wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 05:06 PM EDT

PDB ID	:	6NIN
Title	:	Rhodobacter sphaeroides bc1 with STIGMATELLIN A
Authors	:	Xia, D.; Zhou, F.; Esser, L.
Deposited on	:	2018-12-31
Resolution	:	3.60 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 81894 atoms, of which 40305 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 Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	0	0
			6841	2319	3405	545	556	16			
1	E	428	Total	C	H	N	O	S	0	0	0
			6841	2319	3405	545	556	16			
1	K	428	Total	C	H	N	O	S	0	0	0
			6841	2319	3405	545	556	16			
1	O	428	Total	C	H	N	O	S	0	0	0
			6841	2319	3405	545	556	16			
1	S	428	Total	C	H	N	O	S	0	0	0
			6841	2319	3405	545	556	16			
1	W	428	Total	C	H	N	O	S	0	0	0
			6841	2319	3405	545	556	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	CYS	ALA	engineered mutation	UNP A0A344Q9J3
E	185	CYS	ALA	engineered mutation	UNP A0A344Q9J3
K	185	CYS	ALA	engineered mutation	UNP A0A344Q9J3
O	185	CYS	ALA	engineered mutation	UNP A0A344Q9J3
S	185	CYS	ALA	engineered mutation	UNP A0A344Q9J3
W	185	CYS	ALA	engineered mutation	UNP A0A344Q9J3

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			
2	F	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			
2	L	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	P	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			
2	T	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			
2	X	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	264	GLY	-	expression tag	UNP A0A344Q9J2
B	265	THR	-	expression tag	UNP A0A344Q9J2
B	266	GLY	-	expression tag	UNP A0A344Q9J2
B	267	HIS	-	expression tag	UNP A0A344Q9J2
B	268	HIS	-	expression tag	UNP A0A344Q9J2
B	269	HIS	-	expression tag	UNP A0A344Q9J2
B	270	HIS	-	expression tag	UNP A0A344Q9J2
B	271	HIS	-	expression tag	UNP A0A344Q9J2
B	272	HIS	-	expression tag	UNP A0A344Q9J2
F	264	GLY	-	expression tag	UNP A0A344Q9J2
F	265	THR	-	expression tag	UNP A0A344Q9J2
F	266	GLY	-	expression tag	UNP A0A344Q9J2
F	267	HIS	-	expression tag	UNP A0A344Q9J2
F	268	HIS	-	expression tag	UNP A0A344Q9J2
F	269	HIS	-	expression tag	UNP A0A344Q9J2
F	270	HIS	-	expression tag	UNP A0A344Q9J2
F	271	HIS	-	expression tag	UNP A0A344Q9J2
F	272	HIS	-	expression tag	UNP A0A344Q9J2
L	264	GLY	-	expression tag	UNP A0A344Q9J2
L	265	THR	-	expression tag	UNP A0A344Q9J2
L	266	GLY	-	expression tag	UNP A0A344Q9J2
L	267	HIS	-	expression tag	UNP A0A344Q9J2
L	268	HIS	-	expression tag	UNP A0A344Q9J2
L	269	HIS	-	expression tag	UNP A0A344Q9J2
L	270	HIS	-	expression tag	UNP A0A344Q9J2
L	271	HIS	-	expression tag	UNP A0A344Q9J2
L	272	HIS	-	expression tag	UNP A0A344Q9J2
P	264	GLY	-	expression tag	UNP A0A344Q9J2
P	265	THR	-	expression tag	UNP A0A344Q9J2
P	266	GLY	-	expression tag	UNP A0A344Q9J2
P	267	HIS	-	expression tag	UNP A0A344Q9J2
P	268	HIS	-	expression tag	UNP A0A344Q9J2

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Chain	Residue	Modelled	Actual	Comment	Reference
P	269	HIS	-	expression tag	UNP A0A344Q9J2
P	270	HIS	-	expression tag	UNP A0A344Q9J2
P	271	HIS	-	expression tag	UNP A0A344Q9J2
P	272	HIS	-	expression tag	UNP A0A344Q9J2
T	264	GLY	-	expression tag	UNP A0A344Q9J2
T	265	THR	-	expression tag	UNP A0A344Q9J2
T	266	GLY	-	expression tag	UNP A0A344Q9J2
T	267	HIS	-	expression tag	UNP A0A344Q9J2
T	268	HIS	-	expression tag	UNP A0A344Q9J2
T	269	HIS	-	expression tag	UNP A0A344Q9J2
T	270	HIS	-	expression tag	UNP A0A344Q9J2
T	271	HIS	-	expression tag	UNP A0A344Q9J2
T	272	HIS	-	expression tag	UNP A0A344Q9J2
X	264	GLY	-	expression tag	UNP A0A344Q9J2
X	265	THR	-	expression tag	UNP A0A344Q9J2
X	266	GLY	-	expression tag	UNP A0A344Q9J2
X	267	HIS	-	expression tag	UNP A0A344Q9J2
X	268	HIS	-	expression tag	UNP A0A344Q9J2
X	269	HIS	-	expression tag	UNP A0A344Q9J2
X	270	HIS	-	expression tag	UNP A0A344Q9J2
X	271	HIS	-	expression tag	UNP A0A344Q9J2
X	272	HIS	-	expression tag	UNP A0A344Q9J2

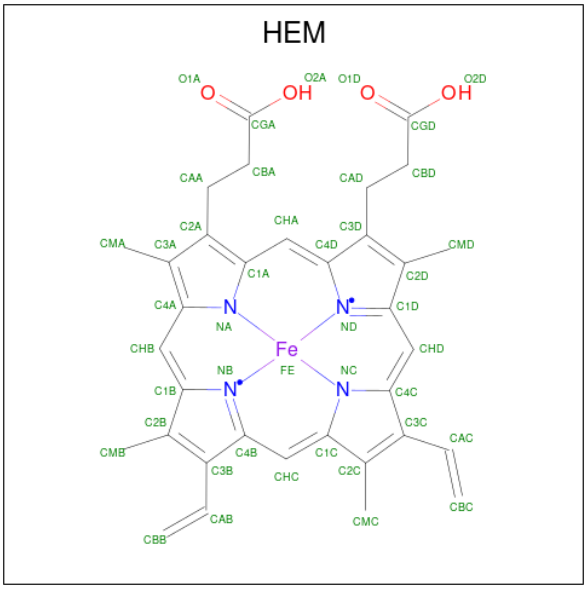
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	179	Total	C	H	N	O	S	0	0	0
			2633	842	1295	236	253	7			
3	G	179	Total	C	H	N	O	S	0	0	0
			2633	842	1295	236	253	7			
3	M	179	Total	C	H	N	O	S	0	0	0
			2633	842	1295	236	253	7			
3	Q	179	Total	C	H	N	O	S	0	0	0
			2633	842	1295	236	253	7			
3	U	179	Total	C	H	N	O	S	0	0	0
			2633	842	1295	236	253	7			
3	Y	179	Total	C	H	N	O	S	0	0	0
			2633	842	1295	236	253	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	70	CYS	LYS	engineered mutation	UNP A0A344Q9J4
G	70	CYS	LYS	engineered mutation	UNP A0A344Q9J4
M	70	CYS	LYS	engineered mutation	UNP A0A344Q9J4
Q	70	CYS	LYS	engineered mutation	UNP A0A344Q9J4
U	70	CYS	LYS	engineered mutation	UNP A0A344Q9J4
Y	70	CYS	LYS	engineered mutation	UNP A0A344Q9J4

- 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
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	O	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	O	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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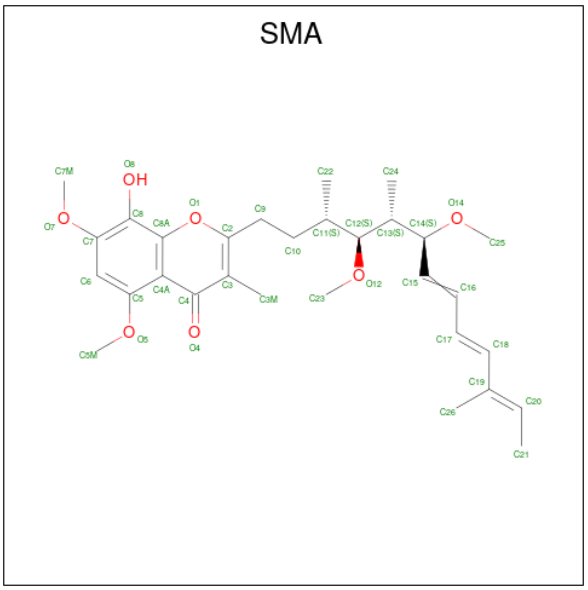
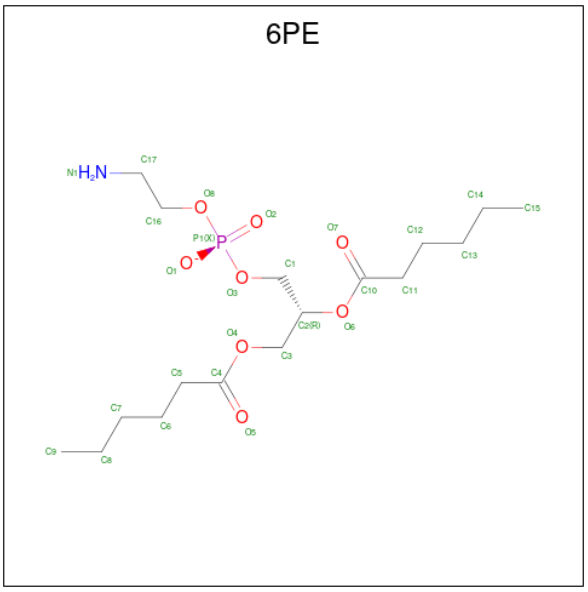
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	S	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	S	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	W	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	W	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 5 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



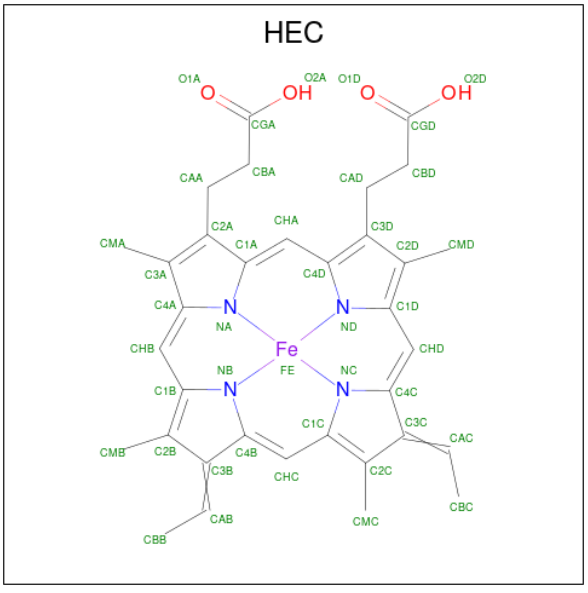
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			79	30	42	7		
5	E	1	Total	C	H	O	0	0
			79	30	42	7		
5	K	1	Total	C	H	O	0	0
			79	30	42	7		
5	O	1	Total	C	H	O	0	0
			79	30	42	7		
5	S	1	Total	C	H	O	0	0
			79	30	42	7		
5	W	1	Total	C	H	O	0	0
			79	30	42	7		

- Molecule 6 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: $C_{17}H_{33}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		
6	E	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		
6	W	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		

- Molecule 7 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	B	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

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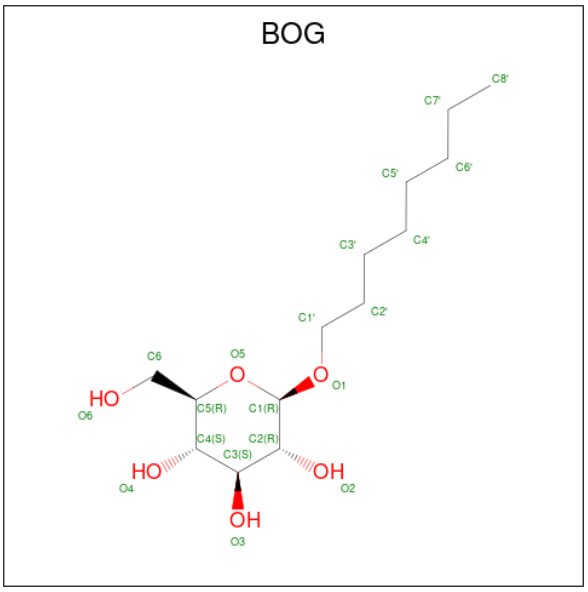
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	F	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
7	L	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
7	P	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
7	T	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
7	X	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 8 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

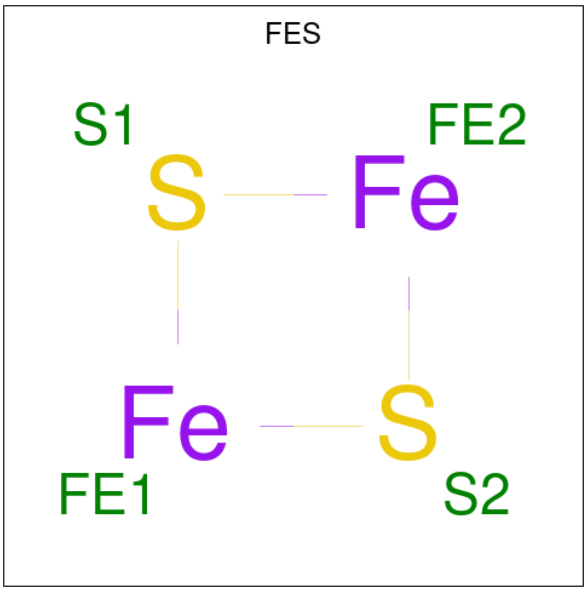
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Sr	0	0
			1	1		
8	F	1	Total	Sr	0	0
			1	1		
8	L	1	Total	Sr	0	0
			1	1		
8	P	1	Total	Sr	0	0
			1	1		
8	T	1	Total	Sr	0	0
			1	1		
8	X	1	Total	Sr	0	0
			1	1		

