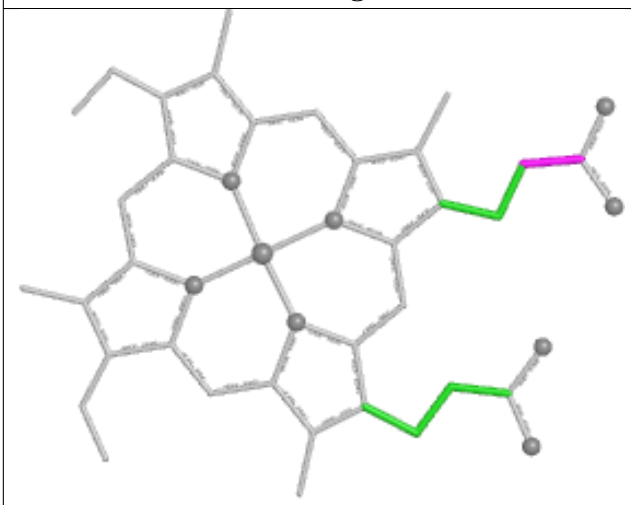

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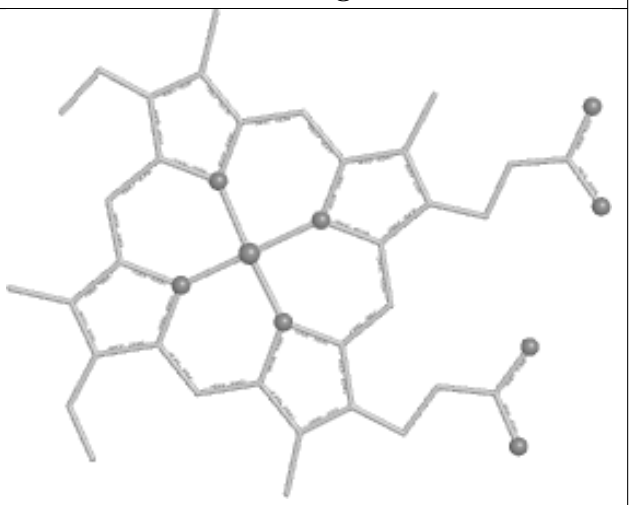
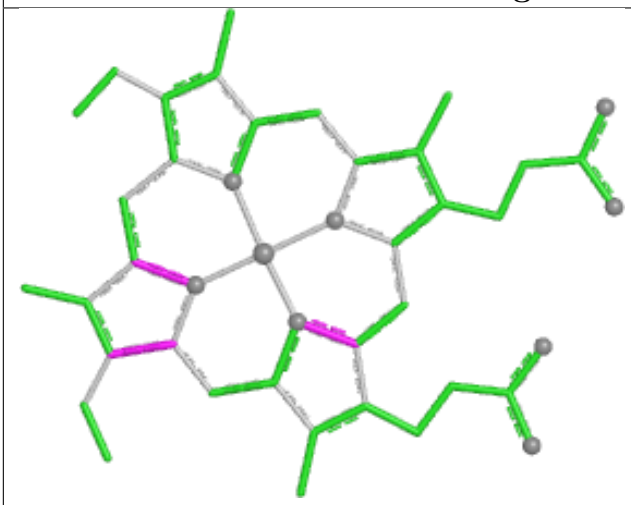


Rings

Ligand HEC A 1004



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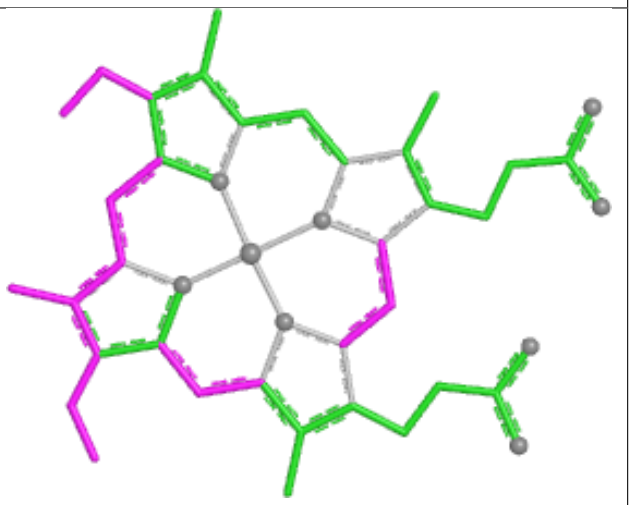

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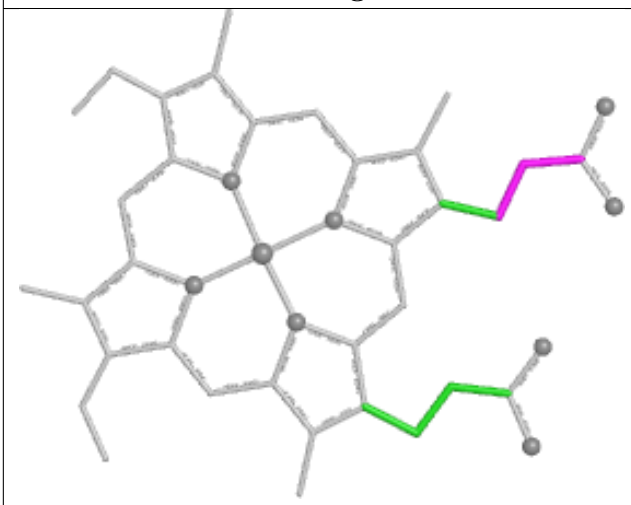

