



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:17 AM UTC

PDB ID : 2CVC / pdb_00002cvc
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

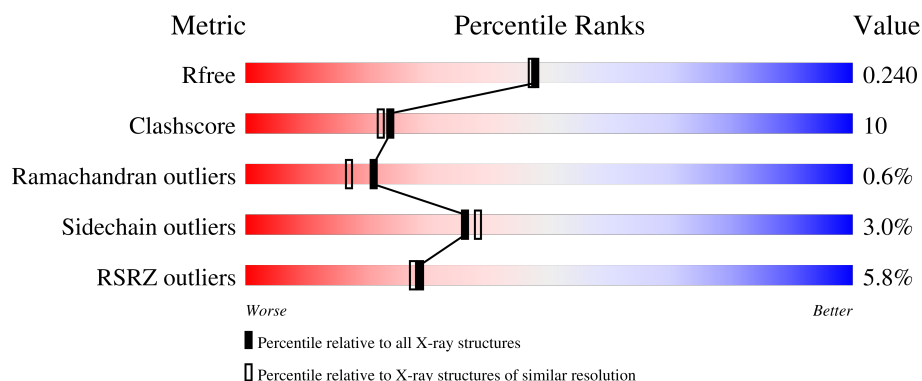
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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% 76% 14% • 8%

2 Entry composition i

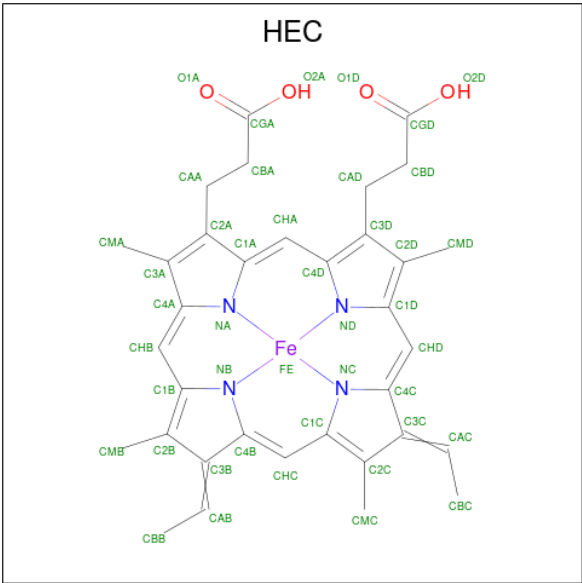
There are 3 unique types of molecules in this entry. The entry contains 4940 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	500	Total	C	N	O	S	0	0	0
			3779	2322	714	699	44			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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

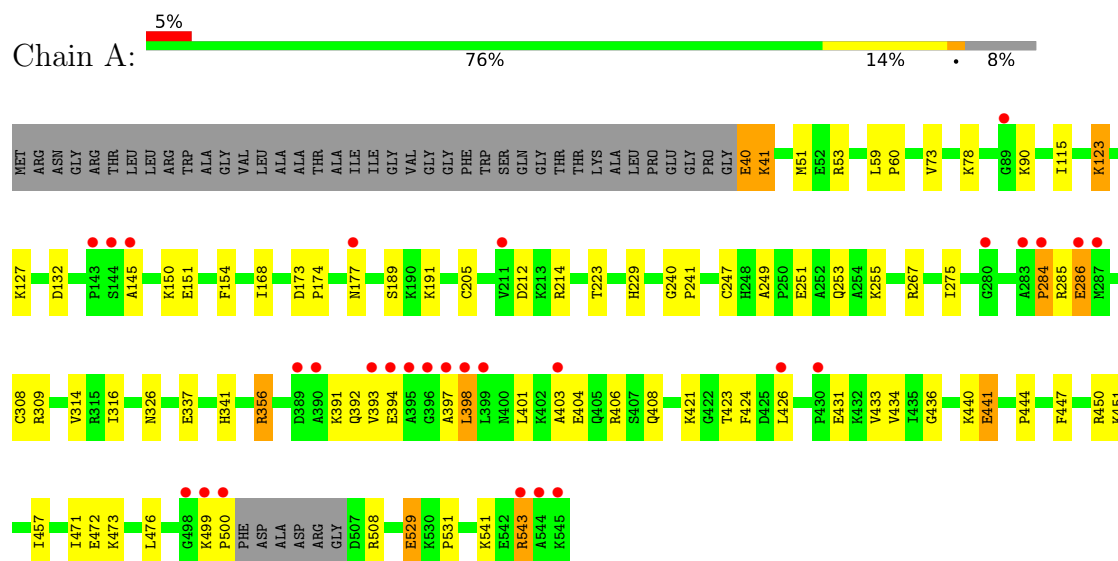
- Molecule 3 is water.

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

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



4 Data and refinement statistics

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 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.35-2.00) 99.9 (29.35-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.32 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.34	0/3860	0.70	1/5196 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	ASP	CB-CA-C	-5.14	110.24	117.23

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	3779	0	3714	78	0
2	A	688	0	480	25	0
3	A	473	0	0	10	0
All	All	4940	0	4194	87	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 10.

All (87) 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
1:A:151:GLU:HG3	2:A:1007:HEC:O1D	1.83	0.78
1:A:309:ARG:HG3	2:A:1004:HEC:O1A	1.90	0.72
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:151:GLU:HG3	2:A:1007:HEC:CGD	2.28	0.64
1:A:499:LYS:H	1:A:500:PRO:HA	1.62	0.64
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
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
2:A:1010:HEC:HMC3	2:A:1010:HEC:HBC3	1.83	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:1002:HEC:HMC1	2:A:1002:HEC:HBC3	1.85	0.59
1:A:151:GLU:HG2	3:A:1188:HOH:O	2.04	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
2:A:1006:HEC:HMC3	2:A:1006:HEC:HBC3	1.88	0.55
2:A:1006:HEC:HMC3	2:A:1006:HEC:CBC	2.36	0.55
1:A:398:LEU:HD22	1:A:398:LEU:N	2.22	0.55
1:A:499:LYS:HB3	1:A:500:PRO:C	2.33	0.54
1:A:398:LEU:C	1:A:401:LEU:HD13	2.34	0.53
1:A:189:SER:HB2	1:A:191:LYS:HE3	1.89	0.53
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1010:HEC:HBD2	3:A:1046:HOH:O	2.13	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:251:GLU:H	1:A:251:GLU:CD	2.21	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
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
2:A:1014:HEC:HMB3	2:A:1014:HEC:HBB3	1.99	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
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
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:1010:HEC:HMC3	2:A:1010:HEC:CBC	2.47	0.43
1:A:150:LYS:HD2	1:A:253:GLN:OE1	2.19	0.43
1:A:316:ILE:HD13	2:A:1008:HEC:HMB3	2.00	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:173:ASP:CG	1:A:174:PRO:HD2	2.45	0.42
1:A:284:PRO:HA	1:A:285:ARG:HA	1.92	0.41
2:A:1002:HEC:HBC3	2:A:1002:HEC:CMC	2.51	0.41
1:A:397:ALA:HB3	1:A:398:LEU:HD22	2.03	0.41
1:A:286:GLU:H	1:A:286:GLU:CD	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	21 17

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%)	36 38

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	127	LYS
1	A	286	GLU
1	A	356	ARG
1	A	394	GLU
1	A	398	LEU
1	A	441	GLU
1	A	529	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	326	ASN
1	A	342	GLN
1	A	392	GLN
1	A	400	ASN
1	A	405	GLN
1	A	427	ASN
1	A	478	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	46,50,50	2.43	15 (32%)	58,82,82	1.81	4 (6%)
2	HEC	A	1014	1	46,50,50	2.38	15 (32%)	58,82,82	1.88	5 (8%)
2	HEC	A	1004	1	46,50,50	2.36	15 (32%)	58,82,82	1.86	6 (10%)
2	HEC	A	1010	1	46,50,50	2.35	17 (36%)	58,82,82	1.92	3 (5%)
2	HEC	A	1013	1	46,50,50	2.36	16 (34%)	58,82,82	1.87	4 (6%)
2	HEC	A	1005	1	46,50,50	2.44	18 (39%)	58,82,82	1.84	4 (6%)
2	HEC	A	1007	1	46,50,50	2.34	15 (32%)	58,82,82	1.94	5 (8%)
2	HEC	A	1002	1	46,50,50	2.36	16 (34%)	58,82,82	1.87	4 (6%)
2	HEC	A	1003	1	46,50,50	2.37	16 (34%)	58,82,82	1.93	5 (8%)
2	HEC	A	1016	1	46,50,50	2.37	16 (34%)	58,82,82	1.88	2 (3%)
2	HEC	A	1001	1	46,50,50	2.33	15 (32%)	58,82,82	1.90	8 (13%)
2	HEC	A	1015	1	46,50,50	1.98	14 (30%)	58,82,82	1.09	4 (6%)
2	HEC	A	1011	1	46,50,50	2.32	15 (32%)	58,82,82	1.89	4 (6%)
2	HEC	A	1009	1	46,50,50	2.32	15 (32%)	58,82,82	1.96	6 (10%)
2	HEC	A	1006	1	46,50,50	2.33	15 (32%)	58,82,82	1.91	6 (10%)
2	HEC	A	1012	1	46,50,50	2.31	16 (34%)	58,82,82	1.86	4 (6%)

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	-	6/14/54/54	-
2	HEC	A	1014	1	-	6/14/54/54	-
2	HEC	A	1004	1	-	7/14/54/54	-
2	HEC	A	1010	1	-	9/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	1013	1	-	6/14/54/54	-
2	HEC	A	1005	1	-	8/14/54/54	-
2	HEC	A	1007	1	-	9/14/54/54	-
2	HEC	A	1002	1	-	6/14/54/54	-
2	HEC	A	1003	1	-	6/14/54/54	-
2	HEC	A	1016	1	-	8/14/54/54	-
2	HEC	A	1001	1	-	7/14/54/54	-
2	HEC	A	1015	1	-	9/14/54/54	-
2	HEC	A	1011	1	-	6/14/54/54	-
2	HEC	A	1009	1	-	6/14/54/54	-
2	HEC	A	1006	1	-	5/14/54/54	-
2	HEC	A	1012	1	-	6/14/54/54	-

