Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 07:26 PM EST

PDB ID	:	2E84
Title	:	Crystal structure of High-Molecular Weight Cytochrome c from Desulfovibrio vulgaris (Miyazaki F) in the presence of zinc ion
Authors	:	Shibata, N.; Suto, K.; Sato, M.; Morimoto, Y.; Kitamura, M.; Higuchi, Y.
Deposited on	:	2007-01-17
Resolution	:	2.70 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

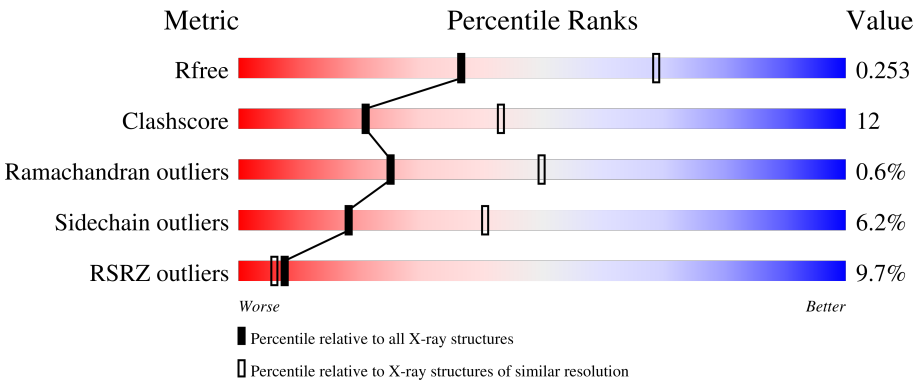
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	556	9% 68% 22% • 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4714 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	513	3813	2337	723	706	47	6	0	0

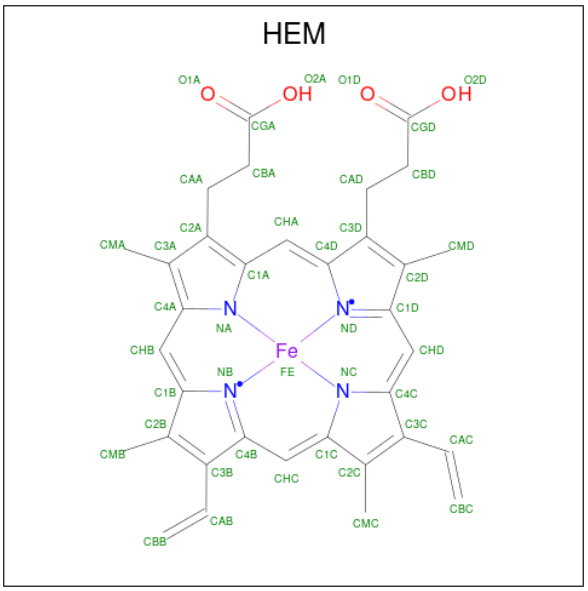
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	4	4	4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	4	4	4	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

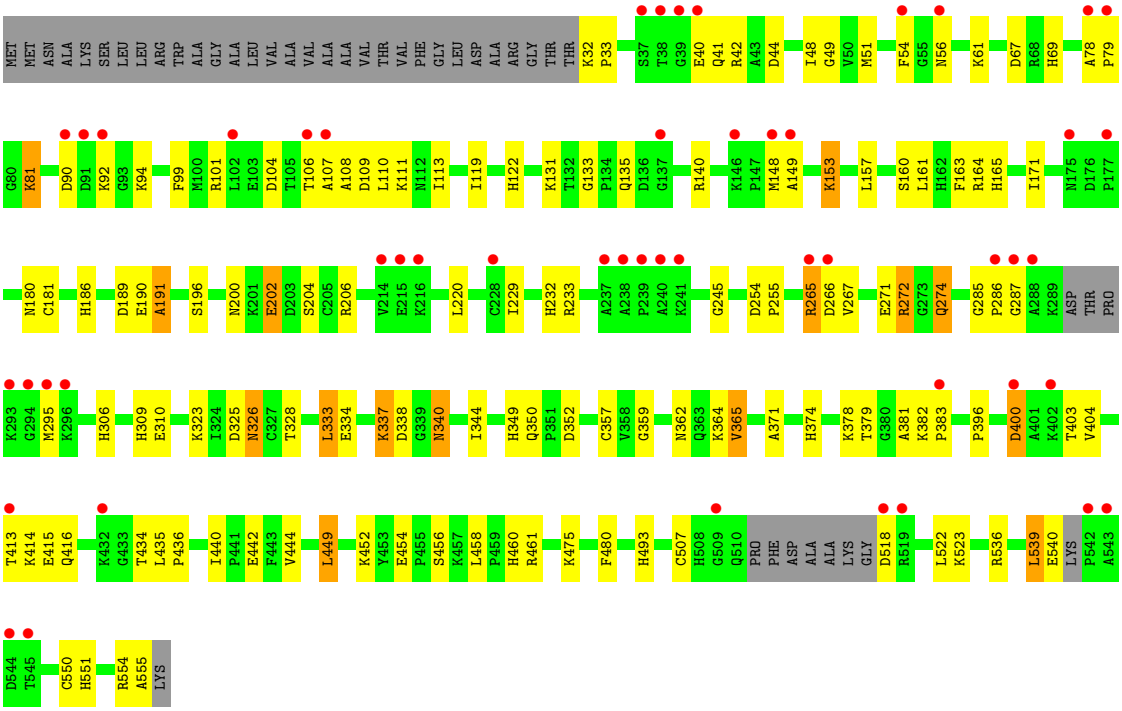
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	205	205	205	0	0

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

Chain A: 9% 68% 22% 8%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.09Å 84.07Å 142.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.20 – 2.70 27.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.20-2.70) 99.6 (27.20-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.259 0.199 , 0.253	Depositor DCC
R_{free} test set	2006 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4714	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, HEM, ZN

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	0/3891	0.49	0/5243

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	3813	0	3751	106	0
2	A	4	0	0	0	0
3	A	4	0	0	0	0
4	A	688	0	480	17	0
5	A	205	0	0	5	0
All	All	4714	0	4231	106	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 (106) 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:413:THR:HG22	1:A:415:GLU:H	1.26	1.01
1:A:79:PRO:HG2	1:A:81:LYS:HB2	1.65	0.78
1:A:229:ILE:O	1:A:233:ARG:HG3	1.87	0.75
1:A:106:THR:HG22	1:A:108:ALA:H	1.50	0.75
1:A:42:ARG:HG3	1:A:148:MET:HE1	1.70	0.74
1:A:507:CYS:O	1:A:518:ASP:HB3	1.87	0.73
1:A:119:ILE:HG13	4:A:1303:HEM:HBC2	1.69	0.72
1:A:41:GLN:HG2	1:A:149:ALA:HB3	1.71	0.71
1:A:165:HIS:HB3	4:A:1304:HEM:HBC2	1.73	0.70
1:A:378:LYS:HG2	1:A:381:ALA:HB3	1.77	0.67
1:A:440:ILE:HG12	4:A:1313:HEM:HBB2	1.78	0.66
1:A:171:ILE:HB	1:A:180:ASN:HD21	1.61	0.65
1:A:454:GLU:HG3	1:A:554:ARG:HE	1.62	0.65
1:A:200:ASN:HA	1:A:202:GLU:OE1	1.97	0.65
1:A:160:SER:O	1:A:164:ARG:HG3	1.99	0.62
1:A:309:HIS:HB3	4:A:1308:HEM:HBC2	1.81	0.62
1:A:48:ILE:HG22	4:A:1303:HEM:HBD1	1.82	0.61
1:A:69:HIS:HB3	4:A:1301:HEM:HBC2	1.82	0.61
1:A:400:ASP:OD2	1:A:400:ASP:N	2.35	0.60
1:A:328:THR:HG22	1:A:344:ILE:HD12	1.85	0.59
1:A:340:ASN:HB2	4:A:1309:HEM:HAD1	1.85	0.59
1:A:337:LYS:HD3	1:A:338:ASP:N	2.17	0.58
1:A:413:THR:HB	1:A:416:GLN:HG3	1.86	0.58
1:A:285:GLY:C	1:A:287:GLY:H	2.07	0.58
1:A:326:ASN:HB2	4:A:1308:HEM:HBD2	1.87	0.56
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.70	0.56
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.20	0.56
1:A:157:LEU:HD22	1:A:161:LEU:HG	1.87	0.56
1:A:272:ARG:O	1:A:272:ARG:HD3	2.04	0.55
1:A:396:PRO:HG2	1:A:404:VAL:HG21	1.87	0.55
1:A:171:ILE:HG22	1:A:180:ASN:OD1	2.06	0.55
1:A:456:SER:HB2	1:A:550:CYS:O	2.06	0.55
1:A:285:GLY:O	1:A:287:GLY:N	2.38	0.54
1:A:49:GLY:HA3	1:A:61:LYS:HD3	1.90	0.54
1:A:449:LEU:HB2	4:A:1316:HEM:O2D	2.08	0.54
1:A:396:PRO:O	5:A:1455:HOH:O	2.18	0.54
1:A:40:GLU:HG2	1:A:148:MET:CE	2.38	0.53
1:A:232:HIS:CE1	1:A:245:GLY:HA3	2.44	0.53
1:A:379:THR:HG23	5:A:1346:HOH:O	2.07	0.53
1:A:371:ALA:O	1:A:536:ARG:HD2	2.09	0.52
1:A:40:GLU:HG2	1:A:148:MET:HE1	1.91	0.52
1:A:51:MET:HE1	1:A:111:LYS:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:OD1	1:A:191:ALA:HB3	2.09	0.52
1:A:265:ARG:HB2	1:A:265:ARG:NH1	2.24	0.52
1:A:206:ARG:NH2	4:A:1307:HEM:O1D	2.42	0.51
1:A:295:MET:HB3	1:A:333:LEU:HD13	1.92	0.51
1:A:265:ARG:HB2	1:A:265:ARG:HH11	1.75	0.51
1:A:163:PHE:HB2	1:A:267:VAL:HG13	1.93	0.51
1:A:32:LYS:HD3	1:A:33:PRO:O	2.11	0.51
1:A:456:SER:CB	1:A:550:CYS:O	2.60	0.50
1:A:365:VAL:HG13	1:A:374:HIS:CB	2.43	0.49
1:A:444:VAL:HG23	1:A:460:HIS:HB2	1.95	0.49
1:A:153:LYS:HD2	1:A:255:PRO:HG3	1.94	0.49
1:A:400:ASP:HB2	1:A:403:THR:OG1	2.12	0.49
1:A:442:GLU:HA	1:A:461:ARG:HB2	1.95	0.49
1:A:374:HIS:HD1	1:A:379:THR:HG1	1.61	0.49
1:A:90:ASP:OD2	1:A:92:LYS:HB2	2.12	0.48
1:A:42:ARG:HG3	1:A:148:MET:CE	2.42	0.48
1:A:109:ASP:O	1:A:113:ILE:HG13	2.13	0.48
1:A:99:PHE:O	1:A:101:ARG:HG2	2.14	0.48
1:A:161:LEU:HD21	4:A:1306:HEM:HMA1	1.95	0.47
1:A:79:PRO:C	1:A:81:LYS:H	2.17	0.47
1:A:254:ASP:OD1	1:A:255:PRO:HD2	2.14	0.47
1:A:539:LEU:CD1	1:A:540:GLU:HG3	2.45	0.47
1:A:554:ARG:O	1:A:555:ALA:HB3	2.15	0.47
1:A:349:HIS:O	1:A:350:GLN:C	2.53	0.47
1:A:357:CYS:HA	4:A:1310:HEM:CHC	2.44	0.47
1:A:449:LEU:HD13	1:A:522:LEU:HD23	1.96	0.47
1:A:458:LEU:O	1:A:460:HIS:N	2.47	0.47
1:A:122:HIS:CE1	1:A:133:GLY:HA3	2.50	0.46
1:A:435:LEU:HB3	1:A:436:PRO:HD2	1.97	0.46
1:A:325:ASP:CG	1:A:326:ASN:H	2.19	0.45
1:A:272:ARG:O	1:A:272:ARG:CD	2.64	0.45
1:A:359:GLY:O	1:A:362:ASN:HB2	2.16	0.45
1:A:206:ARG:NH2	5:A:1333:HOH:O	2.35	0.44
1:A:449:LEU:HD21	1:A:523:LYS:HB2	2.00	0.44
1:A:220:LEU:HB3	5:A:1426:HOH:O	2.18	0.43
1:A:202:GLU:OE1	1:A:272:ARG:HG2	2.18	0.43
1:A:274:GLN:HG2	4:A:1308:HEM:CHB	2.49	0.43
1:A:306:HIS:ND1	1:A:310:GLU:OE2	2.50	0.43
1:A:92:LYS:N	1:A:92:LYS:HD2	2.34	0.43
1:A:364:LYS:HD3	1:A:364:LYS:HA	1.83	0.43
1:A:78:ALA:N	1:A:79:PRO:HD2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:OD1	1:A:94:LYS:N	2.52	0.42
1:A:337:LYS:HE2	1:A:338:ASP:OD1	2.19	0.42
1:A:539:LEU:HD13	1:A:540:GLU:HG3	2.02	0.42
1:A:54:PHE:CB	1:A:107:ALA:HB2	2.49	0.42
1:A:480:PHE:CD2	4:A:1311:HEM:HAA1	2.54	0.42
1:A:54:PHE:HB3	1:A:107:ALA:HB2	2.01	0.42
1:A:382:LYS:HB2	1:A:383:PRO:HD2	2.01	0.42
1:A:413:THR:CG2	1:A:415:GLU:H	2.14	0.42
1:A:181:CYS:HA	4:A:1304:HEM:HHC	2.02	0.42
1:A:285:GLY:C	1:A:287:GLY:N	2.73	0.41
1:A:365:VAL:HG13	1:A:374:HIS:HB3	2.01	0.41
1:A:323:LYS:NZ	5:A:1362:HOH:O	2.50	0.41
1:A:44:ASP:CG	1:A:67:ASP:H	2.17	0.41
1:A:40:GLU:O	1:A:148:MET:HE3	2.20	0.41
1:A:186:HIS:HA	1:A:196:SER:O	2.21	0.41
1:A:232:HIS:NE2	1:A:245:GLY:HA3	2.35	0.41
1:A:378:LYS:CG	1:A:381:ALA:HB3	2.49	0.41
1:A:414:LYS:HD3	1:A:414:LYS:O	2.21	0.41
1:A:365:VAL:HG13	1:A:374:HIS:CG	2.56	0.40
1:A:104:ASP:OD1	1:A:110:LEU:HD21	2.20	0.40
1:A:131:LYS:HD3	4:A:1302:HEM:O2D	2.22	0.40
1:A:181:CYS:HA	4:A:1304:HEM:CHC	2.51	0.40
1:A:434:THR:OG1	1:A:435:LEU:N	2.54	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	505/556 (91%)	459 (91%)	43 (8%)	3 (1%)	25 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ALA
1	A	266	ASP
1	A	286	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	404/434 (93%)	379 (94%)	25 (6%)	18 40

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	81	LYS
1	A	135	GLN
1	A	153	LYS
1	A	190	GLU
1	A	202	GLU
1	A	204	SER
1	A	265	ARG
1	A	271	GLU
1	A	272	ARG
1	A	274	GLN
1	A	326	ASN
1	A	333	LEU
1	A	334	GLU
1	A	337	LYS
1	A	340	ASN
1	A	352	ASP
1	A	365	VAL
1	A	400	ASP
1	A	449	LEU
1	A	452	LYS
1	A	475	LYS
1	A	493	HIS
1	A	539	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	551	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	343	GLN
1	A	465	ASN
1	A	535	ASN

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)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HEM	A	1314	1	41,50,50	1.82	9 (21%)	45,82,82	1.23	6 (13%)
4	HEM	A	1316	1	41,50,50	1.81	9 (21%)	45,82,82	1.33	6 (13%)
4	HEM	A	1313	1	41,50,50	1.79	8 (19%)	45,82,82	1.29	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HEM	A	1308	1	41,50,50	1.71	6 (14%)	45,82,82	1.26	6 (13%)
4	HEM	A	1305	1	41,50,50	1.74	9 (21%)	45,82,82	1.28	6 (13%)
4	HEM	A	1302	1	41,50,50	1.76	8 (19%)	45,82,82	1.30	6 (13%)
4	HEM	A	1303	1	41,50,50	1.77	7 (17%)	45,82,82	1.27	6 (13%)
4	HEM	A	1307	1	41,50,50	1.87	10 (24%)	45,82,82	1.31	6 (13%)
4	HEM	A	1306	1	41,50,50	1.74	7 (17%)	45,82,82	1.31	6 (13%)
4	HEM	A	1312	1	41,50,50	1.80	9 (21%)	45,82,82	1.26	6 (13%)
4	HEM	A	1315	1	41,50,50	1.84	9 (21%)	45,82,82	1.33	7 (15%)
4	HEM	A	1310	1	41,50,50	1.80	9 (21%)	45,82,82	1.31	6 (13%)
4	HEM	A	1301	1	41,50,50	1.80	7 (17%)	45,82,82	1.32	7 (15%)
4	HEM	A	1311	1	41,50,50	1.74	8 (19%)	45,82,82	1.33	6 (13%)
4	HEM	A	1309	1	41,50,50	1.85	8 (19%)	45,82,82	1.38	7 (15%)
4	HEM	A	1304	1	41,50,50	1.74	7 (17%)	45,82,82	1.41	8 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	1314	1	-	8/12/54/54	-
4	HEM	A	1316	1	-	5/12/54/54	-
4	HEM	A	1313	1	-	2/12/54/54	-
4	HEM	A	1308	1	-	4/12/54/54	-
4	HEM	A	1305	1	-	7/12/54/54	-
4	HEM	A	1302	1	-	5/12/54/54	-
4	HEM	A	1303	1	-	7/12/54/54	-
4	HEM	A	1307	1	-	4/12/54/54	-
4	HEM	A	1306	1	-	4/12/54/54	-
4	HEM	A	1312	1	-	4/12/54/54	-
4	HEM	A	1315	1	-	2/12/54/54	-
4	HEM	A	1310	1	-	5/12/54/54	-
4	HEM	A	1301	1	-	5/12/54/54	-
4	HEM	A	1311	1	-	6/12/54/54	-
4	HEM	A	1309	1	-	9/12/54/54	-
4	HEM	A	1304	1	-	4/12/54/54	-