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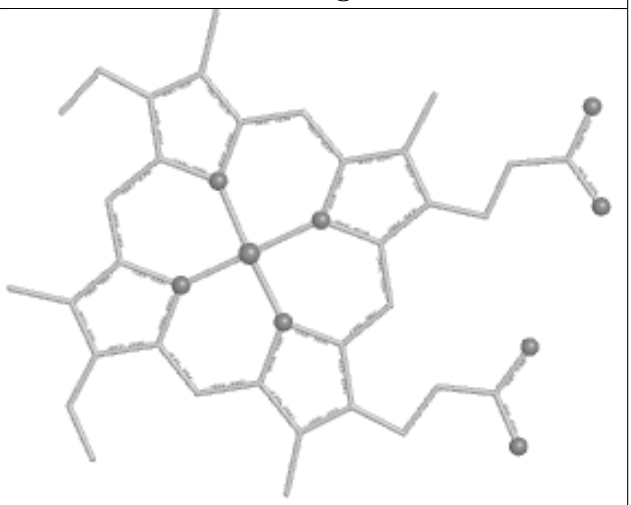
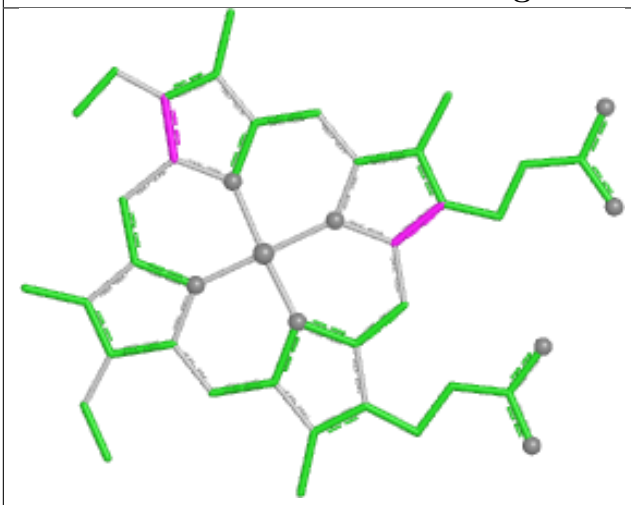


Rings

Ligand HEC A 1001



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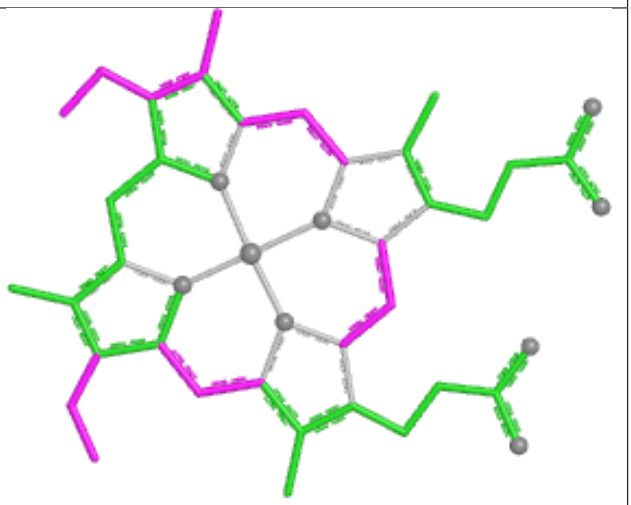
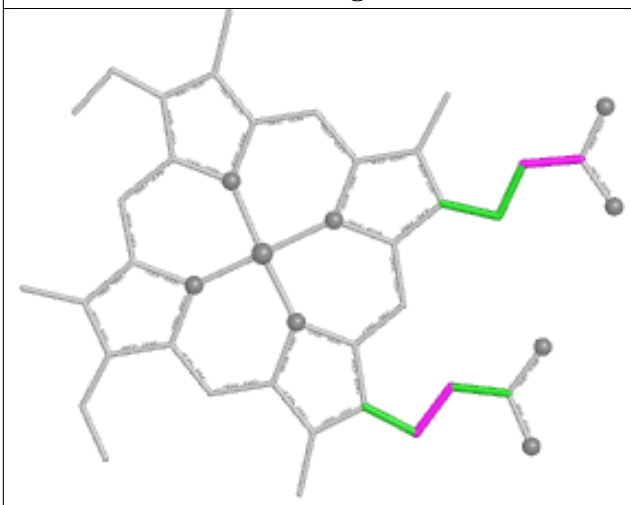
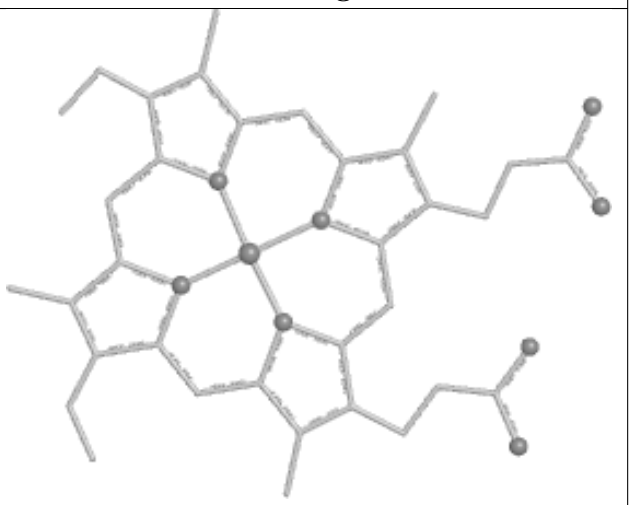