All (249) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1006	HEC	CAC-C3C	5.89	1.54	1.35
2	A	1004	HEC	CAB-C3B	5.77	1.53	1.35
2	A	1008	HEC	CAB-C3B	5.71	1.53	1.35
2	A	1010	HEC	CAC-C3C	5.70	1.53	1.35
2	A	1016	HEC	CAC-C3C	5.67	1.53	1.35
2	A	1002	HEC	CAC-C3C	5.67	1.53	1.35
2	A	1013	HEC	CAC-C3C	5.66	1.53	1.35
2	A	1008	HEC	CAC-C3C	5.66	1.53	1.35
2	A	1014	HEC	CAC-C3C	5.66	1.53	1.35
2	A	1001	HEC	CAC-C3C	5.65	1.53	1.35
2	A	1009	HEC	CAB-C3B	5.65	1.53	1.35
2	A	1003	HEC	CAC-C3C	5.64	1.53	1.35
2	A	1006	HEC	CAB-C3B	5.62	1.53	1.35
2	A	1014	HEC	CAB-C3B	5.61	1.53	1.35
2	A	1005	HEC	CAB-C3B	5.61	1.53	1.35
2	A	1011	HEC	CAB-C3B	5.60	1.53	1.35
2	A	1005	HEC	CAC-C3C	5.57	1.53	1.35
2	A	1003	HEC	CAB-C3B	5.57	1.53	1.35
2	A	1016	HEC	CAB-C3B	5.56	1.53	1.35
2	A	1012	HEC	CAB-C3B	5.56	1.53	1.35
2	A	1004	HEC	CAC-C3C	5.56	1.53	1.35
2	A	1013	HEC	CAB-C3B	5.54	1.53	1.35
2	A	1001	HEC	CAB-C3B	5.54	1.53	1.35
2	A	1010	HEC	CAB-C3B	5.54	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	HEC	CAB-C3B	5.48	1.52	1.35
2	A	1012	HEC	CAC-C3C	5.48	1.52	1.35
2	A	1007	HEC	CAC-C3C	5.47	1.52	1.35
2	A	1007	HEC	CAB-C3B	5.47	1.52	1.35
2	A	1011	HEC	CAC-C3C	5.42	1.52	1.35
2	A	1009	HEC	CAC-C3C	5.42	1.52	1.35
2	A	1005	HEC	C3C-C4C	-4.83	1.37	1.46
2	A	1010	HEC	C3B-C4B	-4.73	1.37	1.46
2	A	1012	HEC	C3B-C4B	-4.47	1.38	1.46
2	A	1013	HEC	C3B-C4B	-4.32	1.38	1.46
2	A	1009	HEC	C3C-C4C	-4.31	1.38	1.46
2	A	1016	HEC	C4B-NB	-4.30	1.31	1.39
2	A	1001	HEC	C1A-C2A	-4.28	1.37	1.45
2	A	1003	HEC	C4A-NA	-4.20	1.31	1.39
2	A	1008	HEC	C1B-NB	-4.18	1.31	1.39
2	A	1004	HEC	C3C-C4C	-4.18	1.38	1.46
2	A	1007	HEC	C1A-NA	-4.17	1.31	1.39
2	A	1014	HEC	C1B-NB	-4.08	1.31	1.39
2	A	1002	HEC	C1C-NC	-4.08	1.31	1.39
2	A	1010	HEC	C4C-NC	-4.07	1.32	1.39
2	A	1008	HEC	C4B-NB	-4.05	1.32	1.39
2	A	1004	HEC	C4D-ND	-4.04	1.32	1.39
2	A	1008	HEC	C3B-C4B	-4.04	1.39	1.46
2	A	1014	HEC	C1A-NA	-4.03	1.32	1.39
2	A	1014	HEC	C1A-C2A	-4.03	1.38	1.45
2	A	1011	HEC	C1A-C2A	-4.03	1.38	1.45
2	A	1006	HEC	C1B-NB	-4.02	1.32	1.39
2	A	1007	HEC	C4B-NB	-4.02	1.32	1.39
2	A	1003	HEC	C1A-NA	-3.97	1.32	1.39
2	A	1010	HEC	C1A-NA	-3.97	1.32	1.39
2	A	1004	HEC	C1C-NC	-3.97	1.32	1.39
2	A	1011	HEC	C4B-NB	-3.96	1.32	1.39
2	A	1001	HEC	C3B-C4B	-3.95	1.39	1.46
2	A	1008	HEC	C1D-ND	-3.92	1.32	1.39
2	A	1011	HEC	C3C-C4C	-3.91	1.39	1.46
2	A	1006	HEC	C1C-NC	-3.91	1.32	1.39
2	A	1011	HEC	C1B-NB	-3.89	1.32	1.39
2	A	1005	HEC	C1A-NA	-3.88	1.32	1.39
2	A	1016	HEC	C3C-C4C	-3.88	1.39	1.46
2	A	1008	HEC	C3C-C4C	-3.87	1.39	1.46
2	A	1015	HEC	C4C-NC	-3.87	1.32	1.39
2	A	1002	HEC	C4A-NA	-3.84	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1013	HEC	C4A-NA	-3.84	1.32	1.39
2	A	1014	HEC	C4D-ND	-3.83	1.32	1.39
2	A	1007	HEC	C3C-C4C	-3.83	1.39	1.46
2	A	1002	HEC	C4D-ND	-3.83	1.32	1.39
2	A	1015	HEC	C3B-C4B	-3.83	1.39	1.46
2	A	1014	HEC	C3B-C4B	-3.82	1.39	1.46
2	A	1005	HEC	C4B-NB	-3.82	1.32	1.39
2	A	1002	HEC	C3B-C4B	-3.82	1.39	1.46
2	A	1008	HEC	C1A-C2A	-3.81	1.38	1.45
2	A	1004	HEC	C1D-ND	-3.81	1.32	1.39
2	A	1016	HEC	C1D-ND	-3.81	1.32	1.39
2	A	1006	HEC	C4B-NB	-3.80	1.32	1.39
2	A	1014	HEC	C3C-C4C	-3.78	1.39	1.46
2	A	1003	HEC	C4A-C3A	-3.78	1.37	1.45
2	A	1016	HEC	C4A-C3A	-3.77	1.37	1.45
2	A	1011	HEC	C4A-C3A	-3.76	1.37	1.45
2	A	1009	HEC	C1B-NB	-3.76	1.32	1.39
2	A	1007	HEC	C4A-C3A	-3.75	1.37	1.45
2	A	1006	HEC	C3C-C4C	-3.73	1.39	1.46
2	A	1001	HEC	C1D-ND	-3.73	1.32	1.39
2	A	1003	HEC	C1B-NB	-3.73	1.32	1.39
2	A	1015	HEC	C1A-NA	-3.70	1.32	1.39
2	A	1005	HEC	C1A-C2A	-3.69	1.38	1.45
2	A	1016	HEC	C4C-NC	-3.68	1.32	1.39
2	A	1005	HEC	C1D-ND	-3.68	1.32	1.39
2	A	1005	HEC	C3B-C4B	-3.67	1.39	1.46
2	A	1006	HEC	C1D-ND	-3.63	1.32	1.39
2	A	1016	HEC	C4D-ND	-3.63	1.32	1.39
2	A	1001	HEC	C4B-NB	-3.63	1.32	1.39
2	A	1006	HEC	C3B-C4B	-3.63	1.39	1.46
2	A	1008	HEC	C1A-NA	-3.62	1.32	1.39
2	A	1003	HEC	C1D-ND	-3.62	1.32	1.39
2	A	1002	HEC	C4B-NB	-3.62	1.32	1.39
2	A	1003	HEC	C4B-NB	-3.62	1.32	1.39
2	A	1002	HEC	C1A-C2A	-3.61	1.38	1.45
2	A	1009	HEC	C4D-ND	-3.60	1.32	1.39
2	A	1005	HEC	C1C-NC	-3.60	1.32	1.39
2	A	1007	HEC	C3B-C4B	-3.58	1.39	1.46
2	A	1010	HEC	C4A-NA	-3.57	1.32	1.39
2	A	1011	HEC	C4A-NA	-3.57	1.32	1.39
2	A	1004	HEC	C1A-NA	-3.56	1.32	1.39
2	A	1001	HEC	C4A-NA	-3.54	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1012	HEC	C4A-C3A	-3.54	1.38	1.45
2	A	1012	HEC	C4C-NC	-3.53	1.33	1.39
2	A	1015	HEC	C1C-NC	-3.53	1.33	1.39
2	A	1009	HEC	C1D-ND	-3.52	1.33	1.39
2	A	1002	HEC	C1B-NB	-3.51	1.33	1.39
2	A	1009	HEC	C4A-NA	-3.51	1.33	1.39
2	A	1013	HEC	C1D-ND	-3.51	1.33	1.39
2	A	1009	HEC	C4B-NB	-3.50	1.33	1.39
2	A	1016	HEC	C1B-NB	-3.50	1.33	1.39
2	A	1004	HEC	C1B-NB	-3.50	1.33	1.39
2	A	1013	HEC	C1C-NC	-3.49	1.33	1.39
2	A	1004	HEC	C1A-C2A	-3.49	1.39	1.45
2	A	1015	HEC	C4A-NA	-3.48	1.33	1.39
2	A	1013	HEC	C1A-C2A	-3.47	1.39	1.45
2	A	1007	HEC	C1B-NB	-3.47	1.33	1.39
2	A	1015	HEC	C1A-C2A	-3.45	1.39	1.45
2	A	1012	HEC	C1A-C2A	-3.43	1.39	1.45
2	A	1002	HEC	C1A-NA	-3.43	1.33	1.39
2	A	1008	HEC	C1C-NC	-3.43	1.33	1.39
2	A	1001	HEC	C1A-NA	-3.42	1.33	1.39
2	A	1007	HEC	C1A-C2A	-3.42	1.39	1.45
2	A	1016	HEC	C1A-C2A	-3.41	1.39	1.45
2	A	1002	HEC	C3C-C4C	-3.41	1.40	1.46
2	A	1011	HEC	C3B-C4B	-3.40	1.40	1.46
2	A	1005	HEC	C4D-ND	-3.40	1.33	1.39
2	A	1013	HEC	C1B-NB	-3.39	1.33	1.39
2	A	1004	HEC	C3B-C4B	-3.39	1.40	1.46
2	A	1011	HEC	C1D-ND	-3.39	1.33	1.39
2	A	1005	HEC	C4A-C3A	-3.38	1.38	1.45
2	A	1012	HEC	C1D-ND	-3.38	1.33	1.39
2	A	1014	HEC	C4A-NA	-3.37	1.33	1.39
2	A	1014	HEC	C4C-NC	-3.37	1.33	1.39
2	A	1013	HEC	C4D-ND	-3.37	1.33	1.39
2	A	1001	HEC	C3C-C4C	-3.37	1.40	1.46
2	A	1003	HEC	C4D-ND	-3.36	1.33	1.39
2	A	1010	HEC	C1C-NC	-3.34	1.33	1.39
2	A	1013	HEC	C4C-NC	-3.34	1.33	1.39
2	A	1013	HEC	C1A-NA	-3.33	1.33	1.39
2	A	1010	HEC	C4D-C3D	-3.33	1.37	1.44
2	A	1014	HEC	C1D-ND	-3.32	1.33	1.39
2	A	1012	HEC	C4D-ND	-3.31	1.33	1.39
2	A	1006	HEC	C4A-C3A	-3.31	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	HEC	C4C-NC	-3.30	1.33	1.39
2	A	1004	HEC	C4B-NB	-3.30	1.33	1.39
2	A	1013	HEC	C3C-C4C	-3.29	1.40	1.46
2	A	1012	HEC	C4B-NB	-3.29	1.33	1.39
2	A	1005	HEC	C4A-NA	-3.29	1.33	1.39
2	A	1007	HEC	C4A-NA	-3.29	1.33	1.39
2	A	1013	HEC	C4B-NB	-3.27	1.33	1.39
2	A	1004	HEC	C4C-NC	-3.26	1.33	1.39
2	A	1008	HEC	C4A-NA	-3.26	1.33	1.39
2	A	1015	HEC	C3C-C4C	-3.26	1.40	1.46
2	A	1007	HEC	C1C-NC	-3.26	1.33	1.39
2	A	1013	HEC	C4D-C3D	-3.25	1.38	1.44
2	A	1012	HEC	C3C-C4C	-3.25	1.40	1.46
2	A	1009	HEC	C1A-NA	-3.25	1.33	1.39
2	A	1009	HEC	C3B-C4B	-3.24	1.40	1.46
2	A	1014	HEC	C1C-NC	-3.24	1.33	1.39
2	A	1002	HEC	C4C-NC	-3.23	1.33	1.39
2	A	1010	HEC	C4B-NB	-3.23	1.33	1.39
2	A	1008	HEC	C4D-ND	-3.22	1.33	1.39
2	A	1006	HEC	C4D-ND	-3.22	1.33	1.39
2	A	1009	HEC	C4C-NC	-3.21	1.33	1.39
2	A	1006	HEC	C4A-NA	-3.20	1.33	1.39
2	A	1010	HEC	C4D-ND	-3.20	1.33	1.39
2	A	1015	HEC	C4D-C3D	-3.20	1.38	1.44
2	A	1009	HEC	C1C-NC	-3.18	1.33	1.39
2	A	1012	HEC	C1B-NB	-3.18	1.33	1.39
2	A	1001	HEC	C4D-ND	-3.17	1.33	1.39
2	A	1002	HEC	C4A-C3A	-3.16	1.39	1.45
2	A	1006	HEC	C4C-NC	-3.16	1.33	1.39
2	A	1001	HEC	C1B-NB	-3.15	1.33	1.39
2	A	1010	HEC	C1D-ND	-3.15	1.33	1.39
2	A	1004	HEC	C4A-NA	-3.14	1.33	1.39
2	A	1003	HEC	C3C-C4C	-3.14	1.40	1.46
2	A	1003	HEC	C1A-C2A	-3.14	1.39	1.45
2	A	1016	HEC	C1A-NA	-3.13	1.33	1.39
2	A	1001	HEC	C1C-NC	-3.09	1.33	1.39
2	A	1011	HEC	C4C-NC	-3.07	1.33	1.39
2	A	1007	HEC	C4D-C3D	-3.06	1.38	1.44
2	A	1007	HEC	C4C-NC	-3.06	1.33	1.39
2	A	1016	HEC	C3B-C4B	-3.03	1.40	1.46
2	A	1014	HEC	C4B-NB	-3.03	1.33	1.39
2	A	1006	HEC	C1A-C2A	-3.02	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1007	HEC	C1D-ND	-3.02	1.33	1.39
2	A	1001	HEC	C4A-C3A	-3.02	1.39	1.45
2	A	1005	HEC	C4D-C3D	-3.01	1.38	1.44
2	A	1008	HEC	C4C-NC	-3.00	1.34	1.39
2	A	1009	HEC	C4A-C3A	-2.99	1.39	1.45
2	A	1009	HEC	C1A-C2A	-2.98	1.40	1.45
2	A	1015	HEC	C4D-ND	-2.97	1.34	1.39
2	A	1008	HEC	C4A-C3A	-2.96	1.39	1.45
2	A	1003	HEC	C1C-NC	-2.96	1.34	1.39
2	A	1001	HEC	C4C-NC	-2.96	1.34	1.39
2	A	1005	HEC	C4C-NC	-2.96	1.34	1.39
2	A	1002	HEC	C1D-ND	-2.95	1.34	1.39
2	A	1015	HEC	C1D-ND	-2.94	1.34	1.39
2	A	1012	HEC	C1C-NC	-2.94	1.34	1.39
2	A	1006	HEC	C1A-NA	-2.94	1.34	1.39
2	A	1013	HEC	C4A-C3A	-2.94	1.39	1.45
2	A	1016	HEC	C4A-NA	-2.92	1.34	1.39
2	A	1012	HEC	C4A-NA	-2.92	1.34	1.39
2	A	1016	HEC	C1C-NC	-2.91	1.34	1.39
2	A	1003	HEC	C3B-C4B	-2.91	1.40	1.46
2	A	1015	HEC	C4A-C3A	-2.90	1.39	1.45
2	A	1014	HEC	C4D-C3D	-2.87	1.38	1.44
2	A	1004	HEC	C4A-C3A	-2.86	1.39	1.45
2	A	1008	HEC	C4D-C3D	-2.81	1.39	1.44
2	A	1012	HEC	C4D-C3D	-2.79	1.39	1.44
2	A	1014	HEC	C4A-C3A	-2.78	1.39	1.45
2	A	1015	HEC	C4B-NB	-2.76	1.34	1.39
2	A	1010	HEC	C1A-C2A	-2.75	1.40	1.45
2	A	1007	HEC	C4D-ND	-2.72	1.34	1.39
2	A	1003	HEC	C4D-C3D	-2.67	1.39	1.44
2	A	1005	HEC	C1B-NB	-2.65	1.34	1.39
2	A	1012	HEC	C1A-NA	-2.61	1.34	1.39
2	A	1010	HEC	C1B-NB	-2.60	1.34	1.39
2	A	1011	HEC	C4D-ND	-2.59	1.34	1.39
2	A	1016	HEC	C4D-C3D	-2.55	1.39	1.44
2	A	1006	HEC	C4D-C3D	-2.54	1.39	1.44
2	A	1010	HEC	C1B-C2B	-2.51	1.37	1.43
2	A	1011	HEC	C1C-NC	-2.50	1.34	1.39
2	A	1009	HEC	C4D-C3D	-2.49	1.39	1.44
2	A	1011	HEC	C1A-NA	-2.47	1.35	1.39
2	A	1010	HEC	C1D-C2D	-2.38	1.37	1.43
2	A	1010	HEC	C3C-C4C	-2.36	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1016	HEC	C1C-C2C	-2.34	1.37	1.43
2	A	1002	HEC	C4D-C3D	-2.32	1.39	1.44
2	A	1015	HEC	C1B-NB	-2.26	1.35	1.39
2	A	1015	HEC	C1D-C2D	-2.22	1.37	1.43
2	A	1013	HEC	C1B-C2B	-2.20	1.38	1.43
2	A	1012	HEC	C1C-C2C	-2.19	1.38	1.43
2	A	1011	HEC	C1C-C2C	-2.19	1.38	1.43
2	A	1010	HEC	C4A-C3A	-2.18	1.41	1.45
2	A	1004	HEC	C4D-C3D	-2.12	1.40	1.44
2	A	1005	HEC	CHD-C4C	2.09	1.42	1.38
2	A	1001	HEC	CHB-C4A	2.08	1.42	1.38
2	A	1005	HEC	C1B-C2B	-2.07	1.38	1.43
2	A	1003	HEC	CHA-C1A	2.02	1.42	1.38
2	A	1005	HEC	CHC-C4B	2.01	1.42	1.38
2	A	1002	HEC	CHD-C4C	2.01	1.42	1.38

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1007	HEC	CBB-CAB-C3B	-8.86	109.72	127.43
2	A	1002	HEC	CBB-CAB-C3B	-8.83	109.79	127.43
2	A	1016	HEC	CBB-CAB-C3B	-8.79	109.87	127.43
2	A	1014	HEC	CBB-CAB-C3B	-8.78	109.88	127.43
2	A	1009	HEC	CBC-CAC-C3C	-8.78	109.89	127.43
2	A	1004	HEC	CBB-CAB-C3B	-8.75	109.94	127.43
2	A	1013	HEC	CBC-CAC-C3C	-8.72	110.01	127.43
2	A	1003	HEC	CBB-CAB-C3B	-8.72	110.02	127.43
2	A	1005	HEC	CBB-CAB-C3B	-8.71	110.03	127.43
2	A	1010	HEC	CBB-CAB-C3B	-8.69	110.07	127.43
2	A	1003	HEC	CBC-CAC-C3C	-8.63	110.18	127.43
2	A	1001	HEC	CBB-CAB-C3B	-8.62	110.20	127.43
2	A	1009	HEC	CBB-CAB-C3B	-8.62	110.20	127.43
2	A	1007	HEC	CBC-CAC-C3C	-8.59	110.27	127.43
2	A	1011	HEC	CBC-CAC-C3C	-8.58	110.28	127.43
2	A	1005	HEC	CBC-CAC-C3C	-8.58	110.28	127.43
2	A	1011	HEC	CBB-CAB-C3B	-8.57	110.30	127.43
2	A	1012	HEC	CBB-CAB-C3B	-8.54	110.36	127.43
2	A	1014	HEC	CBC-CAC-C3C	-8.51	110.42	127.43
2	A	1008	HEC	CBB-CAB-C3B	-8.51	110.42	127.43
2	A	1004	HEC	CBC-CAC-C3C	-8.48	110.49	127.43
2	A	1006	HEC	CBB-CAB-C3B	-8.46	110.53	127.43
2	A	1001	HEC	CBC-CAC-C3C	-8.43	110.58	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1013	HEC	CBB-CAB-C3B	-8.40	110.65	127.43
2	A	1012	HEC	CBC-CAC-C3C	-8.39	110.67	127.43
2	A	1010	HEC	CBC-CAC-C3C	-8.30	110.83	127.43
2	A	1016	HEC	CBC-CAC-C3C	-8.30	110.84	127.43
2	A	1008	HEC	CBC-CAC-C3C	-8.24	110.96	127.43
2	A	1002	HEC	CBC-CAC-C3C	-8.10	111.24	127.43
2	A	1006	HEC	CBC-CAC-C3C	-7.98	111.48	127.43
2	A	1013	HEC	C1D-CHD-C4C	3.04	134.04	124.66
2	A	1006	HEC	CMD-C2D-C1D	2.84	129.74	125.42
2	A	1011	HEC	CMC-C2C-C1C	2.83	129.73	125.42
2	A	1013	HEC	C1B-CHB-C4A	2.66	132.86	124.66
2	A	1015	HEC	CBB-CAB-C3B	-2.64	122.17	127.43
2	A	1009	HEC	C4D-ND-C1D	2.63	110.11	105.82
2	A	1012	HEC	C1D-CHD-C4C	2.47	132.29	124.66
2	A	1009	HEC	C1C-CHC-C4B	2.47	132.28	124.66
2	A	1010	HEC	CHD-C4C-NC	-2.46	121.77	124.45
2	A	1012	HEC	CAA-C2A-C1A	2.44	129.82	124.85
2	A	1008	HEC	C1B-CHB-C4A	2.40	132.06	124.66
2	A	1001	HEC	C1D-CHD-C4C	2.35	131.92	124.66
2	A	1006	HEC	C1B-CHB-C4A	2.34	131.89	124.66
2	A	1007	HEC	C2A-C1A-NA	-2.32	108.08	110.32
2	A	1006	HEC	CAA-C2A-C1A	2.31	129.56	124.85
2	A	1001	HEC	CAD-C3D-C4D	2.30	129.43	124.94
2	A	1015	HEC	CHD-C4C-NC	-2.25	122.01	124.45
2	A	1003	HEC	C1B-CHB-C4A	2.22	131.53	124.66
2	A	1004	HEC	C4D-CHA-C1A	2.22	131.53	124.66
2	A	1014	HEC	C1B-CHB-C4A	2.22	131.51	124.66
2	A	1006	HEC	C1D-CHD-C4C	2.22	131.50	124.66
2	A	1008	HEC	CMD-C2D-C1D	2.20	128.78	125.42
2	A	1007	HEC	C4B-NB-C1B	2.19	109.39	105.82
2	A	1001	HEC	CMD-C2D-C1D	2.18	128.74	125.42
2	A	1005	HEC	C4C-NC-C1C	2.16	109.34	105.82
2	A	1014	HEC	C4A-NA-C1A	2.16	109.33	105.82
2	A	1009	HEC	C4D-CHA-C1A	2.15	131.31	124.66
2	A	1011	HEC	C4D-CHA-C1A	2.12	131.21	124.66
2	A	1002	HEC	CMB-C2B-C1B	2.12	128.65	125.42
2	A	1015	HEC	CHA-C1A-NA	-2.11	122.16	124.45
2	A	1004	HEC	C1C-CHC-C4B	2.10	131.13	124.66
2	A	1003	HEC	C4D-ND-C1D	2.09	109.24	105.82
2	A	1001	HEC	C4A-NA-C1A	2.09	109.22	105.82
2	A	1003	HEC	C1C-CHC-C4B	2.08	131.08	124.66
2	A	1004	HEC	C4D-ND-C1D	2.08	109.21	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1015	HEC	CAA-C2A-C1A	2.07	129.06	124.85
2	A	1002	HEC	C4D-ND-C1D	2.07	109.20	105.82
2	A	1009	HEC	CMC-C2C-C1C	2.06	128.56	125.42
2	A	1005	HEC	C4D-CHA-C1A	2.05	130.99	124.66
2	A	1001	HEC	C4D-CHA-C1A	2.04	130.96	124.66
2	A	1007	HEC	C4A-NA-C1A	2.03	109.13	105.82
2	A	1014	HEC	C1D-CHD-C4C	2.01	130.88	124.66
2	A	1001	HEC	CMA-C3A-C4A	2.01	128.27	124.73
2	A	1004	HEC	C4A-NA-C1A	2.00	109.08	105.82