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	HEM	CBB-CAB	4.99	1.55	1.30
4	A	1310	HEM	CBB-CAB	4.98	1.55	1.30
4	A	1303	HEM	CBB-CAB	4.88	1.54	1.30
4	A	1311	HEM	CBB-CAB	4.88	1.54	1.30
4	A	1316	HEM	CBB-CAB	4.88	1.54	1.30
4	A	1313	HEM	CBB-CAB	4.87	1.54	1.30
4	A	1309	HEM	CBB-CAB	4.86	1.54	1.30
4	A	1307	HEM	CBB-CAB	4.83	1.54	1.30
4	A	1308	HEM	CBB-CAB	4.83	1.54	1.30
4	A	1312	HEM	CBB-CAB	4.83	1.54	1.30
4	A	1304	HEM	CBB-CAB	4.81	1.54	1.30
4	A	1305	HEM	CBB-CAB	4.81	1.54	1.30
4	A	1314	HEM	CBB-CAB	4.79	1.54	1.30
4	A	1306	HEM	CBB-CAB	4.78	1.54	1.30
4	A	1302	HEM	CBB-CAB	4.76	1.53	1.30
4	A	1315	HEM	CBB-CAB	4.75	1.53	1.30
4	A	1307	HEM	C3C-C2C	-4.54	1.34	1.40
4	A	1301	HEM	C3C-CAC	4.52	1.57	1.47
4	A	1304	HEM	C3C-CAC	4.48	1.57	1.47
4	A	1312	HEM	C3C-C2C	-4.46	1.34	1.40
4	A	1314	HEM	C3C-C2C	-4.41	1.34	1.40
4	A	1309	HEM	C3C-CAC	4.37	1.56	1.47
4	A	1313	HEM	C3C-C2C	-4.35	1.34	1.40
4	A	1315	HEM	C3C-CAC	4.25	1.56	1.47
4	A	1307	HEM	C3C-CAC	4.18	1.56	1.47
4	A	1305	HEM	C3C-C2C	-4.10	1.34	1.40
4	A	1306	HEM	C3C-CAC	4.02	1.56	1.47
4	A	1311	HEM	C3C-CAC	4.01	1.56	1.47
4	A	1308	HEM	C3C-CAC	4.01	1.56	1.47
4	A	1309	HEM	CAA-C2A	4.00	1.57	1.52
4	A	1316	HEM	C3C-CAC	3.99	1.56	1.47
4	A	1311	HEM	C3C-C2C	-3.96	1.34	1.40
4	A	1303	HEM	C3C-CAC	3.96	1.55	1.47
4	A	1310	HEM	C3C-CAC	3.95	1.55	1.47
4	A	1302	HEM	C3C-CAC	3.89	1.55	1.47
4	A	1308	HEM	C3C-C2C	-3.87	1.35	1.40
4	A	1309	HEM	C3C-C2C	-3.87	1.35	1.40
4	A	1302	HEM	CBC-CAC	3.85	1.54	1.29
4	A	1312	HEM	C3C-CAC	3.85	1.55	1.47
4	A	1310	HEM	CBC-CAC	3.83	1.54	1.29
4	A	1306	HEM	CBC-CAC	3.83	1.54	1.29
4	A	1314	HEM	C3C-CAC	3.81	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1312	HEM	CBC-CAC	3.80	1.54	1.29
4	A	1316	HEM	CBC-CAC	3.79	1.54	1.29
4	A	1308	HEM	CBC-CAC	3.78	1.54	1.29
4	A	1306	HEM	C3C-C2C	-3.78	1.35	1.40
4	A	1313	HEM	CBC-CAC	3.77	1.54	1.29
4	A	1301	HEM	C3C-C2C	-3.76	1.35	1.40
4	A	1303	HEM	CBC-CAC	3.76	1.54	1.29
4	A	1301	HEM	CBC-CAC	3.74	1.54	1.29
4	A	1307	HEM	CBC-CAC	3.72	1.54	1.29
4	A	1309	HEM	CBC-CAC	3.72	1.54	1.29
4	A	1315	HEM	CBC-CAC	3.72	1.54	1.29
4	A	1311	HEM	CBC-CAC	3.71	1.53	1.29
4	A	1305	HEM	CBC-CAC	3.67	1.53	1.29
4	A	1316	HEM	C3C-C2C	-3.66	1.35	1.40
4	A	1314	HEM	CBC-CAC	3.66	1.53	1.29
4	A	1304	HEM	CBC-CAC	3.62	1.53	1.29
4	A	1305	HEM	C3C-CAC	3.58	1.55	1.47
4	A	1310	HEM	C3C-C2C	-3.54	1.35	1.40
4	A	1315	HEM	C3C-C2C	-3.52	1.35	1.40
4	A	1307	HEM	CAA-C2A	3.40	1.57	1.52
4	A	1303	HEM	C3C-C2C	-3.34	1.35	1.40
4	A	1304	HEM	C3C-C2C	-3.31	1.35	1.40
4	A	1302	HEM	C3C-C2C	-3.25	1.35	1.40
4	A	1313	HEM	C3C-CAC	3.18	1.54	1.47
4	A	1316	HEM	CAA-C2A	3.13	1.56	1.52
4	A	1314	HEM	CAA-C2A	2.88	1.56	1.52
4	A	1304	HEM	C2C-C1C	2.86	1.49	1.42
4	A	1303	HEM	CAA-C2A	2.85	1.56	1.52
4	A	1313	HEM	CAA-C2A	2.76	1.56	1.52
4	A	1315	HEM	C2C-C1C	2.75	1.48	1.42
4	A	1301	HEM	C2C-C1C	2.62	1.48	1.42
4	A	1315	HEM	CAA-C2A	2.60	1.55	1.52
4	A	1313	HEM	CAB-C3B	2.60	1.54	1.47
4	A	1311	HEM	CAB-C3B	2.60	1.54	1.47
4	A	1307	HEM	C2C-C1C	2.60	1.48	1.42
4	A	1301	HEM	CAB-C3B	2.52	1.54	1.47
4	A	1312	HEM	CAB-C3B	2.48	1.54	1.47
4	A	1310	HEM	C2C-C1C	2.48	1.48	1.42
4	A	1309	HEM	CAB-C3B	2.48	1.54	1.47
4	A	1312	HEM	CAA-C2A	2.46	1.55	1.52
4	A	1308	HEM	CAB-C3B	2.45	1.54	1.47
4	A	1314	HEM	CAB-C3B	2.43	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1314	HEM	C2C-C1C	2.41	1.48	1.42
4	A	1301	HEM	O2A-CGA	-2.40	1.22	1.30
4	A	1316	HEM	CAB-C3B	2.36	1.53	1.47
4	A	1310	HEM	CAA-C2A	2.36	1.55	1.52
4	A	1307	HEM	CBA-CGA	2.35	1.56	1.50
4	A	1303	HEM	CAB-C3B	2.34	1.53	1.47
4	A	1303	HEM	C2C-C1C	2.33	1.47	1.42
4	A	1306	HEM	C2C-C1C	2.33	1.47	1.42
4	A	1308	HEM	C2C-C1C	2.33	1.47	1.42
4	A	1305	HEM	C2C-C1C	2.33	1.47	1.42
4	A	1305	HEM	CAB-C3B	2.32	1.53	1.47
4	A	1309	HEM	C2C-C1C	2.29	1.47	1.42
4	A	1312	HEM	C2C-C1C	2.29	1.47	1.42
4	A	1302	HEM	O1A-CGA	2.28	1.29	1.22
4	A	1302	HEM	CAA-C2A	2.28	1.55	1.52
4	A	1302	HEM	C2C-C1C	2.24	1.47	1.42
4	A	1316	HEM	CMD-C2D	2.23	1.55	1.50
4	A	1310	HEM	O2A-CGA	-2.23	1.23	1.30
4	A	1316	HEM	C2C-C1C	2.22	1.47	1.42
4	A	1307	HEM	O1A-CGA	2.20	1.29	1.22
4	A	1313	HEM	C2C-C1C	2.19	1.47	1.42
4	A	1304	HEM	CAB-C3B	2.18	1.53	1.47
4	A	1311	HEM	C2C-C1C	2.17	1.47	1.42
4	A	1310	HEM	CMC-C2C	2.17	1.56	1.51
4	A	1307	HEM	O2A-CGA	-2.16	1.23	1.30
4	A	1313	HEM	O1A-CGA	2.15	1.29	1.22
4	A	1315	HEM	CMD-C2D	2.15	1.55	1.50
4	A	1312	HEM	O2A-CGA	-2.14	1.23	1.30
4	A	1310	HEM	CMD-C2D	2.10	1.55	1.50
4	A	1314	HEM	O1A-CGA	2.09	1.29	1.22
4	A	1307	HEM	CMD-C2D	2.09	1.55	1.50
4	A	1312	HEM	CMD-C2D	2.07	1.55	1.50
4	A	1305	HEM	O2A-CGA	-2.07	1.23	1.30
4	A	1309	HEM	O2A-CGA	-2.07	1.23	1.30
4	A	1311	HEM	CMD-C2D	2.06	1.55	1.50
4	A	1315	HEM	O1A-CGA	2.04	1.28	1.22
4	A	1304	HEM	CMC-C2C	2.04	1.56	1.51
4	A	1314	HEM	O2A-CGA	-2.04	1.23	1.30
4	A	1311	HEM	O2A-CGA	-2.04	1.23	1.30
4	A	1305	HEM	O1A-CGA	2.03	1.28	1.22
4	A	1315	HEM	CMC-C2C	2.02	1.56	1.51
4	A	1316	HEM	O2A-CGA	-2.02	1.24	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1305	HEM	CMD-C2D	2.01	1.55	1.50
4	A	1302	HEM	O2A-CGA	-2.01	1.24	1.30
4	A	1306	HEM	CMC-C2C	2.01	1.56	1.51
4	A	1306	HEM	O1A-CGA	2.01	1.28	1.22

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1313	HEM	C4C-CHD-C1D	4.23	128.14	122.56
4	A	1311	HEM	C4C-CHD-C1D	4.22	128.12	122.56
4	A	1301	HEM	C4C-CHD-C1D	4.20	128.10	122.56
4	A	1309	HEM	C4C-CHD-C1D	4.12	128.00	122.56
4	A	1312	HEM	C4C-CHD-C1D	4.09	127.95	122.56
4	A	1306	HEM	C4C-CHD-C1D	4.08	127.94	122.56
4	A	1303	HEM	C4C-CHD-C1D	4.07	127.93	122.56
4	A	1305	HEM	C4C-CHD-C1D	4.04	127.89	122.56
4	A	1314	HEM	C4C-CHD-C1D	4.01	127.85	122.56
4	A	1315	HEM	C4C-CHD-C1D	4.00	127.83	122.56
4	A	1310	HEM	C4C-CHD-C1D	3.99	127.83	122.56
4	A	1304	HEM	C4C-CHD-C1D	3.96	127.78	122.56
4	A	1308	HEM	C4C-CHD-C1D	3.94	127.75	122.56
4	A	1302	HEM	C4C-CHD-C1D	3.93	127.75	122.56
4	A	1316	HEM	C4C-CHD-C1D	3.91	127.72	122.56
4	A	1307	HEM	C4C-CHD-C1D	3.61	127.32	122.56
4	A	1315	HEM	C4B-CHC-C1C	3.17	126.75	122.56
4	A	1309	HEM	CMA-C3A-C4A	-3.15	123.62	128.46
4	A	1310	HEM	CBB-CAB-C3B	-3.08	112.28	127.62
4	A	1315	HEM	CBB-CAB-C3B	-3.06	112.39	127.62
4	A	1307	HEM	C4B-CHC-C1C	2.98	126.50	122.56
4	A	1305	HEM	CBB-CAB-C3B	-2.97	112.85	127.62
4	A	1310	HEM	CMA-C3A-C4A	-2.96	123.92	128.46
4	A	1306	HEM	CMA-C3A-C4A	-2.94	123.94	128.46
4	A	1304	HEM	C4B-CHC-C1C	2.93	126.42	122.56
4	A	1307	HEM	CBB-CAB-C3B	-2.92	113.08	127.62
4	A	1311	HEM	CMA-C3A-C4A	-2.91	123.99	128.46
4	A	1302	HEM	CMA-C3A-C4A	-2.91	124.00	128.46
4	A	1308	HEM	C4B-CHC-C1C	2.90	126.39	122.56
4	A	1316	HEM	CMA-C3A-C4A	-2.87	124.06	128.46
4	A	1304	HEM	CBB-CAB-C3B	-2.85	113.46	127.62
4	A	1304	HEM	O1A-CGA-CBA	-2.84	113.95	123.08
4	A	1312	HEM	CMA-C3A-C4A	-2.83	124.11	128.46
4	A	1304	HEM	CMA-C3A-C4A	-2.82	124.13	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1305	HEM	C4B-CHC-C1C	2.82	126.27	122.56
4	A	1312	HEM	CBB-CAB-C3B	-2.81	113.64	127.62
4	A	1310	HEM	C4B-CHC-C1C	2.81	126.26	122.56
4	A	1306	HEM	C4B-CHC-C1C	2.81	126.26	122.56
4	A	1309	HEM	C4B-CHC-C1C	2.80	126.25	122.56
4	A	1301	HEM	CBB-CAB-C3B	-2.79	113.73	127.62
4	A	1303	HEM	C4B-CHC-C1C	2.78	126.22	122.56
4	A	1314	HEM	CBB-CAB-C3B	-2.78	113.80	127.62
4	A	1314	HEM	C4B-CHC-C1C	2.78	126.22	122.56
4	A	1307	HEM	CBA-CAA-C2A	2.77	117.35	112.62
4	A	1316	HEM	C4B-CHC-C1C	2.77	126.22	122.56
4	A	1311	HEM	CBB-CAB-C3B	-2.77	113.84	127.62
4	A	1313	HEM	CBB-CAB-C3B	-2.77	113.86	127.62
4	A	1313	HEM	CMA-C3A-C4A	-2.76	124.22	128.46
4	A	1316	HEM	CMC-C2C-C3C	2.75	129.83	124.68
4	A	1301	HEM	C4B-CHC-C1C	2.75	126.19	122.56
4	A	1303	HEM	CBB-CAB-C3B	-2.73	114.01	127.62
4	A	1304	HEM	CBA-CAA-C2A	-2.73	107.96	112.62
4	A	1309	HEM	CBB-CAB-C3B	-2.73	114.04	127.62
4	A	1316	HEM	CBB-CAB-C3B	-2.71	114.12	127.62
4	A	1309	HEM	CMC-C2C-C3C	2.71	129.75	124.68
4	A	1315	HEM	CMA-C3A-C4A	-2.71	124.30	128.46
4	A	1312	HEM	C4B-CHC-C1C	2.71	126.13	122.56
4	A	1302	HEM	C4B-CHC-C1C	2.70	126.12	122.56
4	A	1302	HEM	CBB-CAB-C3B	-2.70	114.18	127.62
4	A	1307	HEM	CMA-C3A-C4A	-2.70	124.32	128.46
4	A	1308	HEM	CBB-CAB-C3B	-2.69	114.23	127.62
4	A	1311	HEM	O1A-CGA-CBA	-2.67	114.49	123.08
4	A	1311	HEM	C4B-CHC-C1C	2.66	126.07	122.56
4	A	1301	HEM	CMA-C3A-C4A	-2.65	124.39	128.46
4	A	1309	HEM	CBA-CAA-C2A	2.64	117.12	112.62
4	A	1306	HEM	CMC-C2C-C3C	2.63	129.60	124.68
4	A	1305	HEM	CMA-C3A-C4A	-2.63	124.42	128.46
4	A	1309	HEM	O1A-CGA-CBA	-2.62	114.65	123.08
4	A	1306	HEM	CBB-CAB-C3B	-2.62	114.58	127.62
4	A	1308	HEM	O1A-CGA-CBA	-2.60	114.72	123.08
4	A	1303	HEM	CMA-C3A-C4A	-2.58	124.49	128.46
4	A	1302	HEM	CMC-C2C-C3C	2.58	129.51	124.68
4	A	1308	HEM	CMA-C3A-C4A	-2.56	124.53	128.46
4	A	1306	HEM	O1A-CGA-CBA	-2.55	114.90	123.08
4	A	1310	HEM	CMC-C2C-C3C	2.54	129.44	124.68
4	A	1314	HEM	CMA-C3A-C4A	-2.54	124.56	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1303	HEM	CMC-C2C-C3C	2.53	129.42	124.68
4	A	1312	HEM	O1A-CGA-CBA	-2.53	114.96	123.08
4	A	1313	HEM	C4B-CHC-C1C	2.53	125.89	122.56
4	A	1315	HEM	CMC-C2C-C3C	2.52	129.40	124.68
4	A	1310	HEM	O1A-CGA-CBA	-2.51	115.01	123.08
4	A	1303	HEM	O1A-CGA-CBA	-2.50	115.04	123.08
4	A	1305	HEM	O1A-CGA-CBA	-2.49	115.09	123.08
4	A	1313	HEM	CMC-C2C-C3C	2.44	129.24	124.68
4	A	1315	HEM	O1A-CGA-CBA	-2.43	115.26	123.08
4	A	1311	HEM	CMC-C2C-C3C	2.43	129.22	124.68
4	A	1301	HEM	O1A-CGA-CBA	-2.40	115.37	123.08
4	A	1308	HEM	CMC-C2C-C3C	2.39	129.16	124.68
4	A	1304	HEM	CMC-C2C-C3C	2.39	129.16	124.68
4	A	1316	HEM	O1A-CGA-CBA	-2.39	115.41	123.08
4	A	1305	HEM	CMC-C2C-C3C	2.37	129.12	124.68
4	A	1313	HEM	O1A-CGA-CBA	-2.36	115.50	123.08
4	A	1302	HEM	O1A-CGA-CBA	-2.36	115.51	123.08
4	A	1301	HEM	CBA-CAA-C2A	-2.34	108.63	112.62
4	A	1314	HEM	CMC-C2C-C3C	2.33	129.04	124.68
4	A	1312	HEM	CMC-C2C-C3C	2.31	128.99	124.68
4	A	1314	HEM	O1A-CGA-CBA	-2.31	115.67	123.08
4	A	1301	HEM	CMC-C2C-C3C	2.29	128.96	124.68
4	A	1307	HEM	O1A-CGA-CBA	-2.04	116.53	123.08
4	A	1315	HEM	CBA-CAA-C2A	2.02	116.07	112.62
4	A	1304	HEM	O2A-CGA-CBA	2.01	120.48	114.03

