Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:46 AM 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 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:

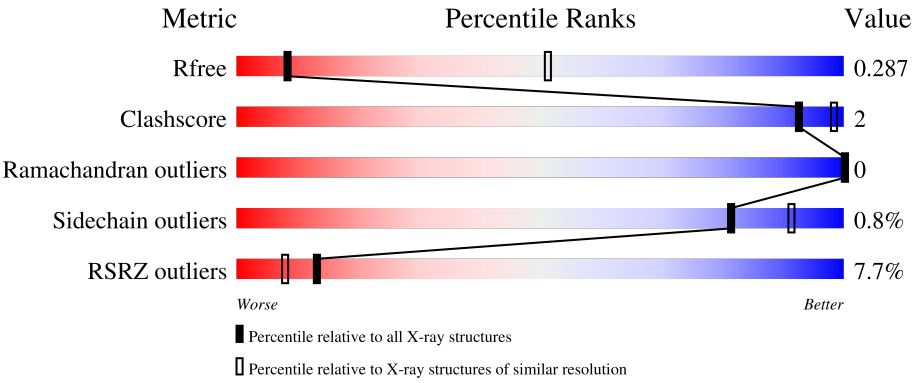
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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.

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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	445	91% 5%
1	E	445	4% 92%
1	K	445	4% 90% 6%
1	O	445	9% 89% 6%
1	S	445	8% 91% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	W	445	4% 91% 5%
2	B	272	8% 93% 6%
2	F	272	6% 94% 6%
2	L	272	5% 91% 6%
2	P	272	12% 93% 6%
2	T	272	23% 92% 6%
2	X	272	11% 93% 6%
3	C	187	6% 94%
3	G	187	5% 93%
3	M	187	12% 95%
3	Q	187	2% 94%
3	U	187	4% 94%
3	Y	187	21% 93%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SMA	S	1003	-	-	-	X
6	6PE	W	1004	-	-	-	X
9	BOG	B	1003	-	-	-	X
9	BOG	F	1002	-	-	-	X
9	BOG	T	1003	-	-	-	X

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			

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

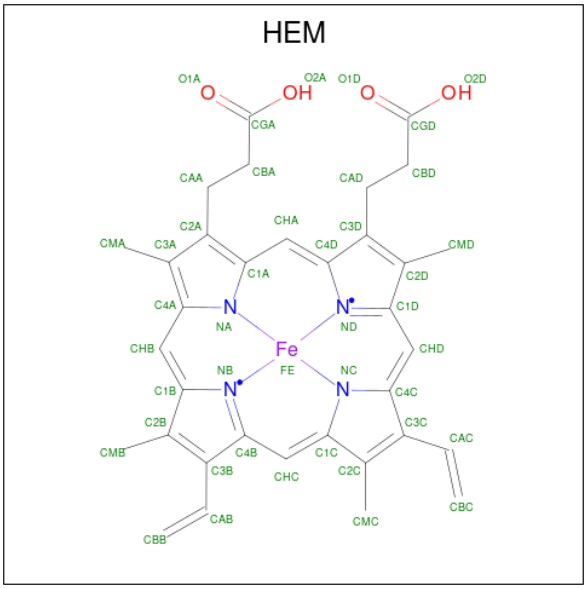
- Molecule 3 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

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: $C_{34}H_{32}FeN_4O_4$).



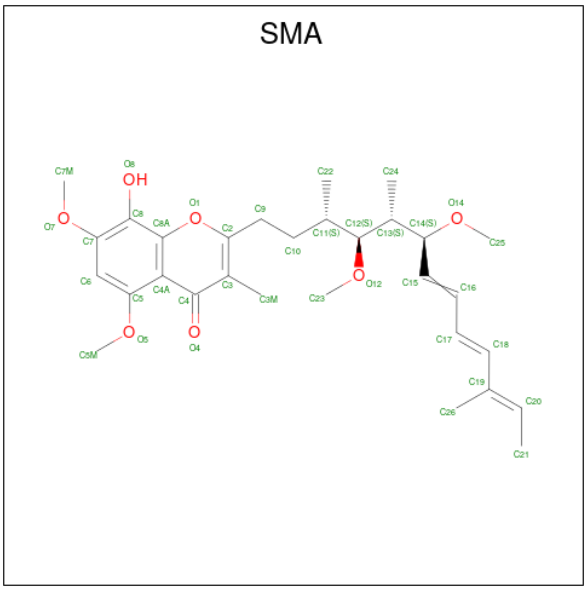
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	K	1	Total	C	Fe	H	N	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		

Continued on next page...