- Molecule 9 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			48	14	28	6		
9	F	1	Total	C	H	O	0	0
			48	14	28	6		
9	L	1	Total	C	H	O	0	0
			48	14	28	6		
9	P	1	Total	C	H	O	0	0
			48	14	28	6		
9	T	1	Total	C	H	O	0	0
			48	14	28	6		
9	X	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Fe S 4 2 2	0	0
10	G	1	Total Fe S 4 2 2	0	0
10	M	1	Total Fe S 4 2 2	0	0
10	Q	1	Total Fe S 4 2 2	0	0
10	U	1	Total Fe S 4 2 2	0	0
10	Y	1	Total Fe S 4 2 2	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	356.66Å 145.75Å 162.22Å 90.00° 104.97° 90.00°	Depositor
Resolution (Å)	28.91 – 3.60	Depositor
% Data completeness (in resolution range)	97.2 (28.91-3.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.48Å)	Xtriage
Refinement program	PHENIX dev_3339	Depositor
R, R_{free}	0.249 , 0.280	Depositor
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.369	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	81894	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2696e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 45 ligands modelled in this entry, 6 are monoatomic - leaving 39 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	K	1001	1	41,50,50	1.46	5 (12%)	45,82,82	1.47	8 (17%)
6	6PE	A	1004	-	26,26,26	0.54	0	29,31,31	0.67	1 (3%)
4	HEM	S	1002	1	41,50,50	1.46	6 (14%)	45,82,82	1.25	5 (11%)
9	BOG	B	1003	-	20,20,20	0.90	0	25,25,25	0.93	0
5	SMA	O	1003	-	38,38,38	1.79	4 (10%)	48,52,52	1.56	9 (18%)
4	HEM	O	1001	1	41,50,50	1.47	6 (14%)	45,82,82	1.47	7 (15%)
9	BOG	L	1003	-	20,20,20	0.89	0	25,25,25	0.99	0
4	HEM	A	1002	1	41,50,50	1.50	6 (14%)	45,82,82	1.47	6 (13%)
4	HEM	W	1001	1	41,50,50	1.45	5 (12%)	45,82,82	1.39	8 (17%)
7	HEC	X	1001	2	32,50,50	2.11	3 (9%)	24,82,82	1.52	4 (16%)
9	BOG	F	1002	-	20,20,20	0.90	0	25,25,25	0.92	0
9	BOG	X	1003	-	20,20,20	0.92	0	25,25,25	0.93	0
6	6PE	E	1004	-	26,26,26	0.55	0	29,31,31	0.78	1 (3%)
5	SMA	A	1003	-	38,38,38	1.75	2 (5%)	48,52,52	1.48	9 (18%)
4	HEM	A	1001	1	41,50,50	1.47	5 (12%)	45,82,82	1.42	7 (15%)
4	HEM	E	1001	1	41,50,50	1.46	7 (17%)	45,82,82	1.36	5 (11%)
10	FES	C	1001	3	0,4,4	-	-	-		
4	HEM	W	1002	1	41,50,50	1.55	5 (12%)	45,82,82	1.33	6 (13%)
5	SMA	W	1003	-	38,38,38	1.72	4 (10%)	48,52,52	1.54	9 (18%)
9	BOG	T	1003	-	20,20,20	0.88	0	25,25,25	0.99	0
10	FES	M	1001	3	0,4,4	-	-	-		
5	SMA	E	1003	-	38,38,38	1.64	3 (7%)	48,52,52	1.62	10 (20%)
6	6PE	W	1004	-	26,26,26	0.55	0	29,31,31	0.70	0
7	HEC	B	1001	2	32,50,50	2.10	4 (12%)	24,82,82	1.44	1 (4%)
4	HEM	E	1002	1	41,50,50	1.49	5 (12%)	45,82,82	1.48	7 (15%)
5	SMA	S	1003	-	38,38,38	1.75	3 (7%)	48,52,52	1.56	9 (18%)
10	FES	U	1001	3	0,4,4	-	-	-		
10	FES	G	1001	3	0,4,4	-	-	-		
7	HEC	F	1001	2	32,50,50	2.08	3 (9%)	24,82,82	1.56	3 (12%)
4	HEM	S	1001	1	41,50,50	1.48	7 (17%)	45,82,82	1.48	7 (15%)
9	BOG	P	1002	-	20,20,20	0.92	0	25,25,25	0.90	0
4	HEM	O	1002	1	41,50,50	1.47	5 (12%)	45,82,82	1.36	4 (8%)
7	HEC	P	1001	2	32,50,50	2.08	3 (9%)	24,82,82	1.55	6 (25%)
5	SMA	K	1003	-	38,38,38	1.72	3 (7%)	48,52,52	1.50	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	HEC	T	1001	2	32,50,50	2.09	3 (9%)	24,82,82	1.51	3 (12%)
10	FES	Y	1001	3	0,4,4	-	-	-		
10	FES	Q	1001	3	0,4,4	-	-	-		
4	HEM	K	1002	1	41,50,50	1.53	4 (9%)	45,82,82	1.37	6 (13%)
7	HEC	L	1001	2	32,50,50	2.16	4 (12%)	24,82,82	1.43	2 (8%)

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	K	1001	1	-	2/12/54/54	-
6	6PE	A	1004	-	-	19/30/30/30	-
4	HEM	S	1002	1	-	2/12/54/54	-
9	BOG	B	1003	-	-	2/11/31/31	0/1/1/1
5	SMA	O	1003	-	-	5/34/34/34	0/2/2/2
4	HEM	O	1001	1	-	2/12/54/54	-
9	BOG	L	1003	-	-	2/11/31/31	0/1/1/1
4	HEM	A	1002	1	-	2/12/54/54	-
4	HEM	W	1001	1	-	2/12/54/54	-
7	HEC	X	1001	2	-	2/10/54/54	-
9	BOG	F	1002	-	-	2/11/31/31	0/1/1/1
9	BOG	X	1003	-	-	4/11/31/31	0/1/1/1
6	6PE	E	1004	-	-	12/30/30/30	-
5	SMA	A	1003	-	-	5/34/34/34	0/2/2/2
4	HEM	A	1001	1	-	2/12/54/54	-
4	HEM	E	1001	1	-	2/12/54/54	-
10	FES	C	1001	3	-	-	0/1/1/1
4	HEM	W	1002	1	-	2/12/54/54	-
5	SMA	W	1003	-	-	5/34/34/34	0/2/2/2
9	BOG	T	1003	-	-	0/11/31/31	0/1/1/1
10	FES	M	1001	3	-	-	0/1/1/1
5	SMA	E	1003	-	-	5/34/34/34	0/2/2/2
6	6PE	W	1004	-	-	12/30/30/30	-
7	HEC	B	1001	2	-	2/10/54/54	-
4	HEM	E	1002	1	-	3/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SMA	S	1003	-	-	5/34/34/34	0/2/2/2
10	FES	U	1001	3	-	-	0/1/1/1
10	FES	G	1001	3	-	-	0/1/1/1
7	HEC	F	1001	2	-	4/10/54/54	-
4	HEM	S	1001	1	-	2/12/54/54	-
9	BOG	P	1002	-	-	3/11/31/31	0/1/1/1
4	HEM	O	1002	1	-	2/12/54/54	-
7	HEC	P	1001	2	-	2/10/54/54	-
5	SMA	K	1003	-	-	5/34/34/34	0/2/2/2
7	HEC	T	1001	2	-	4/10/54/54	-
10	FES	Y	1001	3	-	-	0/1/1/1
10	FES	Q	1001	3	-	-	0/1/1/1
4	HEM	K	1002	1	-	4/12/54/54	-
7	HEC	L	1001	2	-	4/10/54/54	-

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1003	SMA	C20-C19	8.64	1.40	1.33
5	S	1003	SMA	C20-C19	8.19	1.40	1.33
5	A	1003	SMA	C20-C19	8.11	1.40	1.33
5	K	1003	SMA	C20-C19	7.94	1.39	1.33
5	W	1003	SMA	C20-C19	7.89	1.39	1.33

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1003	SMA	O5-C5-C4A	4.52	122.14	115.85
5	W	1003	SMA	C5M-O5-C5	-4.29	111.06	117.53
5	W	1003	SMA	O5-C5-C4A	4.21	121.71	115.85
5	S	1003	SMA	O5-C5-C4A	4.18	121.68	115.85
5	S	1003	SMA	O7-C7-C8	4.10	118.67	114.54

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1004	6PE	C16-O8-P1-O1
6	A	1004	6PE	C16-O8-P1-O2

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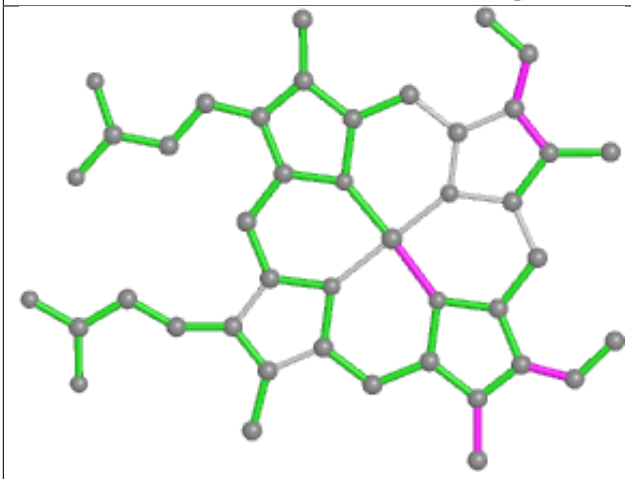
Mol	Chain	Res	Type	Atoms
6	A	1004	6PE	O8-C16-C17-N1
6	E	1004	6PE	C1-O3-P1-O2
6	E	1004	6PE	C1-O3-P1-O8

There are no ring outliers.

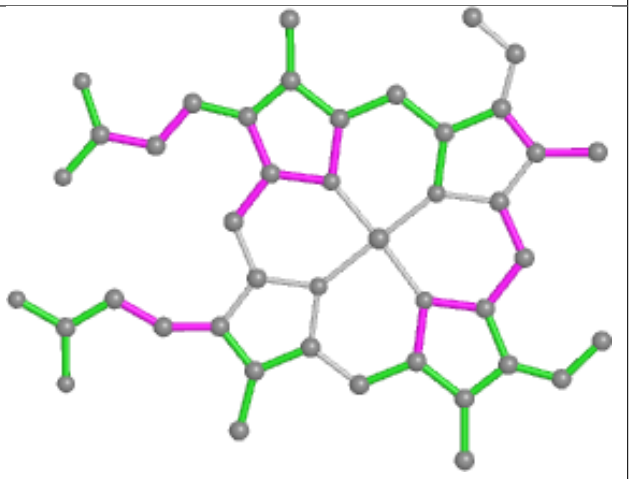
No monomer is involved in short contacts.

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.

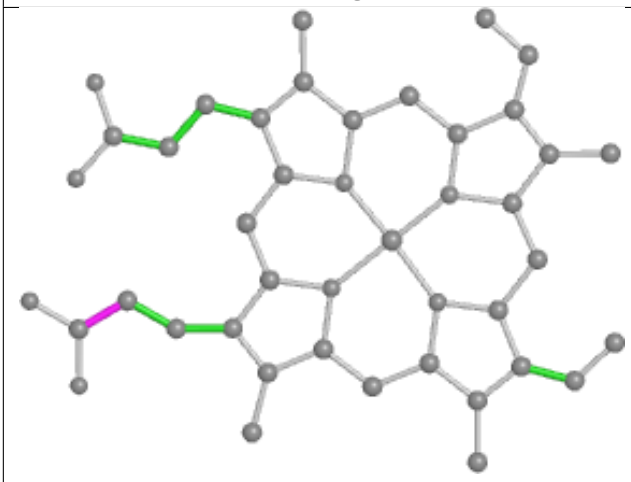
Ligand HEM K 1001



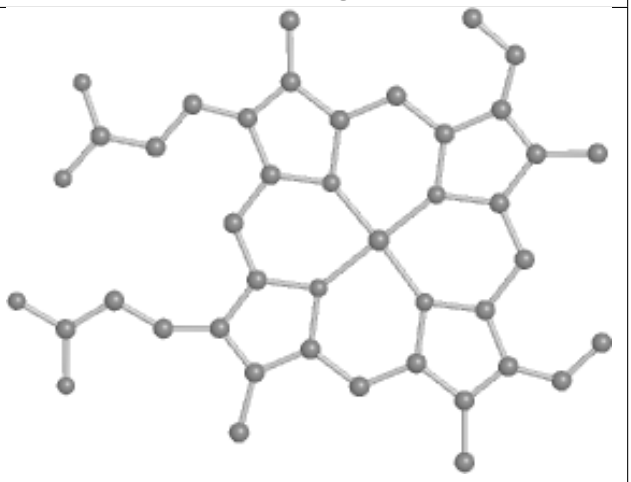
Bond lengths



Bond angles

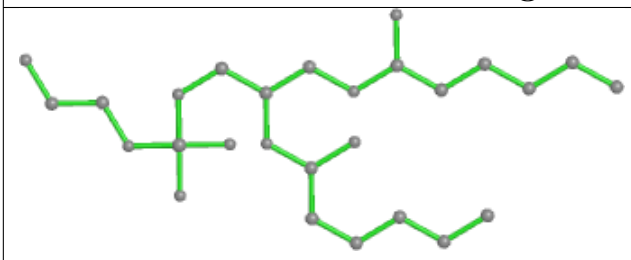


Torsions



Rings

Ligand 6PE A 1004



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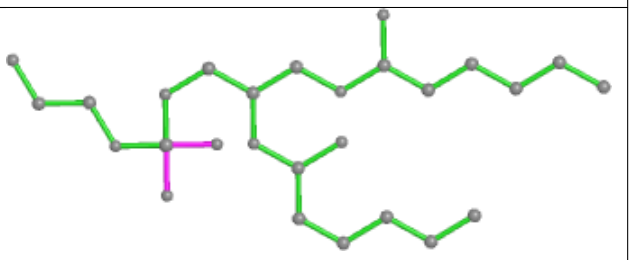
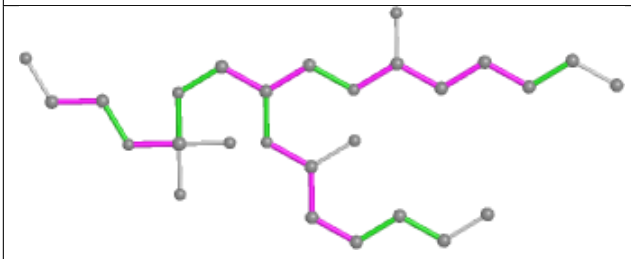


Bond angles



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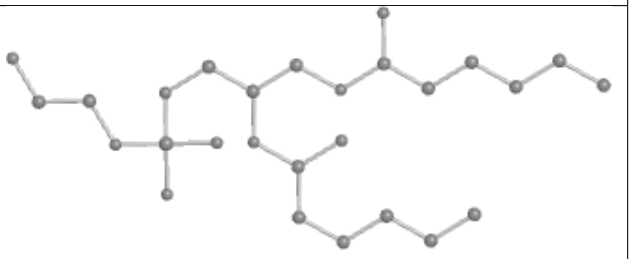
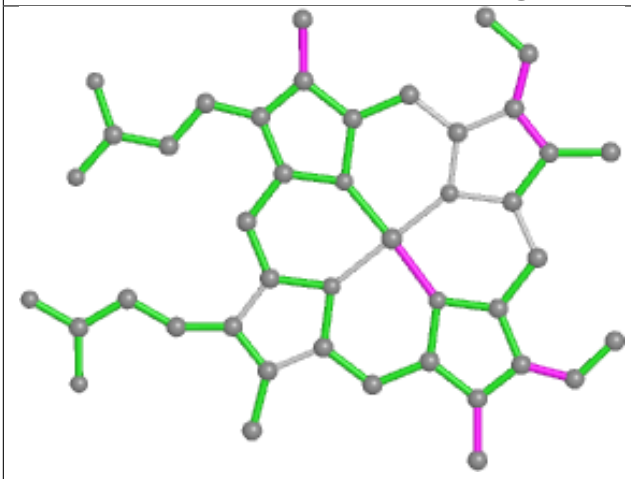
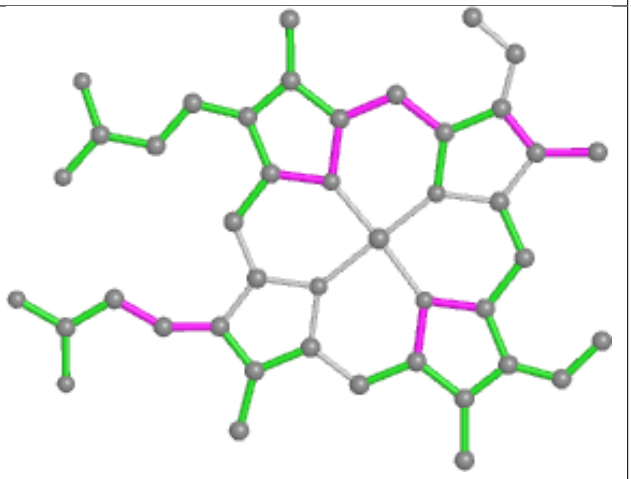