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	HEM	C2B-C3B-CAB-CBB
4	A	1302	HEM	C2B-C3B-CAB-CBB
4	A	1303	HEM	C2B-C3B-CAB-CBB
4	A	1303	HEM	C4B-C3B-CAB-CBB
4	A	1304	HEM	C2B-C3B-CAB-CBB
4	A	1304	HEM	C4B-C3B-CAB-CBB
4	A	1305	HEM	C2B-C3B-CAB-CBB
4	A	1305	HEM	C4B-C3B-CAB-CBB
4	A	1307	HEM	C2B-C3B-CAB-CBB
4	A	1307	HEM	C4B-C3B-CAB-CBB
4	A	1308	HEM	C2B-C3B-CAB-CBB
4	A	1309	HEM	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1309	HEM	C3A-C2A-CAA-CBA
4	A	1309	HEM	C2B-C3B-CAB-CBB
4	A	1309	HEM	C4B-C3B-CAB-CBB
4	A	1310	HEM	C2B-C3B-CAB-CBB
4	A	1311	HEM	C2A-CAA-CBA-CGA
4	A	1311	HEM	C2B-C3B-CAB-CBB
4	A	1312	HEM	C2B-C3B-CAB-CBB
4	A	1313	HEM	C2B-C3B-CAB-CBB
4	A	1314	HEM	C2B-C3B-CAB-CBB
4	A	1314	HEM	C4B-C3B-CAB-CBB
4	A	1315	HEM	C2B-C3B-CAB-CBB
4	A	1316	HEM	C2B-C3B-CAB-CBB
4	A	1316	HEM	C4B-C3B-CAB-CBB
4	A	1303	HEM	C3D-CAD-CBD-CGD
4	A	1305	HEM	C2A-CAA-CBA-CGA
4	A	1309	HEM	C3D-CAD-CBD-CGD
4	A	1301	HEM	C3D-CAD-CBD-CGD
4	A	1301	HEM	C4B-C3B-CAB-CBB
4	A	1302	HEM	C4B-C3B-CAB-CBB
4	A	1308	HEM	C4B-C3B-CAB-CBB
4	A	1310	HEM	C4B-C3B-CAB-CBB
4	A	1311	HEM	C4B-C3B-CAB-CBB
4	A	1312	HEM	C4B-C3B-CAB-CBB
4	A	1313	HEM	C4B-C3B-CAB-CBB
4	A	1315	HEM	C4B-C3B-CAB-CBB
4	A	1316	HEM	C3D-CAD-CBD-CGD
4	A	1306	HEM	C2B-C3B-CAB-CBB
4	A	1314	HEM	C2A-CAA-CBA-CGA
4	A	1316	HEM	CAD-CBD-CGD-O1D
4	A	1309	HEM	CAA-CBA-CGA-O1A
4	A	1314	HEM	CAD-CBD-CGD-O2D
4	A	1306	HEM	C4B-C3B-CAB-CBB
4	A	1312	HEM	CAD-CBD-CGD-O2D
4	A	1314	HEM	CAD-CBD-CGD-O1D
4	A	1302	HEM	C3D-CAD-CBD-CGD
4	A	1314	HEM	CAA-CBA-CGA-O2A
4	A	1314	HEM	CAA-CBA-CGA-O1A
4	A	1305	HEM	CAD-CBD-CGD-O1D
4	A	1309	HEM	CAA-CBA-CGA-O2A
4	A	1302	HEM	CAD-CBD-CGD-O1D
4	A	1311	HEM	CAD-CBD-CGD-O1D
4	A	1307	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1312	HEM	CAD-CBD-CGD-O1D
4	A	1308	HEM	CAA-CBA-CGA-O2A
4	A	1307	HEM	CAD-CBD-CGD-O2D
4	A	1311	HEM	CAD-CBD-CGD-O2D
4	A	1308	HEM	CAA-CBA-CGA-O1A
4	A	1305	HEM	CAA-CBA-CGA-O1A
4	A	1310	HEM	CAA-CBA-CGA-O2A
4	A	1303	HEM	CAD-CBD-CGD-O2D
4	A	1306	HEM	CAD-CBD-CGD-O1D
4	A	1316	HEM	CAD-CBD-CGD-O2D
4	A	1302	HEM	CAD-CBD-CGD-O2D
4	A	1305	HEM	CAD-CBD-CGD-O2D
4	A	1310	HEM	C3D-CAD-CBD-CGD
4	A	1305	HEM	CAA-CBA-CGA-O2A
4	A	1306	HEM	CAD-CBD-CGD-O2D
4	A	1303	HEM	CAD-CBD-CGD-O1D
4	A	1301	HEM	CAA-CBA-CGA-O2A
4	A	1310	HEM	CAA-CBA-CGA-O1A
4	A	1303	HEM	CAA-CBA-CGA-O2A
4	A	1314	HEM	C3D-CAD-CBD-CGD
4	A	1304	HEM	CAD-CBD-CGD-O2D
4	A	1301	HEM	CAA-CBA-CGA-O1A
4	A	1309	HEM	CAD-CBD-CGD-O2D
4	A	1304	HEM	CAD-CBD-CGD-O1D
4	A	1309	HEM	CAD-CBD-CGD-O1D
4	A	1303	HEM	CAA-CBA-CGA-O1A
4	A	1311	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1316	HEM	1	0
4	A	1313	HEM	1	0
4	A	1308	HEM	3	0
4	A	1302	HEM	1	0
4	A	1303	HEM	2	0
4	A	1307	HEM	1	0
4	A	1306	HEM	1	0
4	A	1310	HEM	1	0
4	A	1301	HEM	1	0
4	A	1311	HEM	1	0

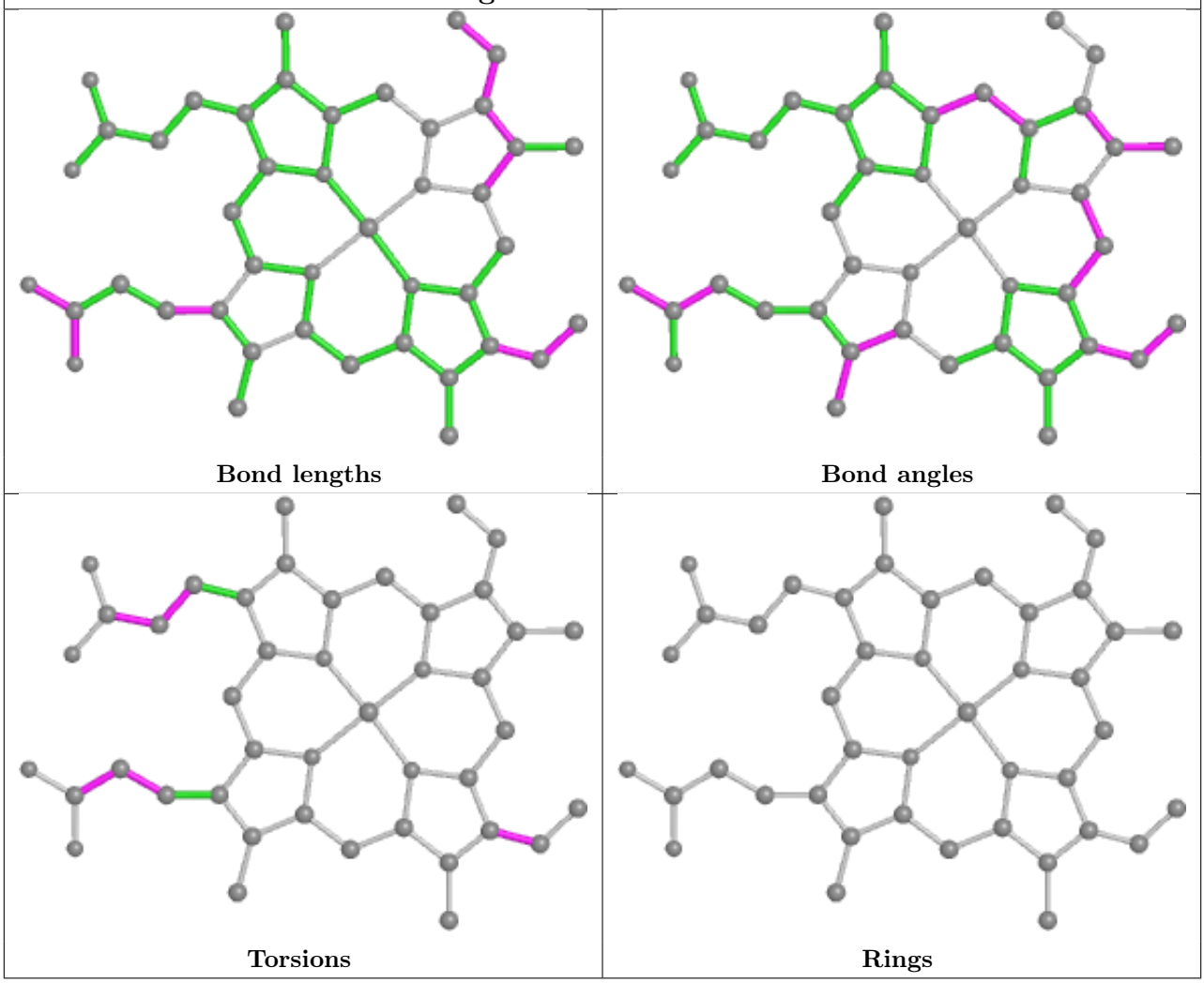
Continued on next page...

Continued from previous page...

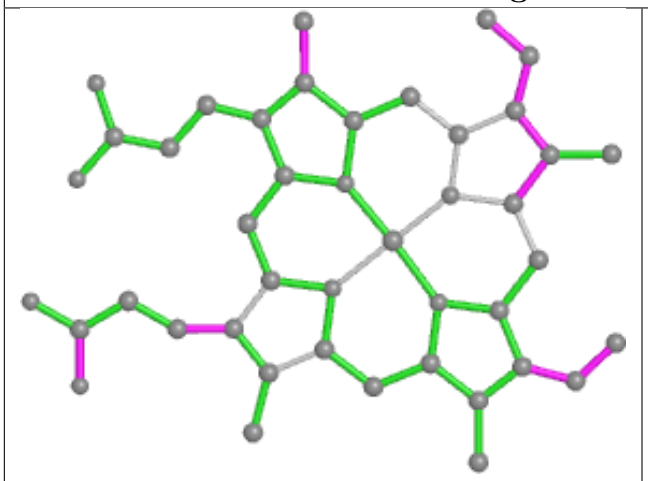
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1309	HEM	1	0
4	A	1304	HEM	3	0

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.