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	HEC	C2B-C3B-CAB-CBB
2	A	1001	HEC	C4B-C3B-CAB-CBB
2	A	1001	HEC	C2C-C3C-CAC-CBC
2	A	1001	HEC	C4C-C3C-CAC-CBC
2	A	1002	HEC	C2B-C3B-CAB-CBB
2	A	1002	HEC	C4B-C3B-CAB-CBB
2	A	1002	HEC	C2C-C3C-CAC-CBC
2	A	1002	HEC	C4C-C3C-CAC-CBC
2	A	1003	HEC	C2B-C3B-CAB-CBB
2	A	1003	HEC	C4B-C3B-CAB-CBB
2	A	1003	HEC	C2C-C3C-CAC-CBC
2	A	1003	HEC	C4C-C3C-CAC-CBC
2	A	1004	HEC	C2B-C3B-CAB-CBB
2	A	1004	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	C4C-C3C-CAC-CBC
2	A	1005	HEC	C2B-C3B-CAB-CBB
2	A	1005	HEC	C4B-C3B-CAB-CBB
2	A	1005	HEC	C2C-C3C-CAC-CBC
2	A	1005	HEC	C4C-C3C-CAC-CBC
2	A	1006	HEC	C2B-C3B-CAB-CBB
2	A	1006	HEC	C4B-C3B-CAB-CBB
2	A	1006	HEC	C4C-C3C-CAC-CBC
2	A	1007	HEC	C2B-C3B-CAB-CBB
2	A	1007	HEC	C4B-C3B-CAB-CBB
2	A	1007	HEC	C2C-C3C-CAC-CBC
2	A	1007	HEC	C4C-C3C-CAC-CBC
2	A	1008	HEC	C2B-C3B-CAB-CBB
2	A	1008	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
2	A	1008	HEC	C2C-C3C-CAC-CBC
2	A	1008	HEC	C4C-C3C-CAC-CBC
2	A	1009	HEC	C2B-C3B-CAB-CBB
2	A	1009	HEC	C4B-C3B-CAB-CBB
2	A	1009	HEC	C2C-C3C-CAC-CBC
2	A	1009	HEC	C4C-C3C-CAC-CBC
2	A	1010	HEC	C2B-C3B-CAB-CBB
2	A	1010	HEC	C4B-C3B-CAB-CBB
2	A	1010	HEC	C2C-C3C-CAC-CBC
2	A	1010	HEC	C4C-C3C-CAC-CBC
2	A	1011	HEC	C2B-C3B-CAB-CBB
2	A	1011	HEC	C4B-C3B-CAB-CBB
2	A	1011	HEC	C2C-C3C-CAC-CBC
2	A	1011	HEC	C4C-C3C-CAC-CBC
2	A	1012	HEC	C2B-C3B-CAB-CBB
2	A	1012	HEC	C4B-C3B-CAB-CBB
2	A	1012	HEC	C2C-C3C-CAC-CBC
2	A	1012	HEC	C4C-C3C-CAC-CBC
2	A	1013	HEC	C2B-C3B-CAB-CBB
2	A	1013	HEC	C4B-C3B-CAB-CBB
2	A	1013	HEC	C2C-C3C-CAC-CBC
2	A	1013	HEC	C4C-C3C-CAC-CBC
2	A	1014	HEC	C2B-C3B-CAB-CBB
2	A	1014	HEC	C4B-C3B-CAB-CBB
2	A	1014	HEC	C2C-C3C-CAC-CBC
2	A	1014	HEC	C4C-C3C-CAC-CBC
2	A	1015	HEC	C2B-C3B-CAB-CBB
2	A	1015	HEC	C4B-C3B-CAB-CBB
2	A	1015	HEC	C2C-C3C-CAC-CBC
2	A	1015	HEC	C4C-C3C-CAC-CBC
2	A	1016	HEC	C2C-C3C-CAC-CBC
2	A	1016	HEC	C4C-C3C-CAC-CBC
2	A	1001	HEC	C3D-CAD-CBD-CGD
2	A	1010	HEC	C2A-CAA-CBA-CGA
2	A	1015	HEC	C1A-C2A-CAA-CBA
2	A	1007	HEC	C3D-CAD-CBD-CGD
2	A	1015	HEC	C3A-C2A-CAA-CBA
2	A	1016	HEC	C4B-C3B-CAB-CBB
2	A	1004	HEC	C2C-C3C-CAC-CBC
2	A	1016	HEC	C2B-C3B-CAB-CBB
2	A	1009	HEC	CAD-CBD-CGD-O2D
2	A	1004	HEC	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
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
2	A	1016	HEC	CAA-CBA-CGA-O2A
2	A	1015	HEC	C2A-CAA-CBA-CGA
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

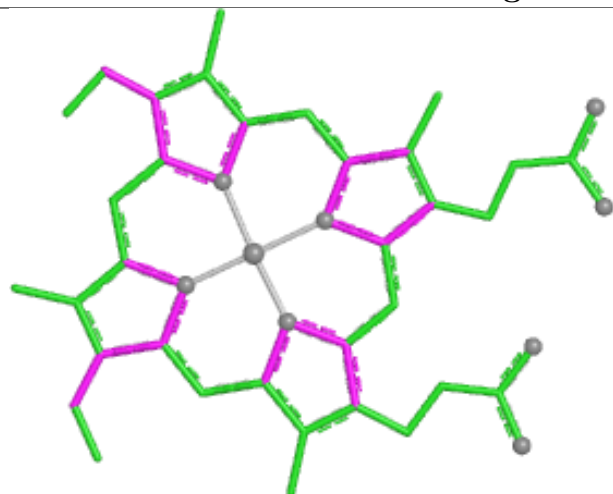
There are no ring outliers.

10 monomers are involved in 25 short contacts:

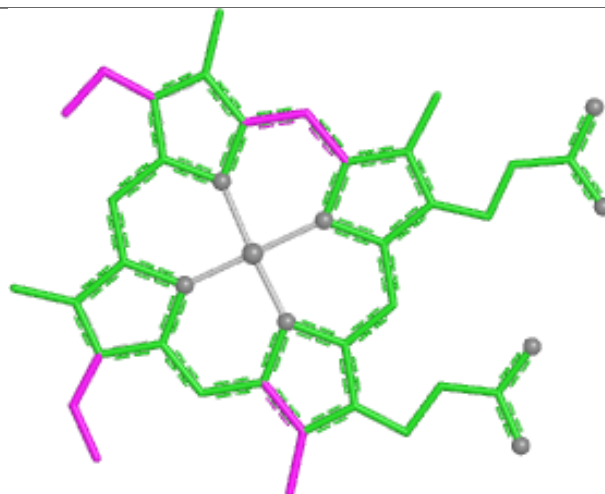
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1008	HEC	1	0
2	A	1014	HEC	2	0
2	A	1004	HEC	4	0
2	A	1010	HEC	3	0
2	A	1007	HEC	2	0
2	A	1002	HEC	2	0
2	A	1015	HEC	5	0
2	A	1009	HEC	1	0
2	A	1006	HEC	2	0
2	A	1012	HEC	3	0

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 than 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.

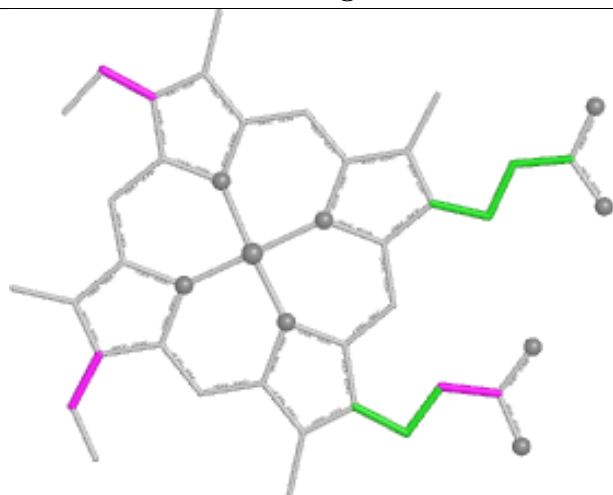
Ligand HEC A 1008



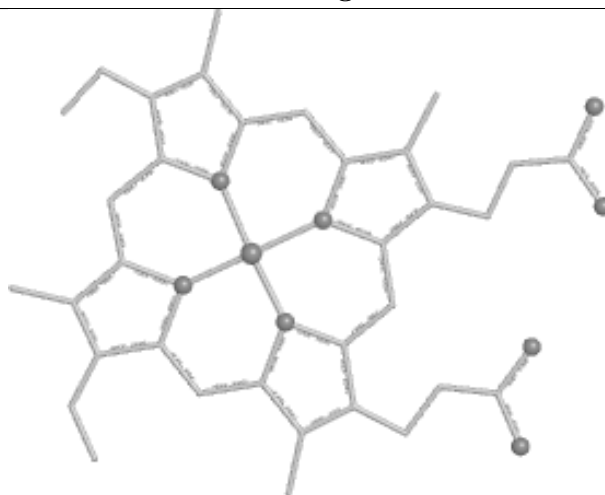
Bond lengths



Bond angles

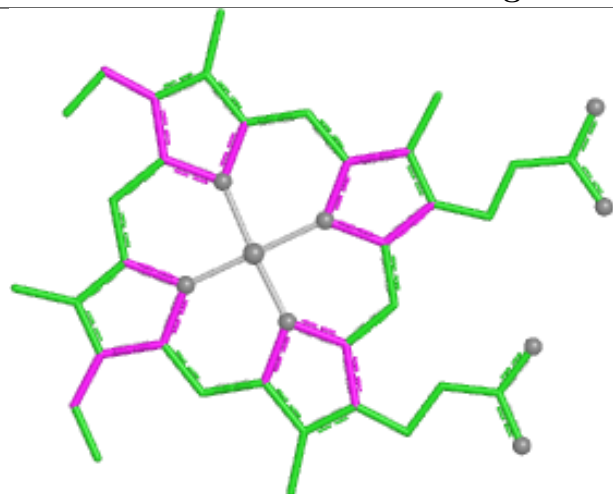


Torsions

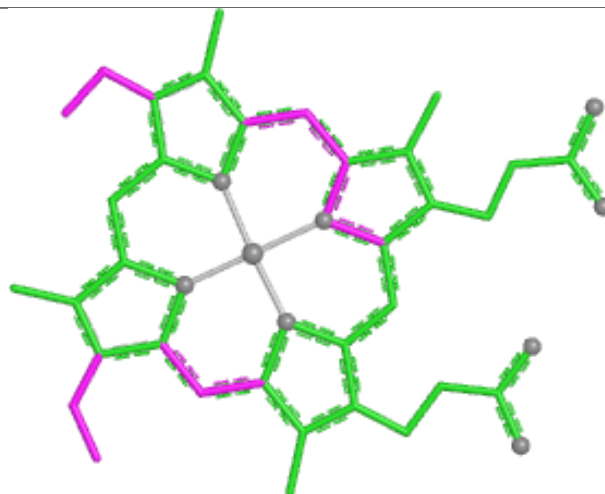


Rings

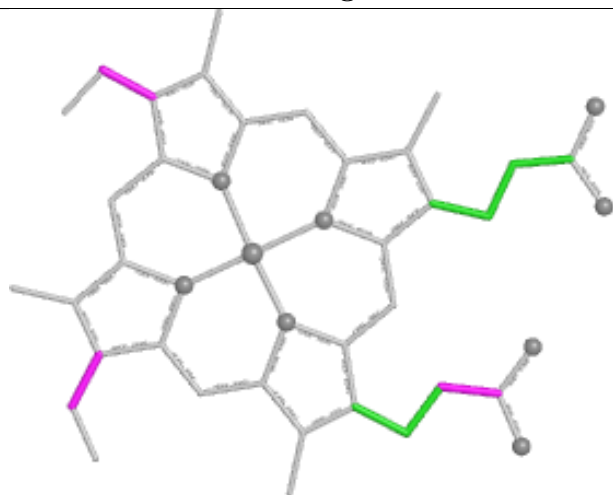
Ligand HEC A 1014



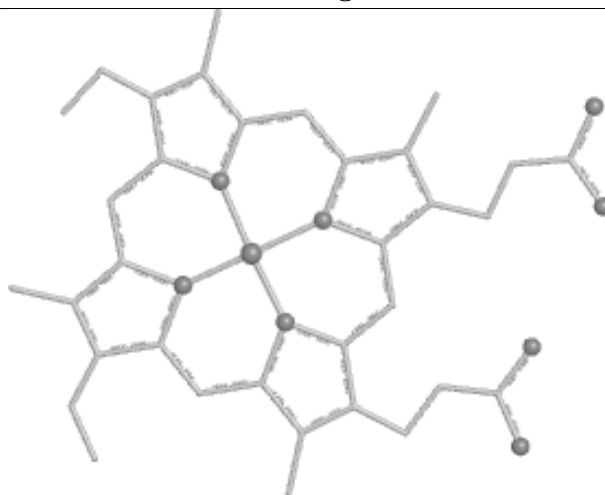
Bond lengths



Bond angles

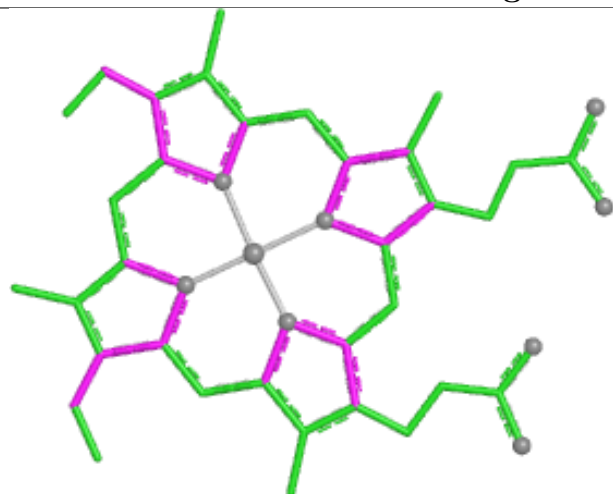


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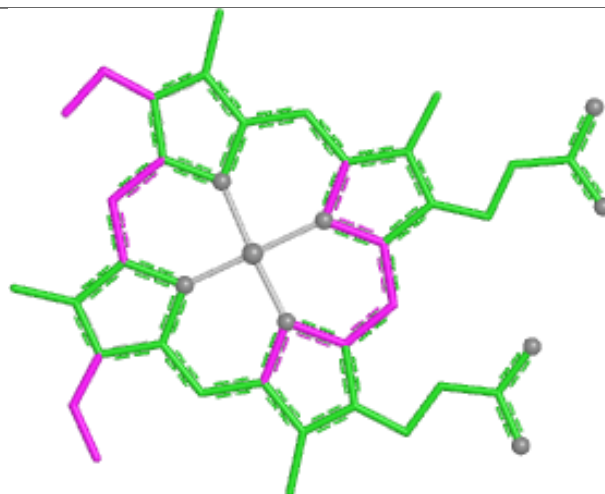


Rings

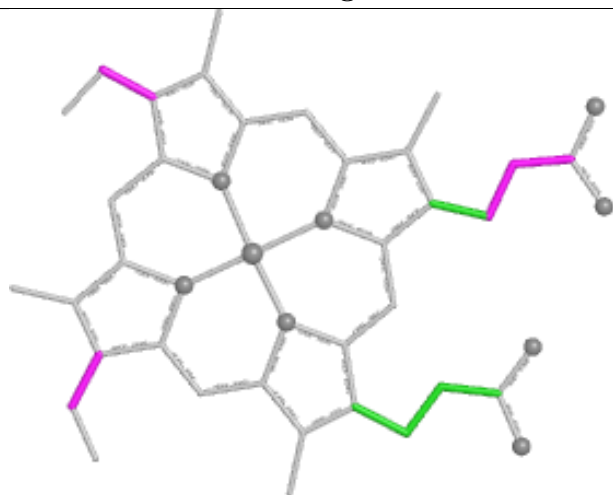
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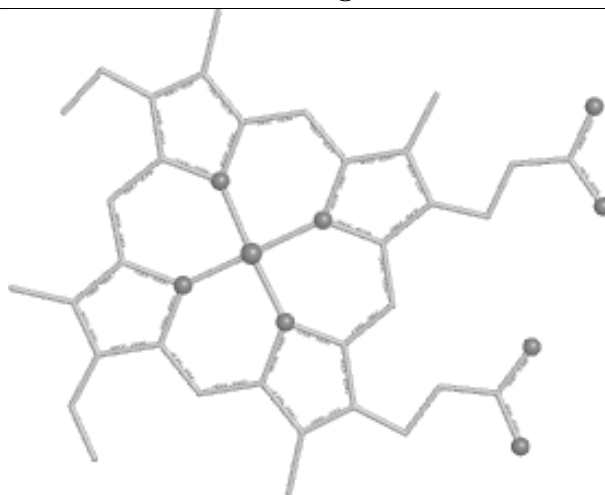
Bond lengths