Continued from previous page...

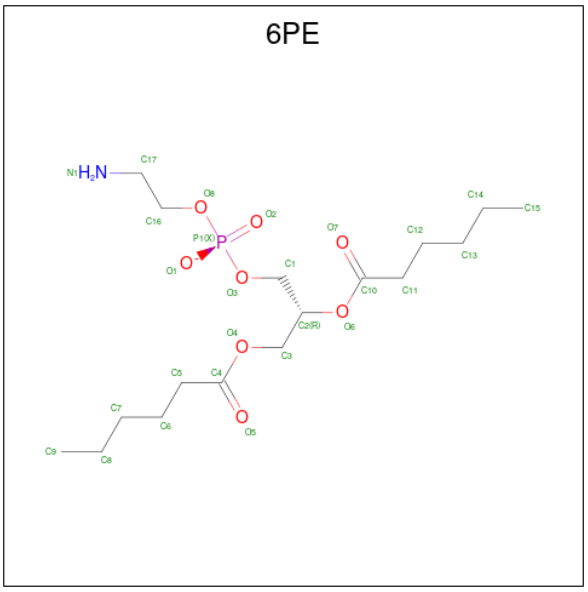
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	S	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	S	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	W	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	W	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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



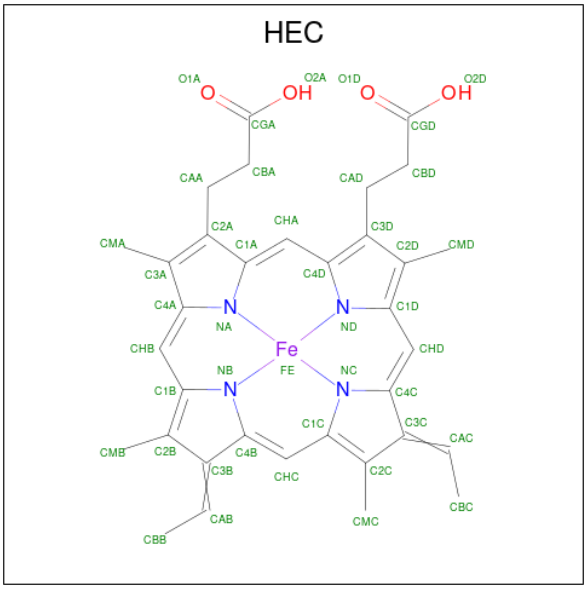
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			79	30	42	7		
5	E	1	Total	C	H	O	0	0
			79	30	42	7		
5	K	1	Total	C	H	O	0	0
			79	30	42	7		
5	O	1	Total	C	H	O	0	0
			79	30	42	7		
5	S	1	Total	C	H	O	0	0
			79	30	42	7		
5	W	1	Total	C	H	O	0	0
			79	30	42	7		

- 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		

Continued on next page...

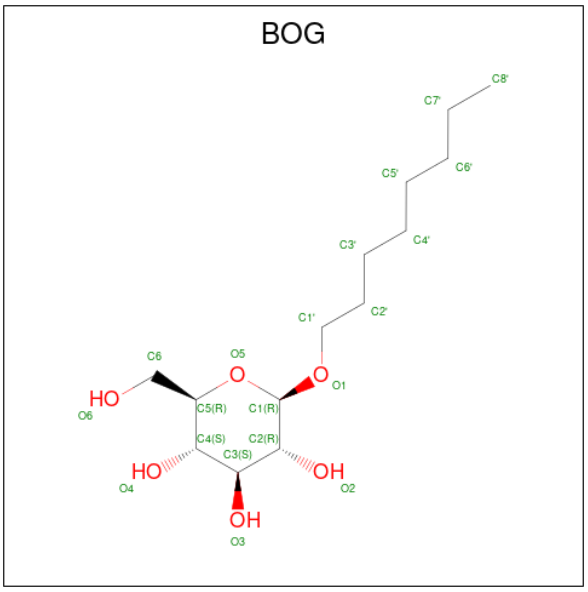
Continued from previous page...

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).