Bond angles

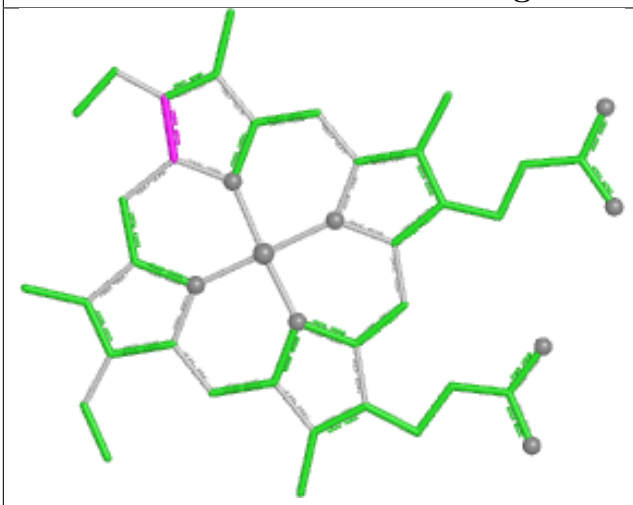


Torsions

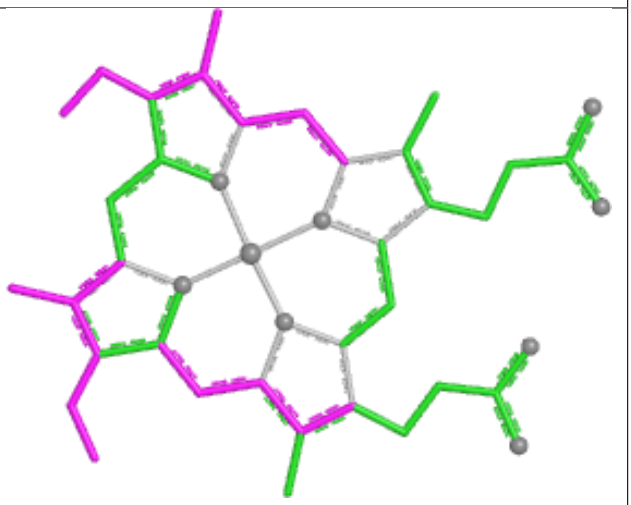


Rings

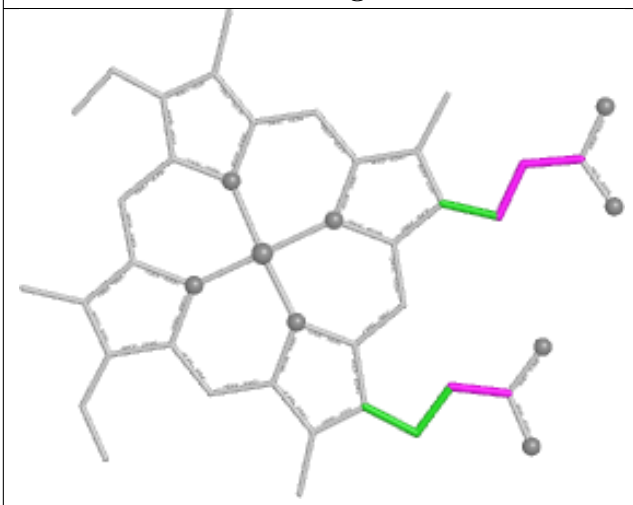
Ligand HEC A 1010



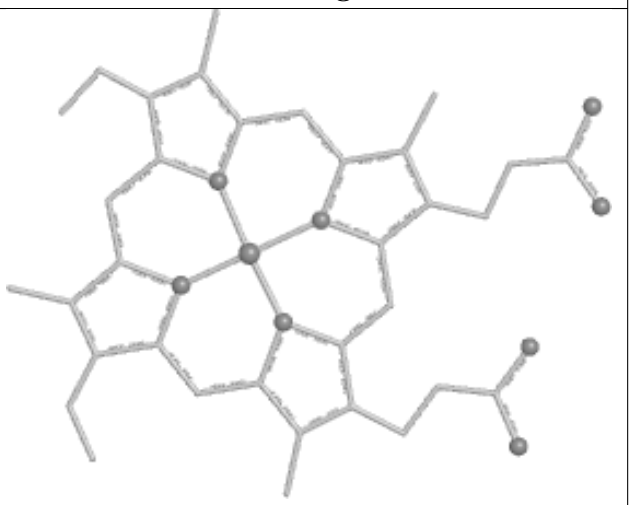
Bond lengths



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 (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	500/545 (91%)	-0.08	28 (5%) 24 23	25, 39, 75, 105	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ALA	8.6
1	A	144	SER	7.7
1	A	544	ALA	7.4
1	A	543	ARG	6.8
1	A	545	LYS	6.4
1	A	500	PRO	5.3
1	A	284	PRO	5.2
1	A	499	LYS	4.8
1	A	403	ALA	4.8
1	A	393	VAL	4.3
1	A	395	ALA	3.9
1	A	40	GLU	3.5
1	A	211	VAL	3.5
1	A	282	ASP	3.0
1	A	507	ASP	2.9
1	A	212	ASP	2.8
1	A	404	GLU	2.7
1	A	286	GLU	2.7
1	A	396	GLY	2.5
1	A	41	LYS	2.4
1	A	498	GLY	2.4
1	A	143	PRO	2.4
1	A	146	ALA	2.3
1	A	236	LYS	2.3
1	A	133	GLY	2.2
1	A	237	ALA	2.2
1	A	190	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	542	GLU	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)

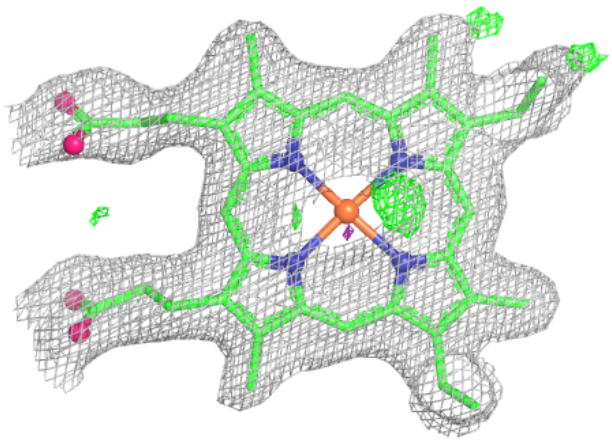
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

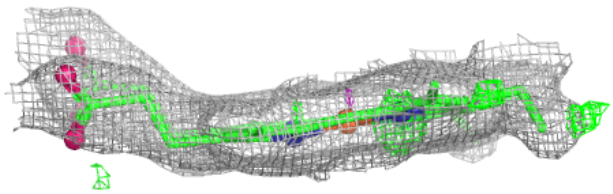
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	A	1013	43/43	0.94	0.14	23,42,64,76	0
2	HEC	A	1015	43/43	0.94	0.15	24,35,76,89	0
2	HEC	A	1014	43/43	0.95	0.11	25,38,59,72	0
2	HEC	A	1010	43/43	0.96	0.12	18,29,59,77	0
2	HEC	A	1016	43/43	0.96	0.12	24,33,44,49	0
2	HEC	A	1006	43/43	0.97	0.09	20,30,44,49	0
2	HEC	A	1009	43/43	0.97	0.09	19,33,50,65	0
2	HEC	A	1003	43/43	0.97	0.08	17,30,37,42	0
2	HEC	A	1011	43/43	0.97	0.10	22,28,38,58	0
2	HEC	A	1004	43/43	0.98	0.08	22,31,41,61	0
2	HEC	A	1005	43/43	0.98	0.08	21,30,50,72	0
2	HEC	A	1012	43/43	0.98	0.11	18,27,36,44	0
2	HEC	A	1002	43/43	0.98	0.10	21,29,40,50	0
2	HEC	A	1007	43/43	0.98	0.10	20,29,43,56	0
2	HEC	A	1008	43/43	0.98	0.10	18,29,41,47	0
2	HEC	A	1001	43/43	0.98	0.12	20,28,37,40	0