Bond angles

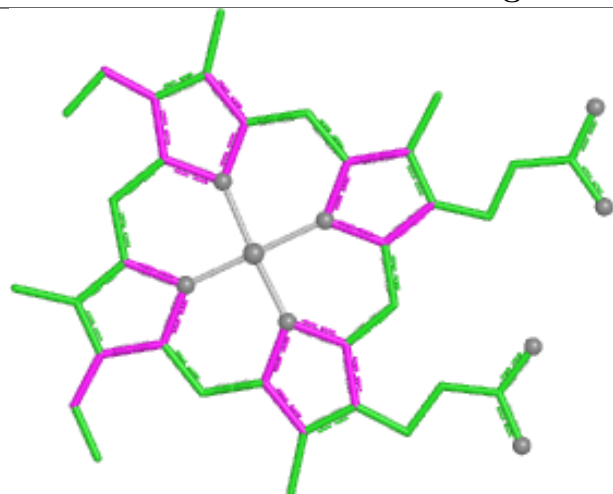


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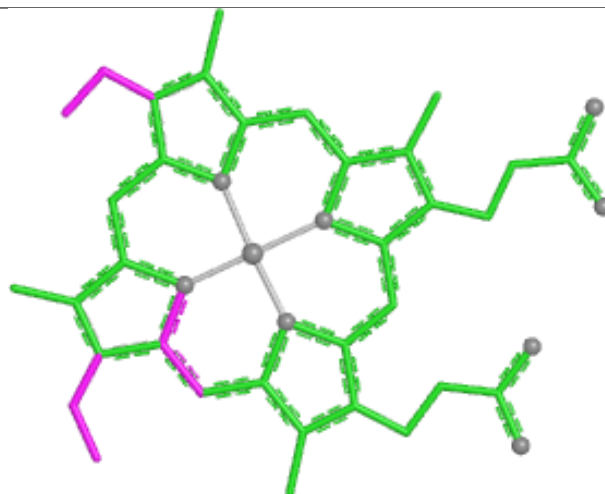


Rings

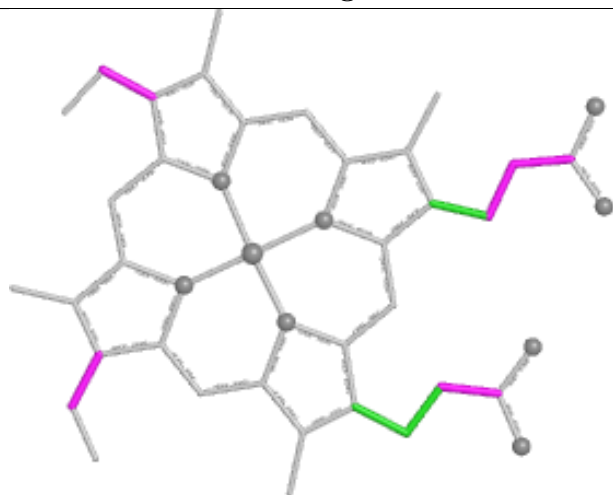
Ligand HEC A 1010



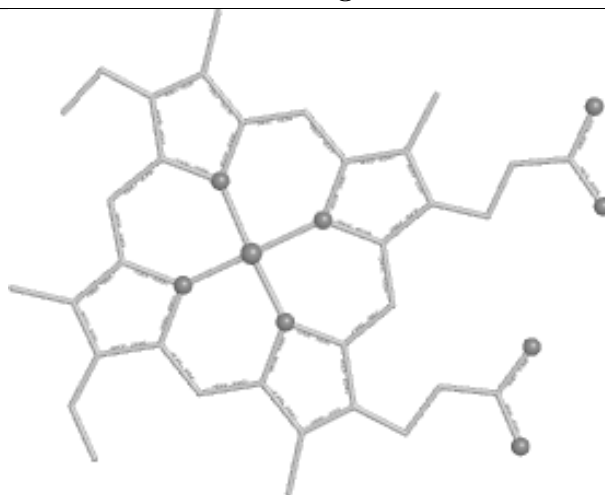
Bond lengths



Bond angles

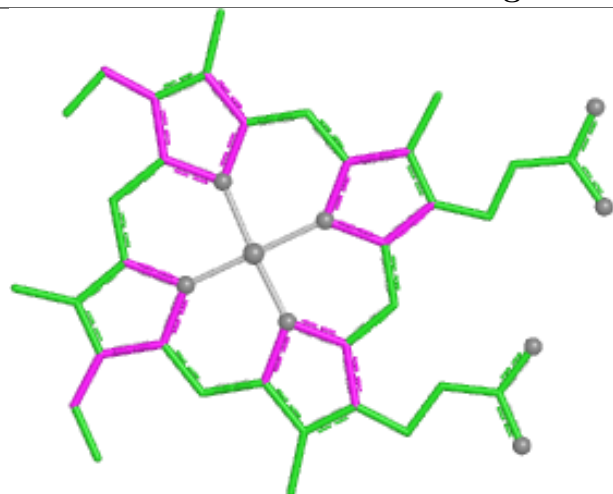


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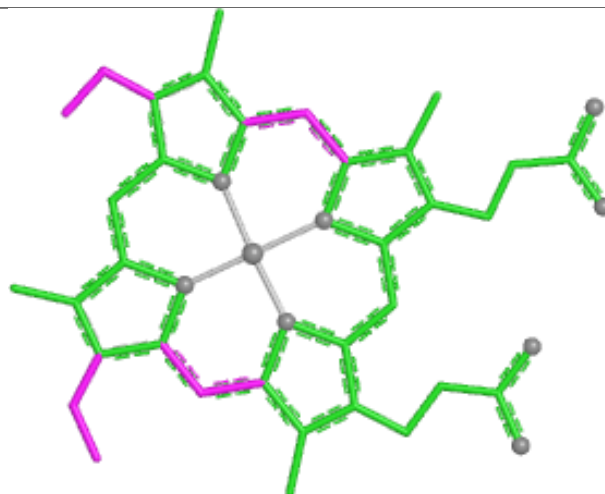