Rings

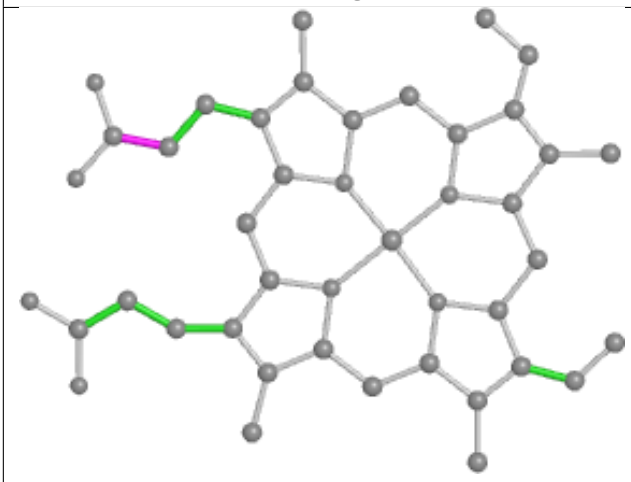
Ligand HEM S 1002



Bond lengths



Bond angles



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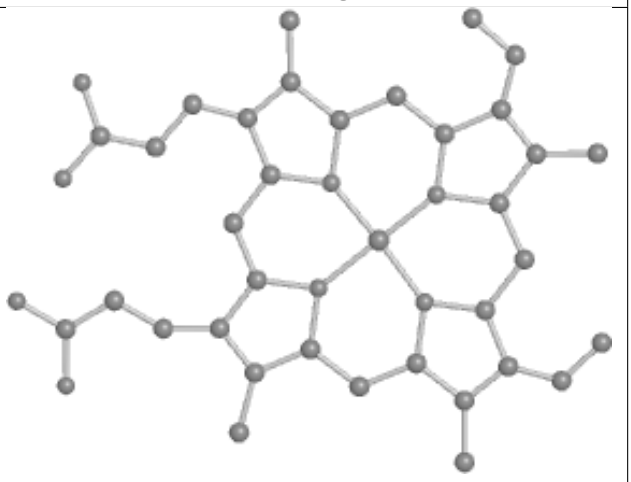
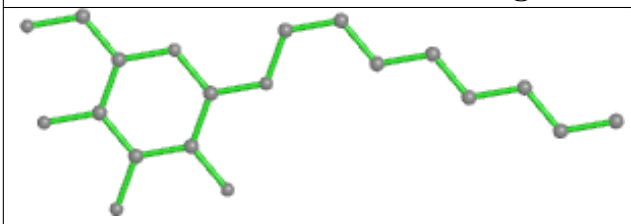
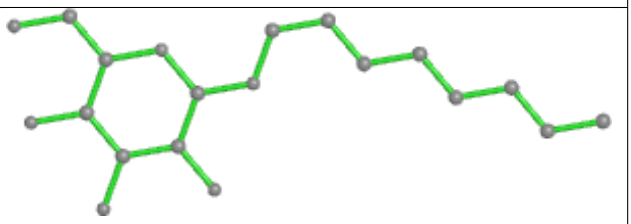


Rings

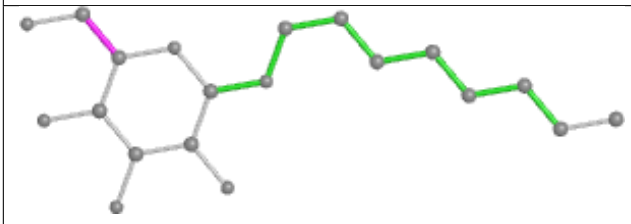
Ligand BOG B 1003



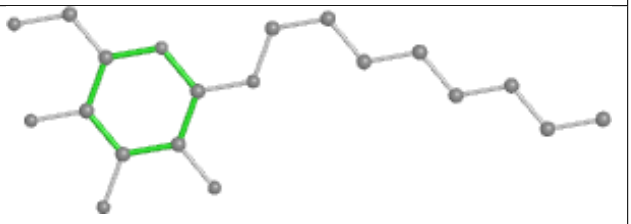
Bond lengths



Bond angles

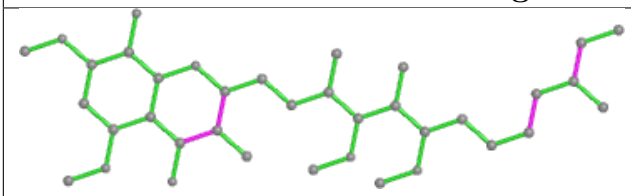


Torsions

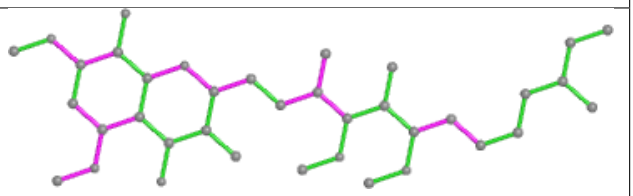


Rings

Ligand SMA O 1003



Bond lengths



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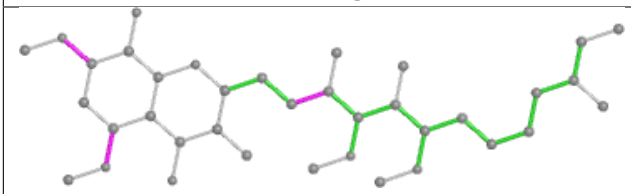

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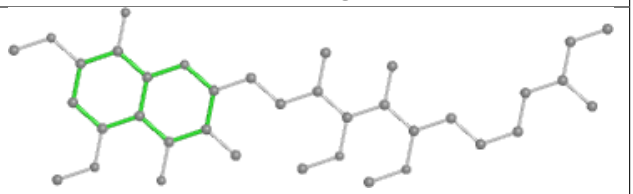
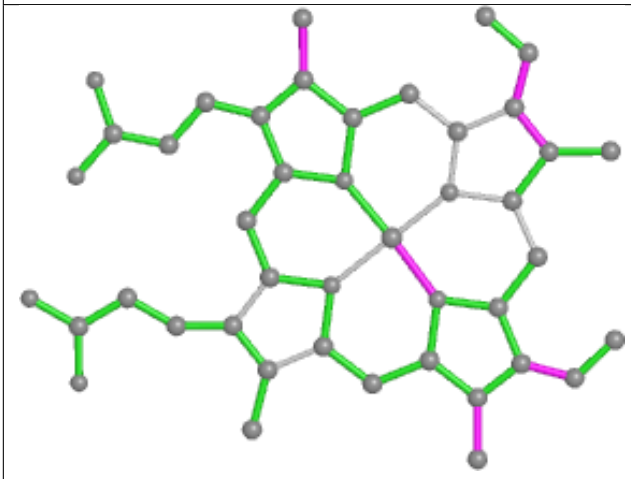


Rings

Ligand HEM O 1001



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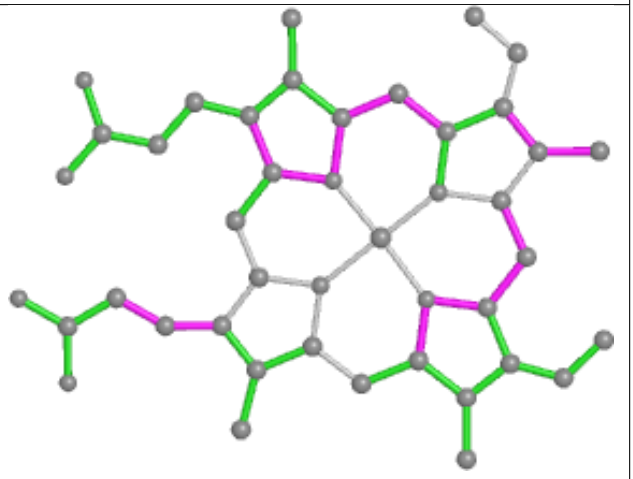

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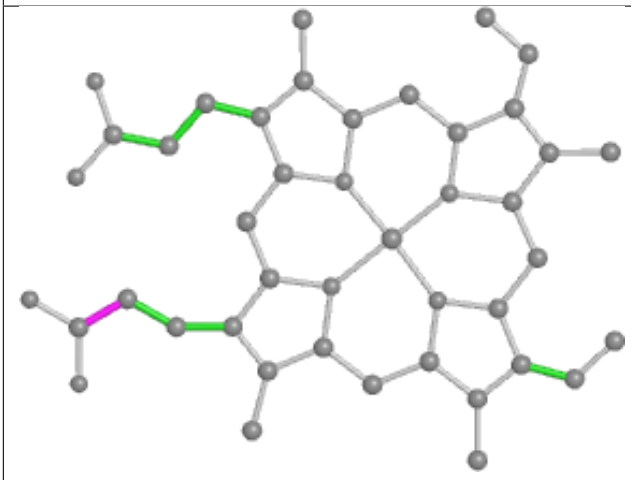

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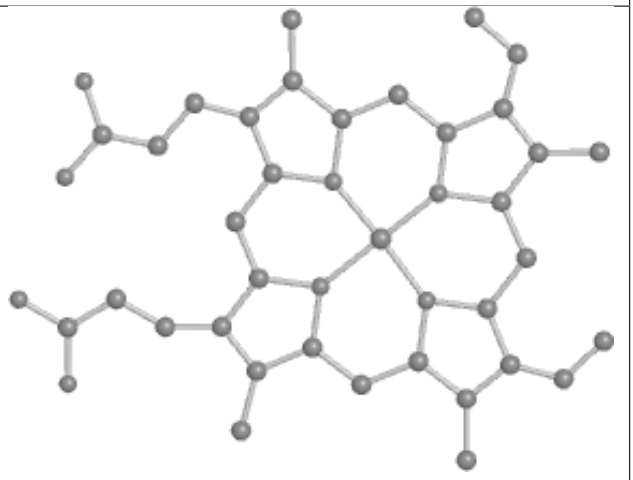
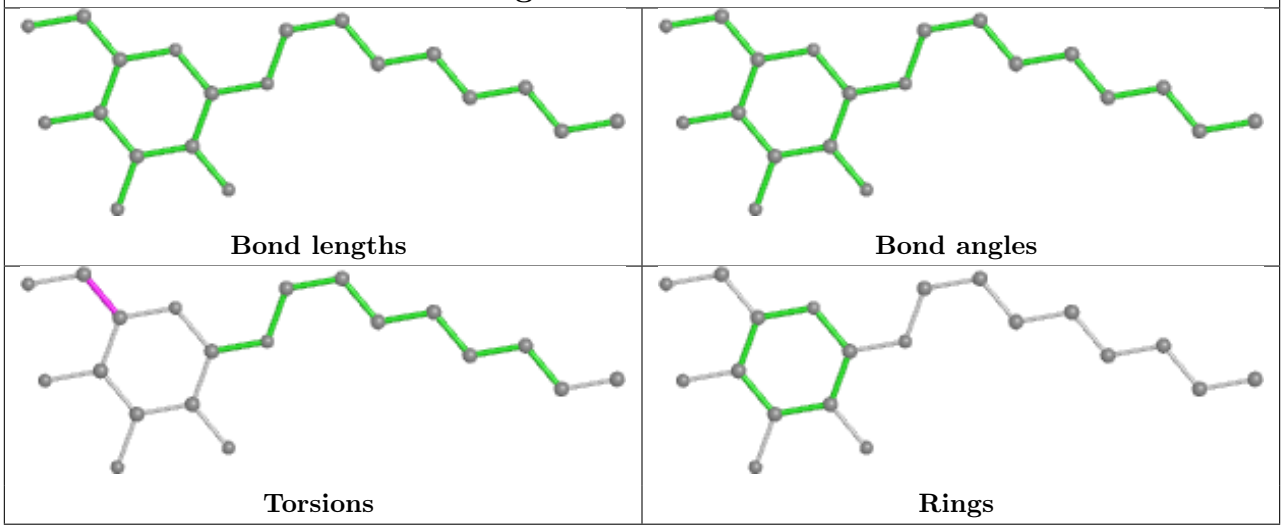
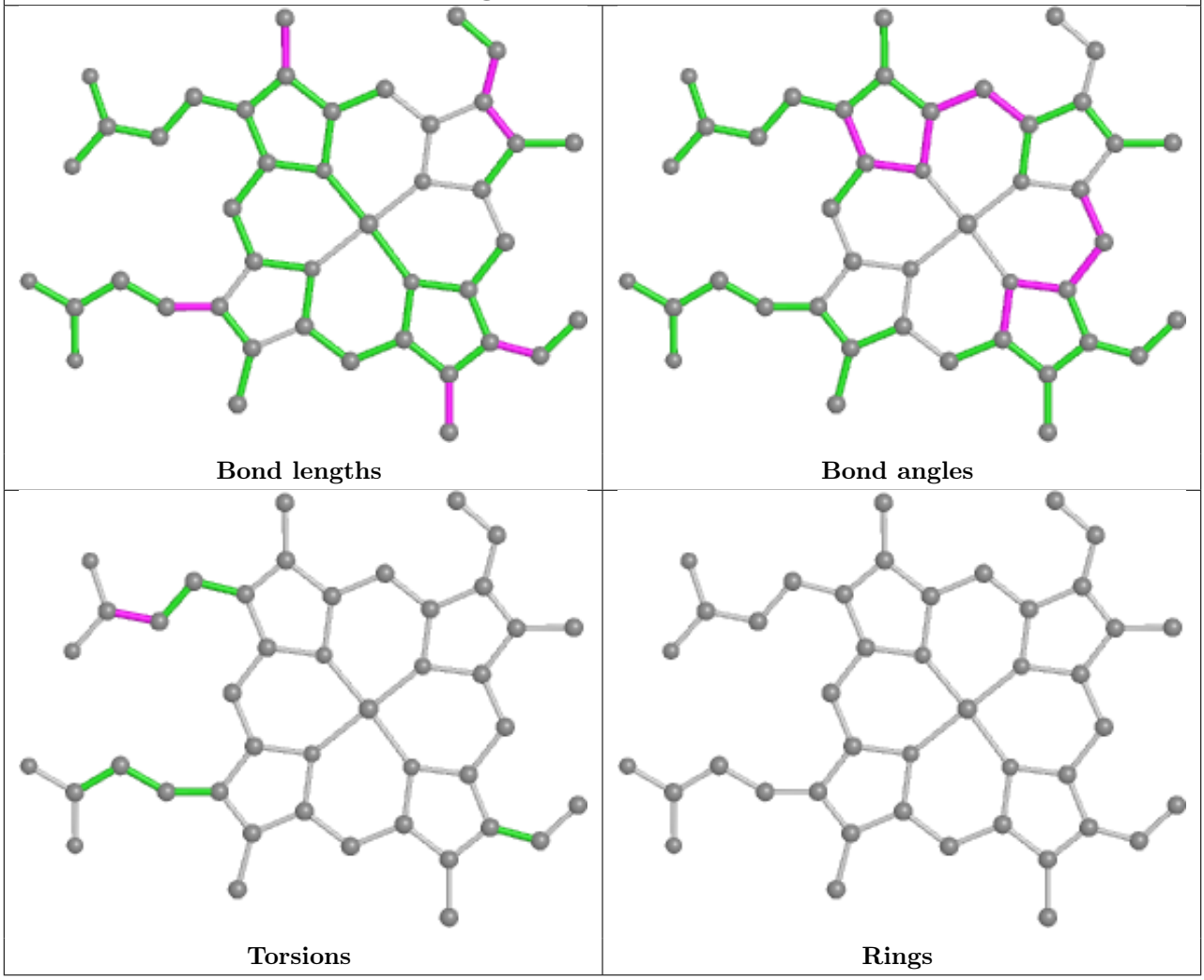