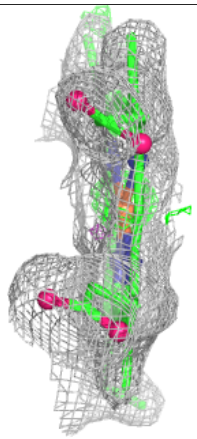
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC A 1013:

$2mF_o$-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 1015:

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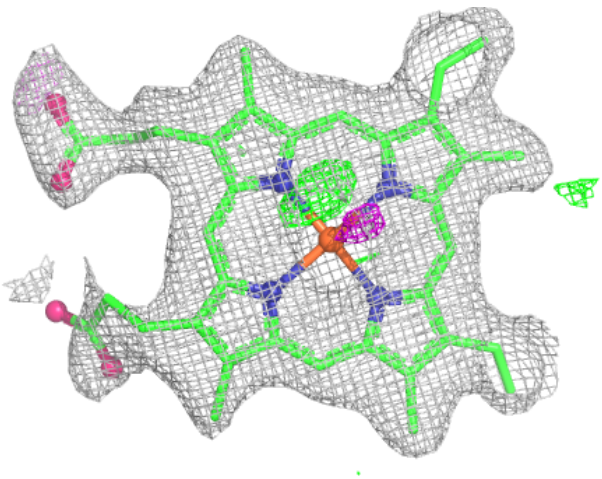
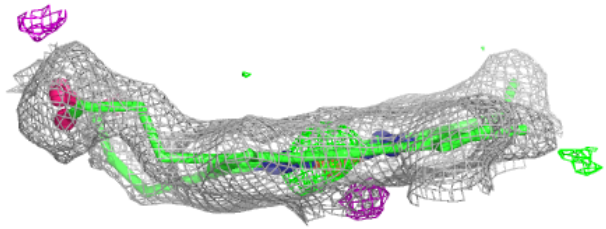
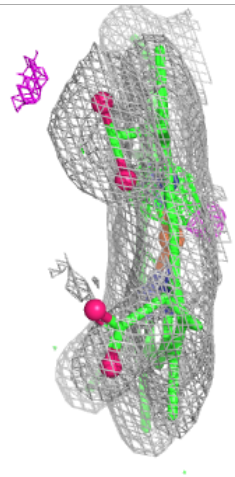
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC A 1014:

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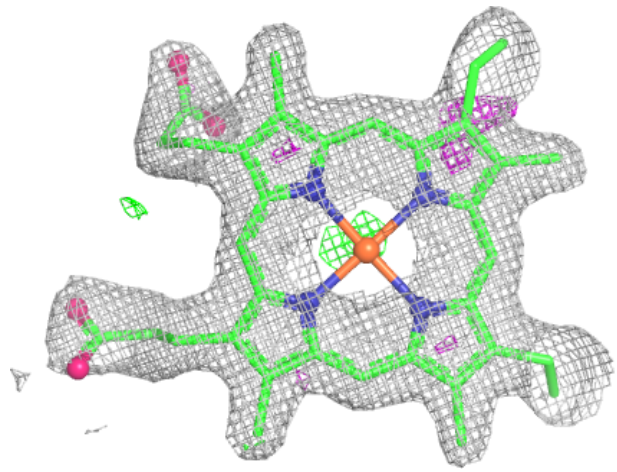
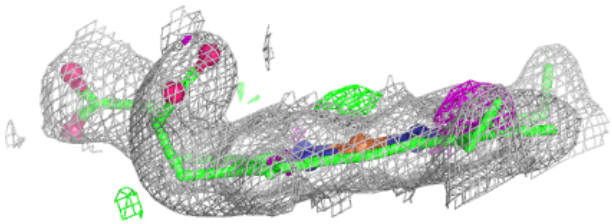
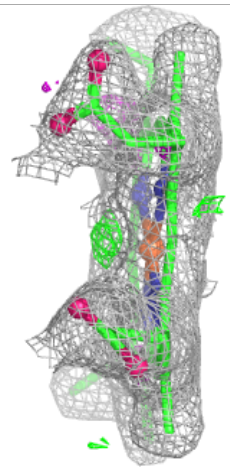
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC A 1010:

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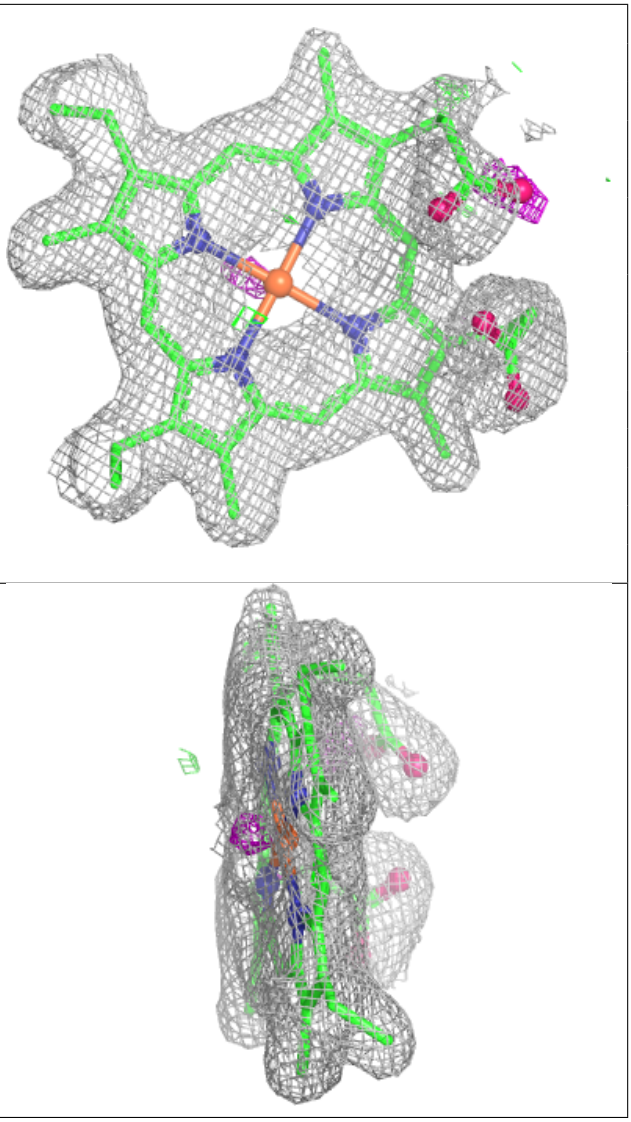
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 1016:

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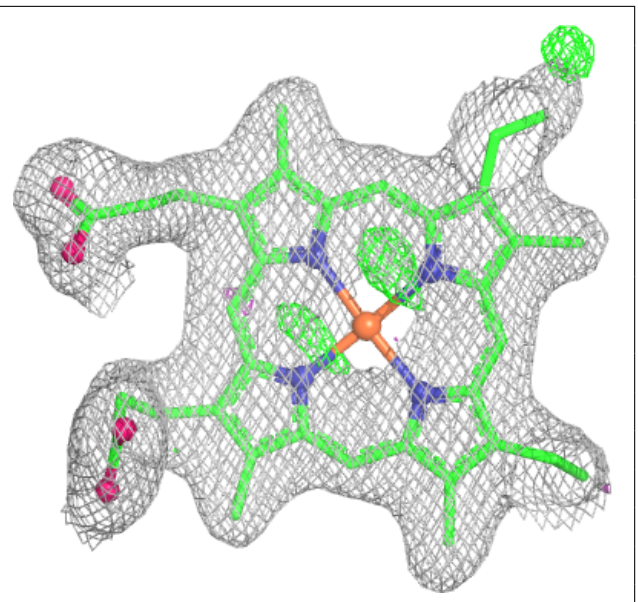
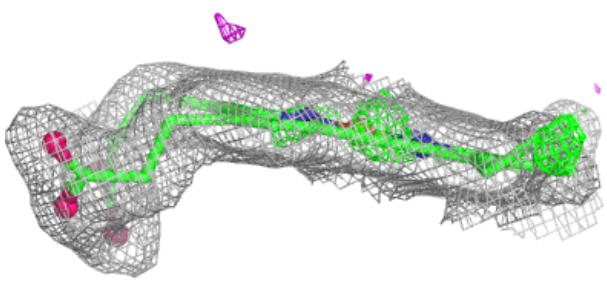
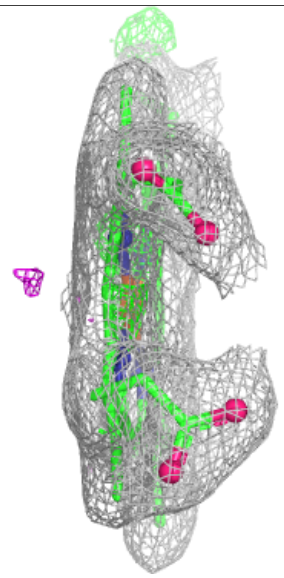
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

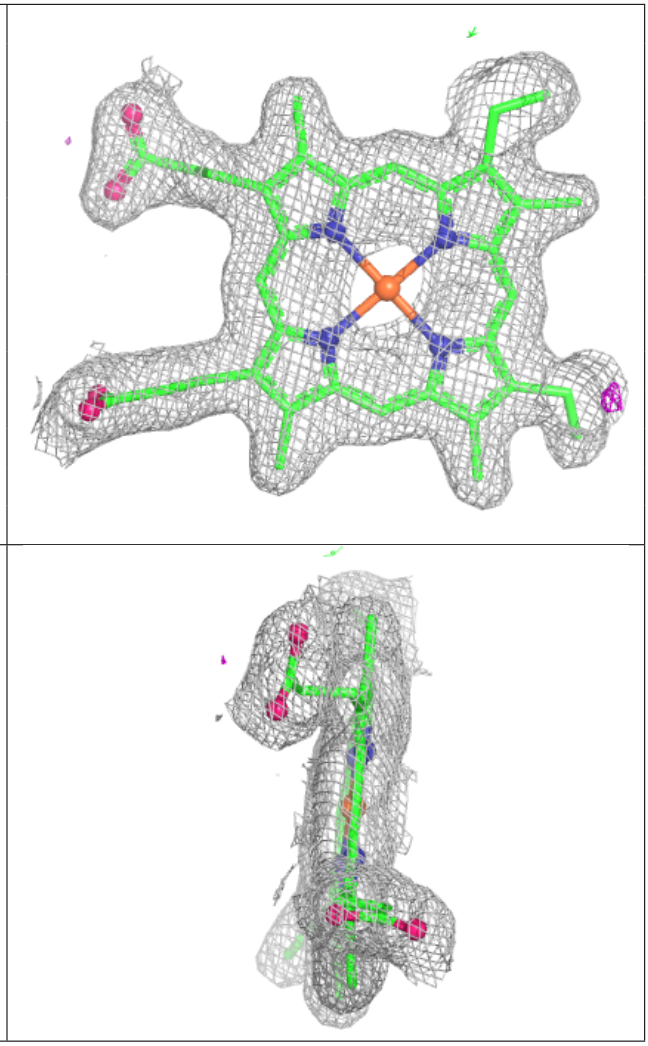






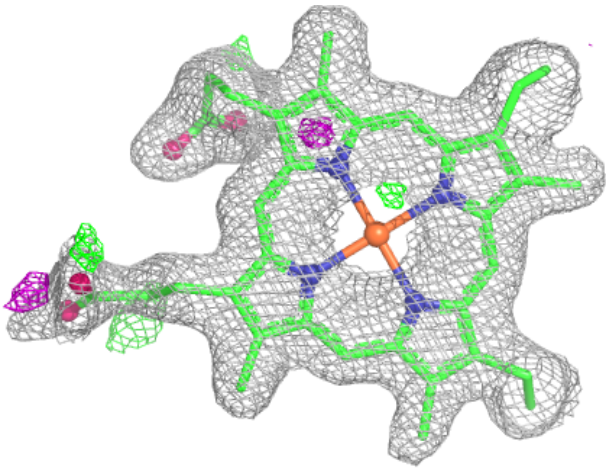
Electron density around HEC A 1006:

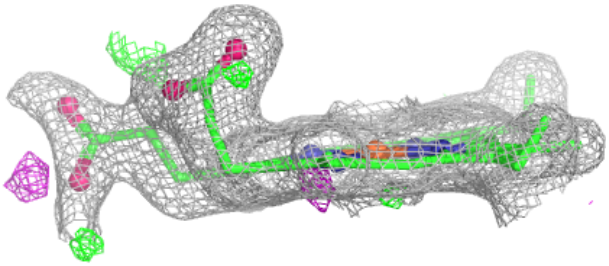
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