Rings

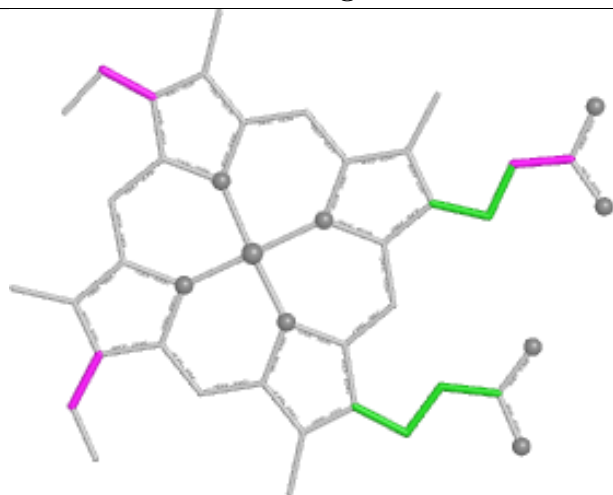
Ligand HEC A 1013



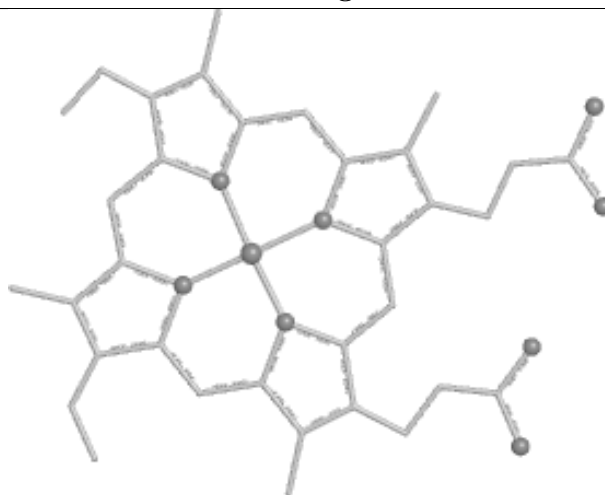
Bond lengths



Bond angles

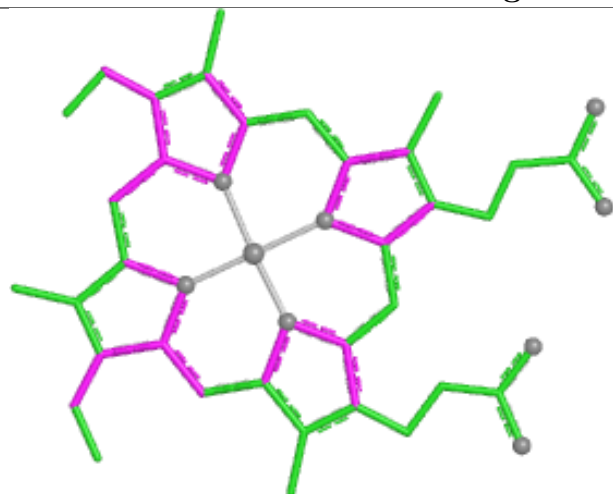


Torsions

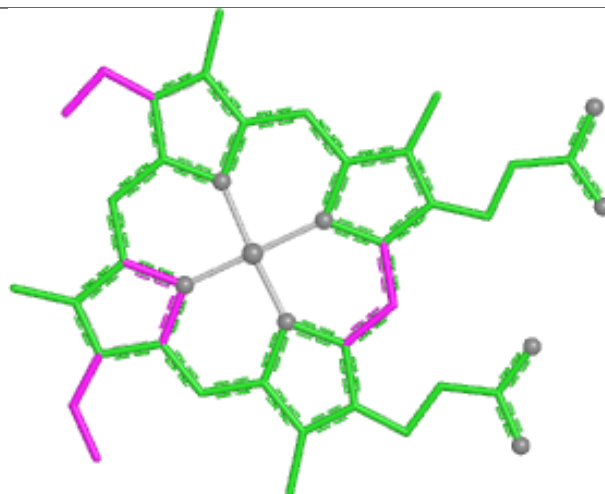


Rings

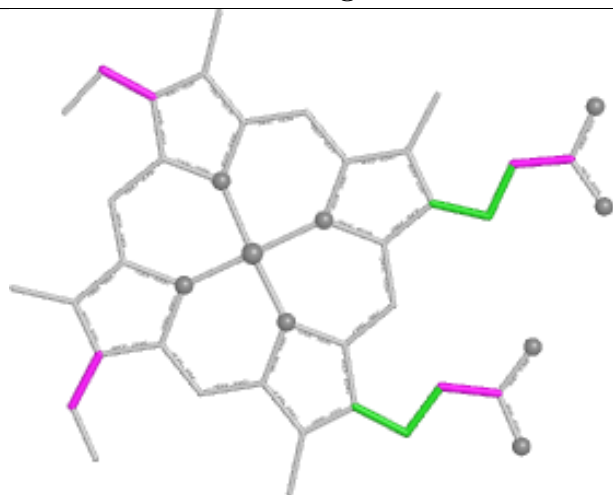
Ligand HEC A 1005



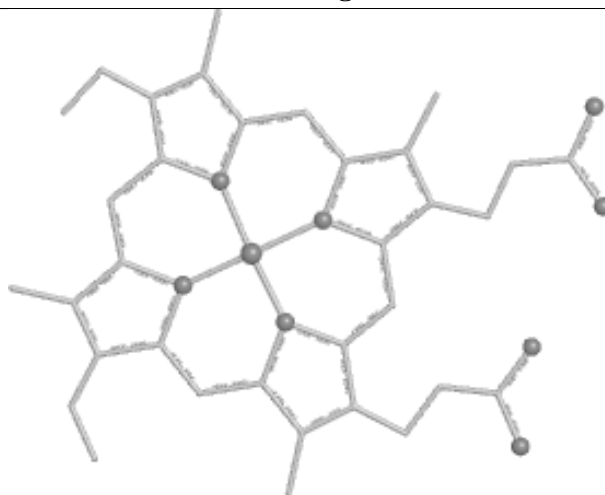
Bond lengths



Bond angles

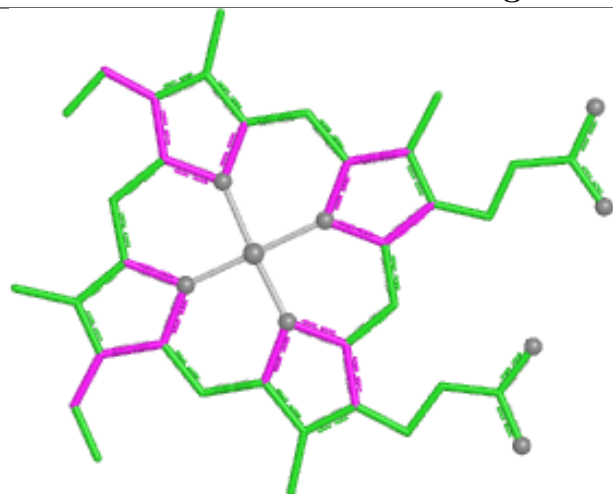


Torsions

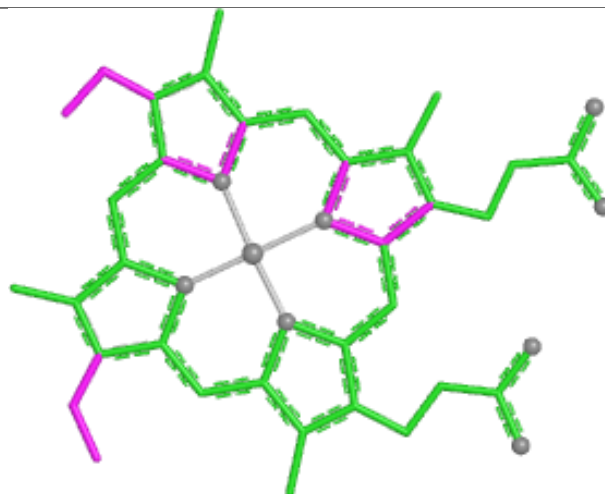


Rings

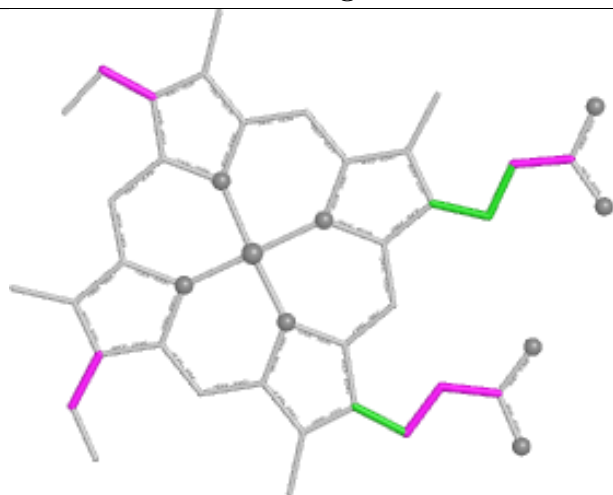
Ligand HEC A 1007



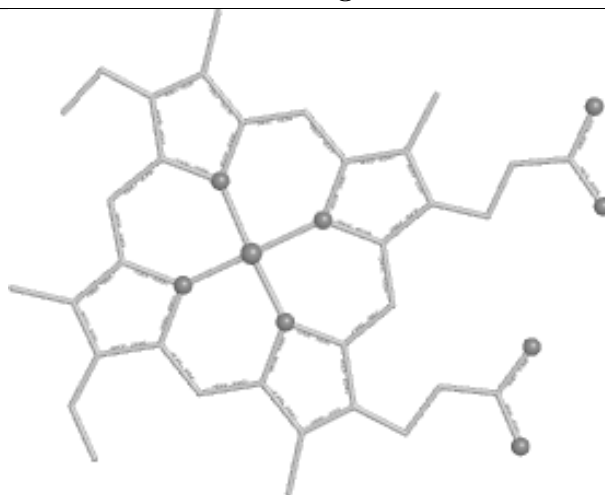
Bond lengths



Bond angles

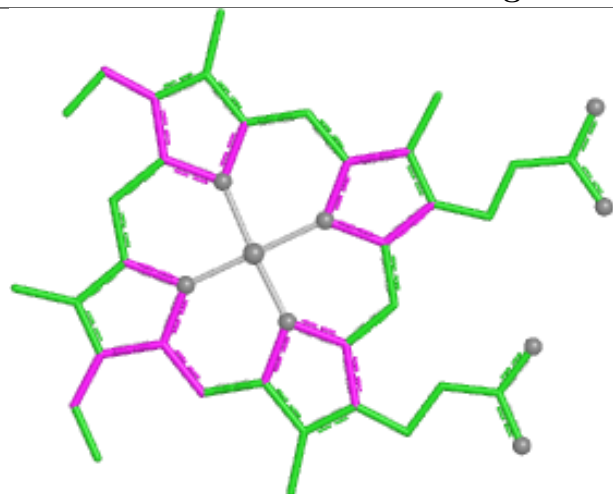


Torsions

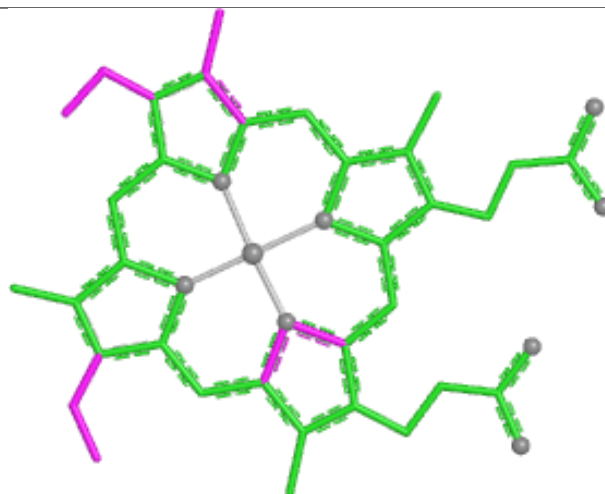


Rings

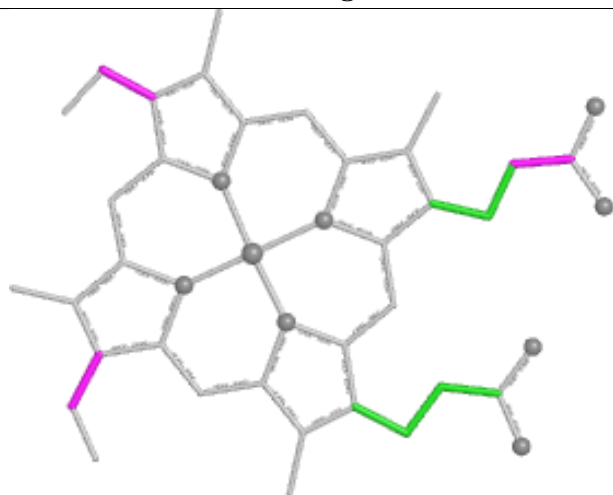
Ligand HEC A 1002



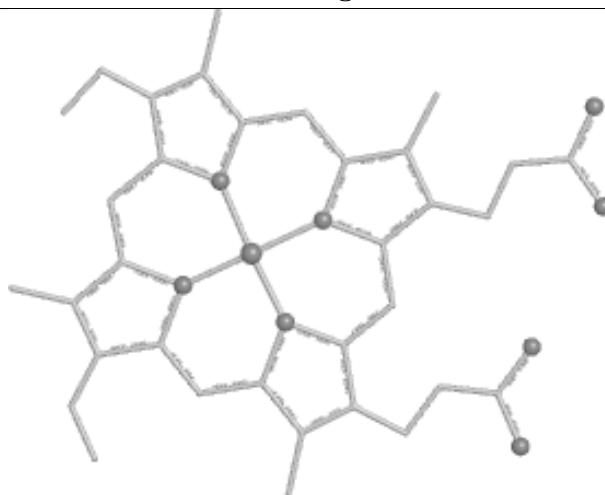
Bond lengths



Bond angles

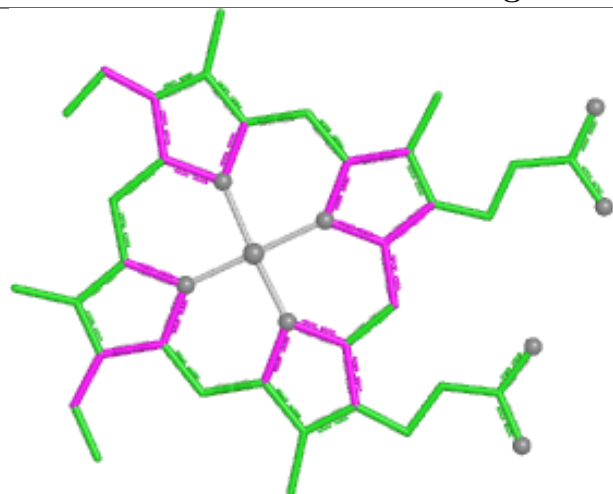


Torsions

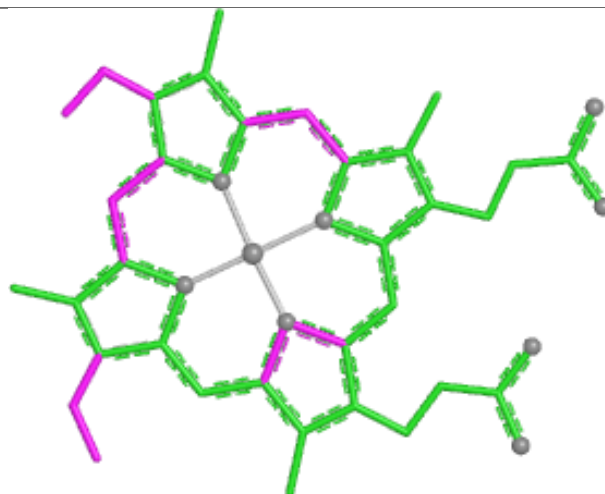


Rings

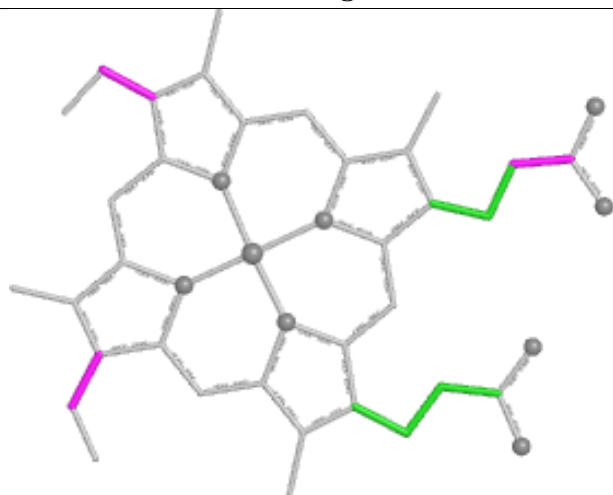
Ligand HEC A 1003



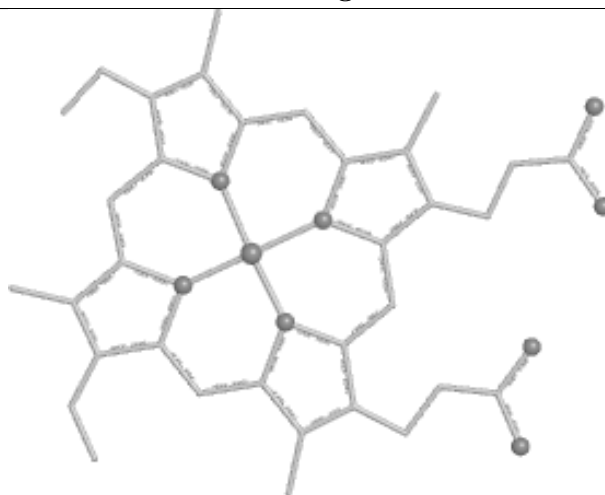
Bond lengths



Bond angles

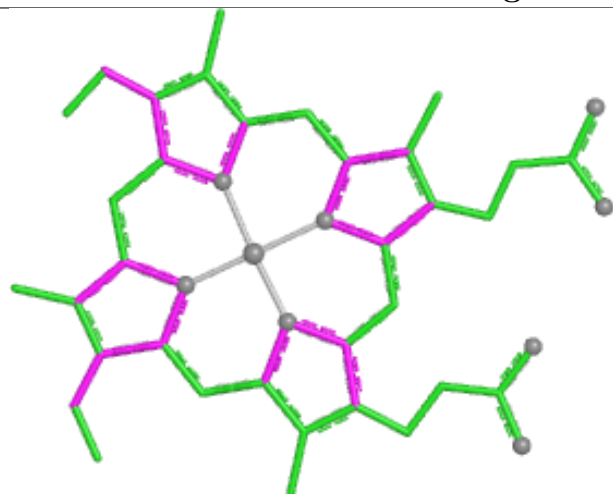


Torsions

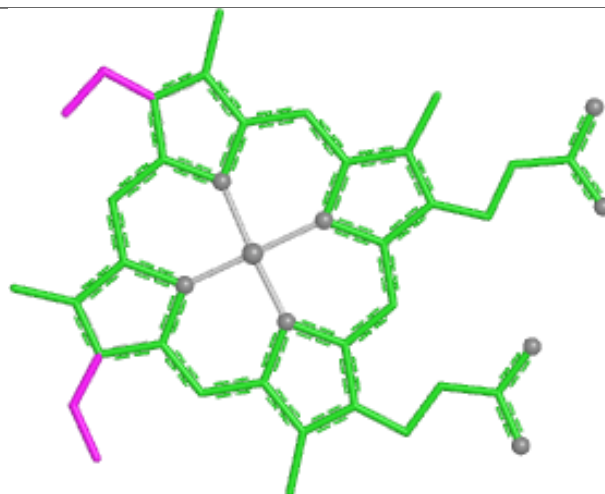


Rings

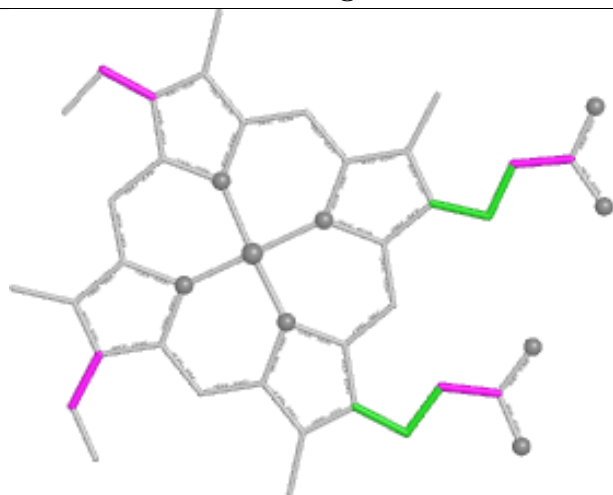
Ligand HEC A 1016



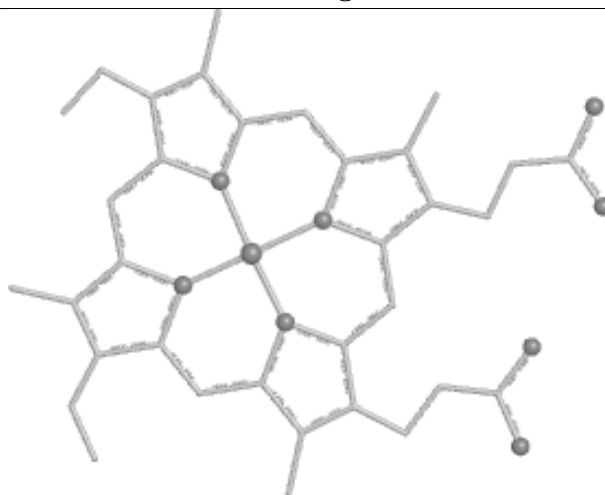
Bond lengths



Bond angles

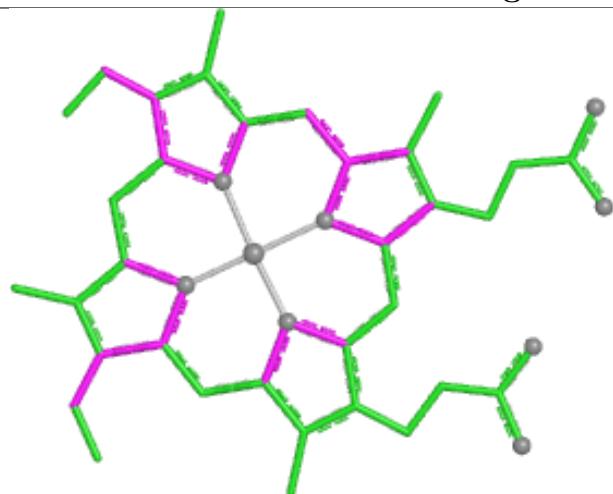


Torsions

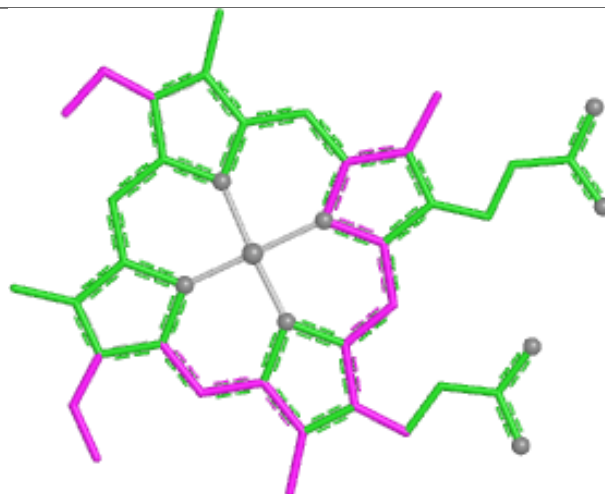


Rings

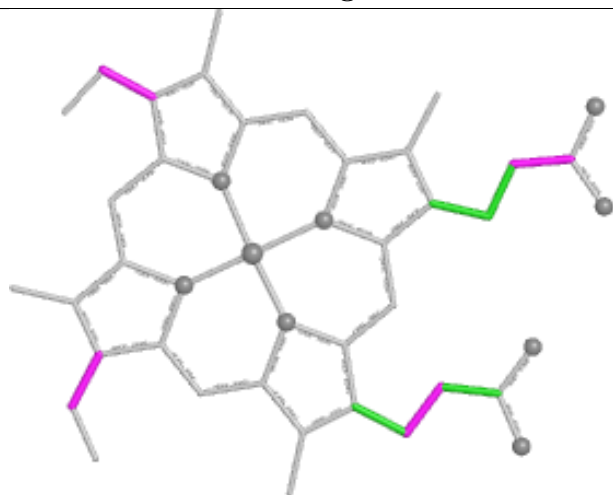
Ligand HEC A 1001



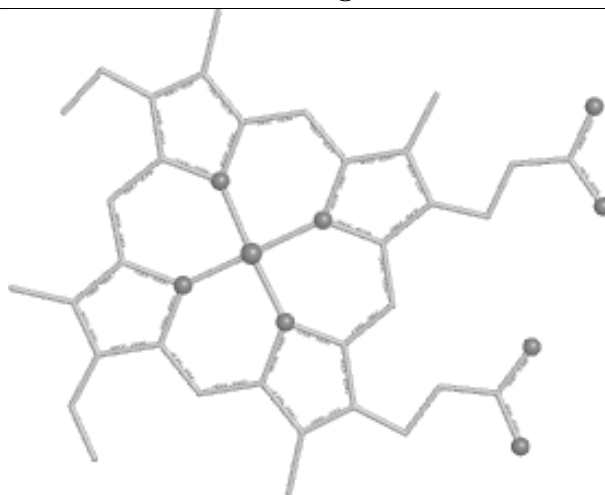
Bond lengths



Bond angles

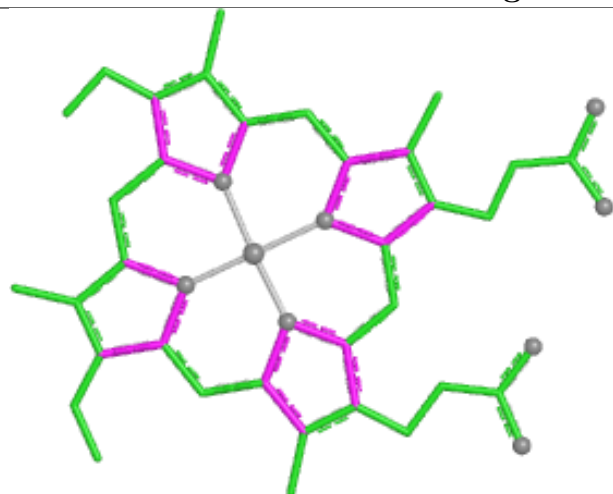


Torsions

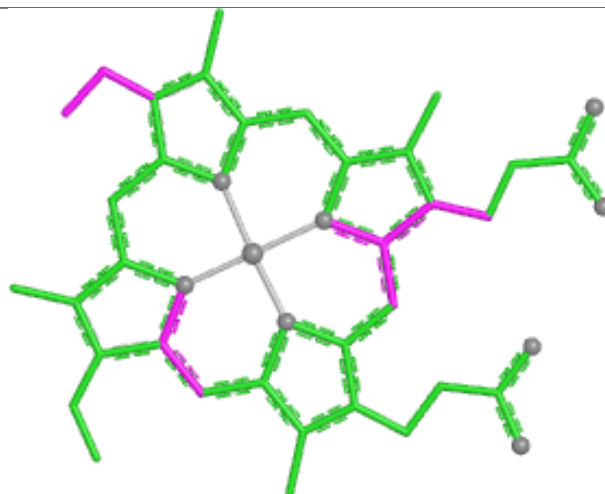