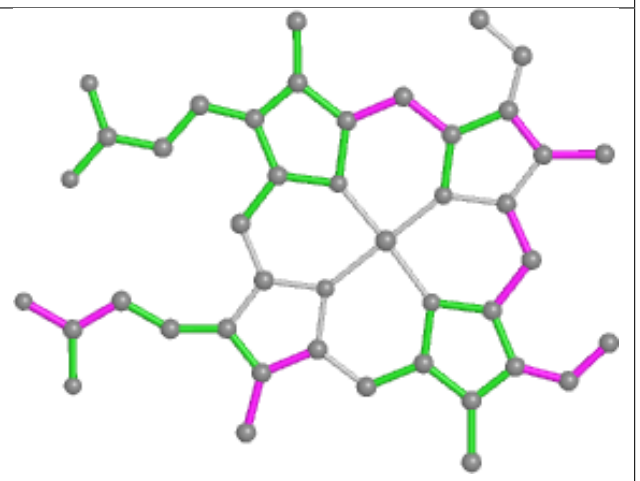
Ligand HEM A 1314



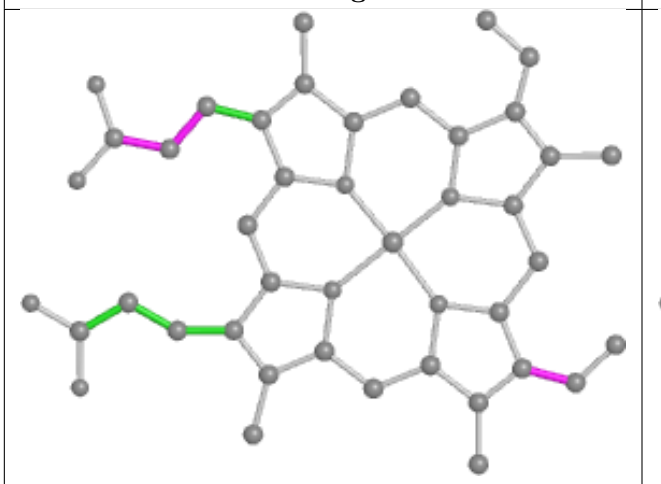
Ligand HEM A 1316



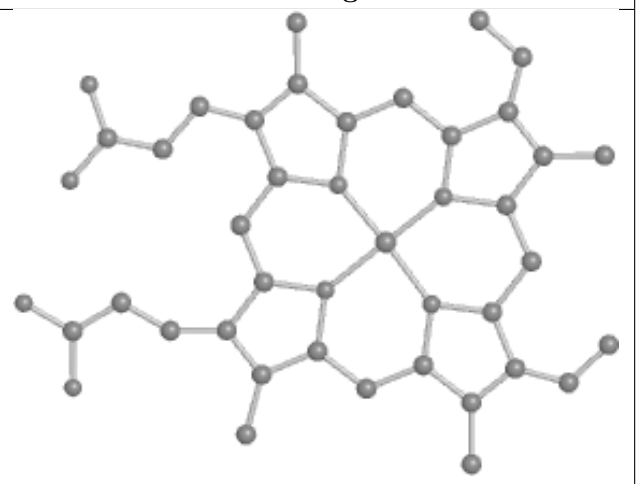
Bond lengths



Bond angles

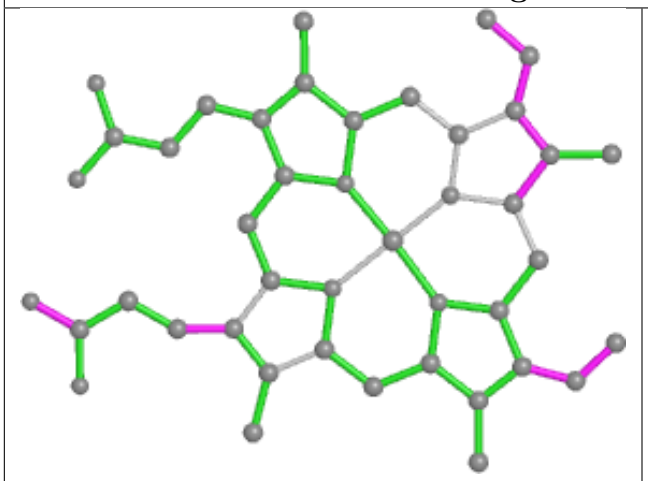


Torsions

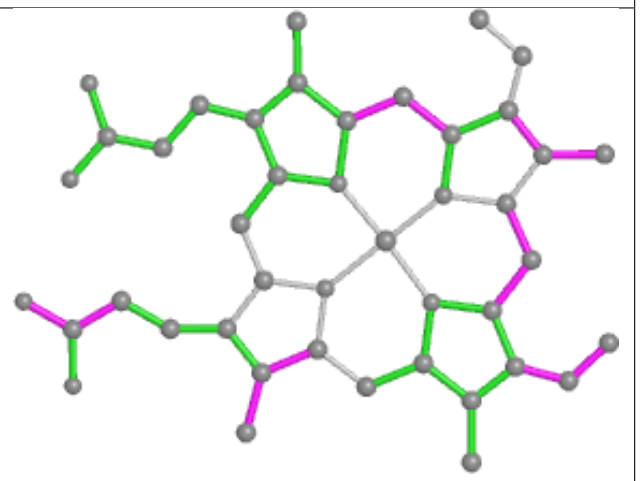


Rings

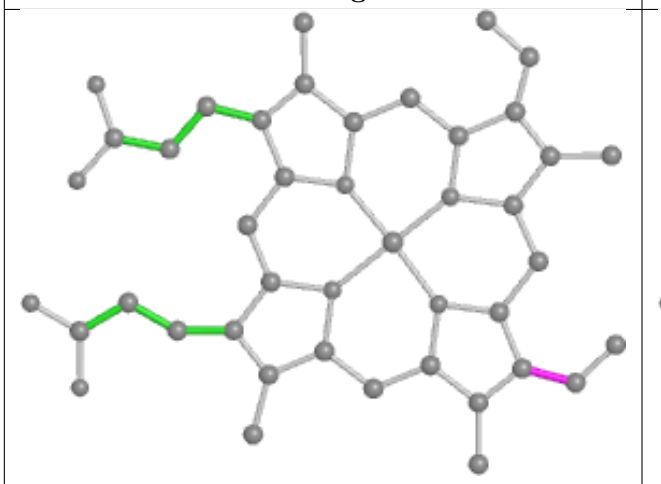
Ligand HEM A 1313



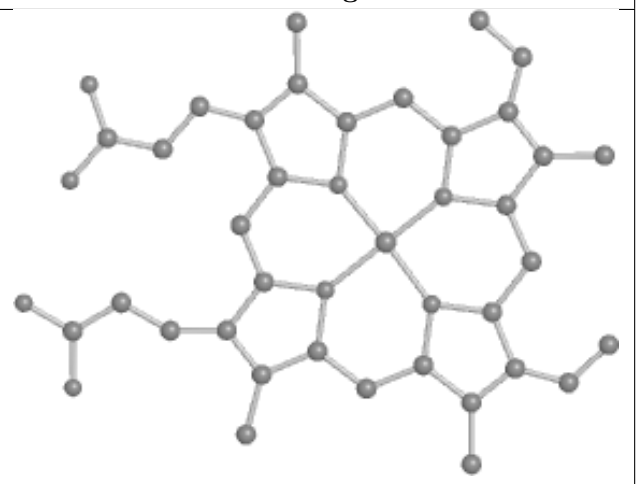
Bond lengths



Bond angles

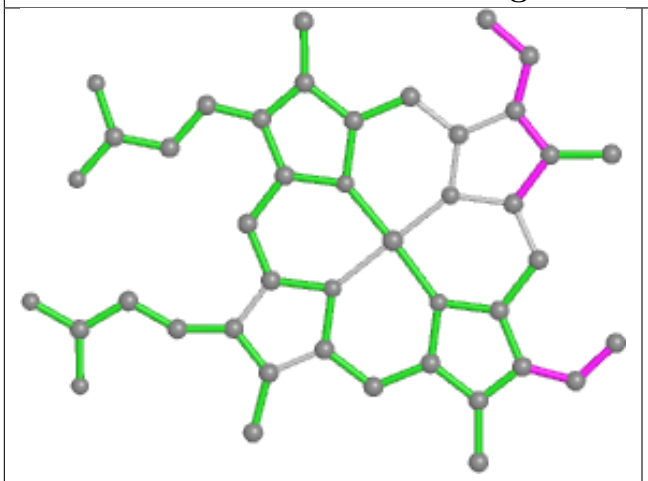


Torsions

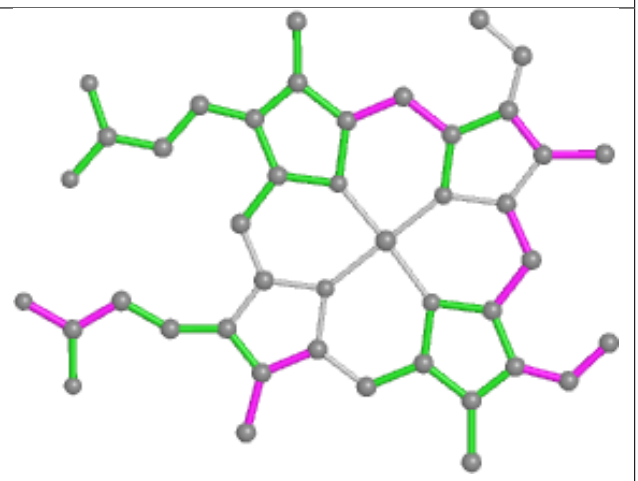


Rings

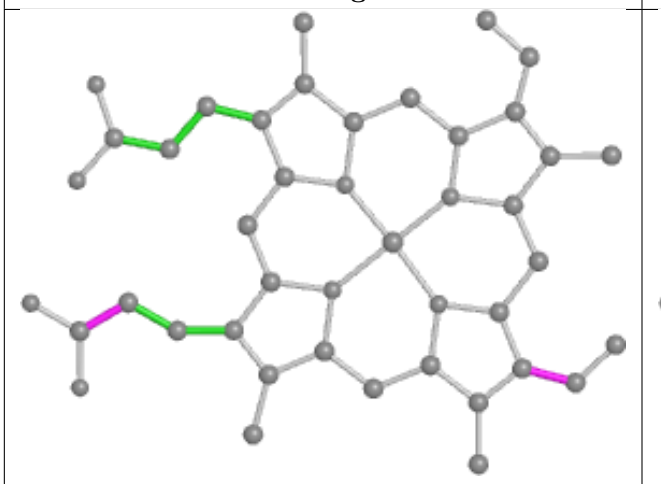
Ligand HEM A 1308



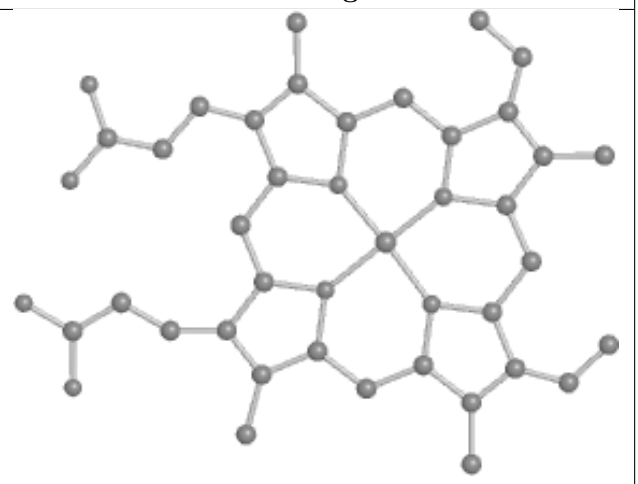
Bond lengths



Bond angles

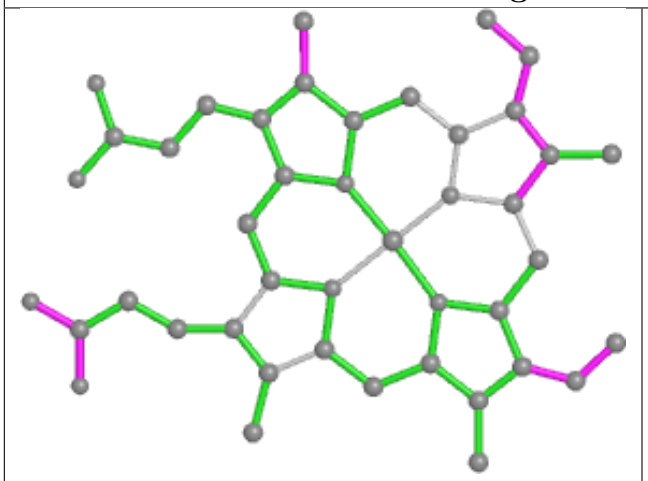


Torsions

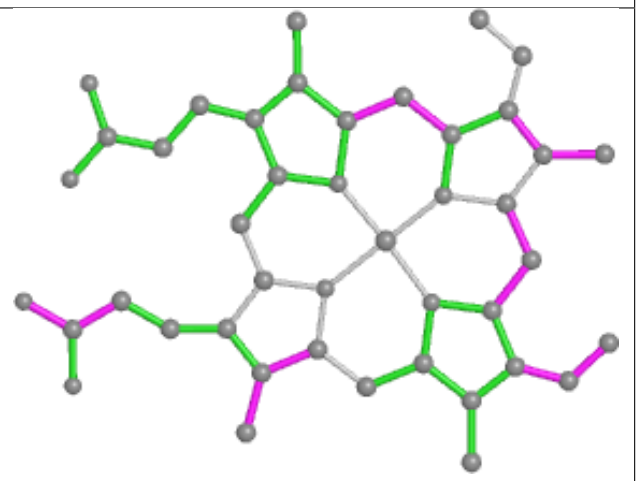


Rings

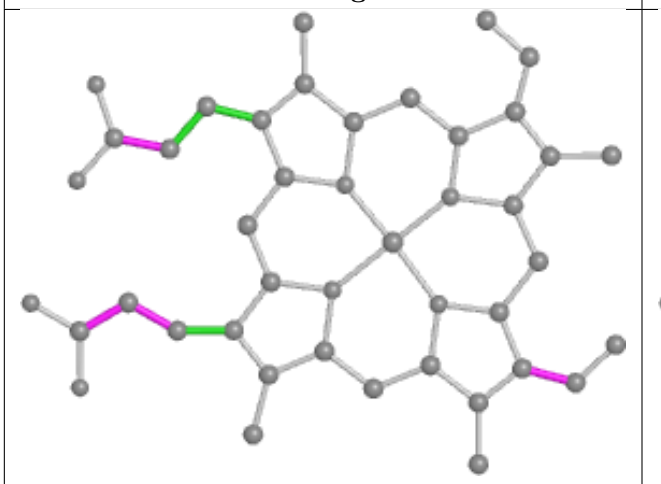
Ligand HEM A 1305



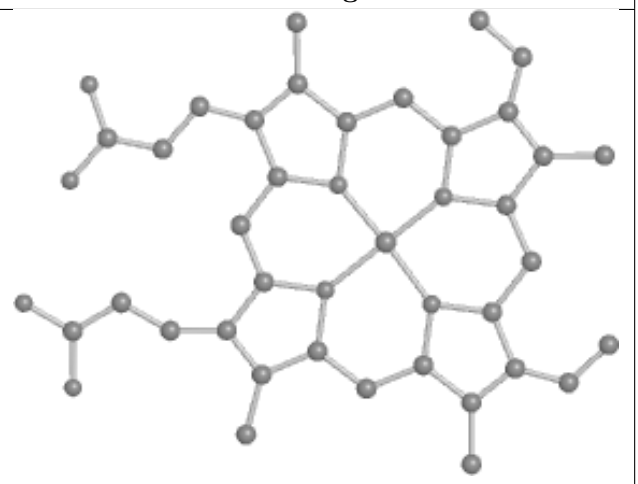
Bond lengths



Bond angles

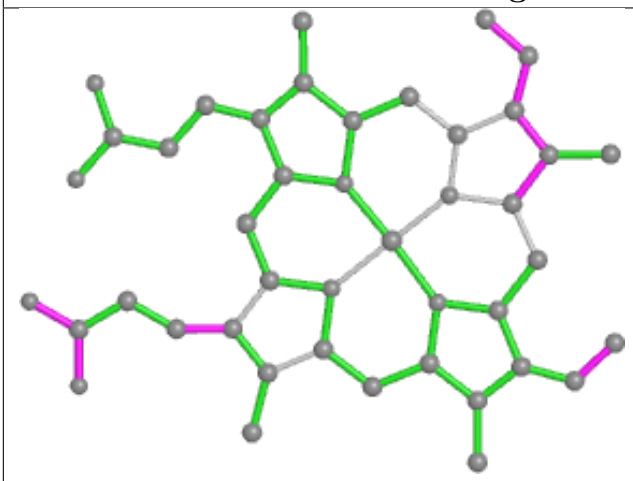


Torsions

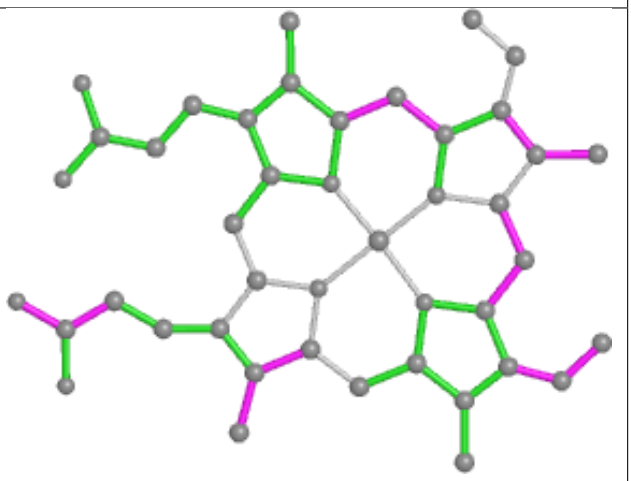


Rings

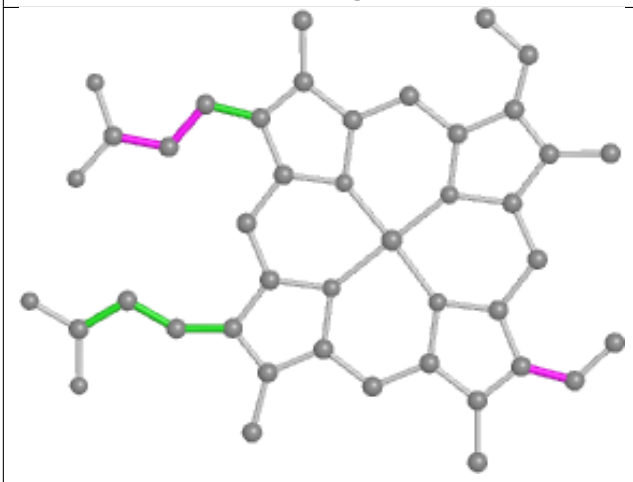
Ligand HEM A 1302



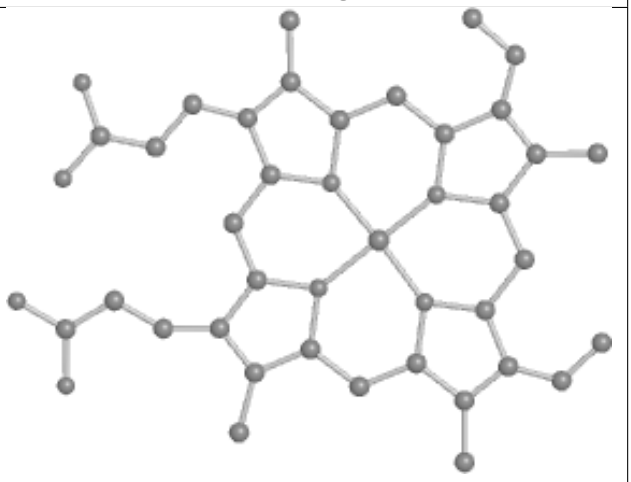
Bond lengths



Bond angles

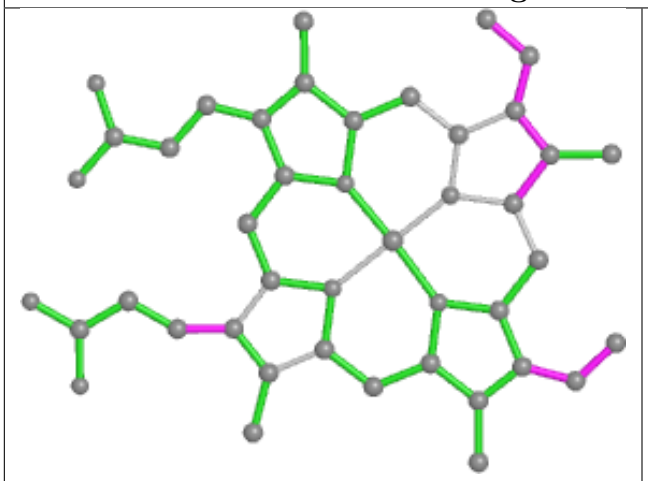


Torsions

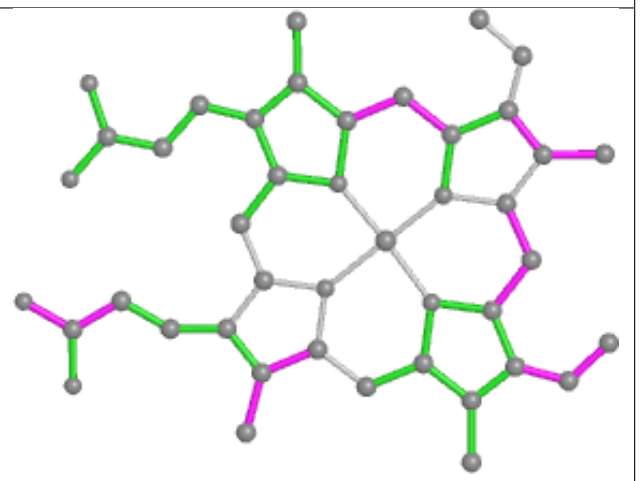


Rings

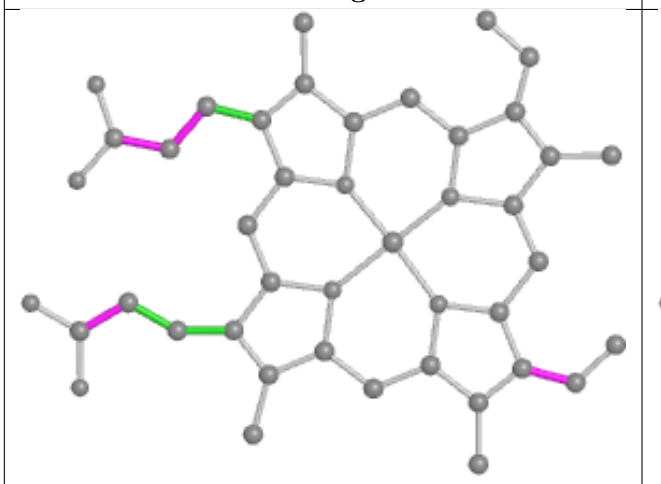
Ligand HEM A 1303



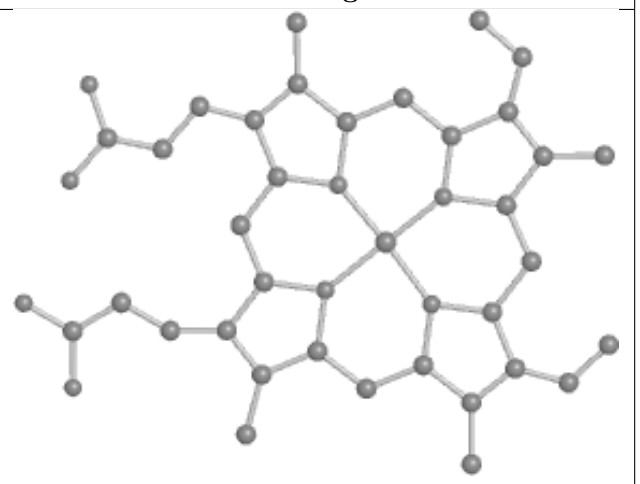
Bond lengths



Bond angles

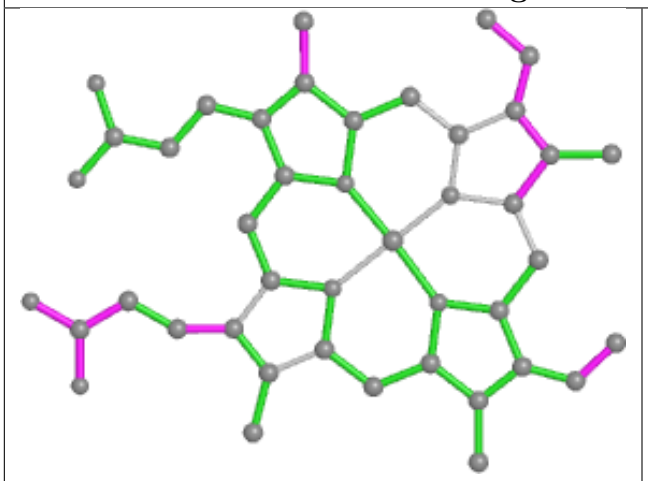


Torsions

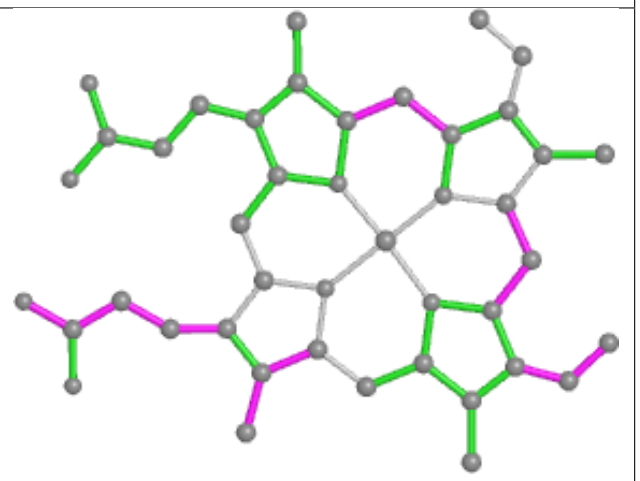


Rings

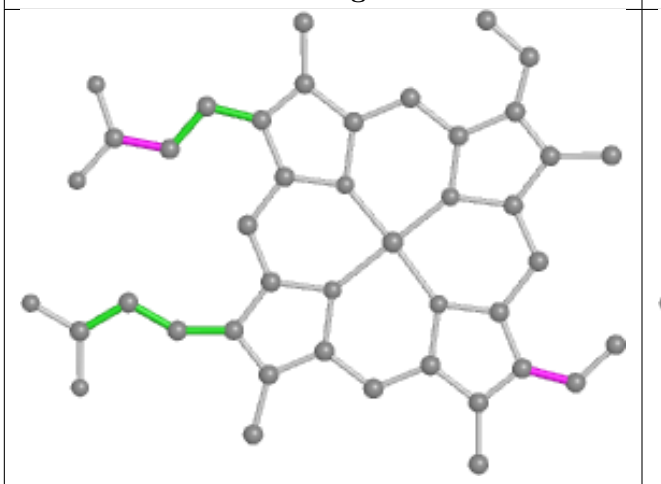
Ligand HEM A 1307



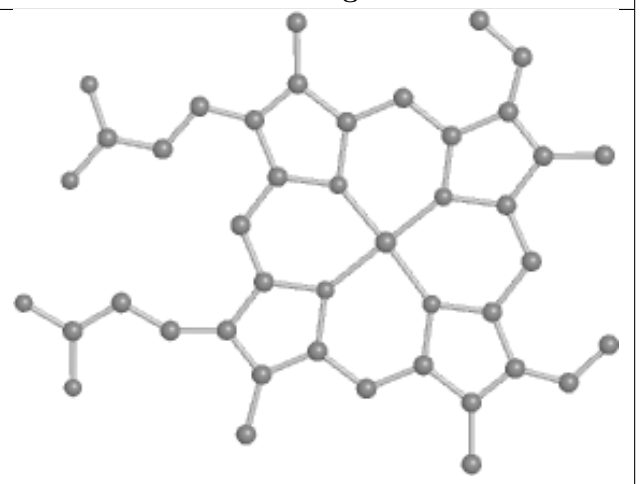
Bond lengths



Bond angles

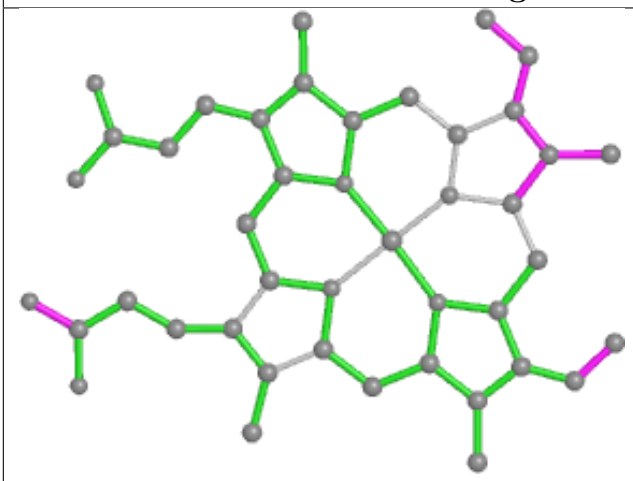


Torsions

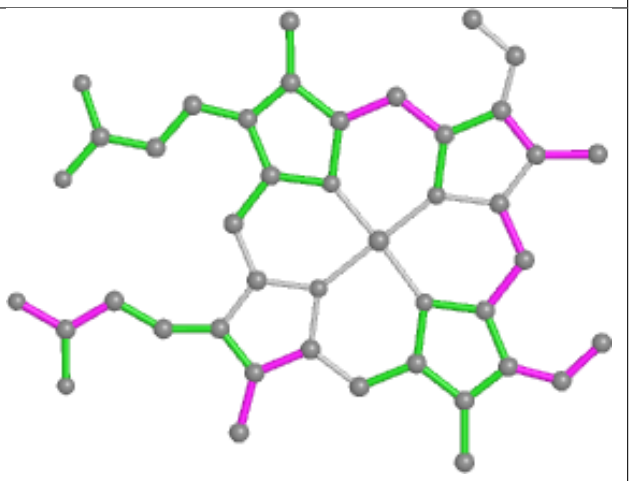


Rings

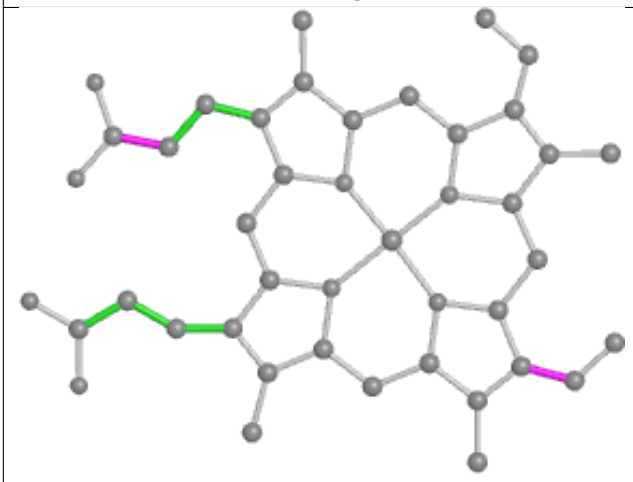