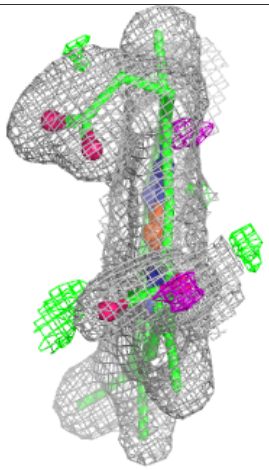


Electron density around HEC A 1009:

$2mF_o$-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 1003:

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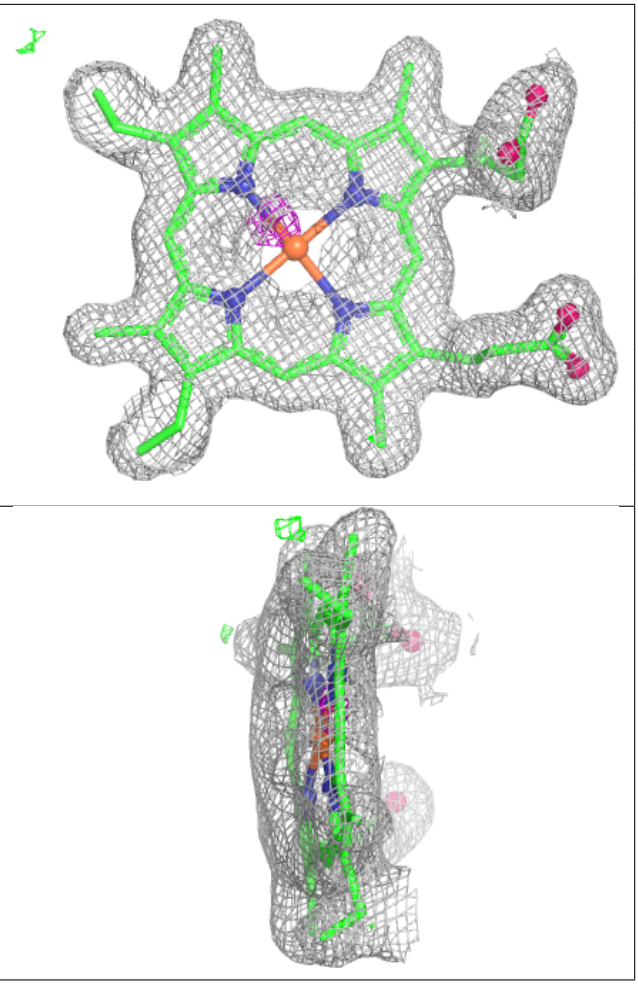
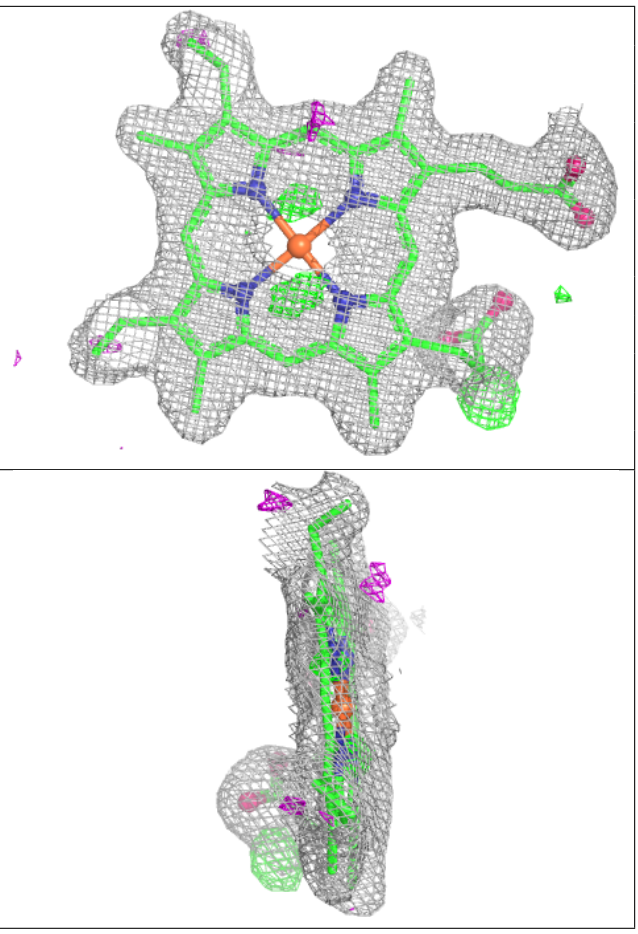
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 1011:

$2mF_o$-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 1004:

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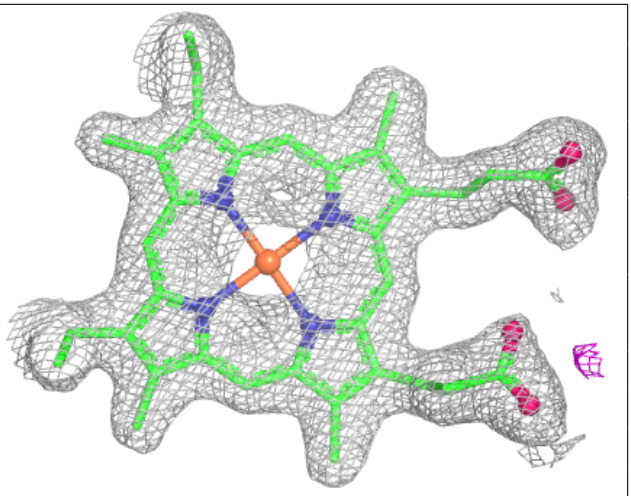
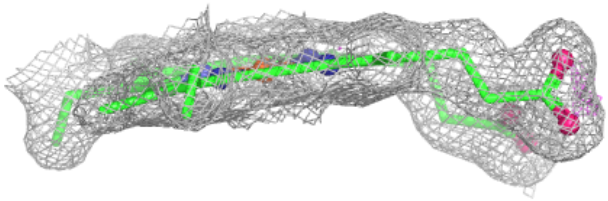
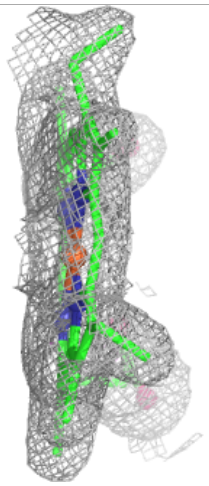
and green (positive)