Rings

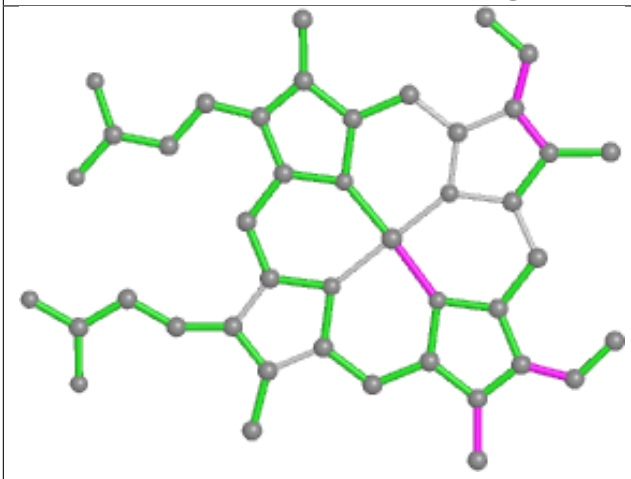
Ligand BOG L 1003



Ligand HEM A 1002



Ligand HEM W 1001



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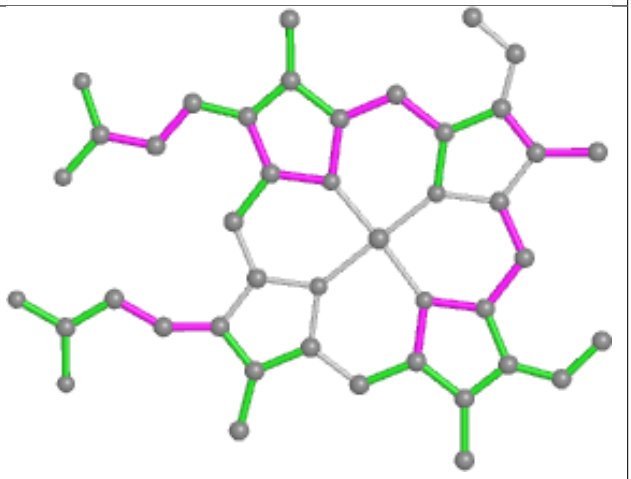

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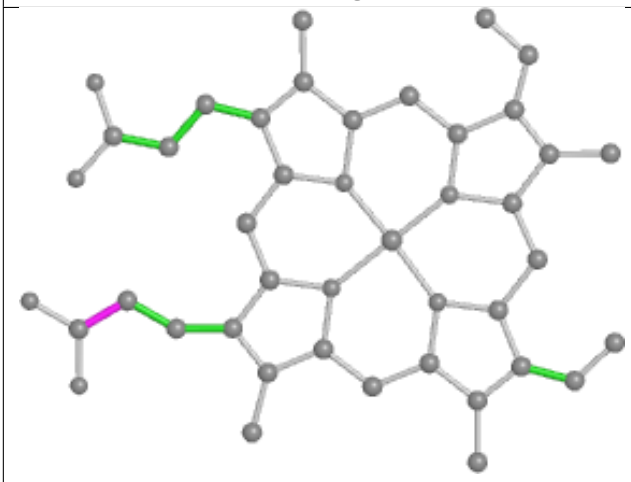

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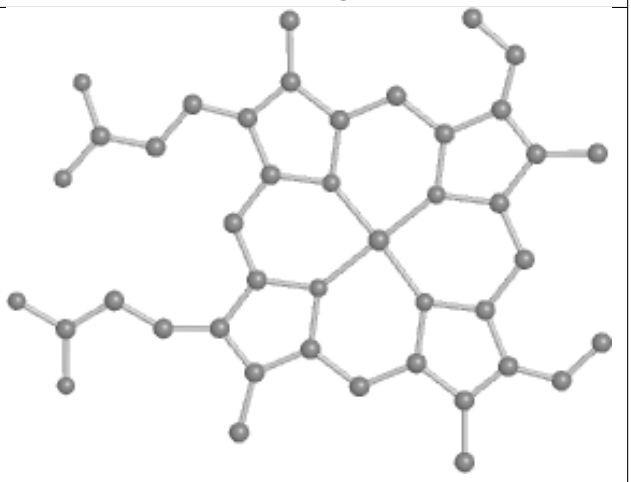
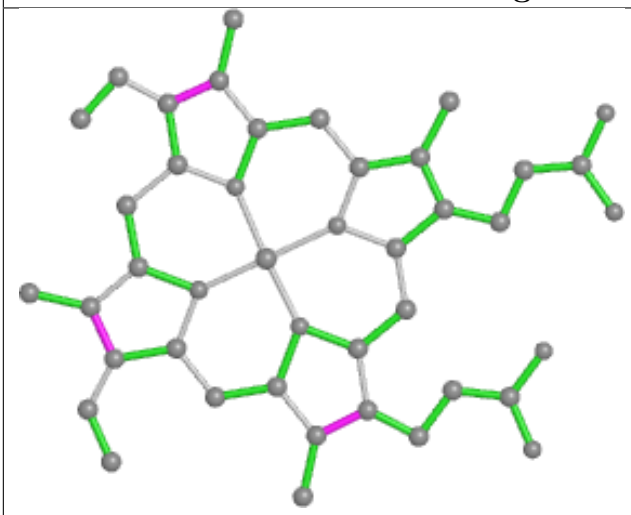
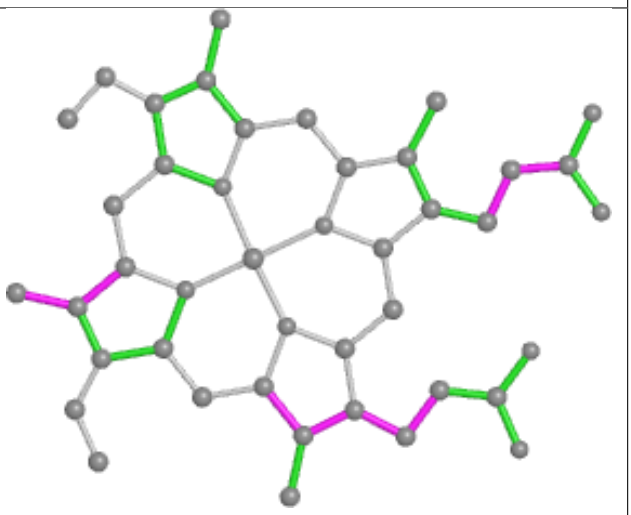