Ligand HEM A 1306



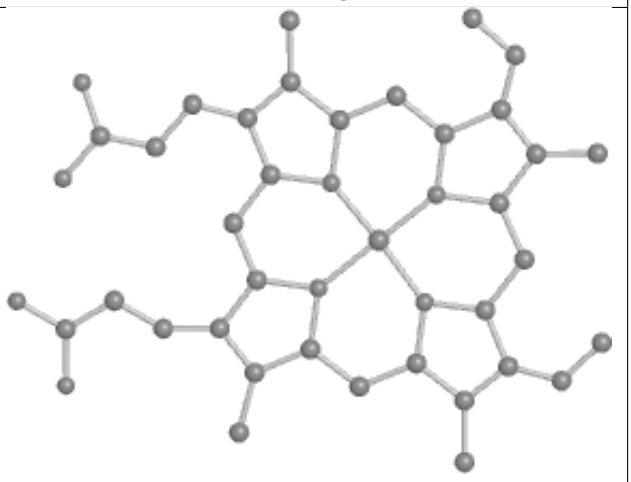
Bond lengths



Bond angles

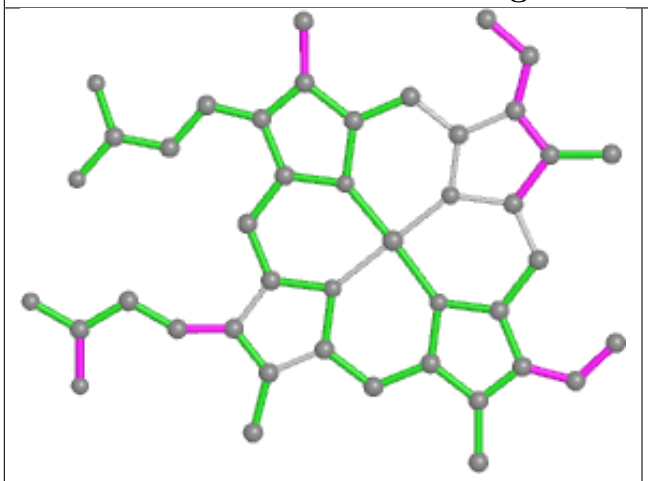


Torsions

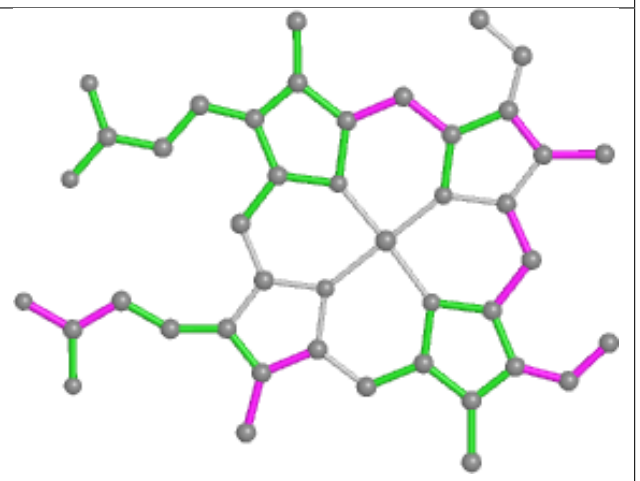


Rings

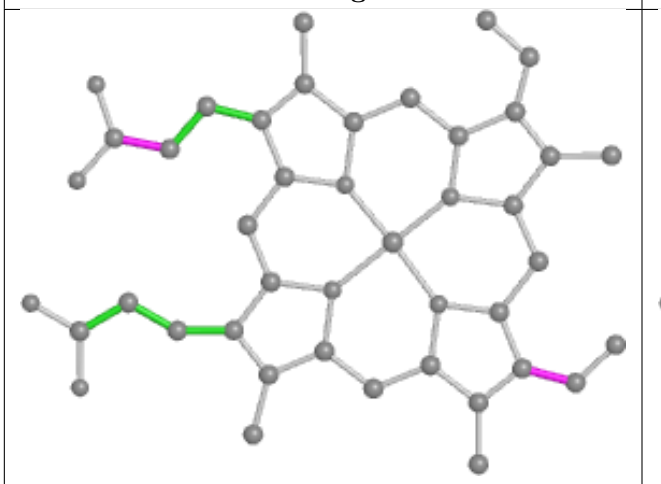
Ligand HEM A 1312



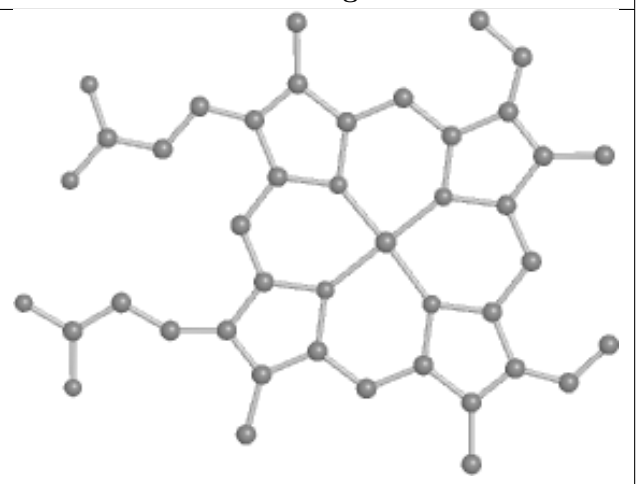
Bond lengths



Bond angles

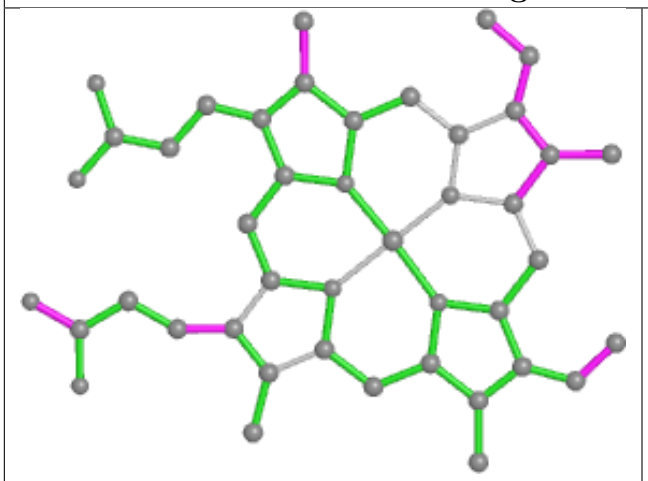


Torsions

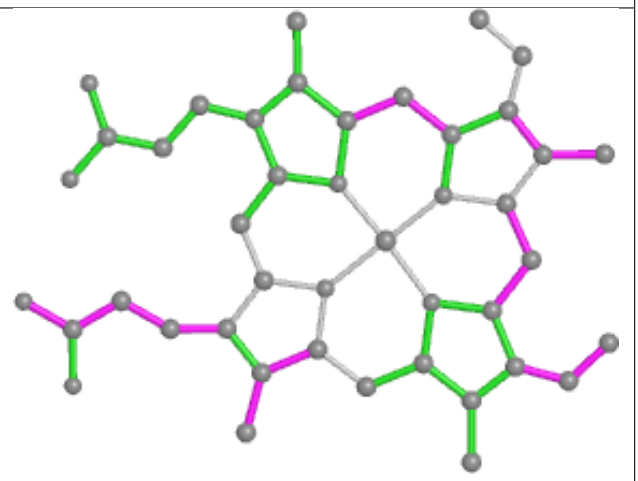


Rings

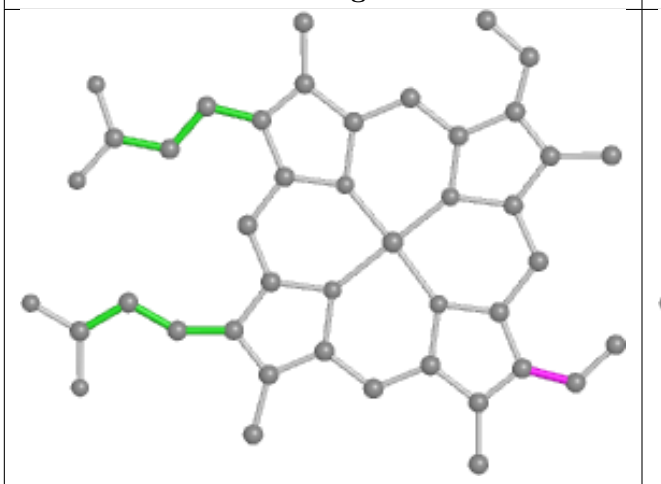
Ligand HEM A 1315



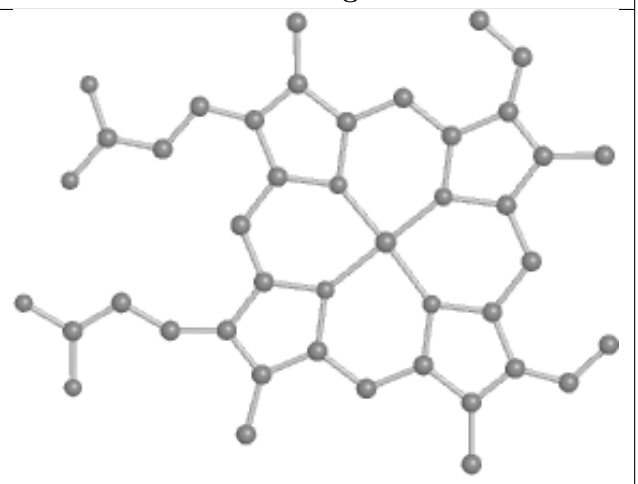
Bond lengths



Bond angles

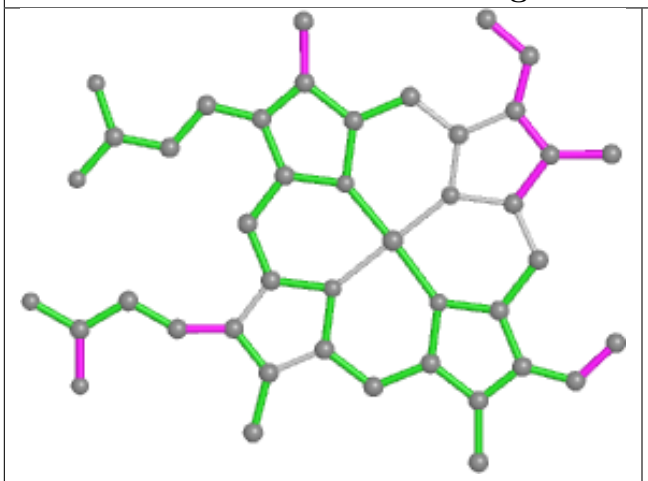


Torsions

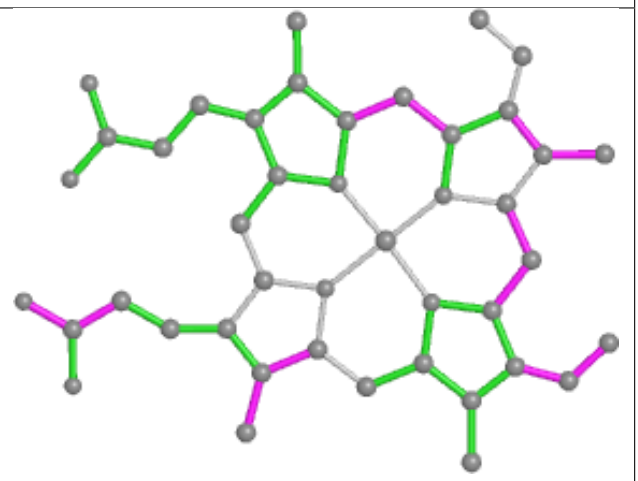


Rings

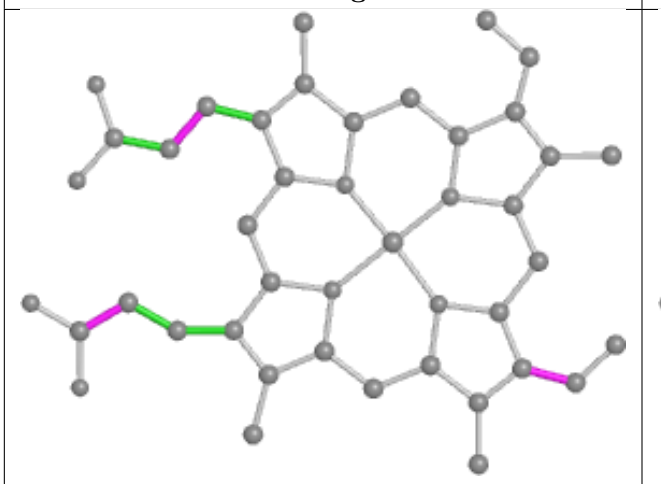
Ligand HEM A 1310



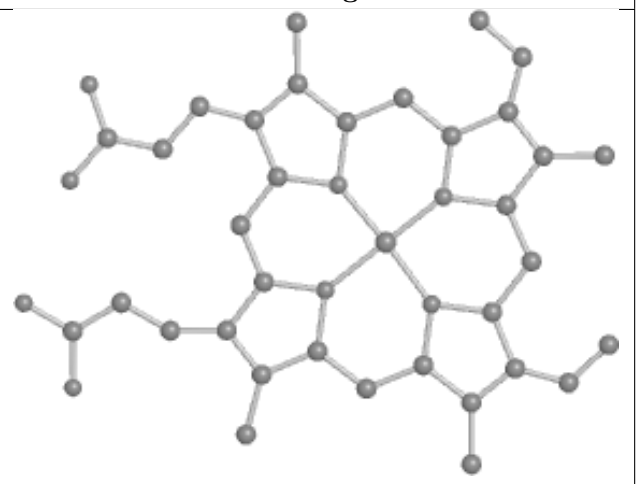
Bond lengths



Bond angles

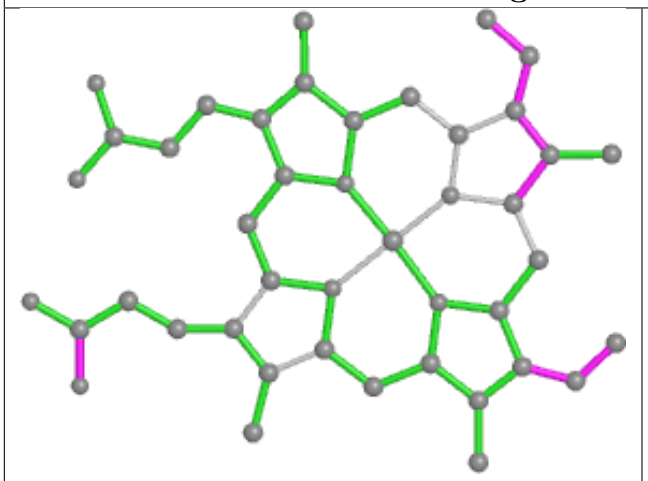


Torsions

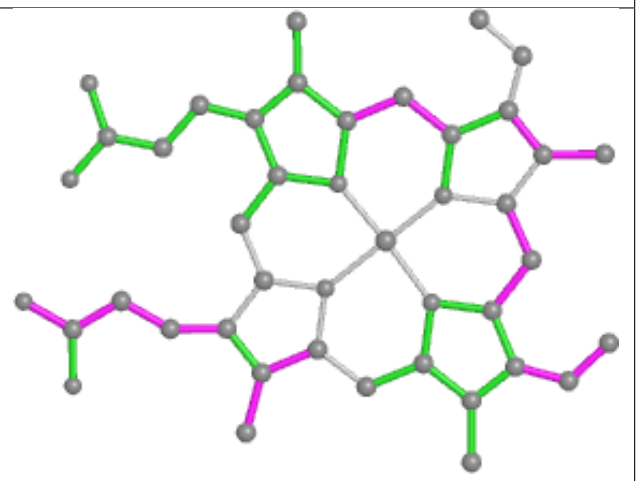


Rings

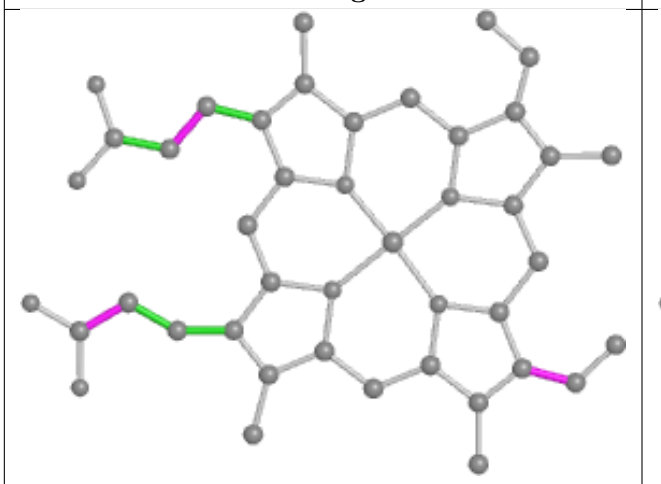
Ligand HEM A 1301



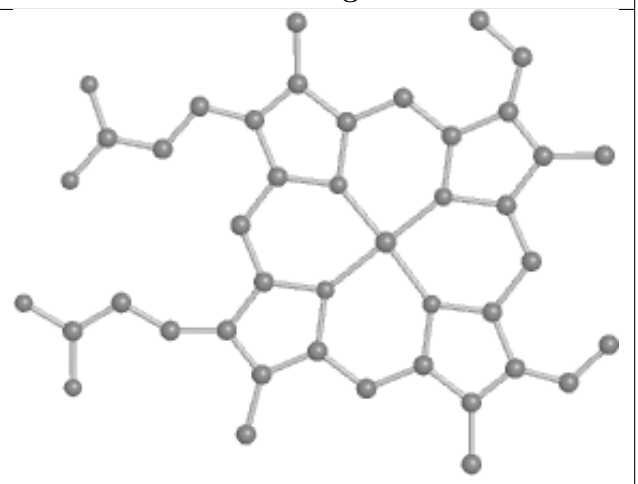
Bond lengths



Bond angles

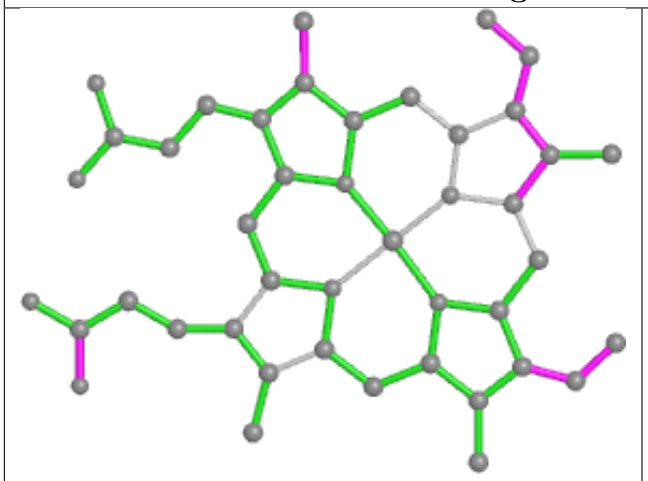


Torsions

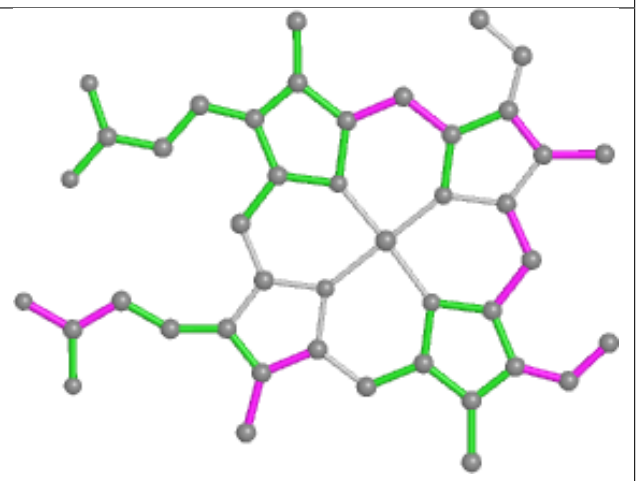


Rings

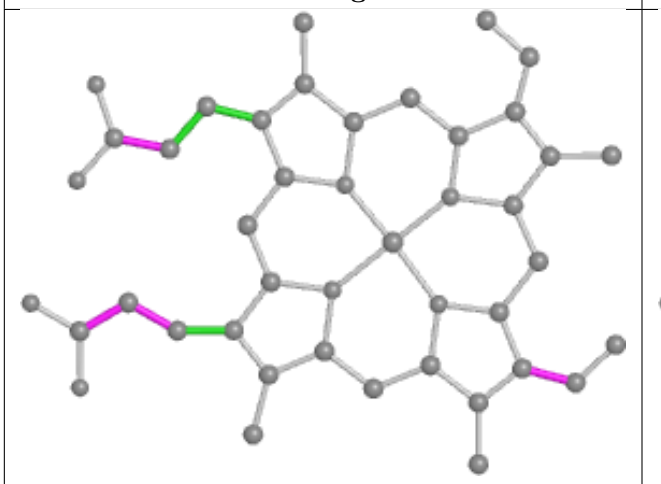
Ligand HEM A 1311



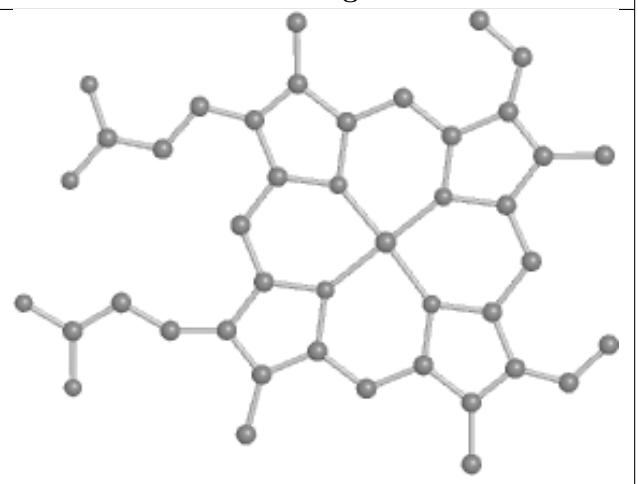
Bond lengths



Bond angles

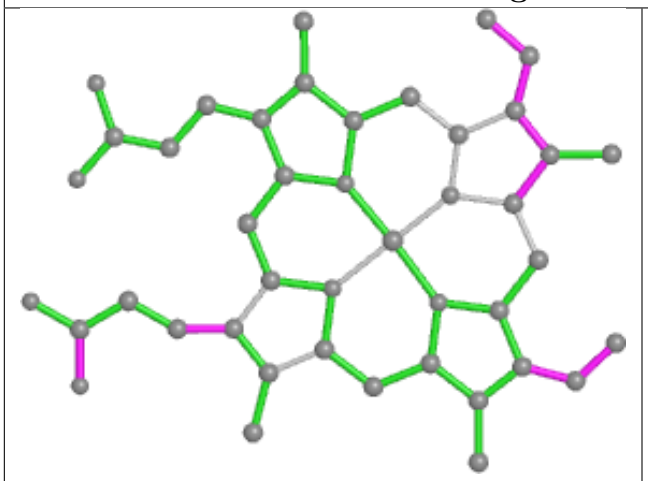


Torsions

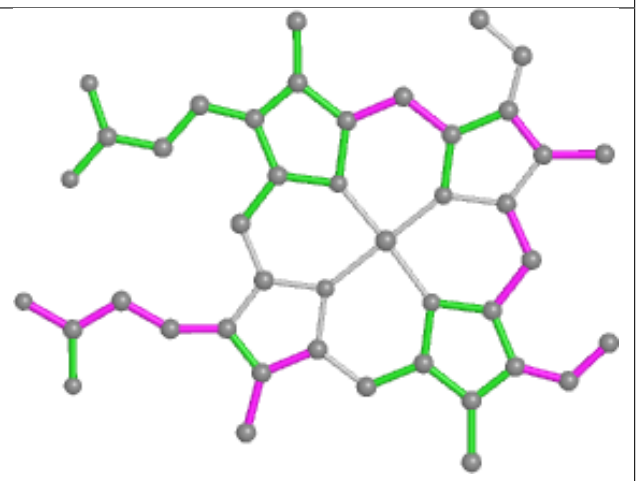


Rings

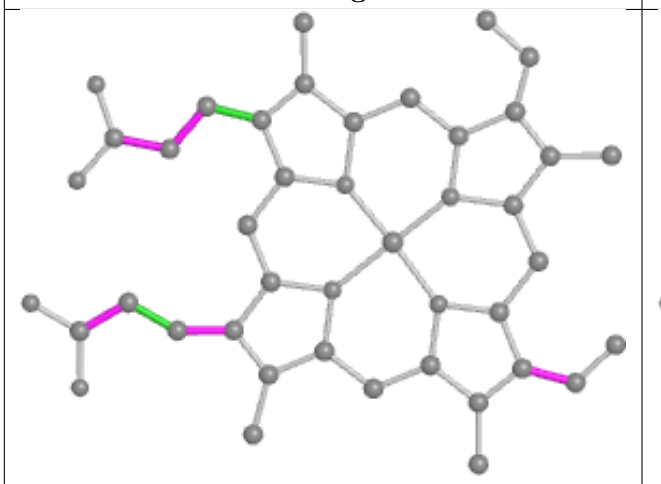
Ligand HEM A 1309



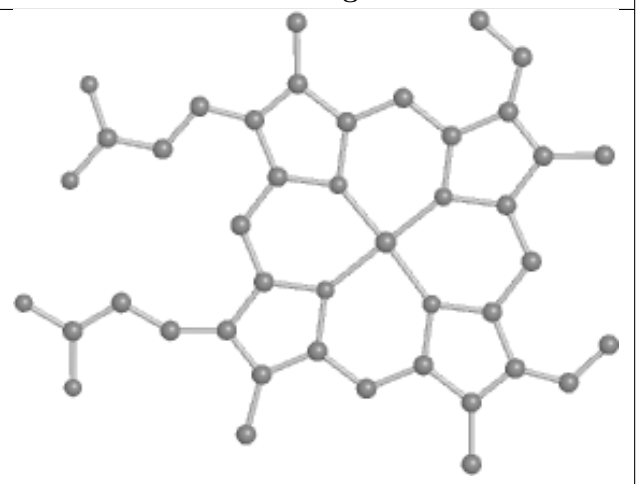
Bond lengths



Bond angles

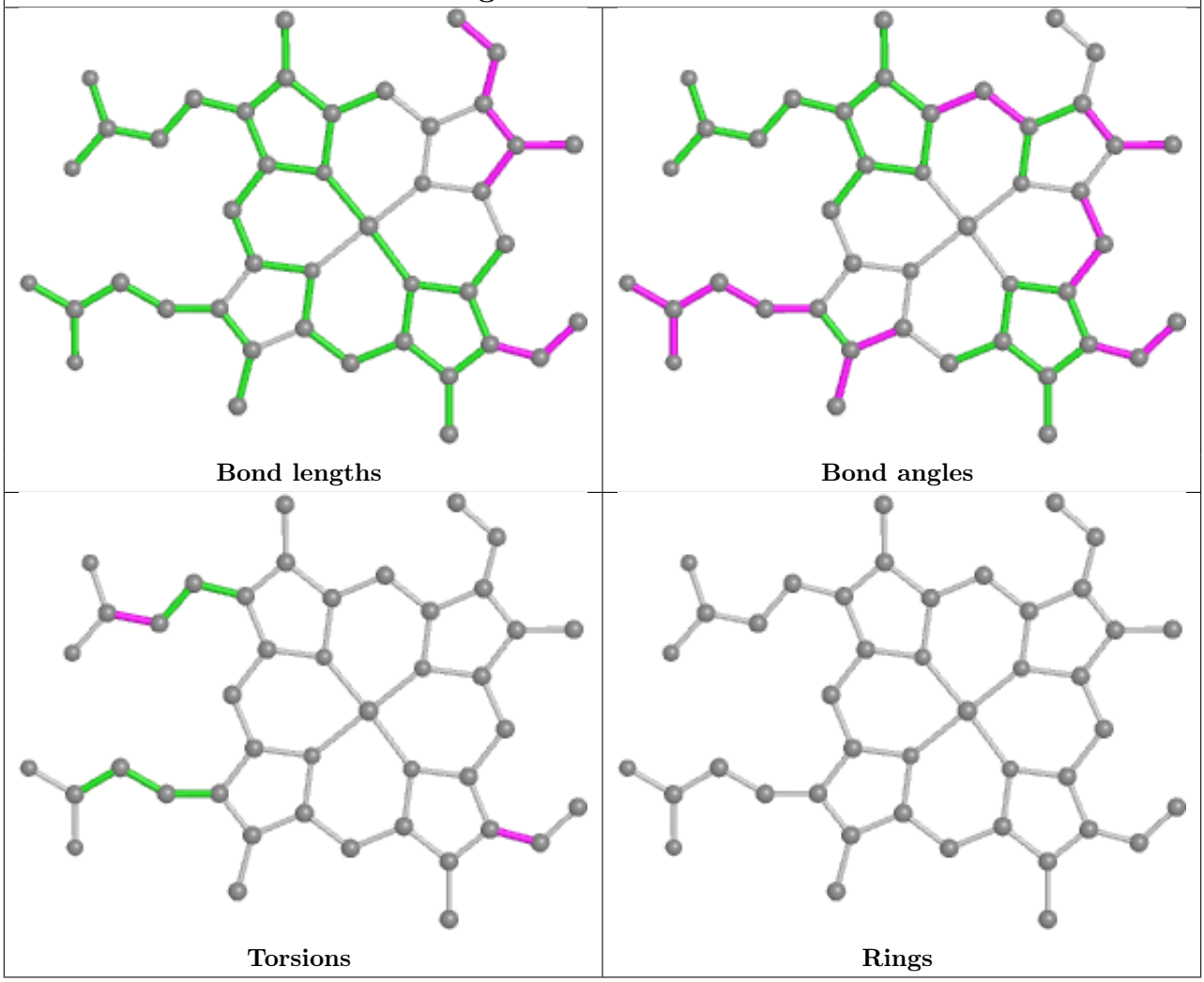


Torsions



Rings

Ligand HEM A 1304



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	513/556 (92%)	0.27	50 (9%) 7 6	16, 37, 74, 101	3 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	ASP	4.6
1	A	56	ASN	4.4