Electron density around HEC A 1005:

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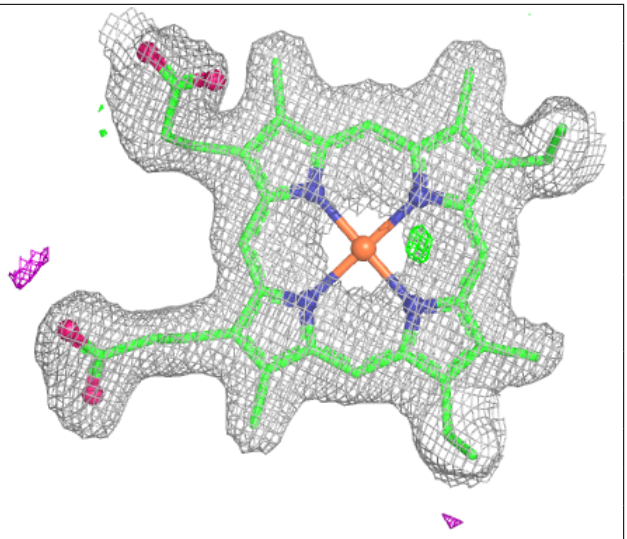
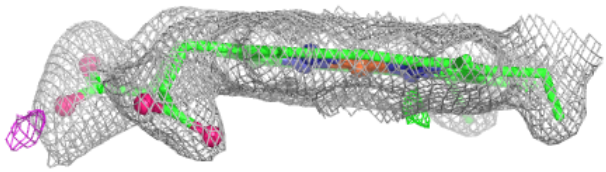
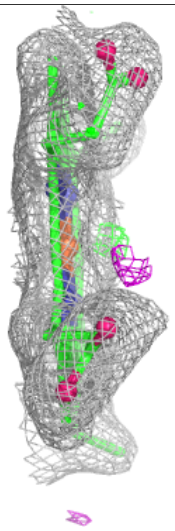
and green (positive)







Electron density around HEC A 1012:

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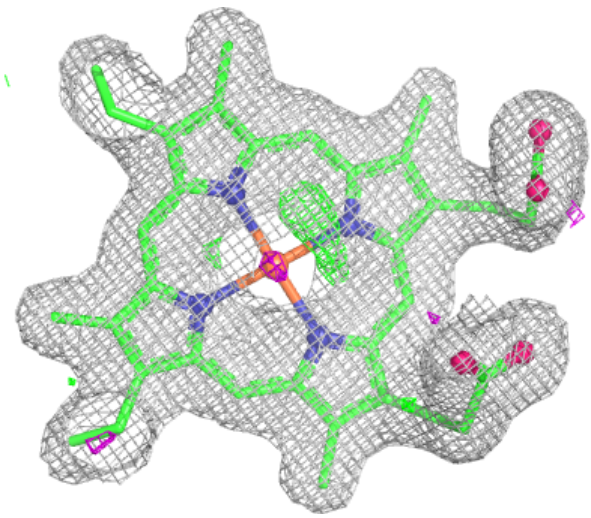
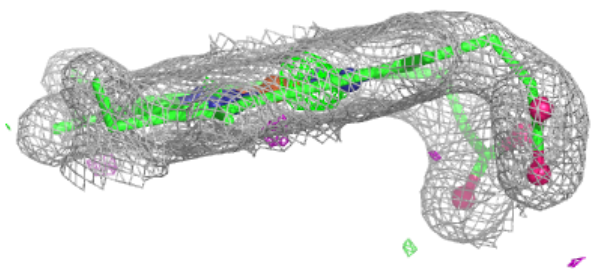
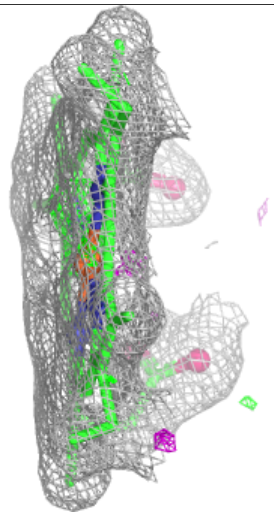
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC A 1002:

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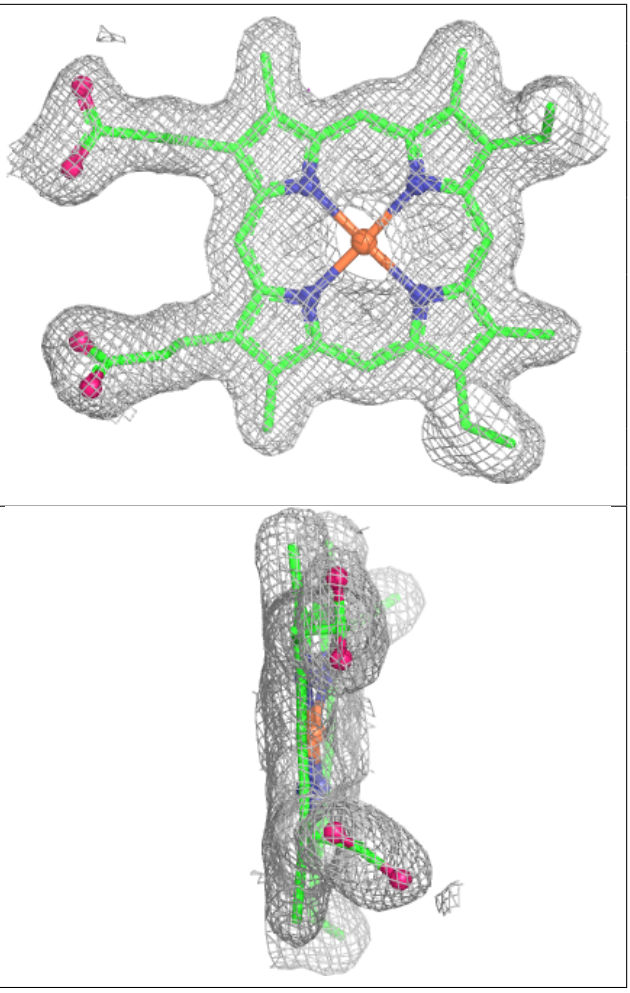
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC A 1007:

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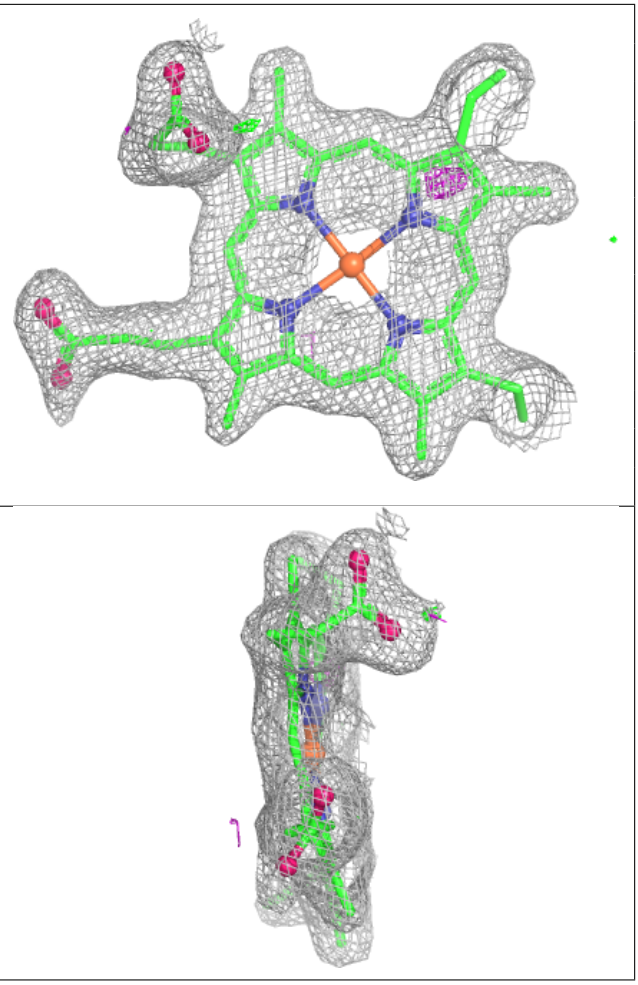

Electron density around HEC A 1008:

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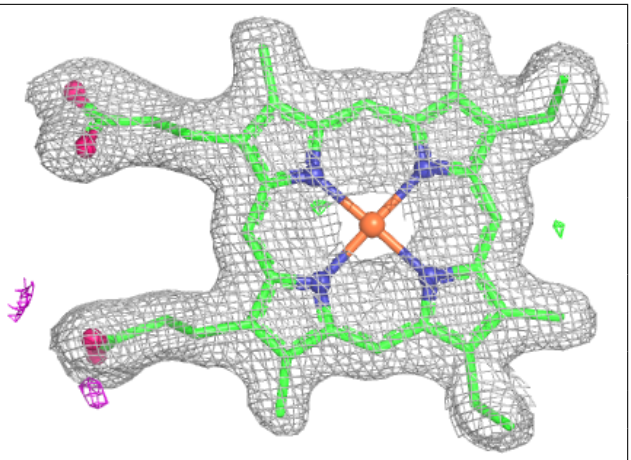
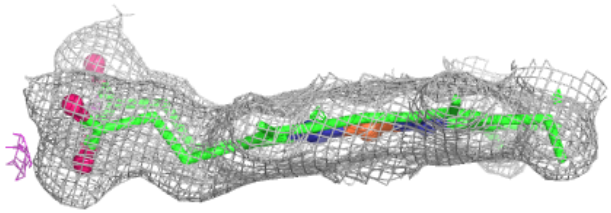
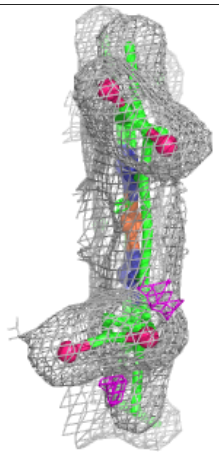
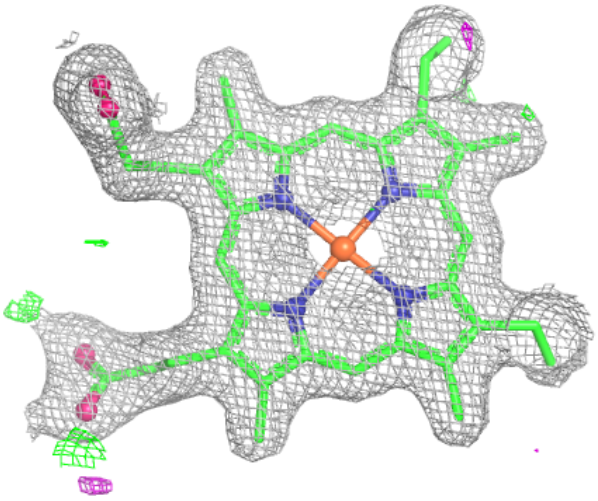


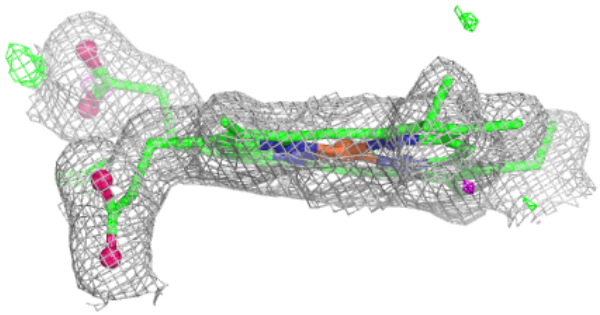


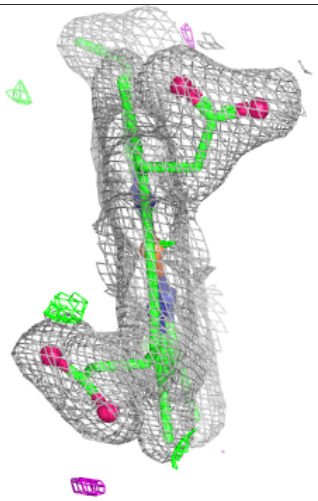


Electron density around HEC A 1001:

$2mF_o$-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.