Rings

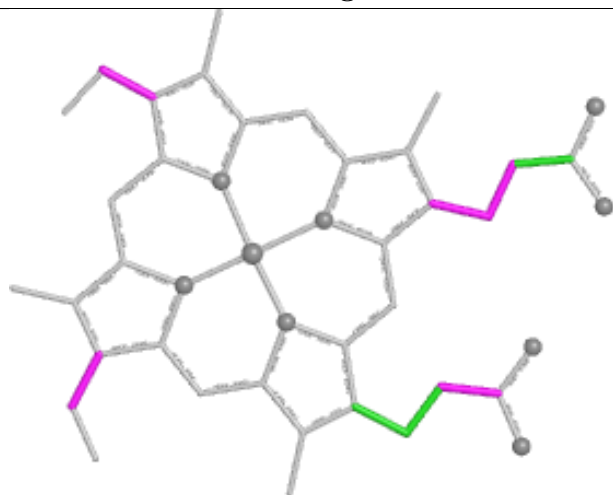
Ligand HEC A 1015



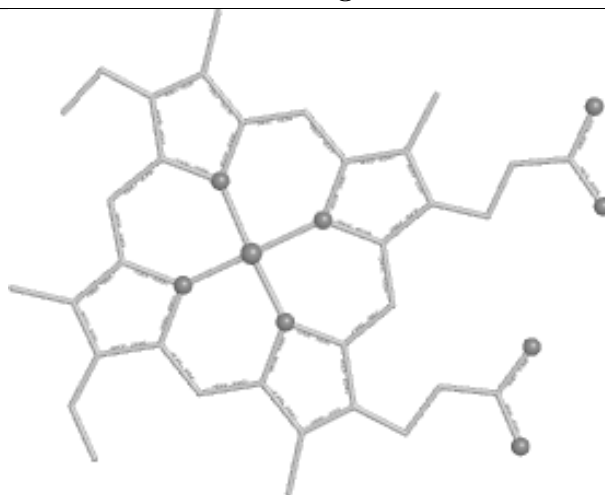
Bond lengths



Bond angles

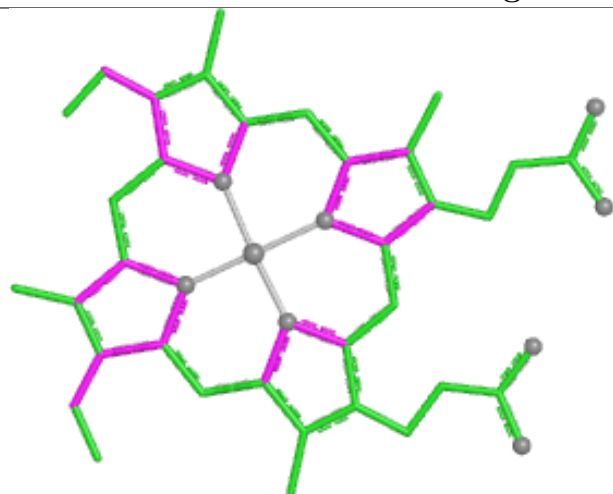


Torsions

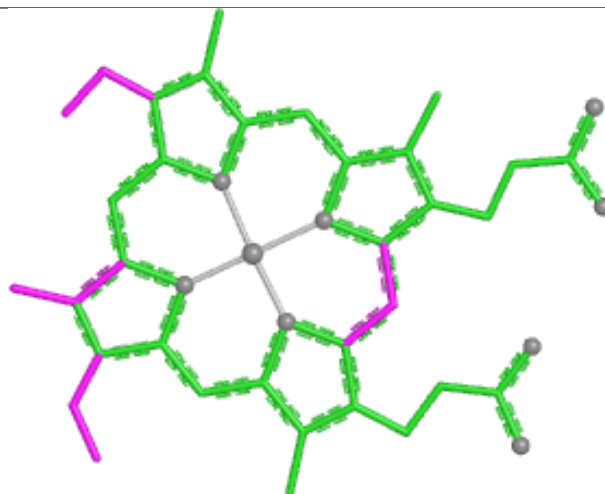


Rings

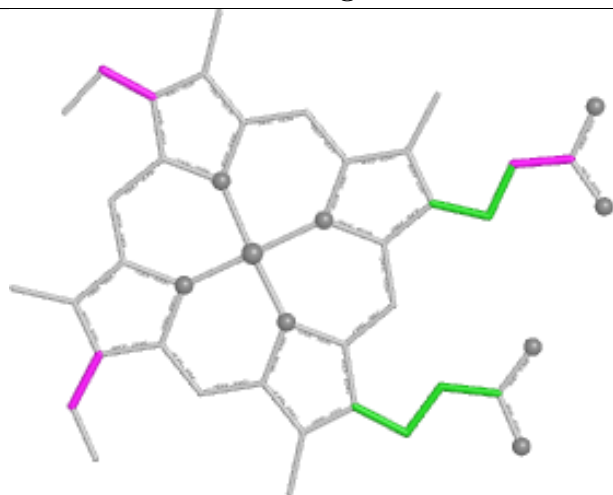
Ligand HEC A 1011



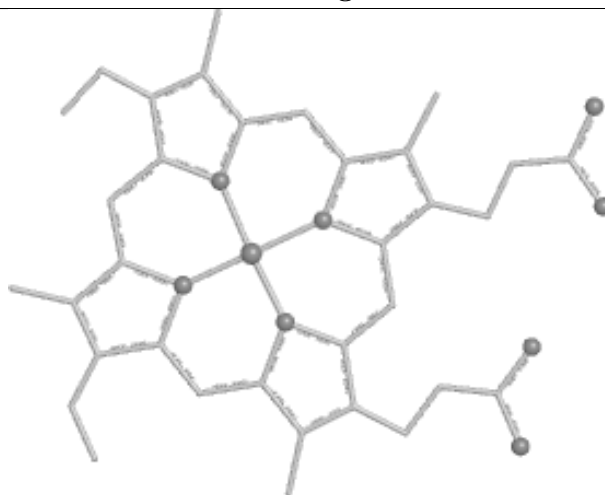
Bond lengths



Bond angles

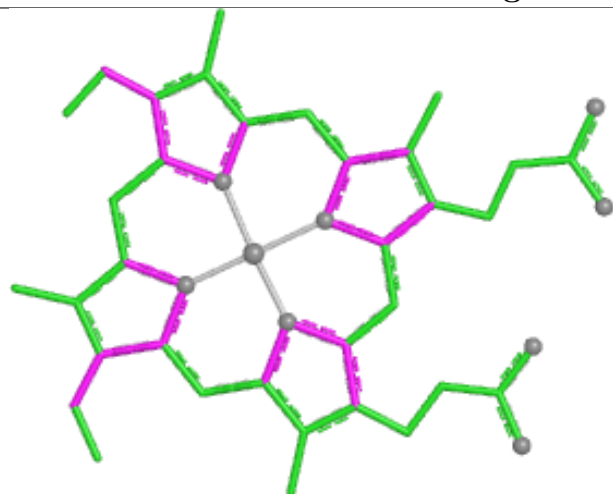


Torsions

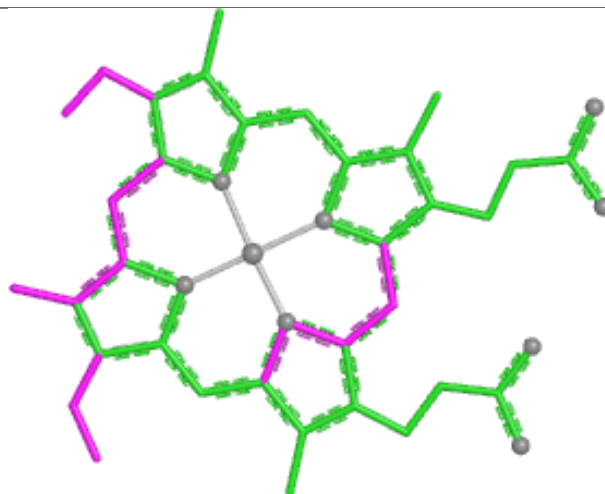


Rings

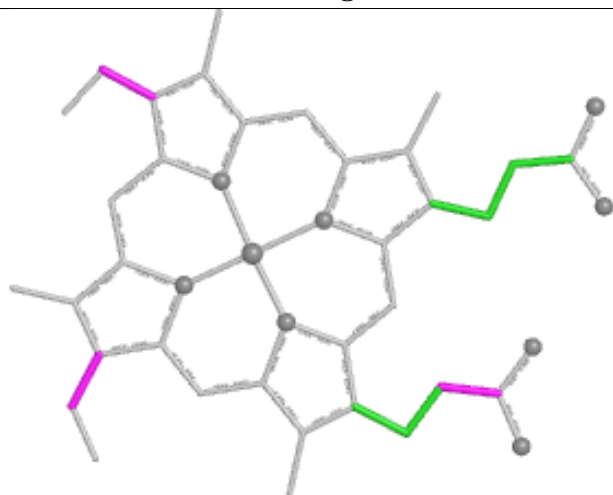
Ligand HEC A 1009



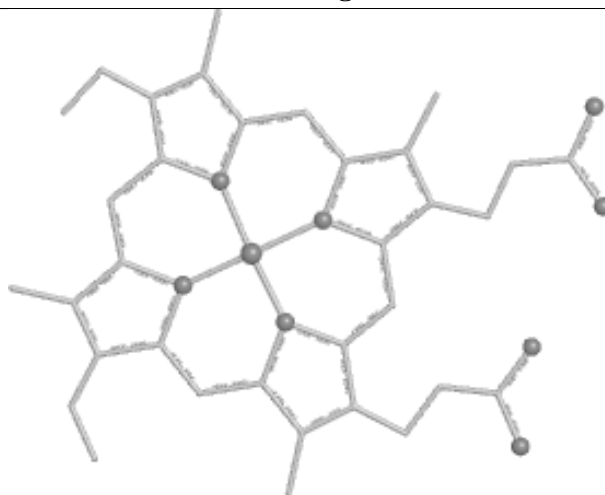
Bond lengths



Bond angles

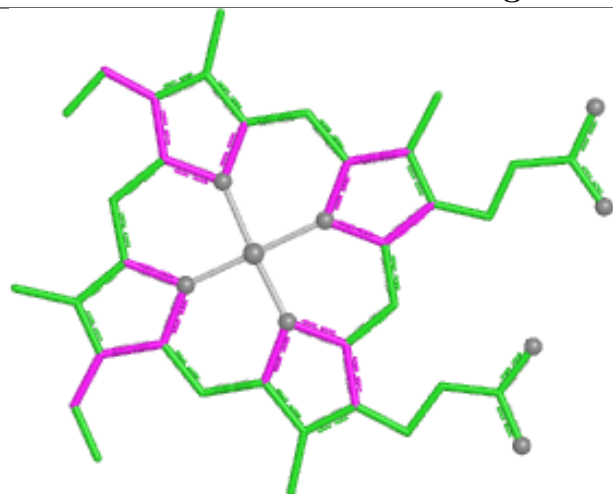


Torsions

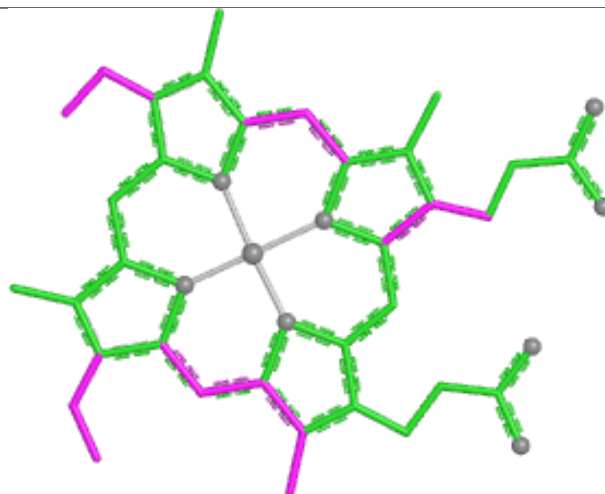


Rings

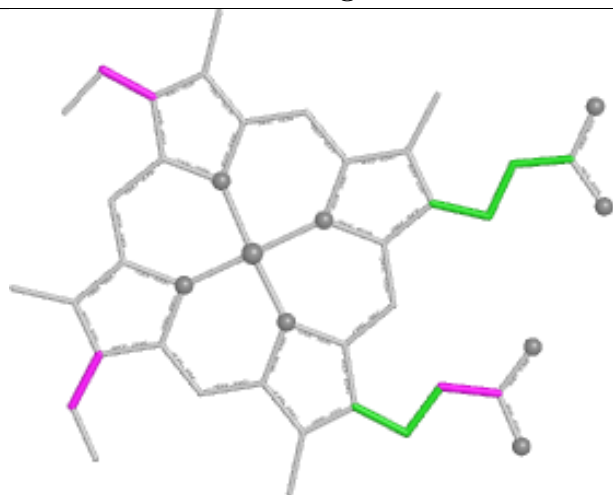
Ligand HEC A 1006



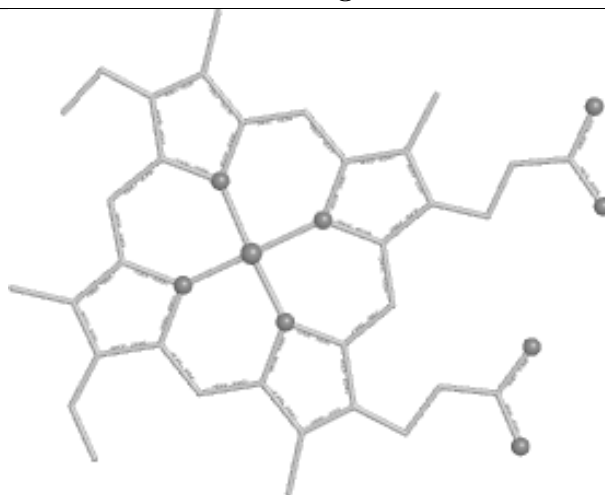
Bond lengths



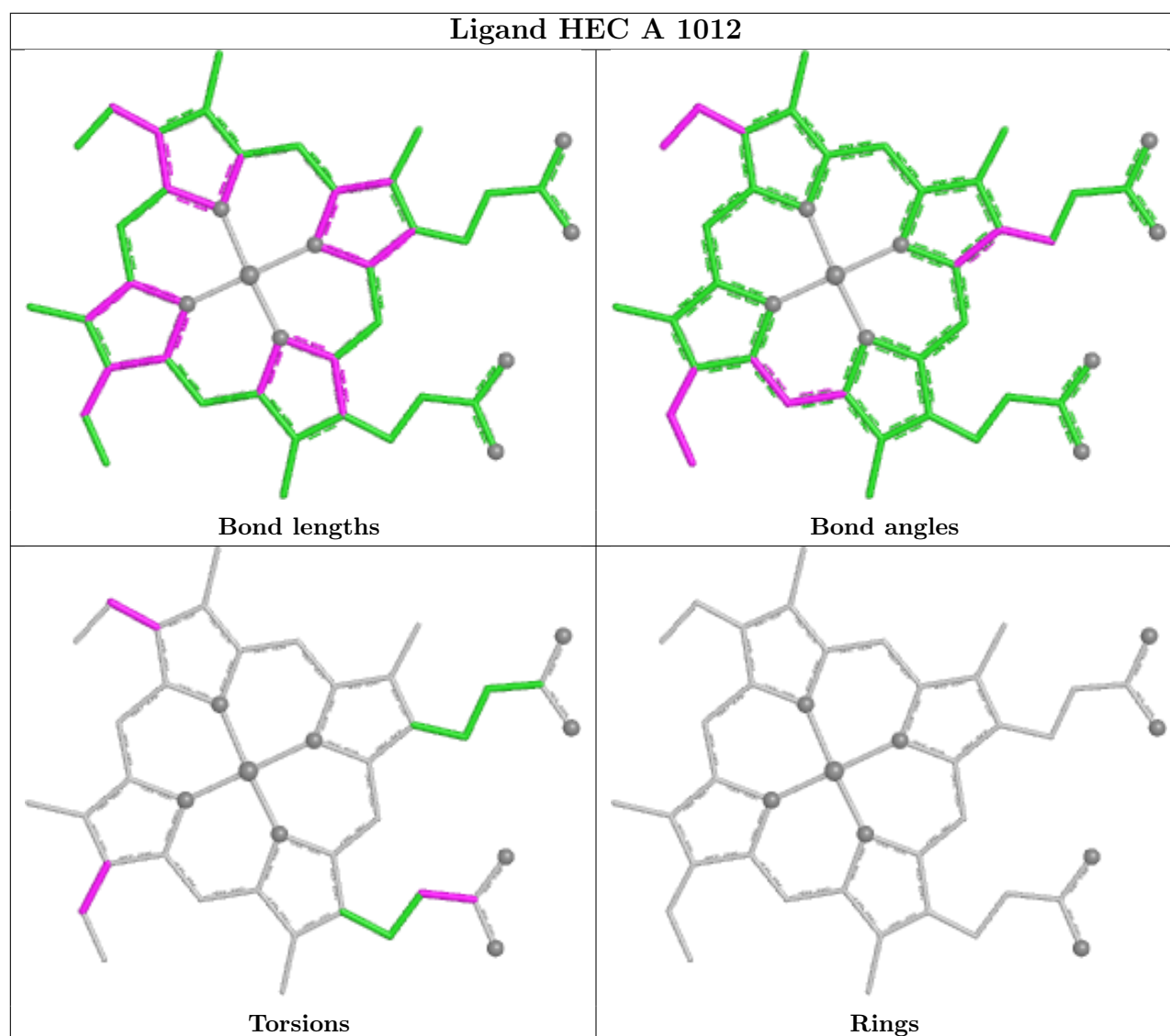
Bond angles



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, 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%)	0.31	29 (5%)	29 27	25, 39, 75, 105	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	ALA	4.8
1	A	144	SER	4.4
1	A	498	GLY	4.4
1	A	500	PRO	4.1
1	A	393	VAL	3.9
1	A	544	ALA	3.4
1	A	397	ALA	2.9
1	A	177	ASN	2.8
1	A	395	ALA	2.8
1	A	284	PRO	2.7
1	A	280	GLY	2.7
1	A	543	ARG	2.7
1	A	89	GLY	2.7
1	A	390	ALA	2.7
1	A	403	ALA	2.7
1	A	143	PRO	2.7
1	A	399	LEU	2.6
1	A	145	ALA	2.6
1	A	287	MET	2.6
1	A	398	LEU	2.6
1	A	286	GLU	2.5
1	A	430	PRO	2.5
1	A	396	GLY	2.5
1	A	211	VAL	2.4
1	A	394	GLU	2.4
1	A	499	LYS	2.4
1	A	426	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	389	ASP	2.2
1	A	545	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