1	A	543	ALA	3.9
1	A	545	THR	3.9
1	A	544	ASP	3.7
1	A	295	MET	3.7
1	A	519	ARG	3.6
1	A	266	ASP	3.6
1	A	239	PRO	3.6
1	A	38	THR	3.5
1	A	293	LYS	3.5
1	A	54	PHE	3.4
1	A	214	VAL	3.3
1	A	149	ALA	3.3
1	A	39	GLY	3.2
1	A	287	GLY	3.2
1	A	542	PRO	3.1
1	A	294	GLY	3.0
1	A	241	LYS	2.9
1	A	265	ARG	2.9
1	A	79	PRO	2.8
1	A	402	LYS	2.8
1	A	296	LYS	2.7
1	A	240	ALA	2.7
1	A	400	ASP	2.6
1	A	146	LYS	2.6
1	A	92	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	383	PRO	2.5
1	A	413	THR	2.5
1	A	175	ASN	2.5
1	A	91	ASP	2.5
1	A	78	ALA	2.5
1	A	137	GLY	2.5
1	A	107	ALA	2.4
1	A	288	ALA	2.4
1	A	102	LEU	2.3
1	A	216	LYS	2.3
1	A	237	ALA	2.3
1	A	509	GLY	2.2
1	A	106	THR	2.2
1	A	215	GLU	2.2
1	A	177	PRO	2.2
1	A	40	GLU	2.2
1	A	90	ASP	2.2
1	A	148	MET	2.2
1	A	286	PRO	2.1
1	A	432	LYS	2.1
1	A	228	CYS	2.1
1	A	238	ALA	2.0
1	A	37	SER	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.

Continued on next page...

Continued from previous page...

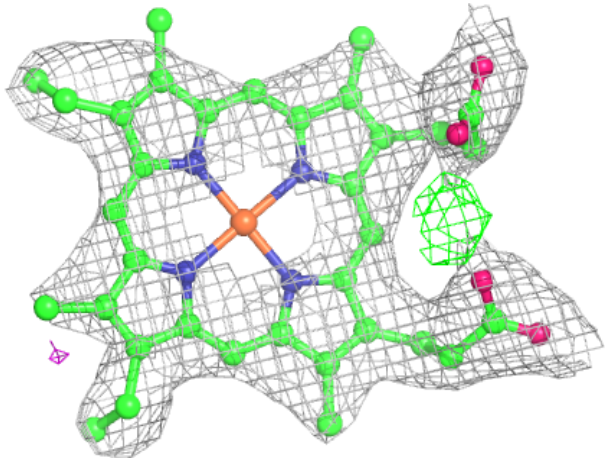
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

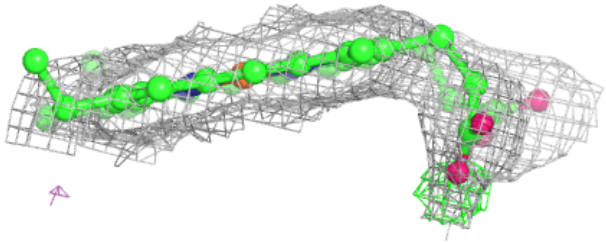
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	A	562	1/1	0.68	0.14	60,60,60,60	0
3	NA	A	561	1/1	0.92	0.37	29,29,29,29	0
2	ZN	A	560	1/1	0.92	0.07	53,53,53,53	0
3	NA	A	563	1/1	0.92	0.14	42,42,42,42	0
4	HEM	A	1303	43/43	0.94	0.17	29,48,61,65	0
4	HEM	A	1315	43/43	0.94	0.19	9,24,51,62	0
4	HEM	A	1304	43/43	0.95	0.18	12,28,38,44	0
4	HEM	A	1306	43/43	0.95	0.20	21,35,43,53	0
4	HEM	A	1307	43/43	0.95	0.17	18,29,53,62	0
4	HEM	A	1313	43/43	0.95	0.18	8,27,51,64	0
4	HEM	A	1314	43/43	0.95	0.18	25,32,57,60	0
4	HEM	A	1302	43/43	0.95	0.18	16,28,56,62	0
4	HEM	A	1305	43/43	0.96	0.15	22,36,55,68	0
4	HEM	A	1308	43/43	0.96	0.17	9,21,43,48	0
4	HEM	A	1309	43/43	0.96	0.17	7,25,55,70	0
4	HEM	A	1312	43/43	0.97	0.17	16,25,39,47	0