Rings

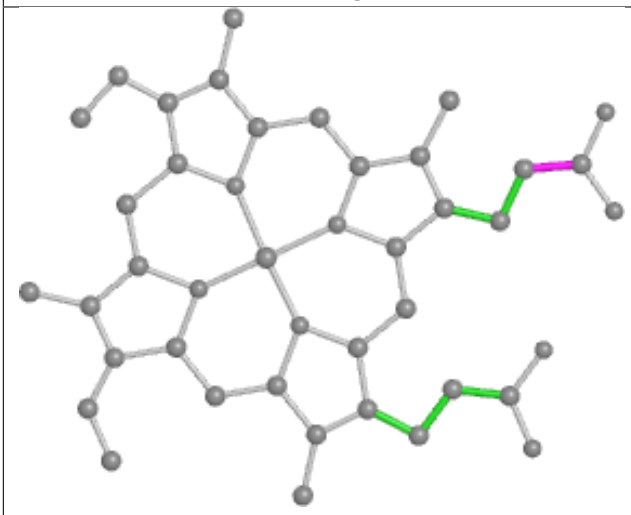
Ligand HEC X 1001



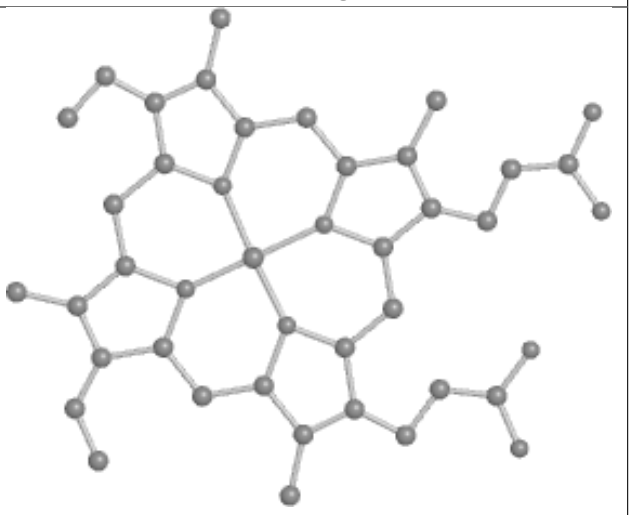
Bond lengths



Bond angles

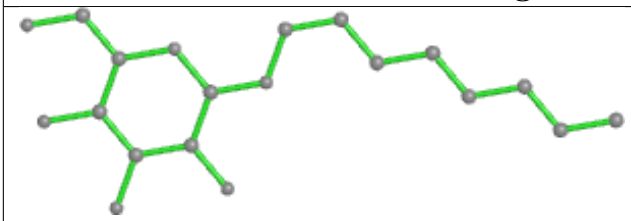


Torsions

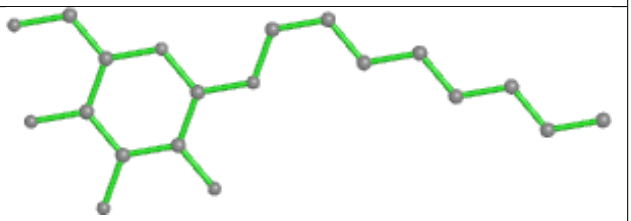


Rings

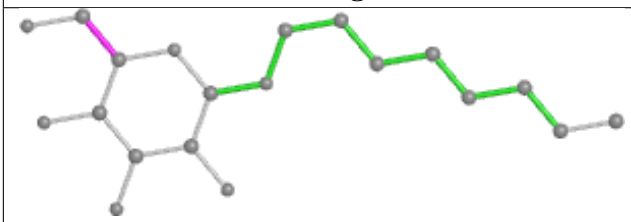
Ligand BOG F 1002



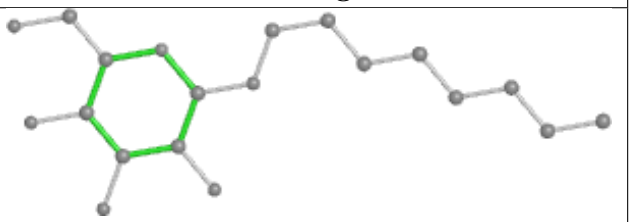
Bond lengths



Bond angles

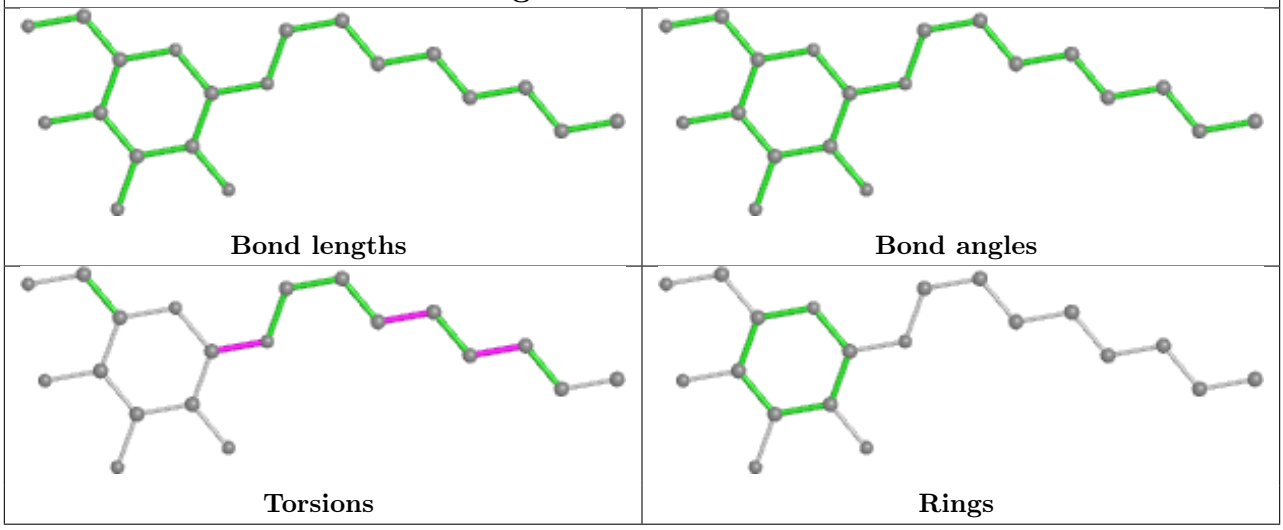


Torsions

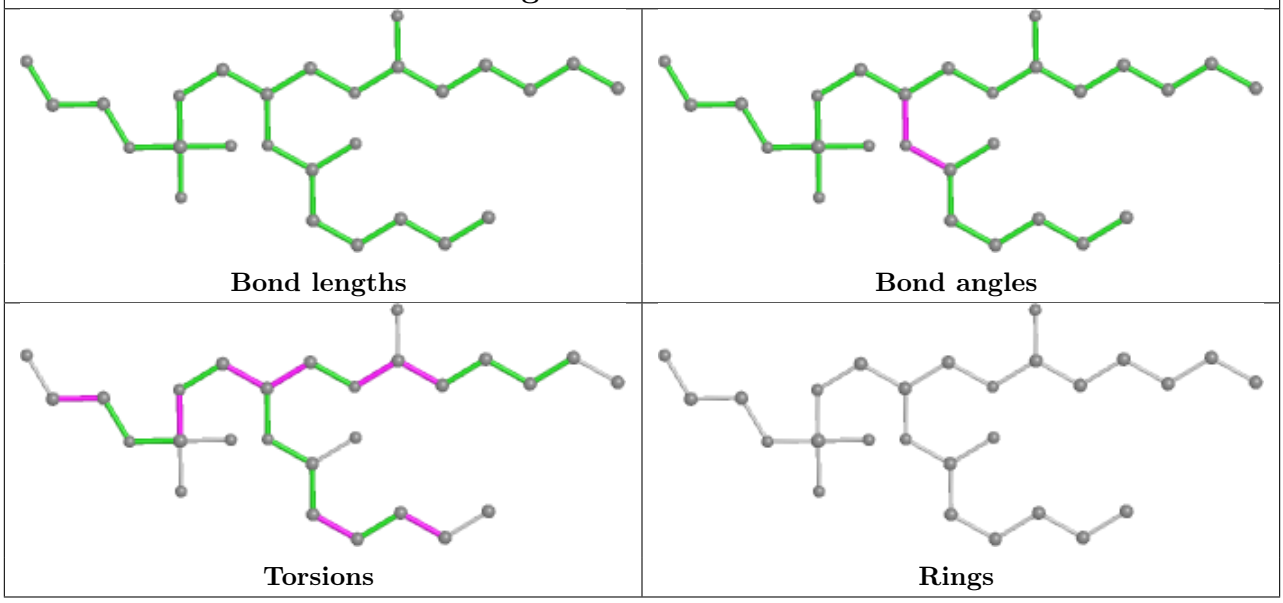


Rings

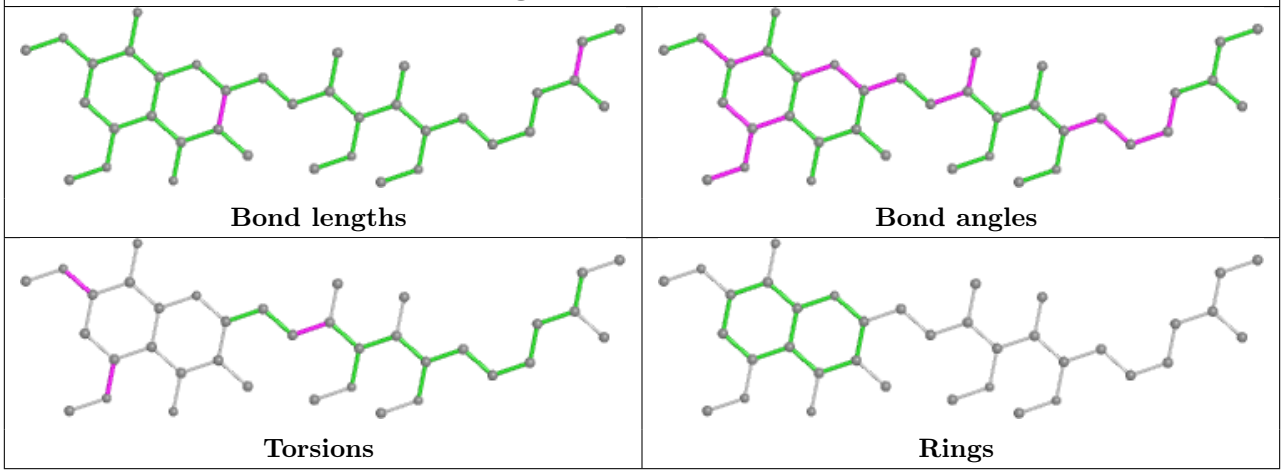
Ligand BOG X 1003



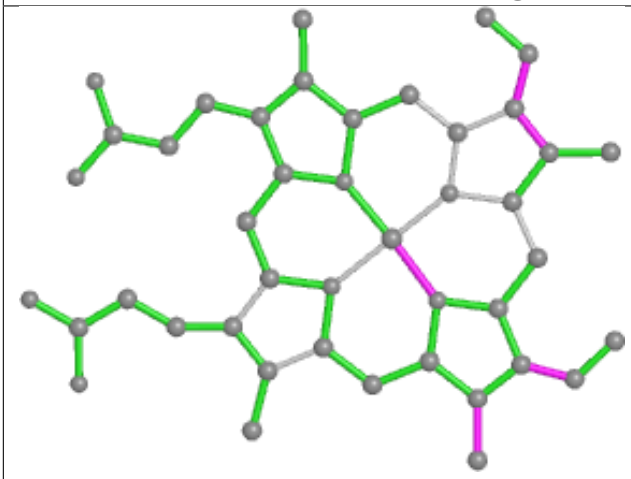
Ligand 6PE E 1004



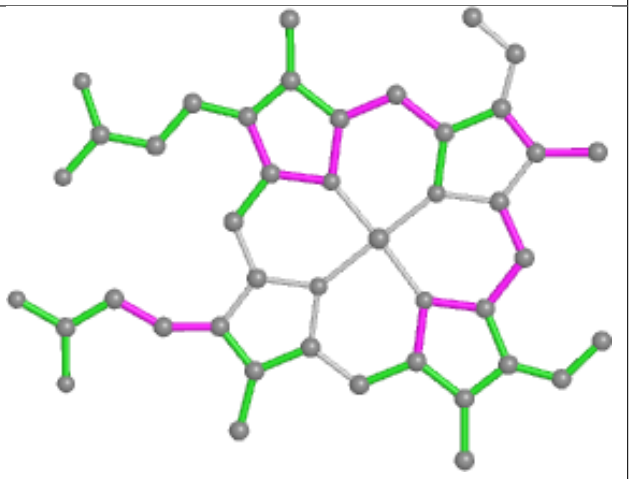
Ligand SMA A 1003



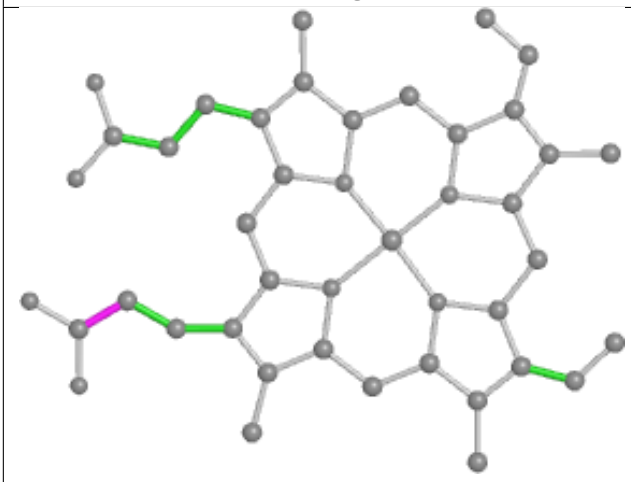
Ligand HEM A 1001



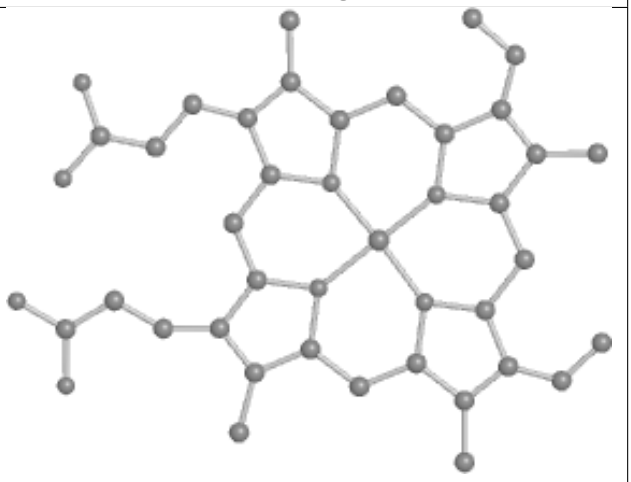
Bond lengths



Bond angles

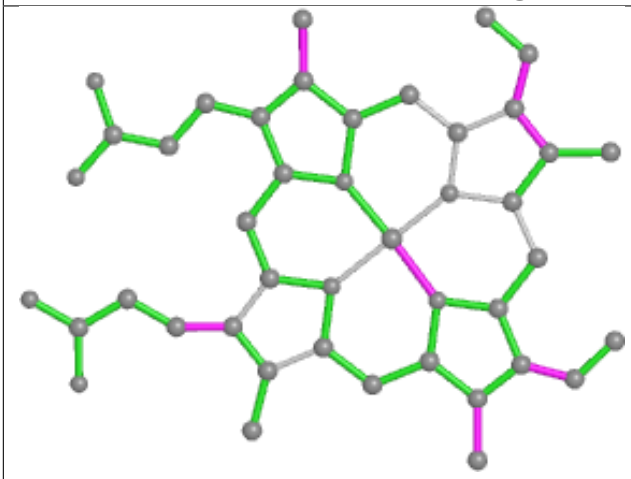


Torsions



Rings

Ligand HEM E 1001



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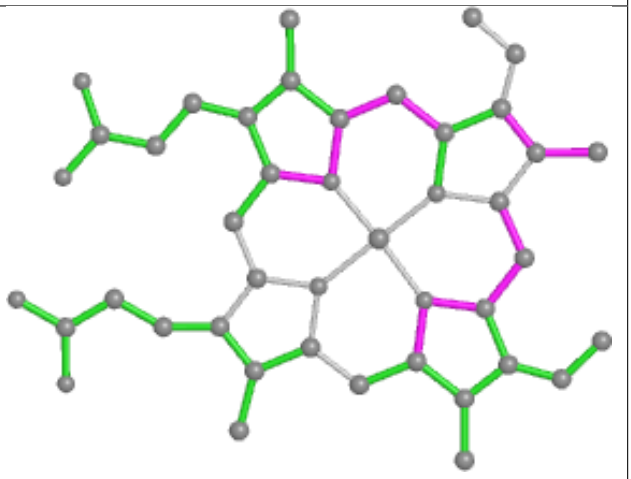
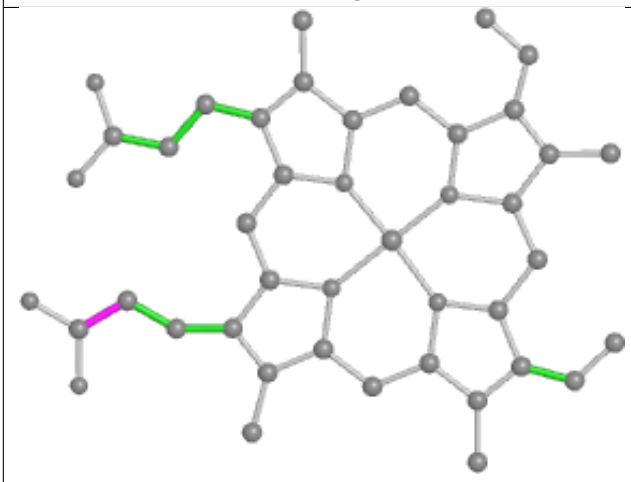
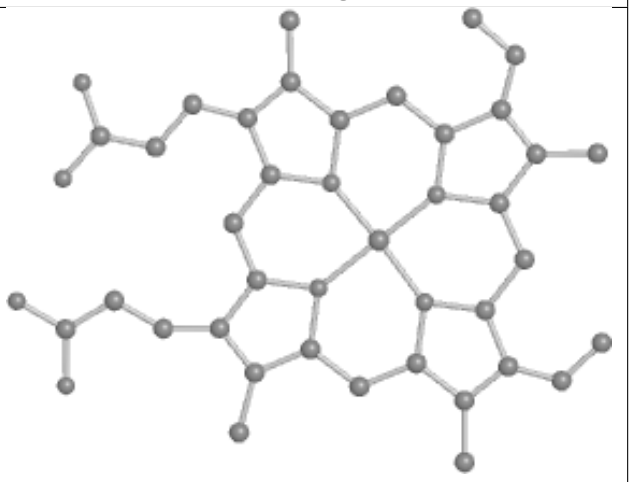


Bond angles

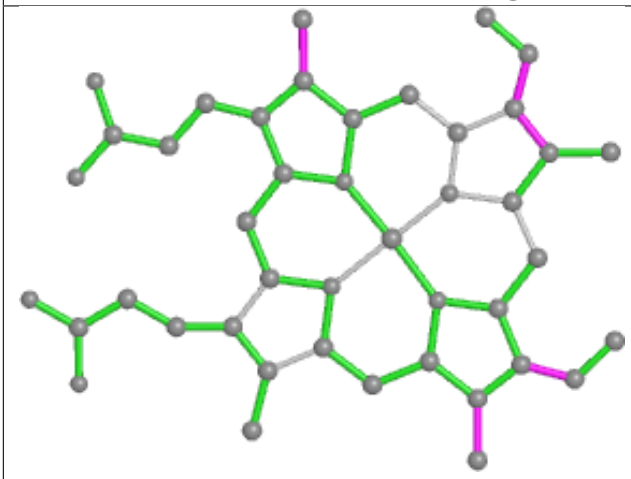


Torsions



Rings

Ligand HEM W 1002



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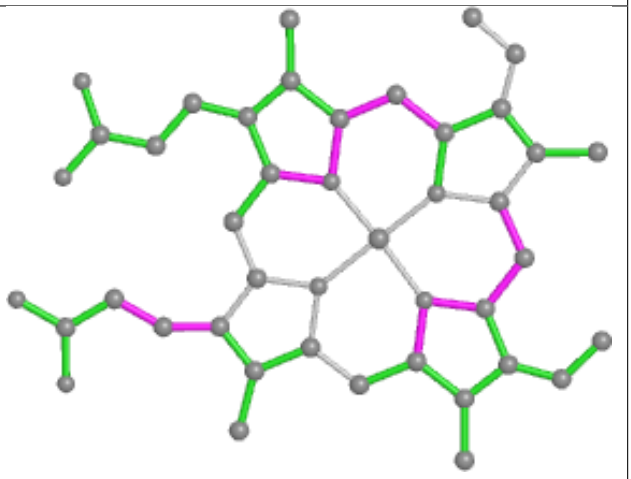
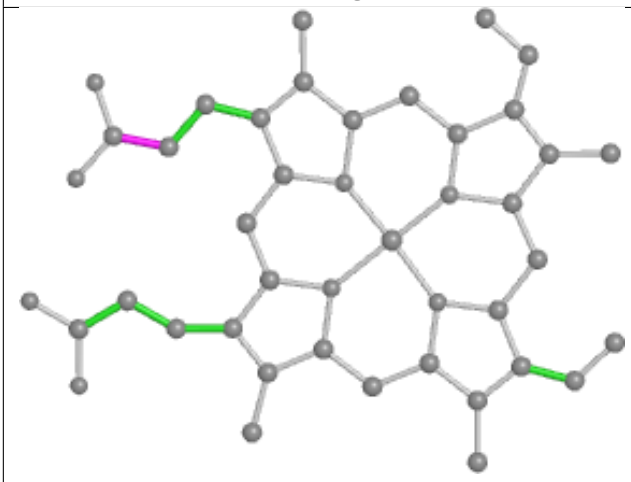
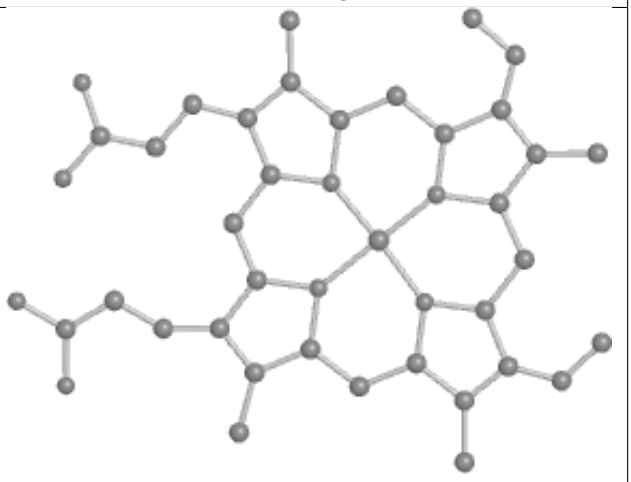


Bond angles

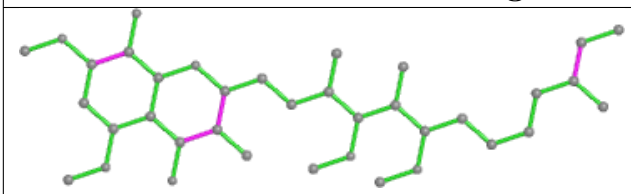


Torsions



Rings

Ligand SMA W 1003



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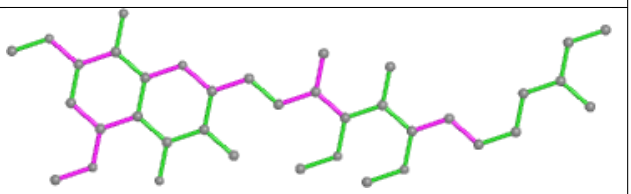
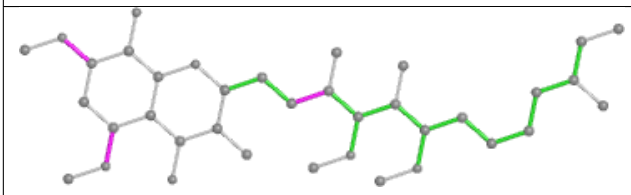
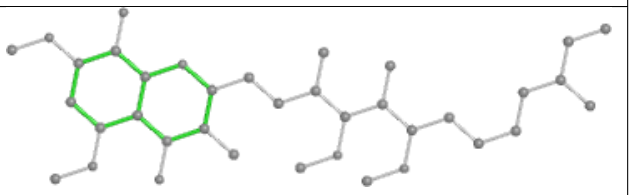