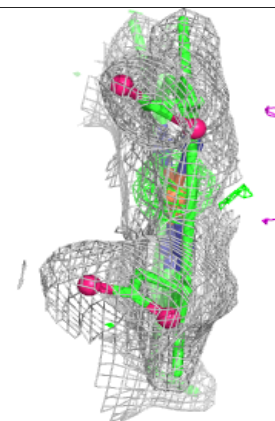
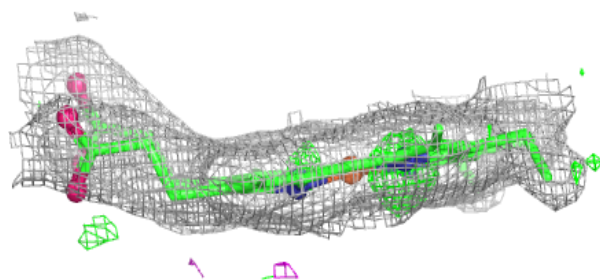
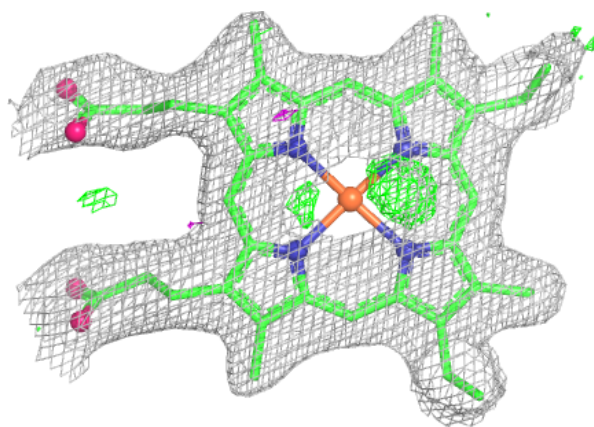
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	A	1013	43/43	0.96	0.10	23,42,64,76	0
2	HEC	A	1014	43/43	0.96	0.09	25,38,59,72	0
2	HEC	A	1010	43/43	0.97	0.09	18,29,59,77	0
2	HEC	A	1011	43/43	0.97	0.08	22,28,38,58	0
2	HEC	A	1015	43/43	0.97	0.09	24,35,76,89	0
2	HEC	A	1016	43/43	0.97	0.08	24,33,44,49	0
2	HEC	A	1007	43/43	0.98	0.07	20,29,43,56	0
2	HEC	A	1008	43/43	0.98	0.07	18,29,41,47	0
2	HEC	A	1009	43/43	0.98	0.08	19,33,50,65	0
2	HEC	A	1001	43/43	0.98	0.06	20,28,37,40	0
2	HEC	A	1002	43/43	0.98	0.07	21,29,40,50	0
2	HEC	A	1012	43/43	0.98	0.06	18,27,36,44	0
2	HEC	A	1003	43/43	0.98	0.06	17,30,37,42	0
2	HEC	A	1004	43/43	0.98	0.06	22,31,41,61	0
2	HEC	A	1005	43/43	0.98	0.06	21,30,50,72	0
2	HEC	A	1006	43/43	0.98	0.06	20,30,44,49	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.

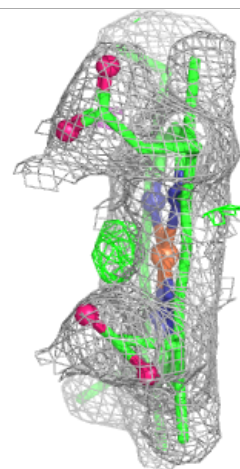
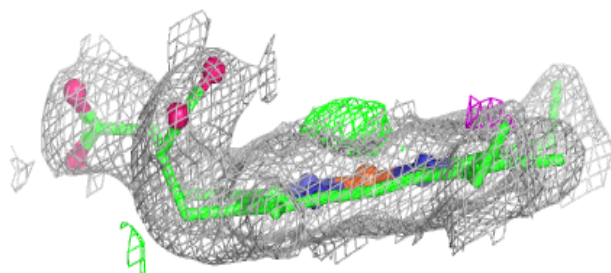
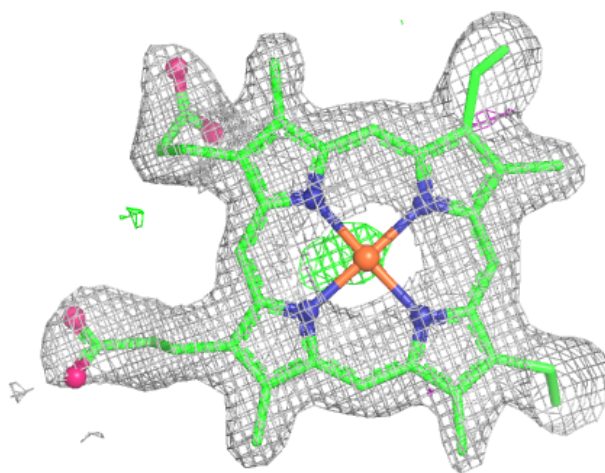
Electron density around HEC A 1013:

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



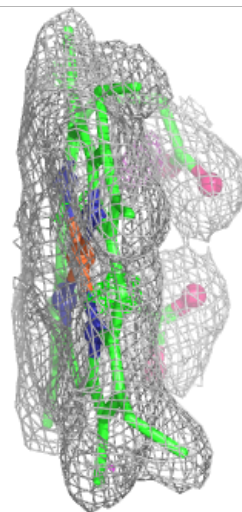
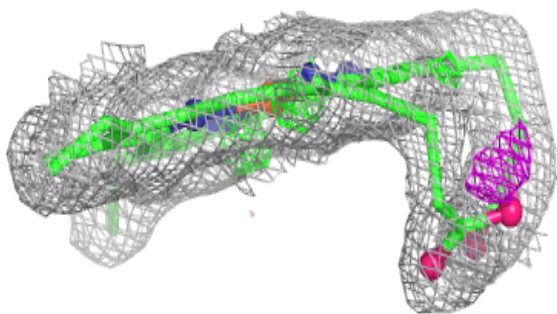
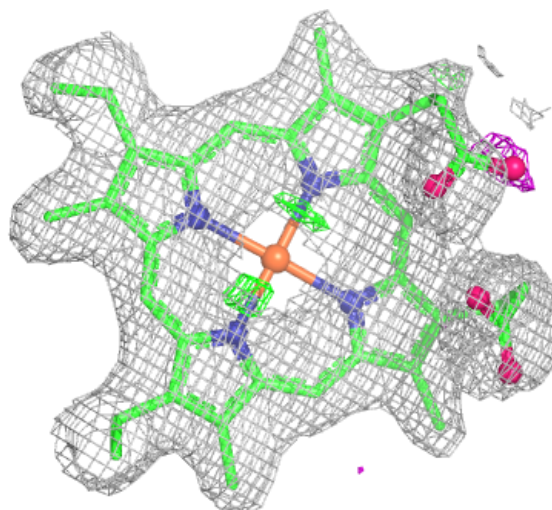
Electron density around HEC A 1014:

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



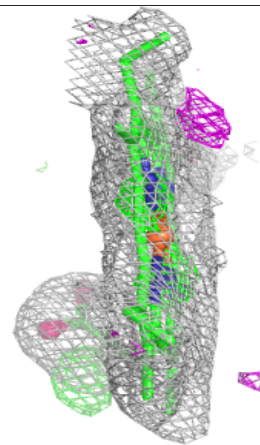
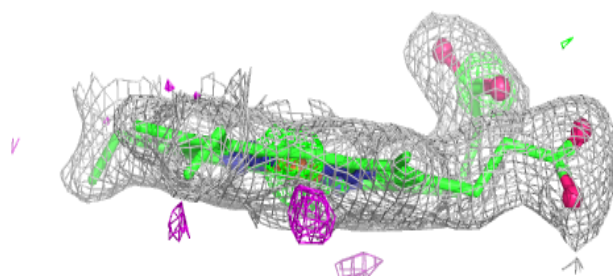
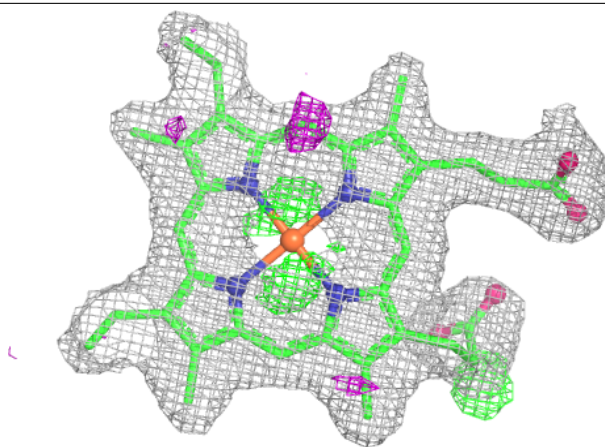
Electron density around HEC A 1010:

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



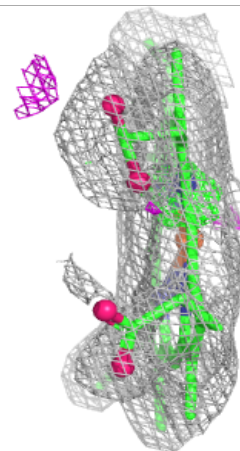
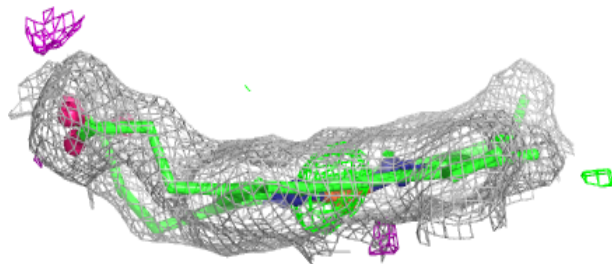
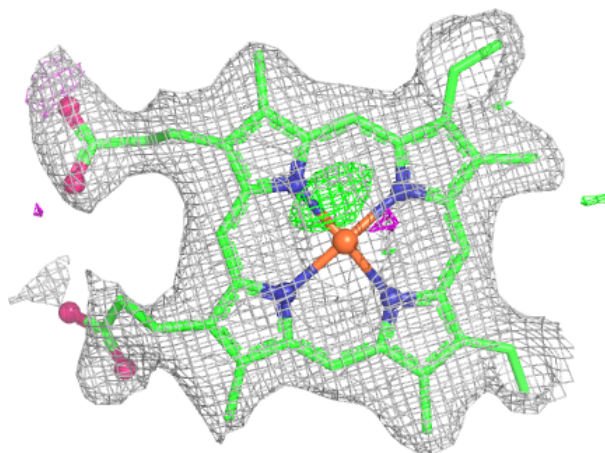
Electron density around HEC A 1011:

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



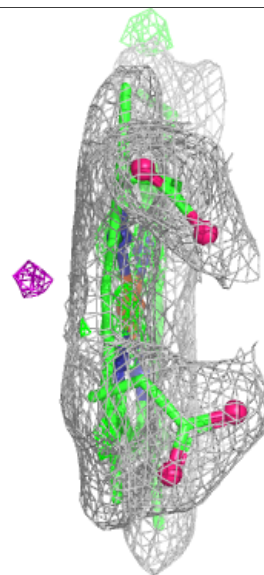
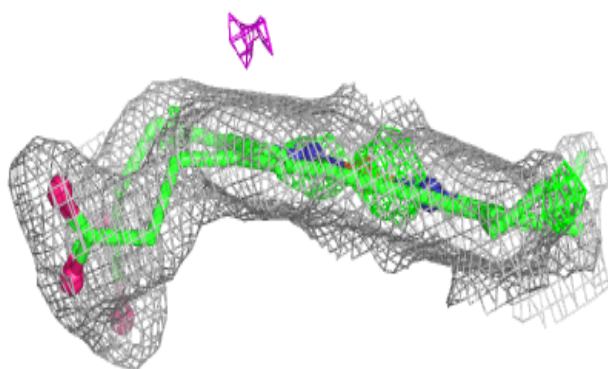
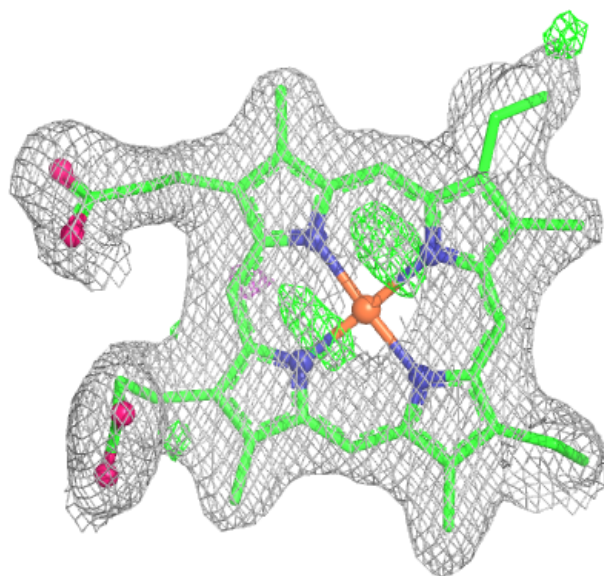
Electron density around HEC A 1015:

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



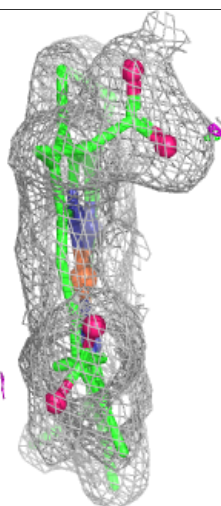
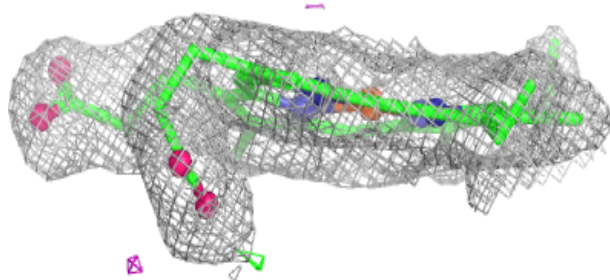
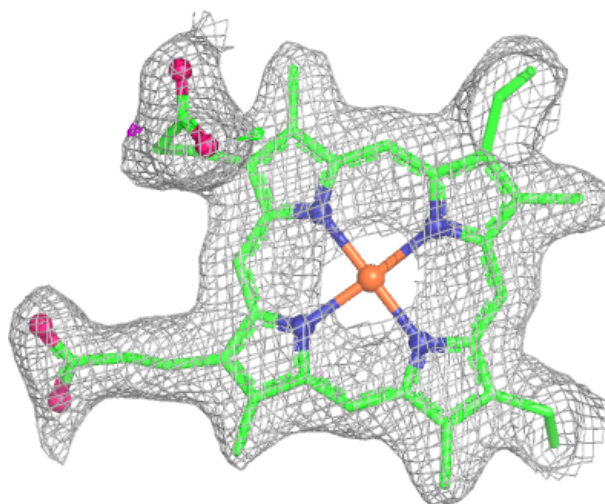
Electron density around HEC A 1016:

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and green (positive)



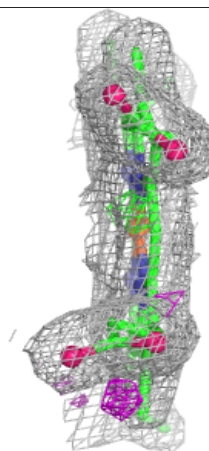
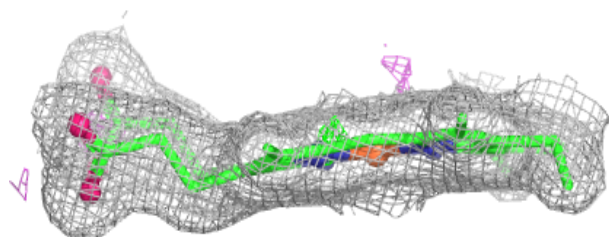
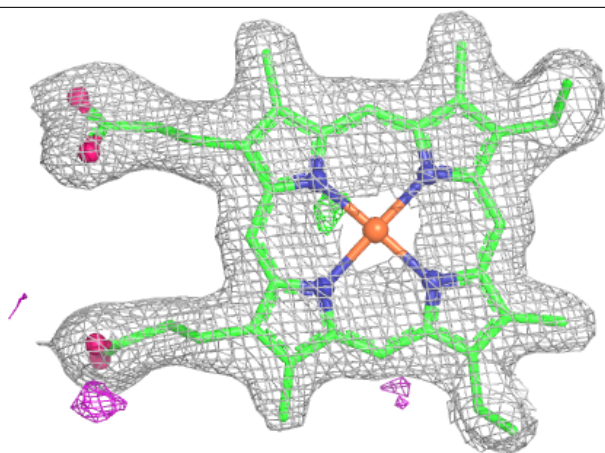
Electron density around HEC A 1007:

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



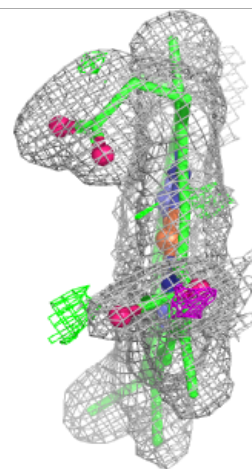
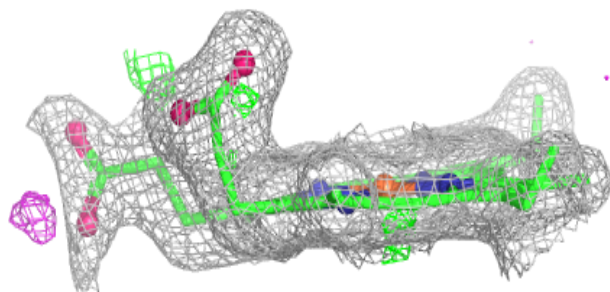
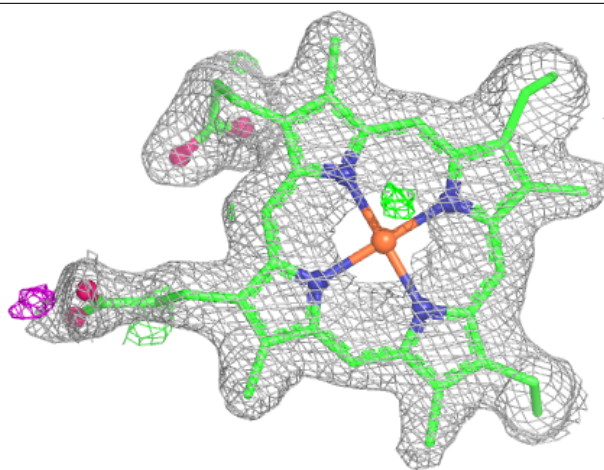
Electron density around HEC A 1008:

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



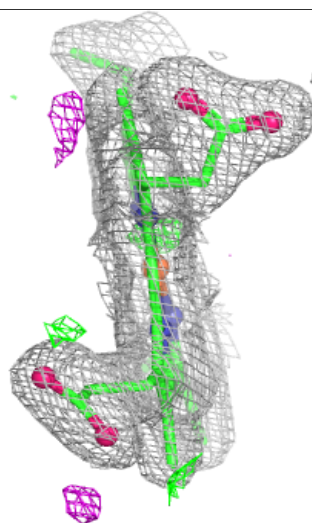
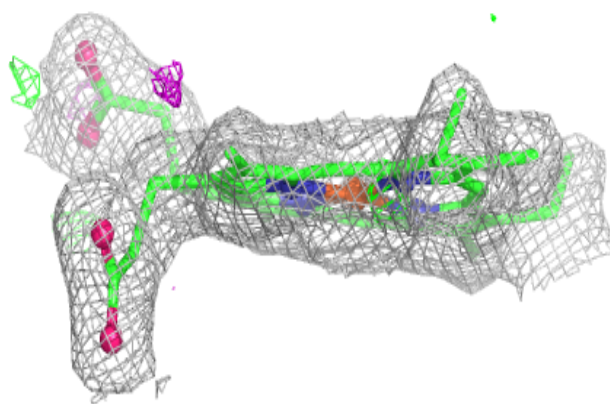
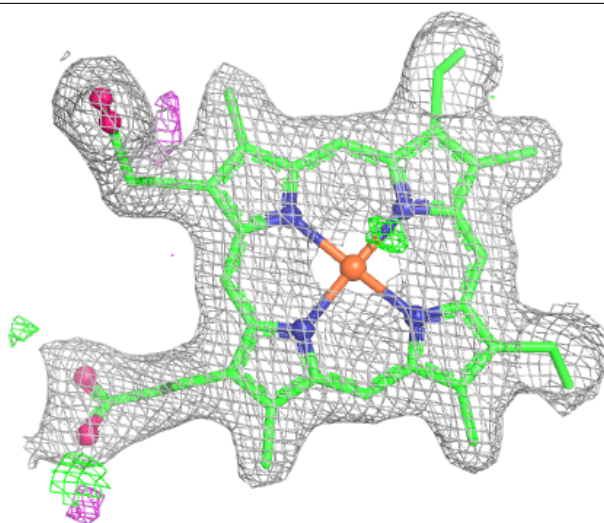
Electron density around HEC A 1009:

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



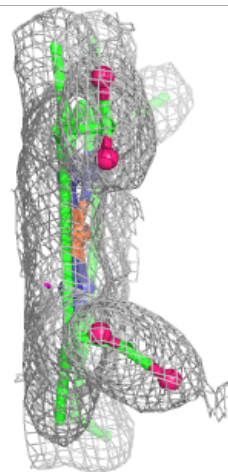
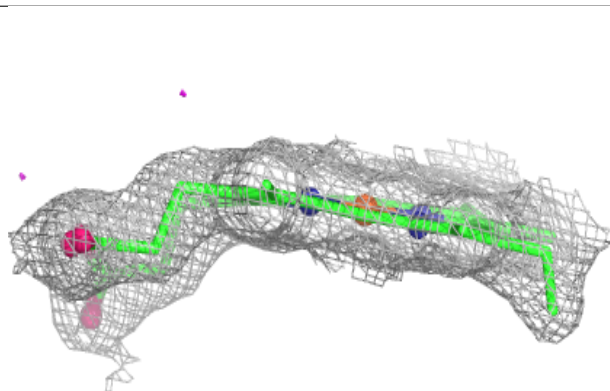
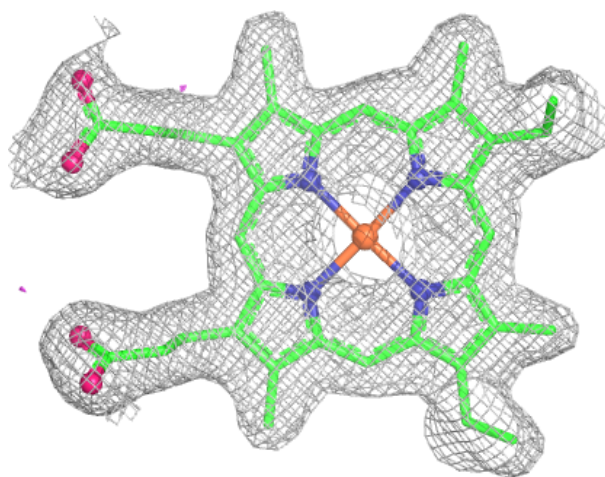
Electron density around HEC A 1001:

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



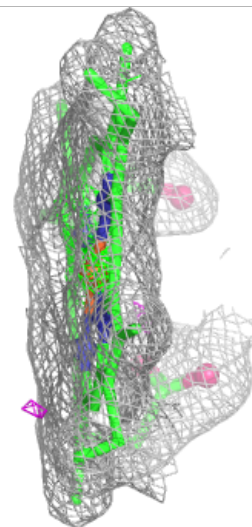
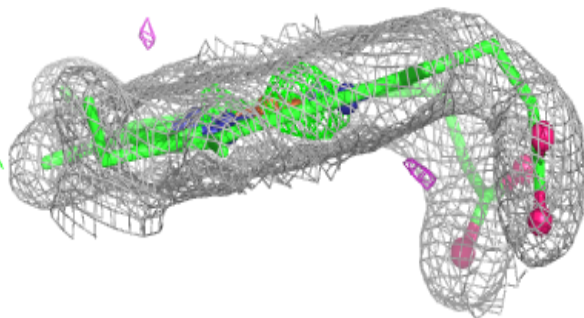
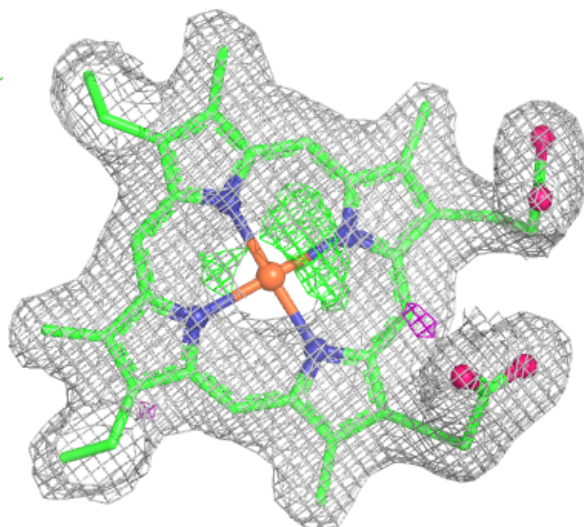
Electron density around HEC A 1002:

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



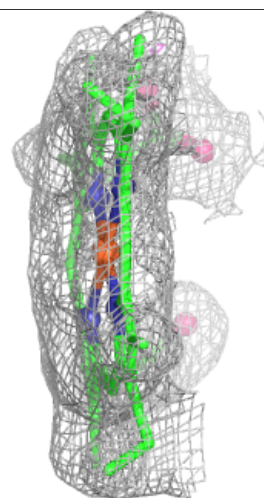
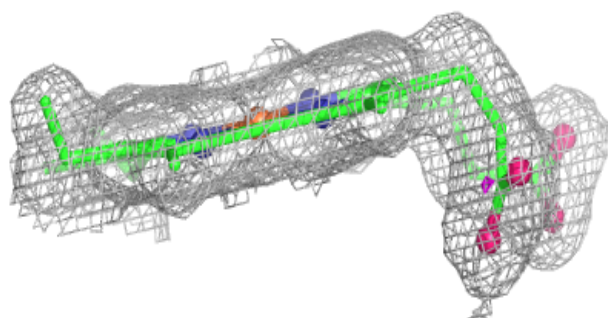
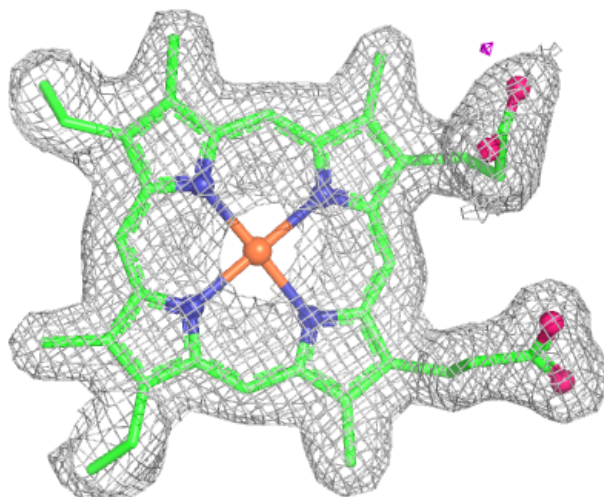
Electron density around HEC A 1012:

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



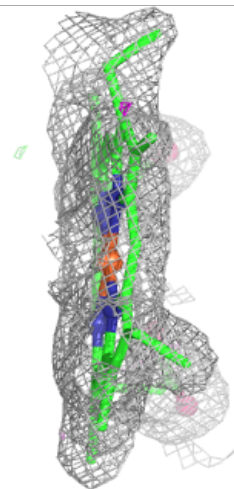
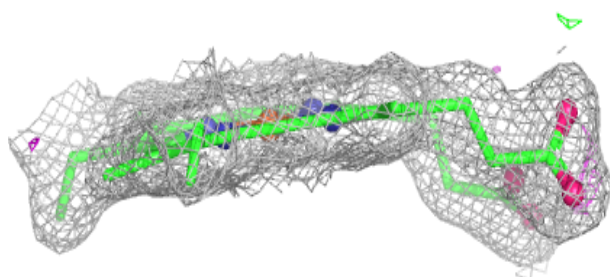
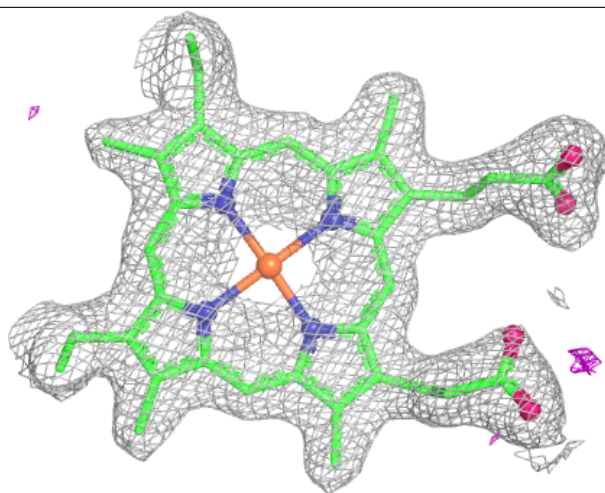
Electron density around HEC A 1003:

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



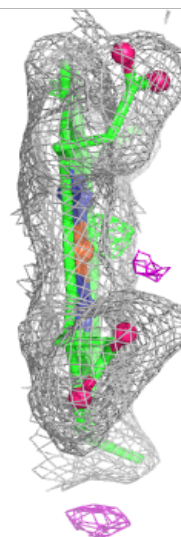
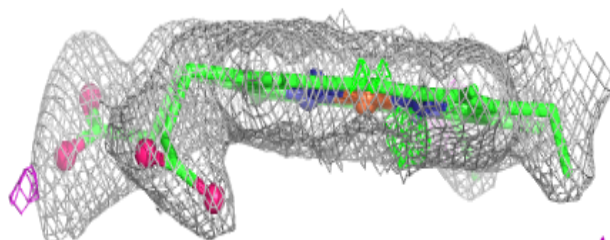
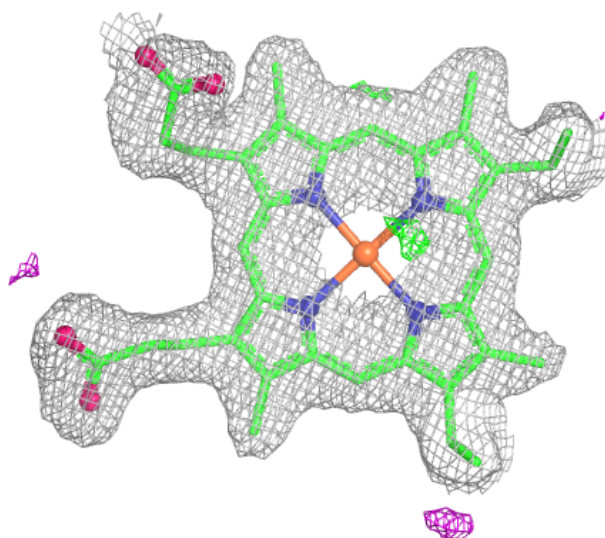
Electron density around HEC A 1004:

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



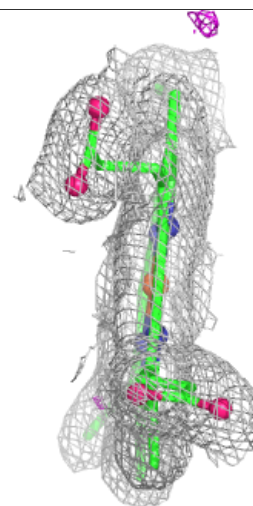
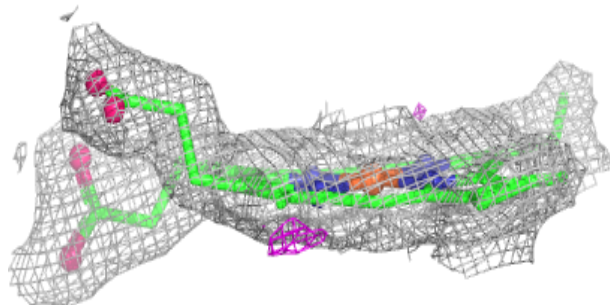
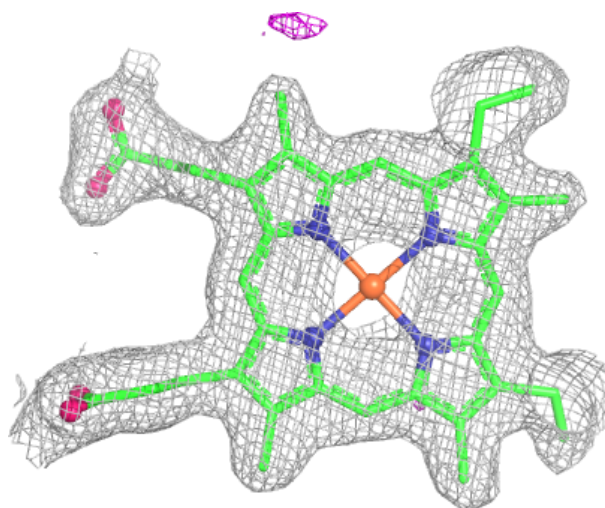
Electron density around HEC A 1005:

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



Electron density around HEC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.