4	HEM	A	1301	43/43	0.97	0.18	17,28,34,45	0
4	HEM	A	1310	43/43	0.97	0.16	9,24,39,50	0
4	HEM	A	1311	43/43	0.97	0.16	10,20,55,62	0
4	HEM	A	1316	43/43	0.97	0.13	11,26,32,32	0
3	NA	A	564	1/1	0.98	0.50	22,22,22,22	0
2	ZN	A	557	1/1	0.99	0.06	28,28,28,28	0
2	ZN	A	558	1/1	0.99	0.11	28,28,28,28	0
2	ZN	A	559	1/1	0.99	0.07	28,28,28,28	0

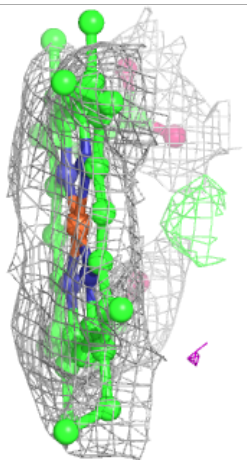
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 1303:

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

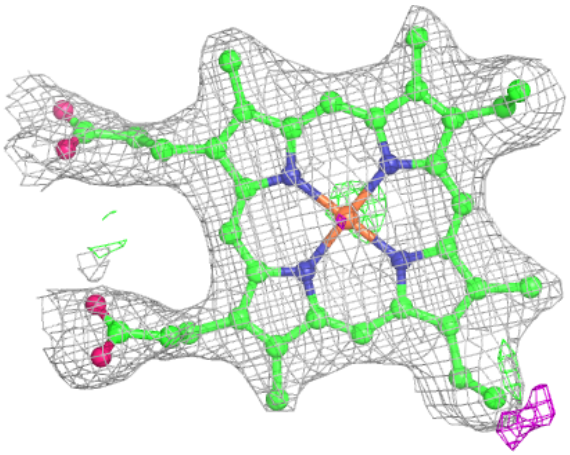


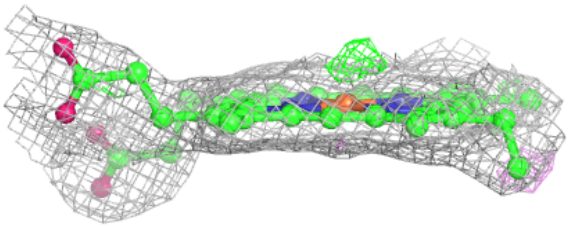


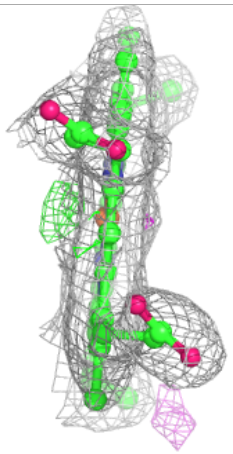


Electron density around HEM A 1315:

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

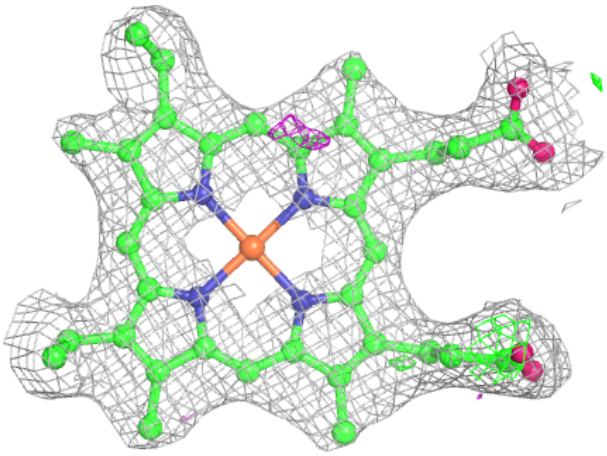


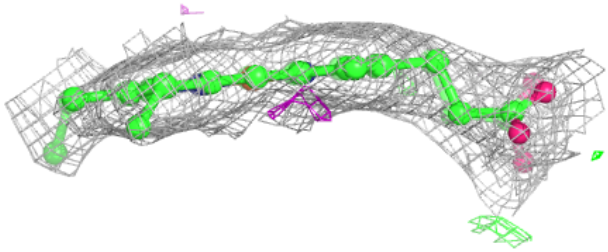


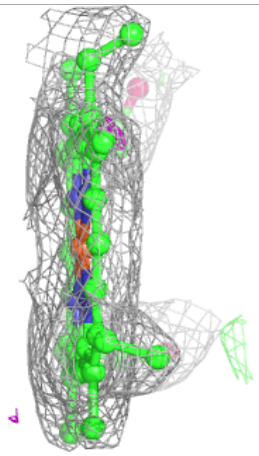


Electron density around HEM A 1304:

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

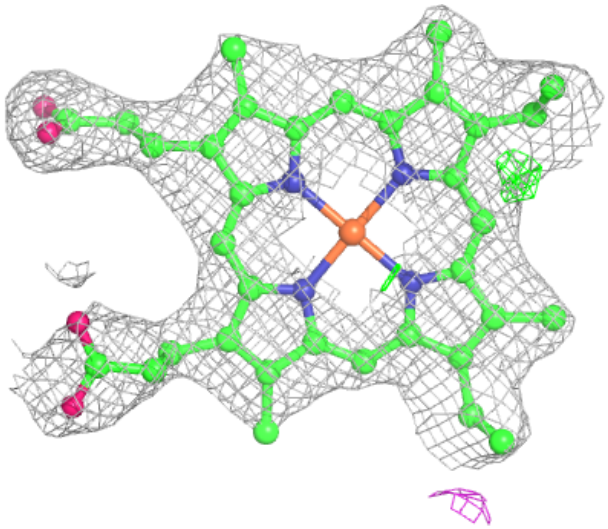


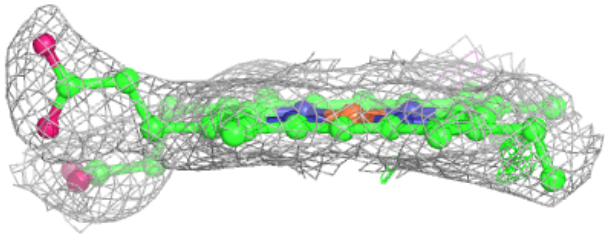


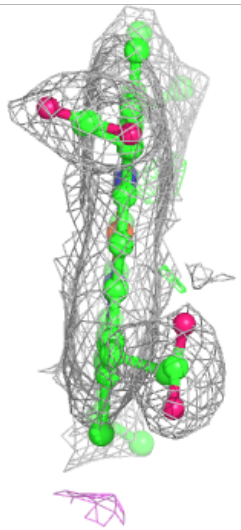


Electron density around HEM A 1306:

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

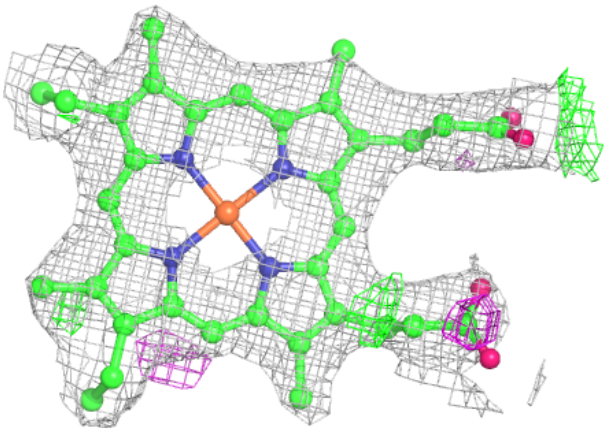


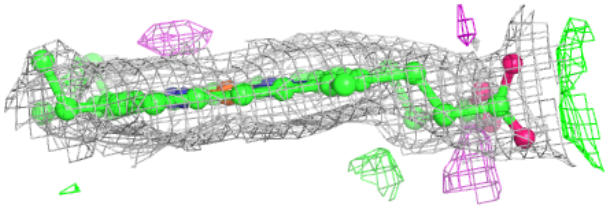


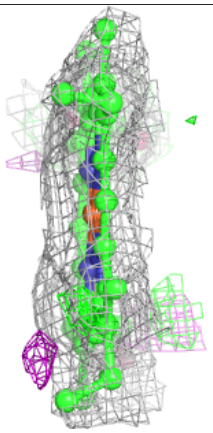


Electron density around HEM A 1307:

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

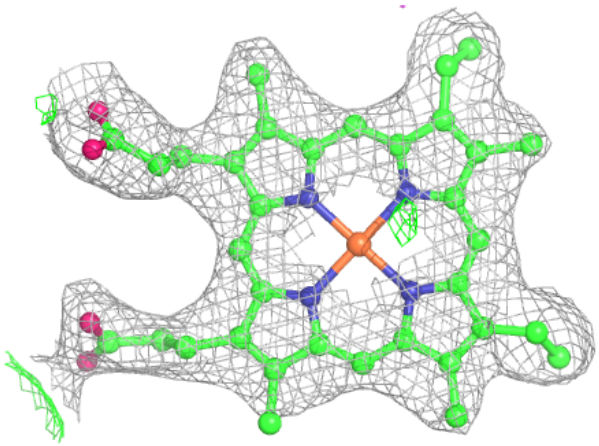


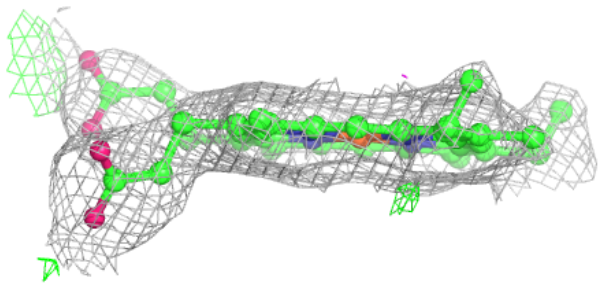


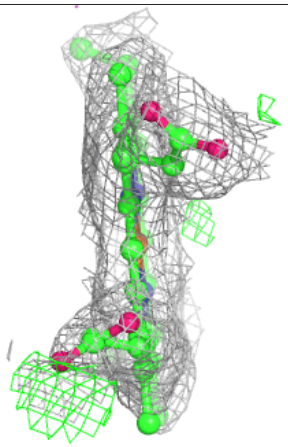


Electron density around HEM A 1313:

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

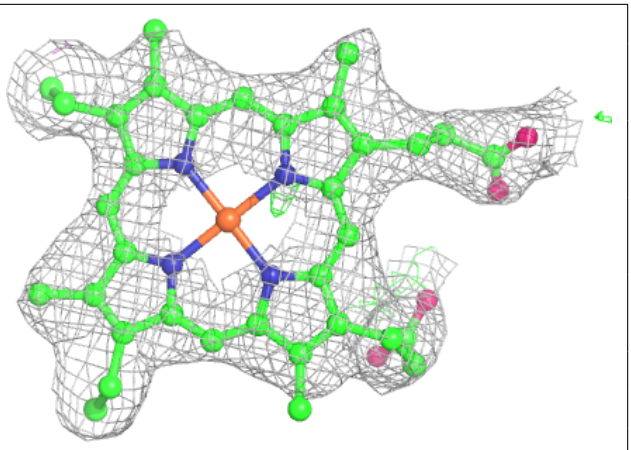


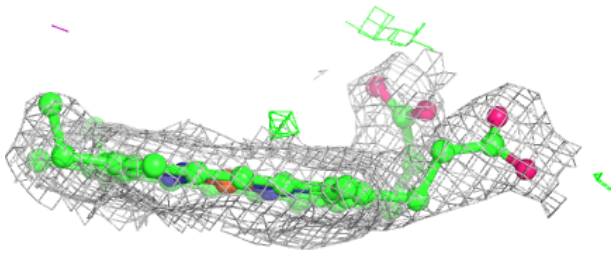


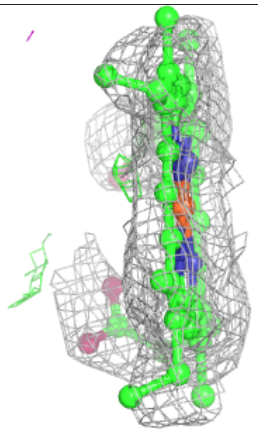


Electron density around HEM A 1314:

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

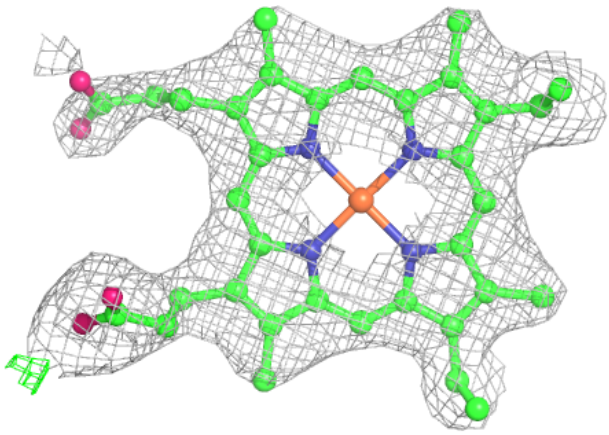


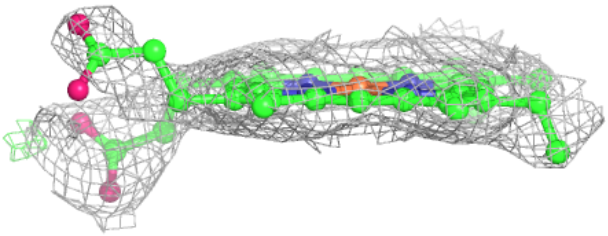


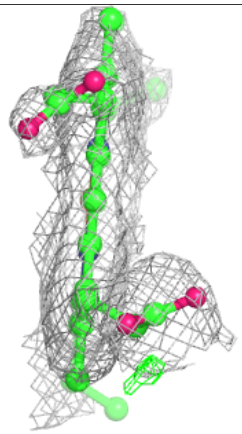


Electron density around HEM A 1302:

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

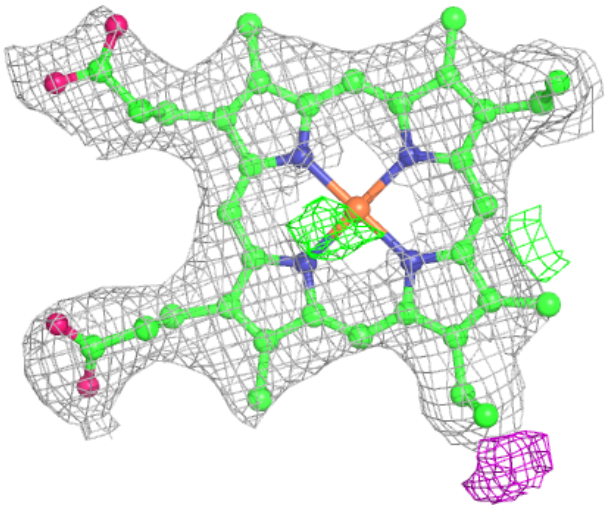


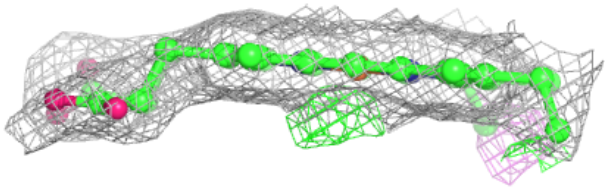




Electron density around HEM A 1305:

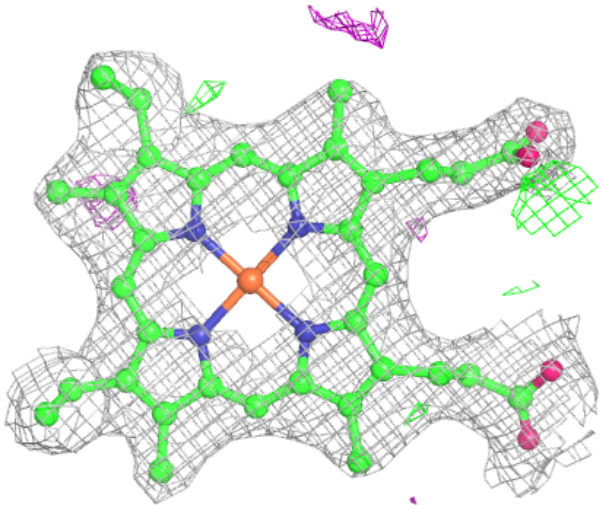
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

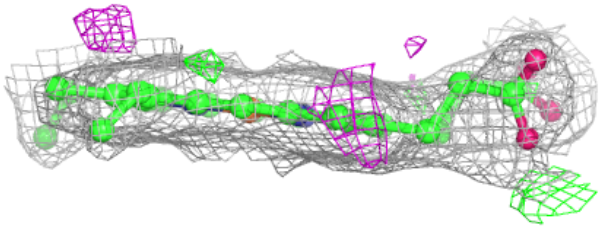


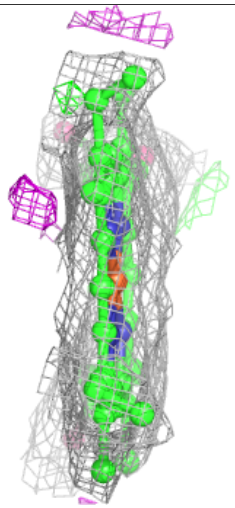


Electron density around HEM A 1308:

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

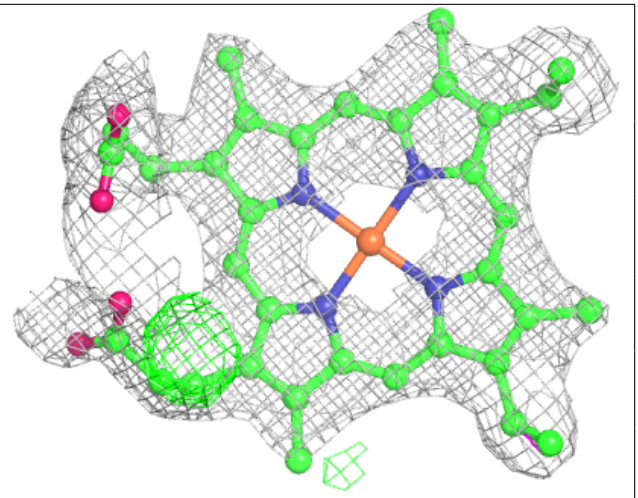


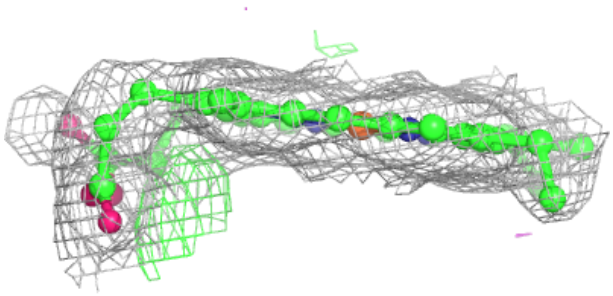


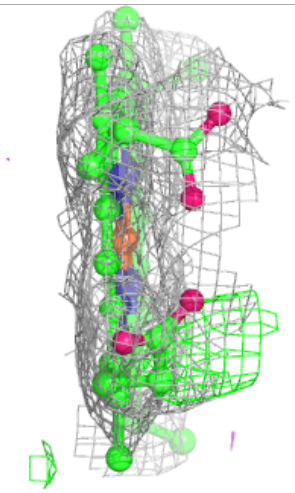


Electron density around HEM A 1309:

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

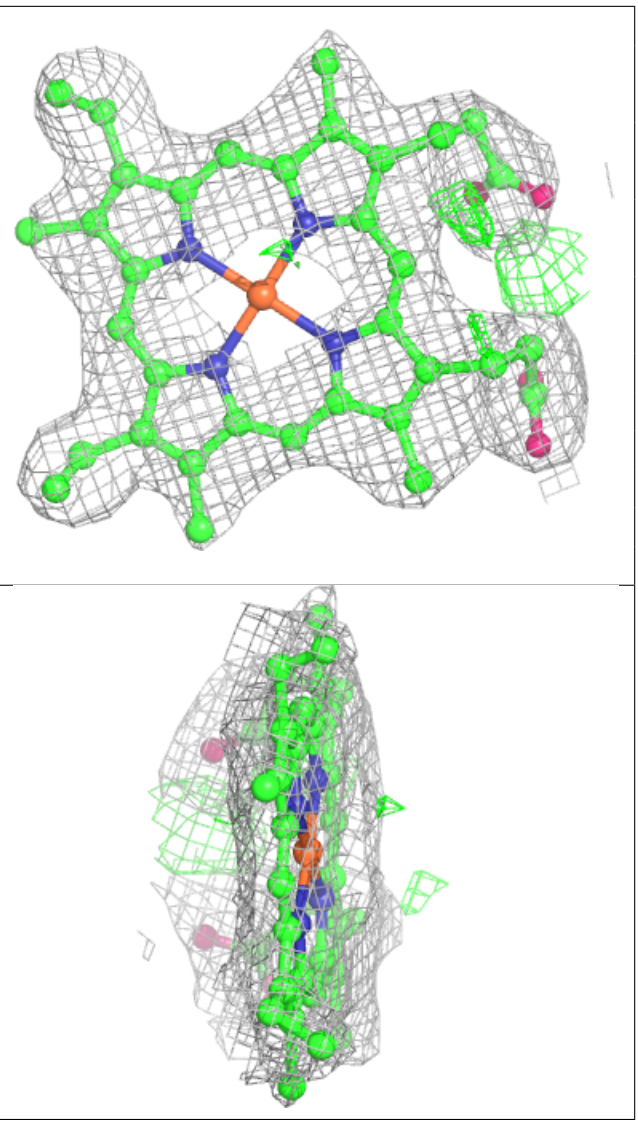






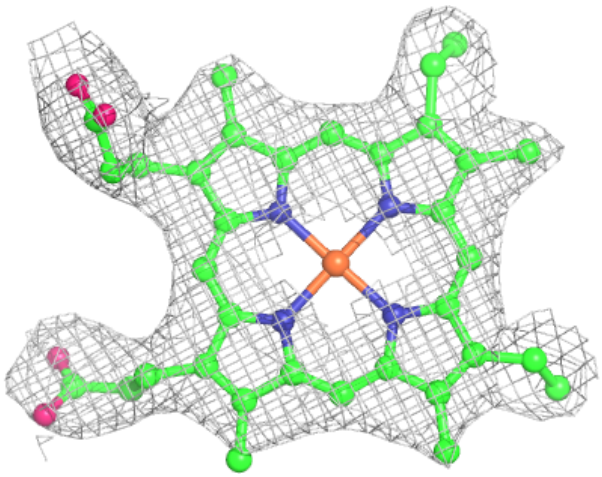
Electron density around HEM A 1312:

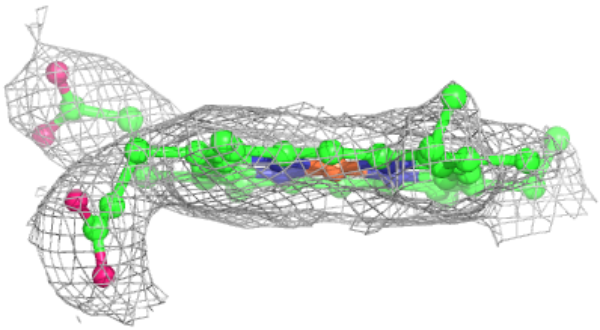
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

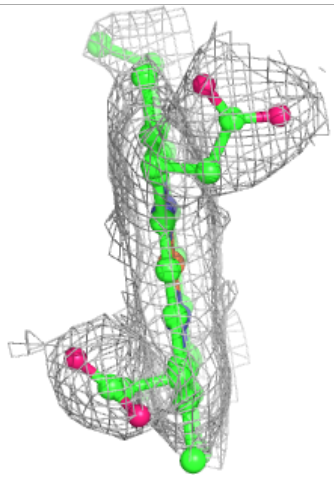


Electron density around HEM A 1301:

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

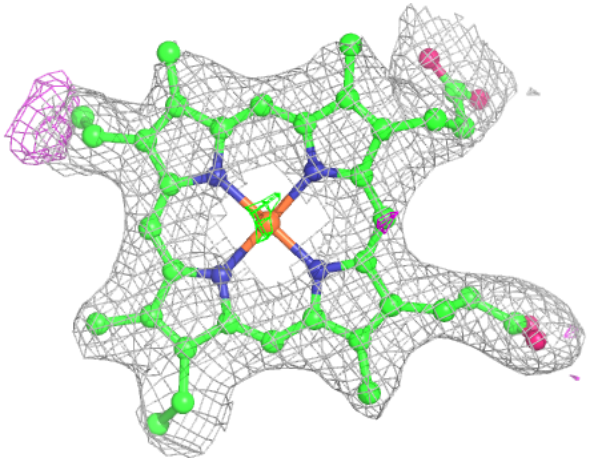


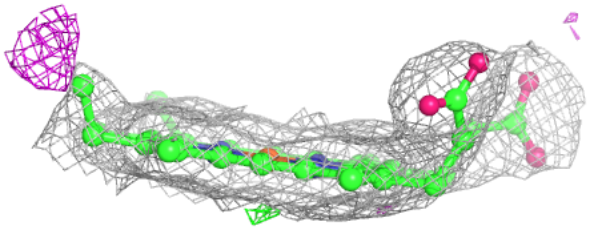


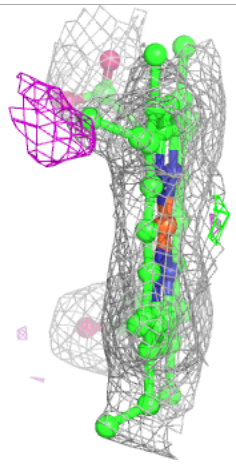


Electron density around HEM A 1310:

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

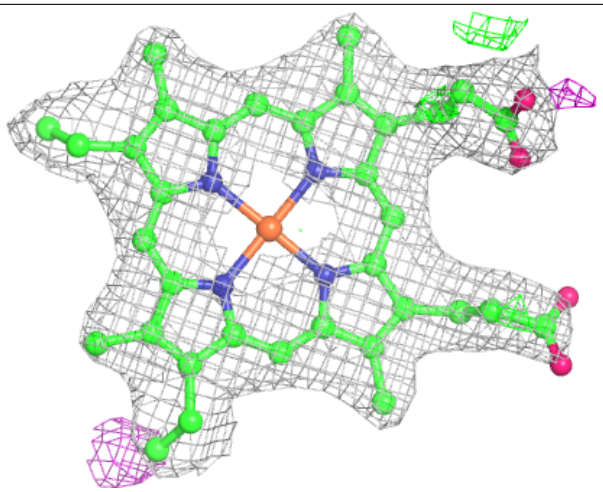


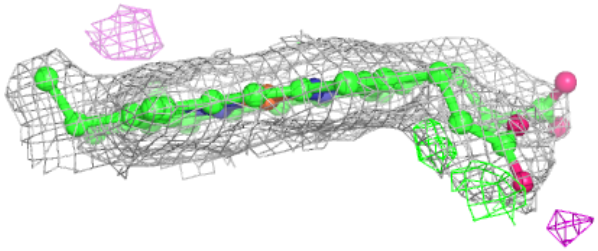


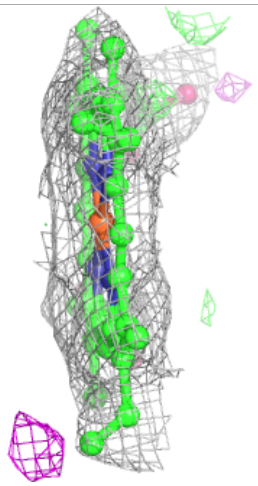


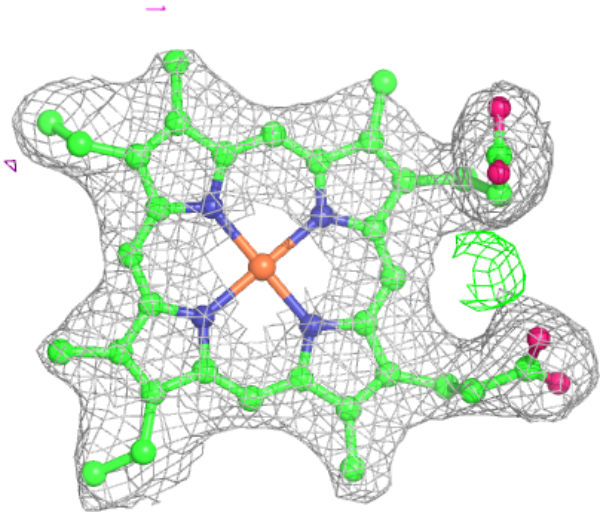
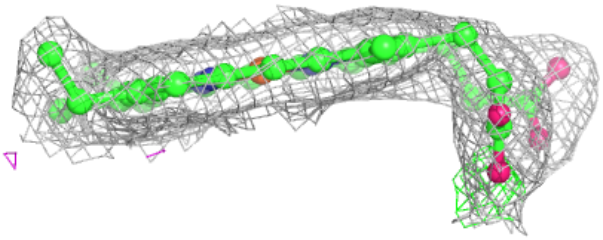
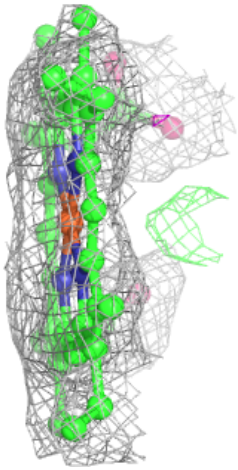
Electron density around HEM A 1311:

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







Electron density around HEM A 1316: 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.