Bond angles

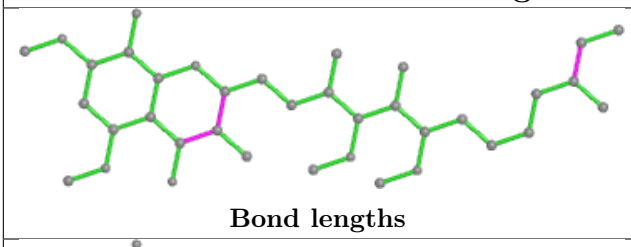


Torsions



Rings

Ligand SMA E 1003



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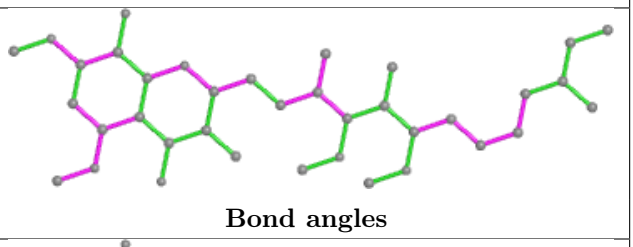
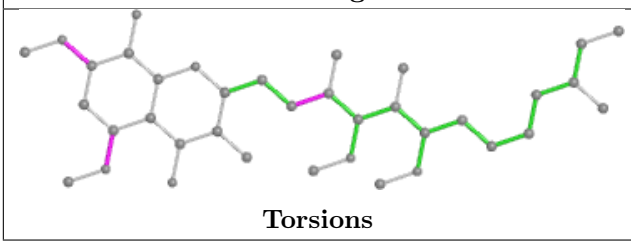
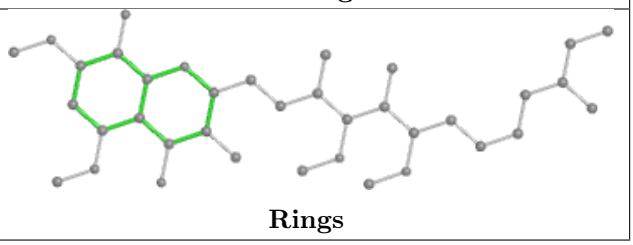


Bond angles

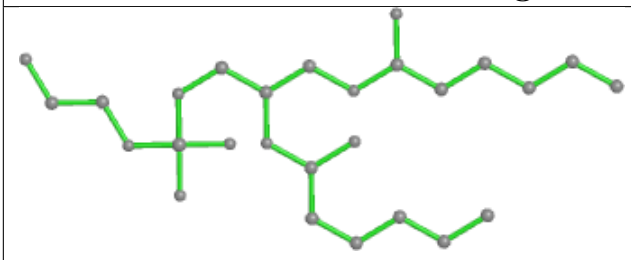


Torsions

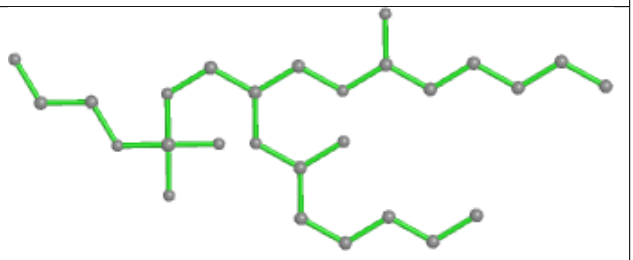


Rings

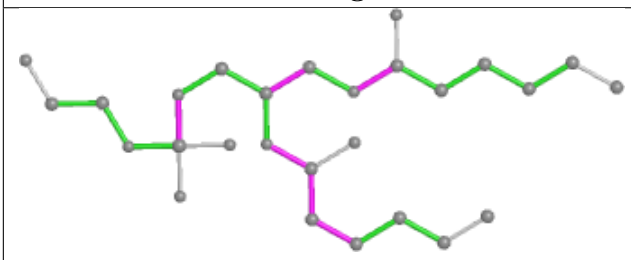
Ligand 6PE W 1004



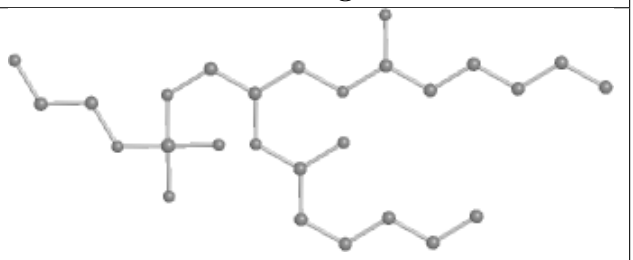
Bond lengths



Bond angles

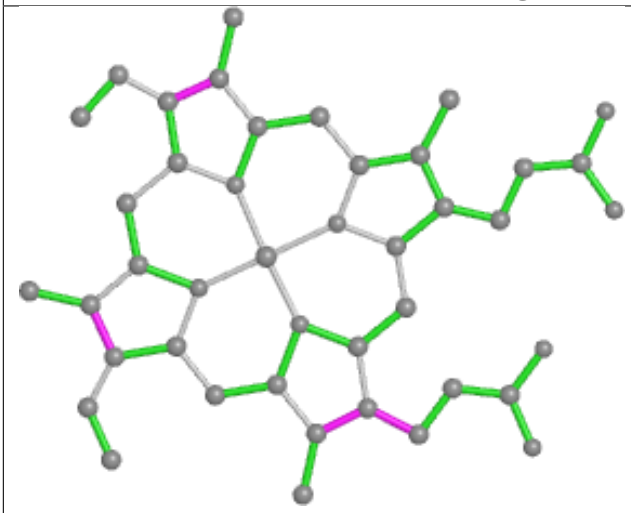


Torsions



Rings

Ligand HEC B 1001



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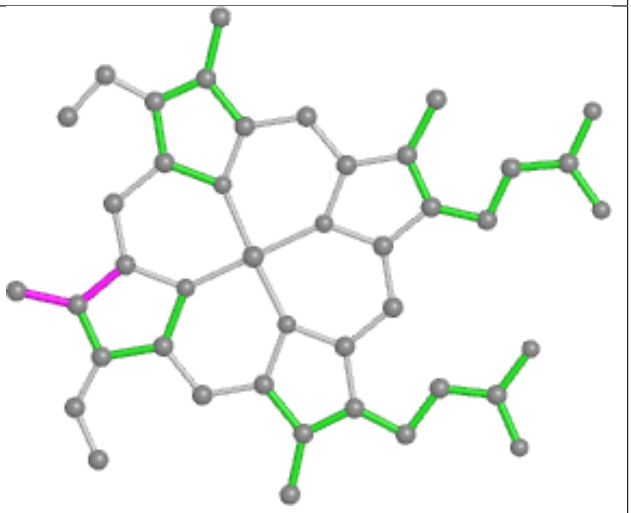
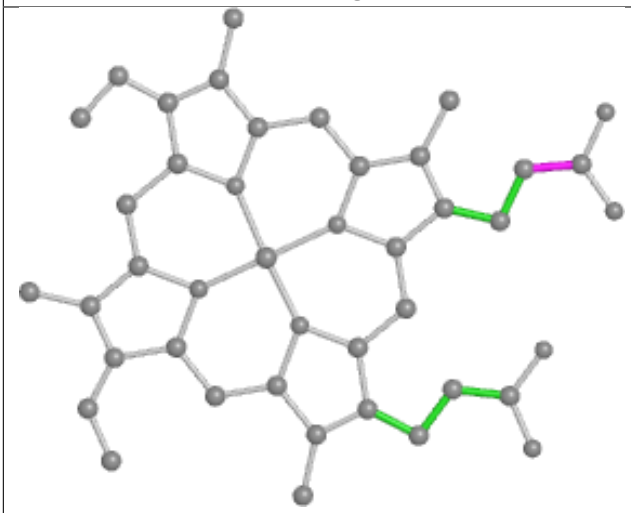


Bond angles



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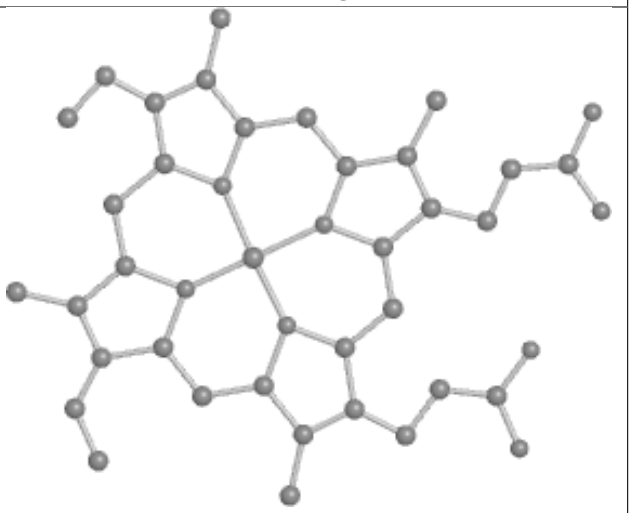
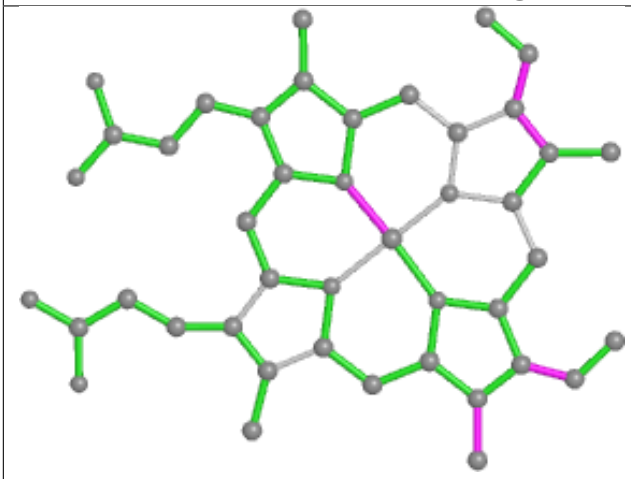


Rings

Ligand HEM E 1002



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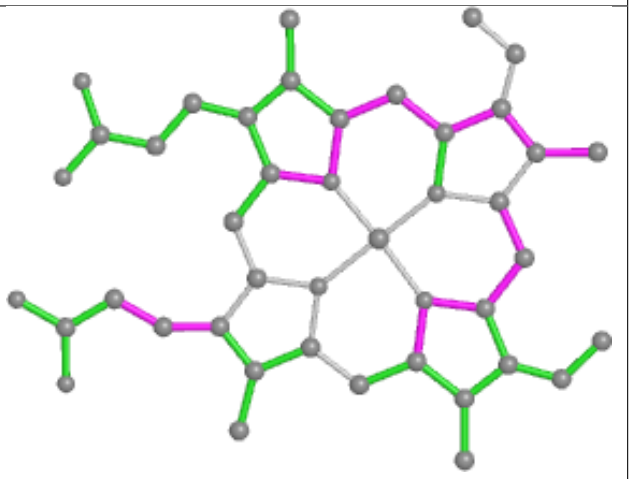
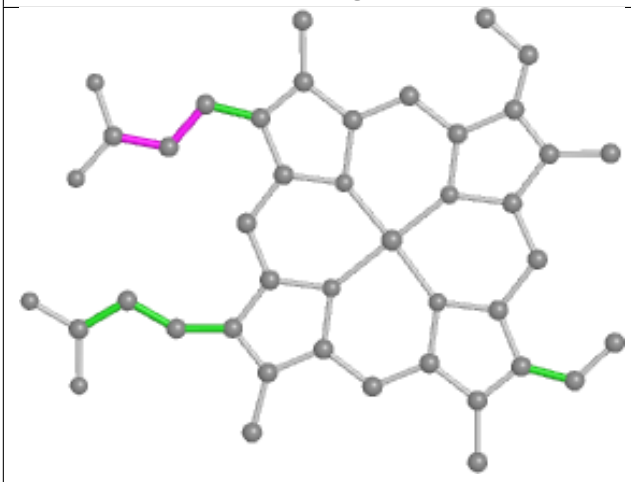
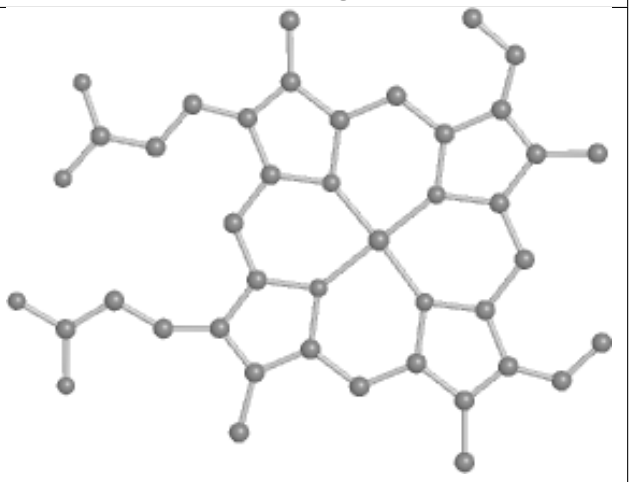


Bond angles

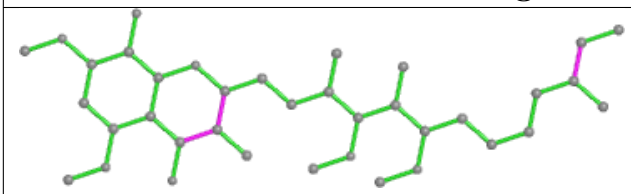


Torsions

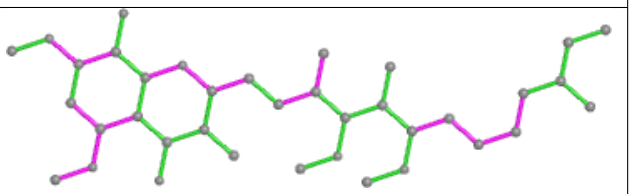


Rings

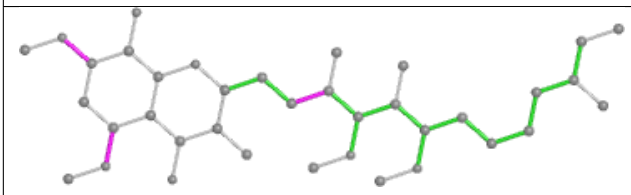
Ligand SMA S 1003



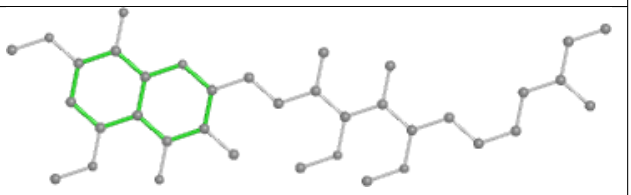
Bond lengths



Bond angles

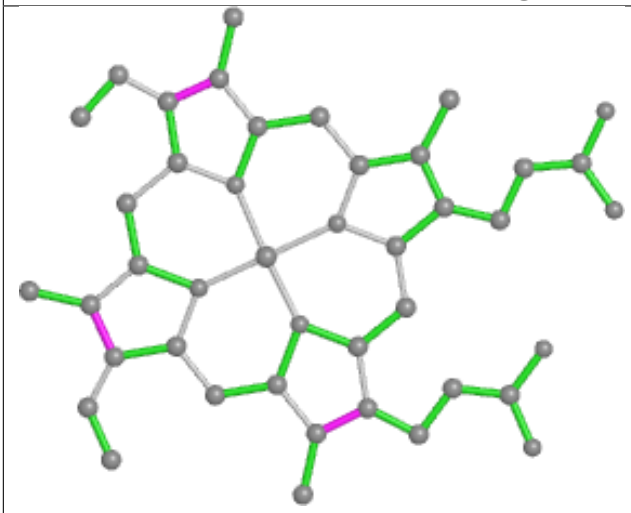


Torsions

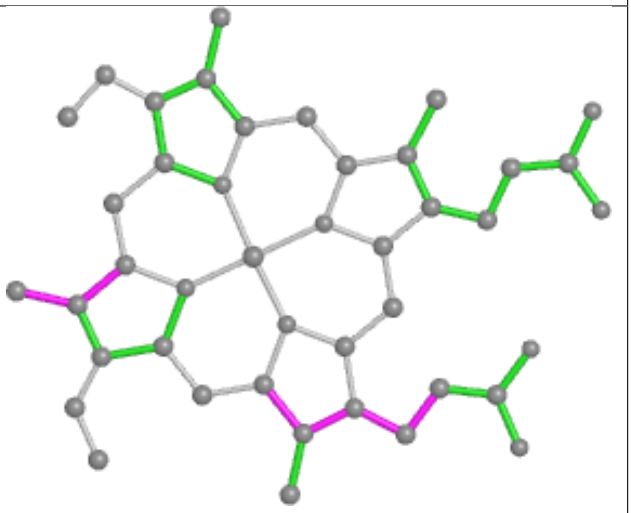


Rings

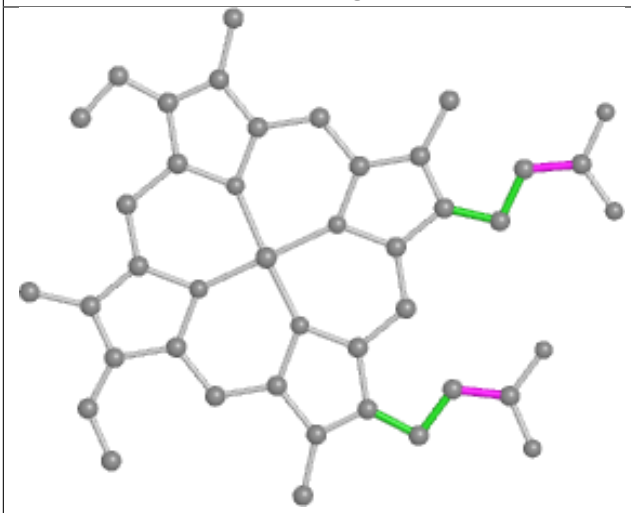
Ligand HEC F 1001



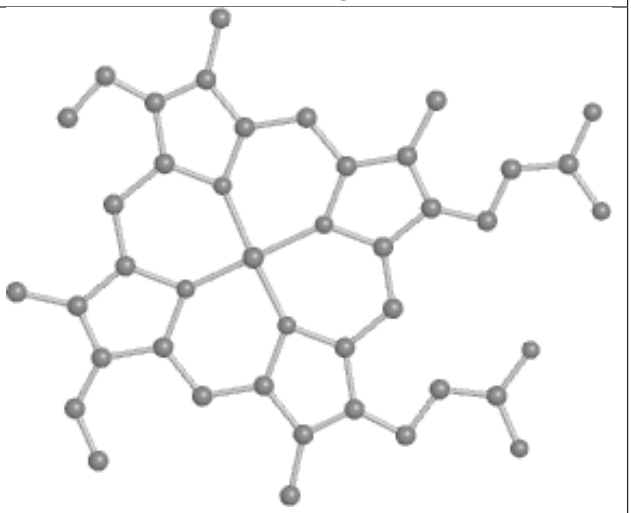
Bond lengths



Bond angles

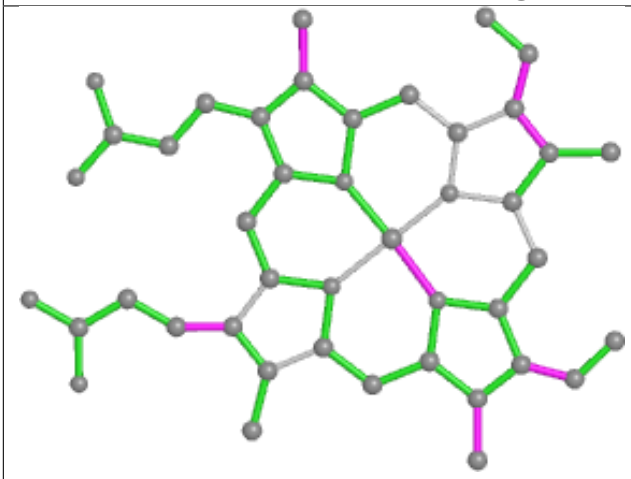


Torsions



Rings

Ligand HEM S 1001



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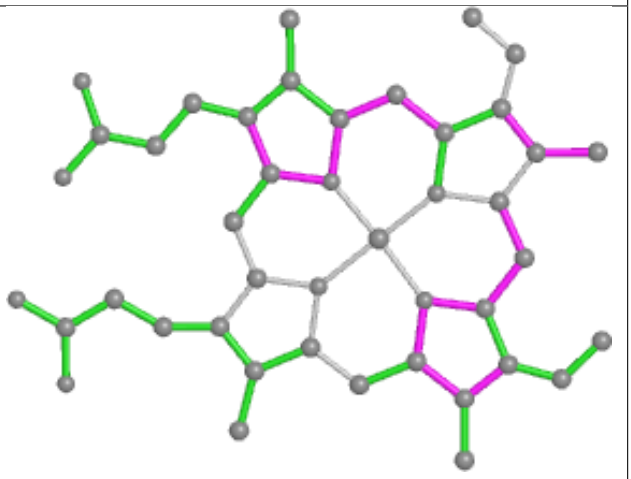
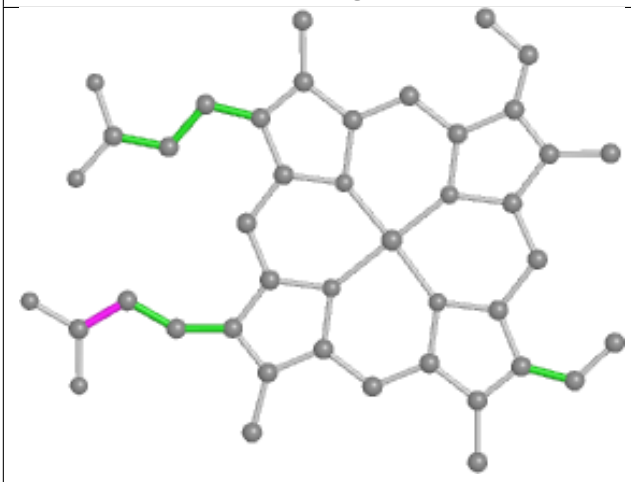
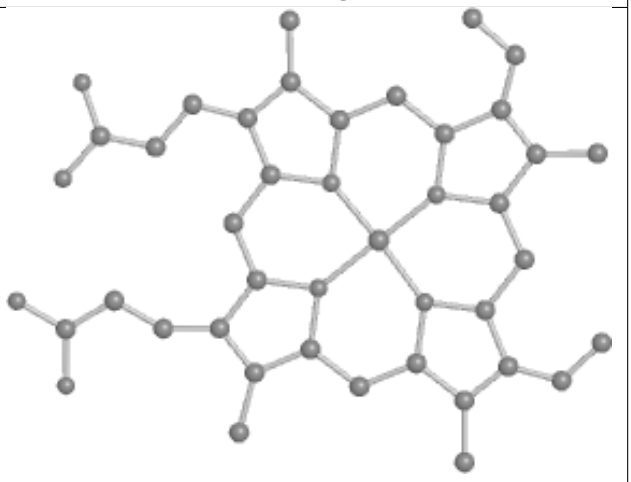


Bond angles

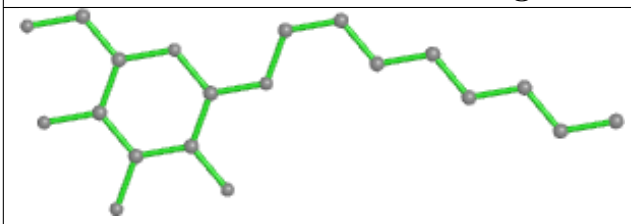


Torsions

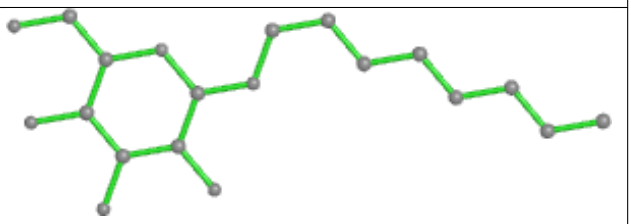


Rings

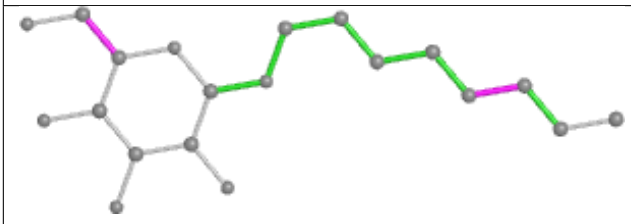
Ligand BOG P 1002



Bond lengths



Bond angles



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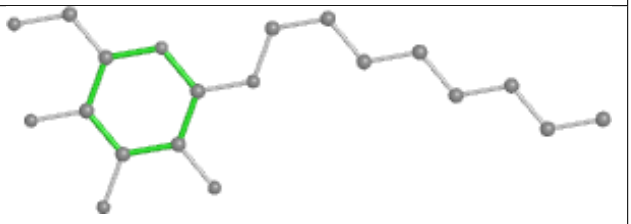
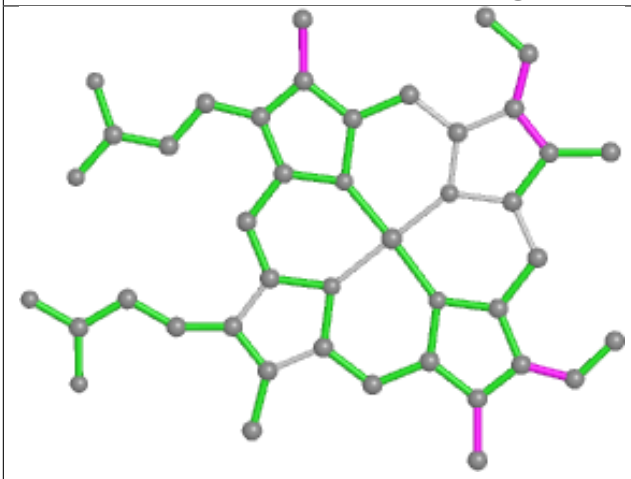
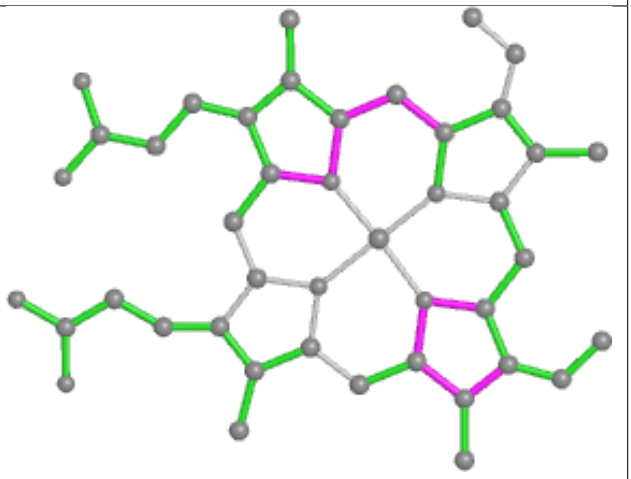


Rings

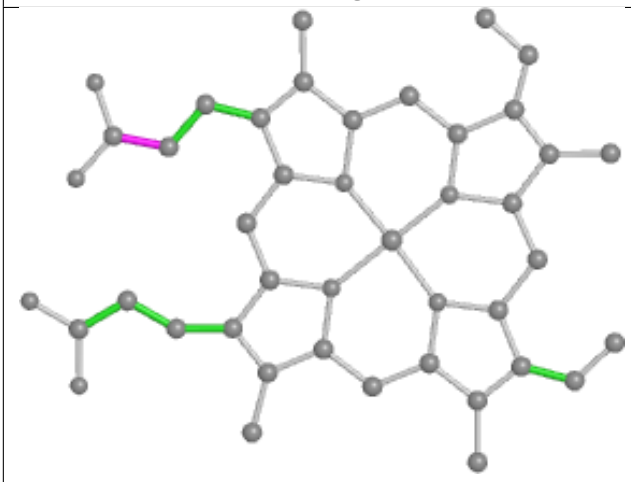
Ligand HEM O 1002



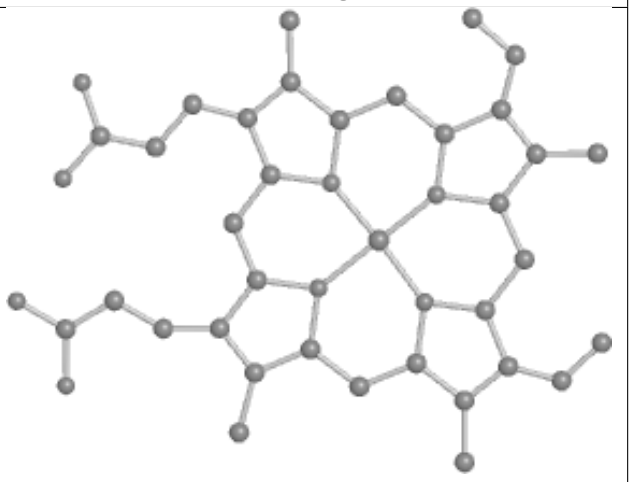
Bond lengths



Bond angles

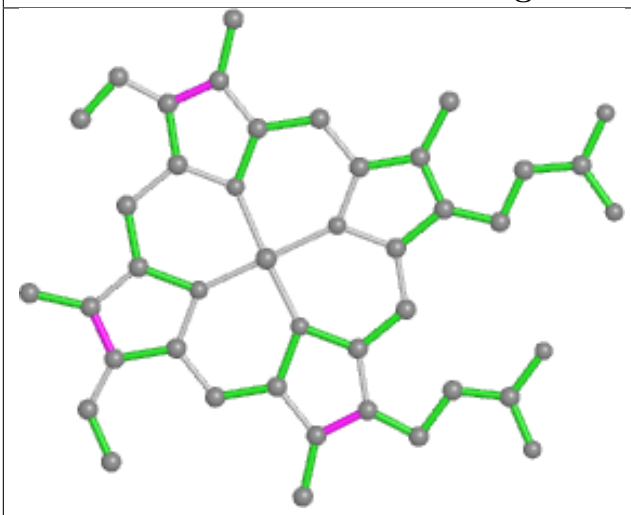


Torsions

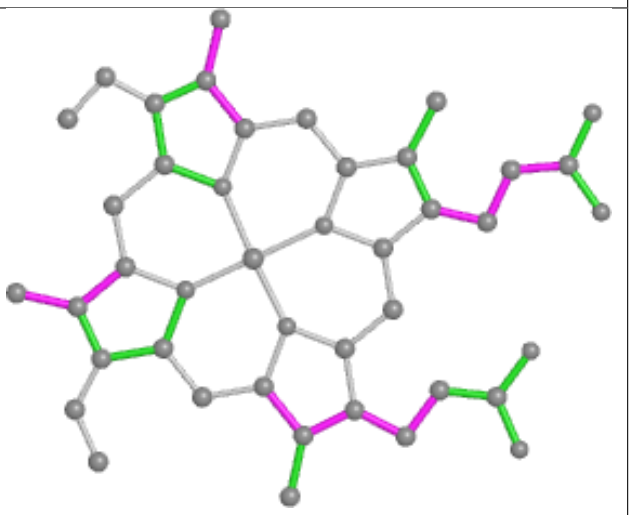


Rings

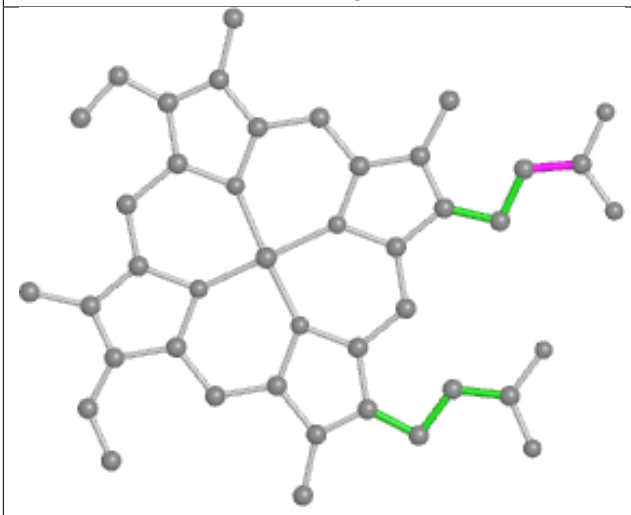
Ligand HEC P 1001



Bond lengths



Bond angles



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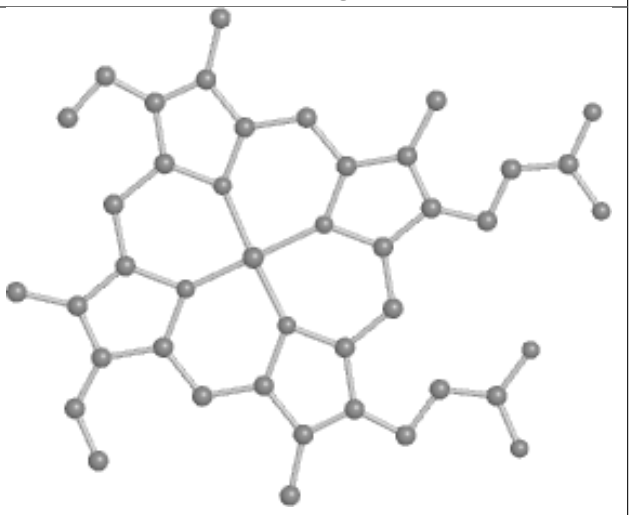
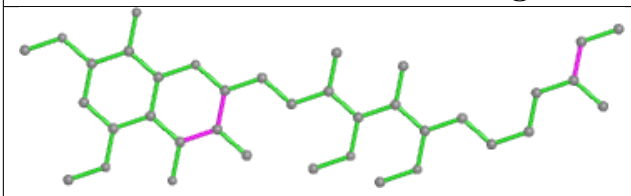
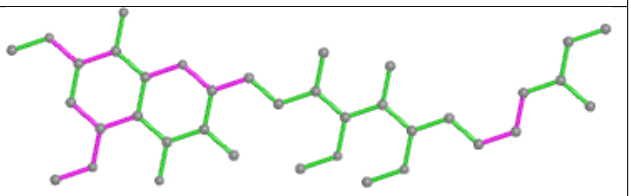


Rings

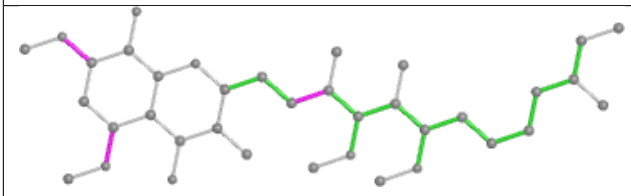
Ligand SMA K 1003



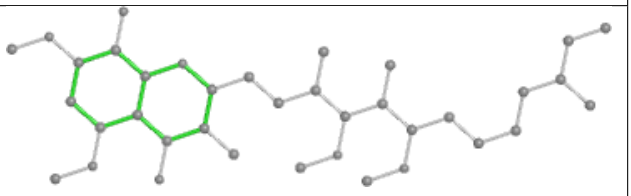
Bond lengths



Bond angles

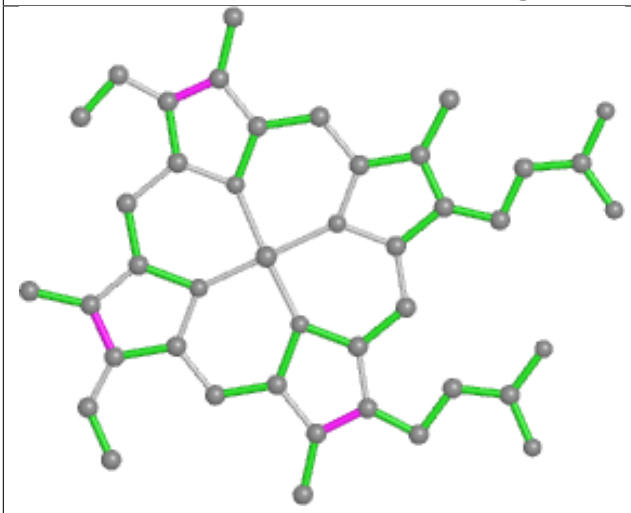


Torsions

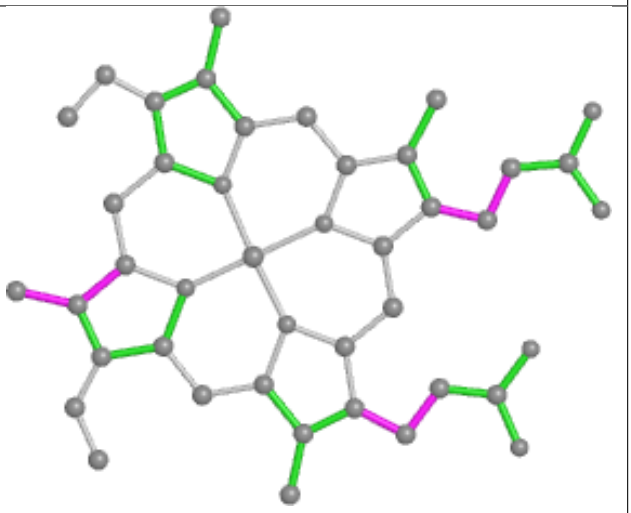


Rings

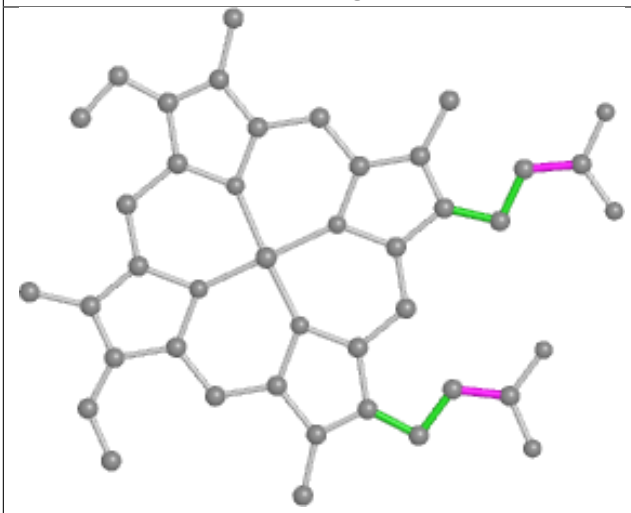
Ligand HEC T 1001



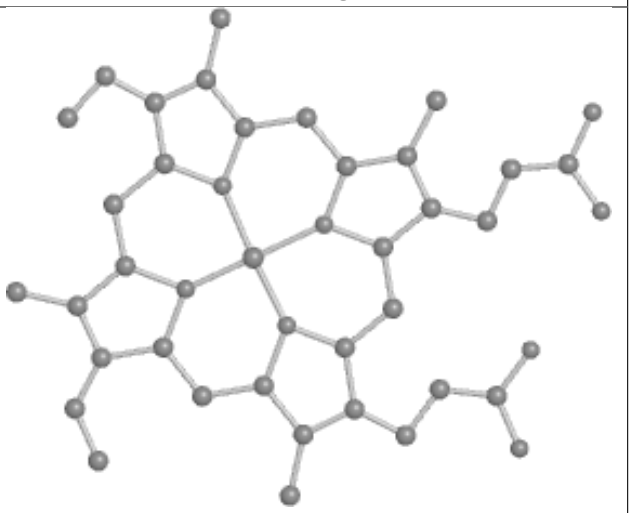
Bond lengths



Bond angles

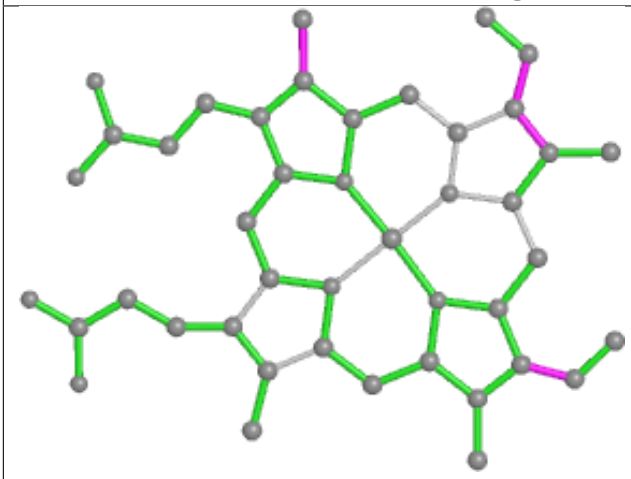


Torsions

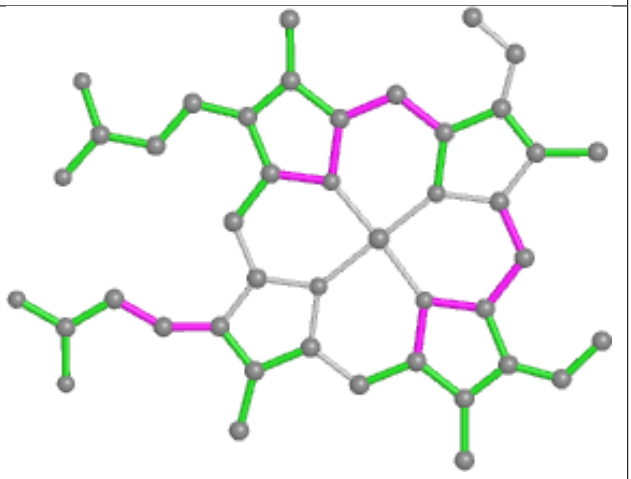


Rings

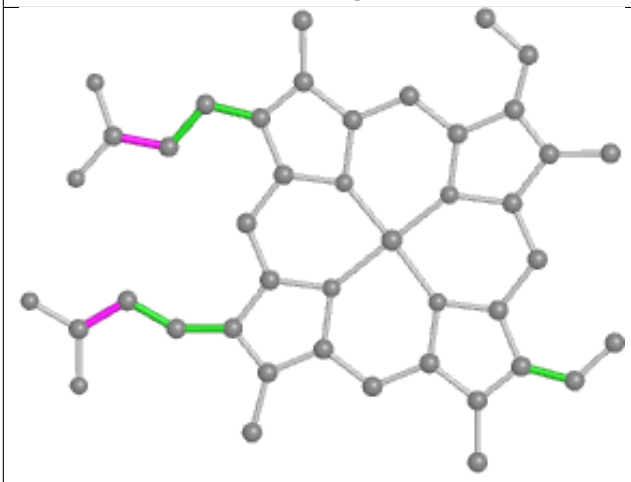
Ligand HEM K 1002



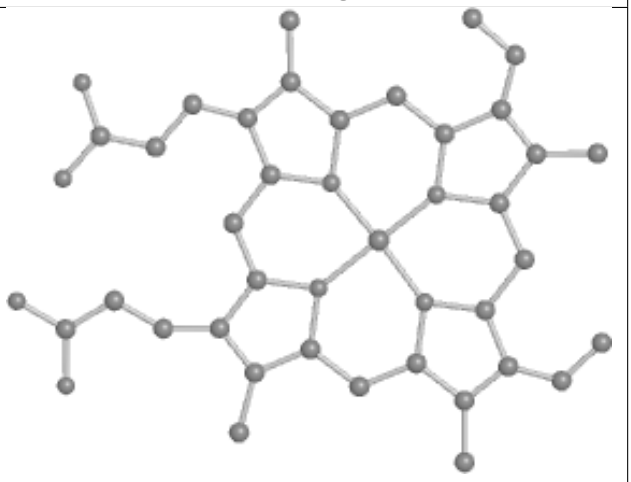
Bond lengths



Bond angles

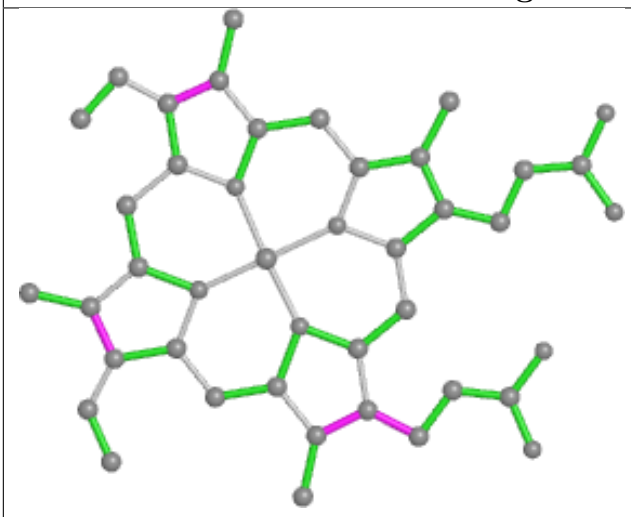


Torsions

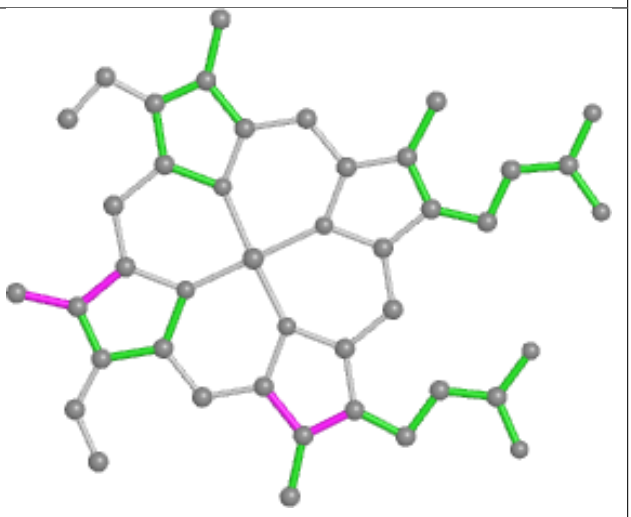


Rings

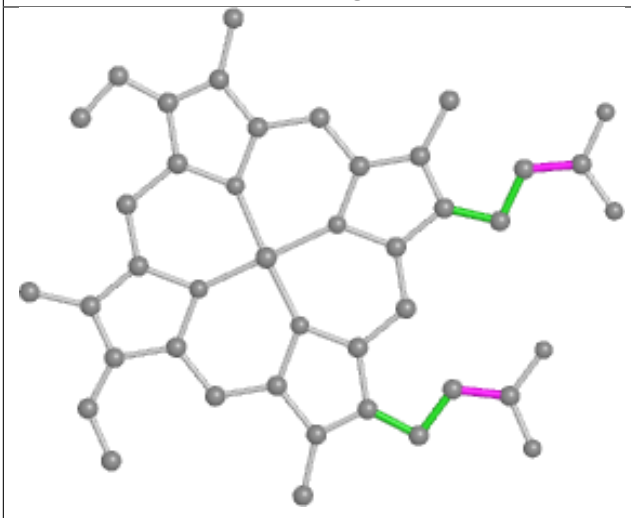
Ligand HEC L 1001



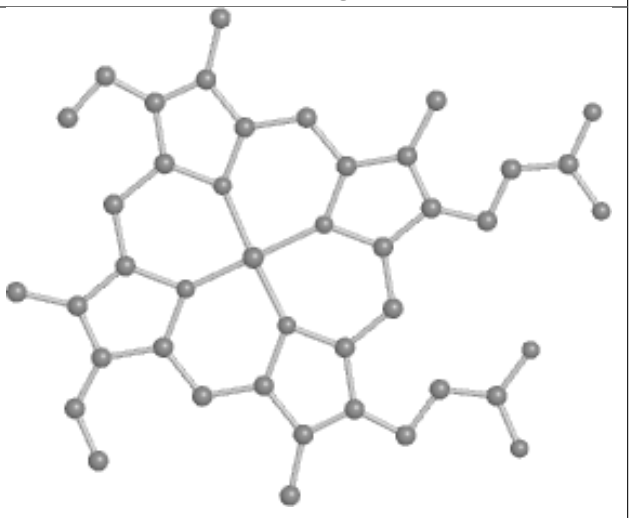
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.