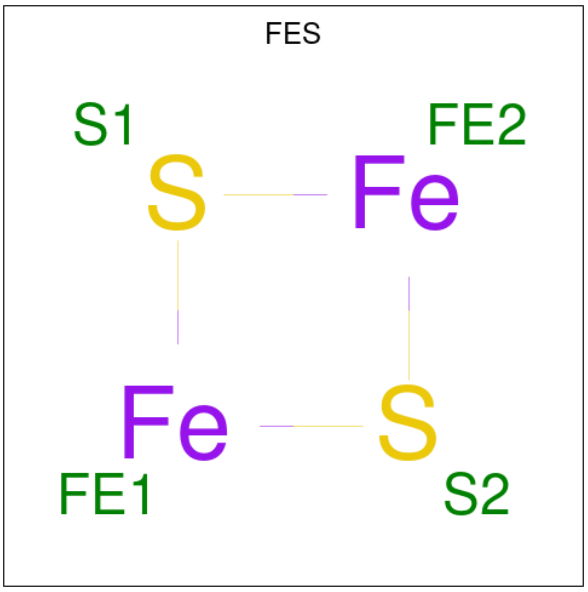
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Sr	0	0
			1	1		
8	F	1	Total	Sr	0	0
			1	1		
8	L	1	Total	Sr	0	0
			1	1		
8	P	1	Total	Sr	0	0
			1	1		
8	T	1	Total	Sr	0	0
			1	1		
8	X	1	Total	Sr	0	0
			1	1		

- 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).



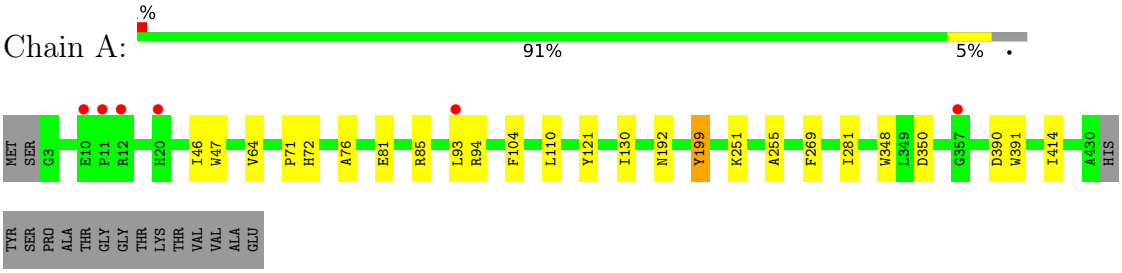
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Fe S 4 2 2	0	0
10	G	1	Total Fe S 4 2 2	0	0
10	M	1	Total Fe S 4 2 2	0	0
10	Q	1	Total Fe S 4 2 2	0	0
10	U	1	Total Fe S 4 2 2	0	0
10	Y	1	Total Fe S 4 2 2	0	0

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.

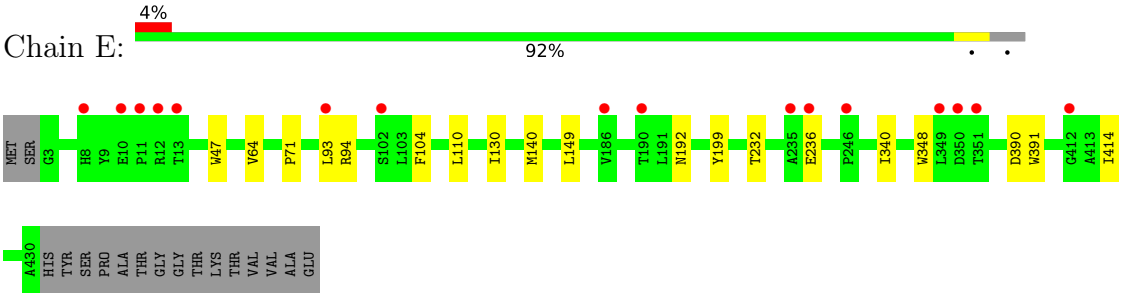
• Molecule 1: Cytochrome b

Chain A:



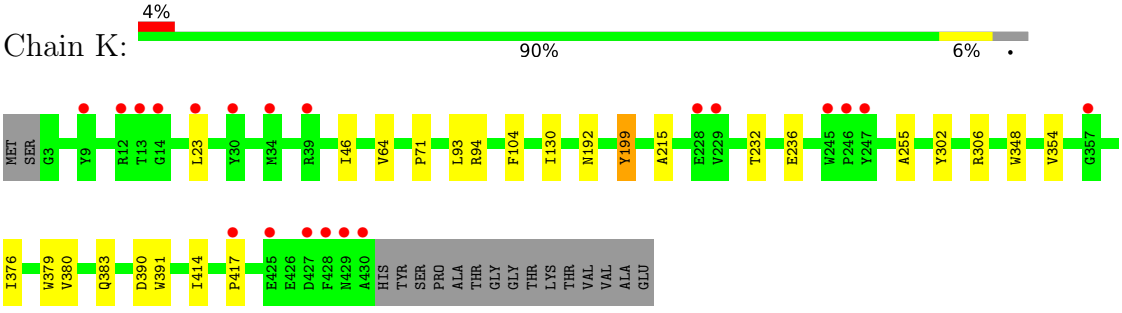
• Molecule 1: Cytochrome b

Chain E:



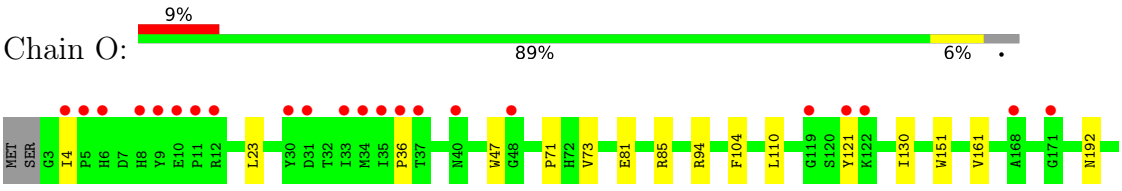
• Molecule 1: Cytochrome b

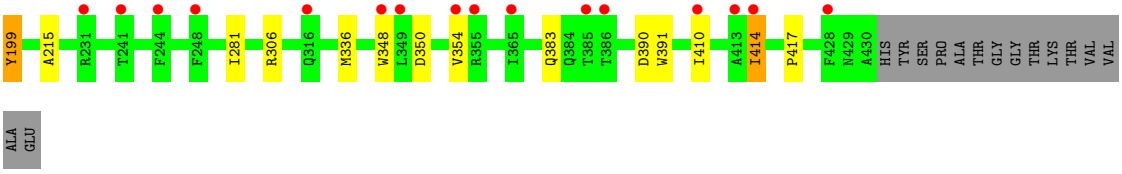
Chain K:



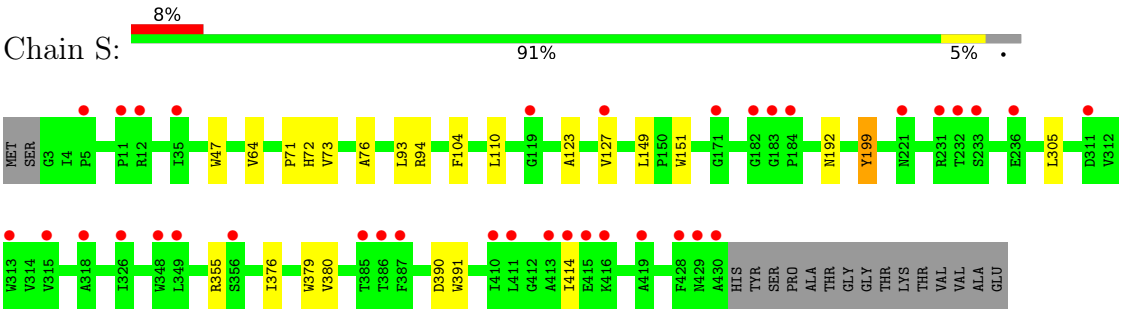
• Molecule 1: Cytochrome b

Chain O:

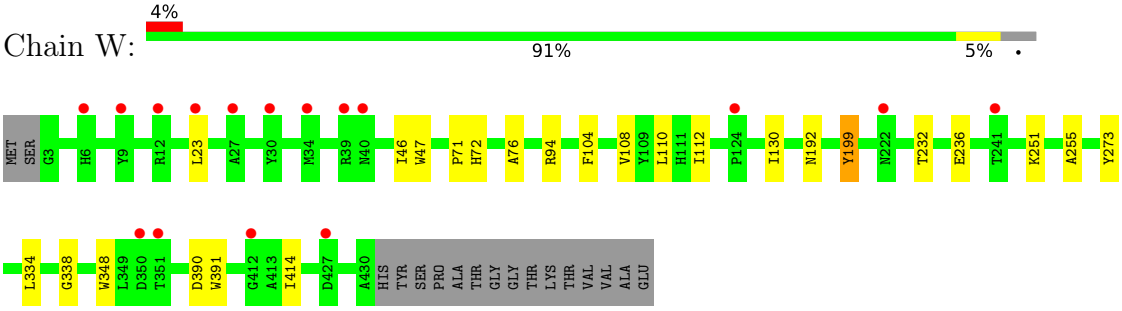




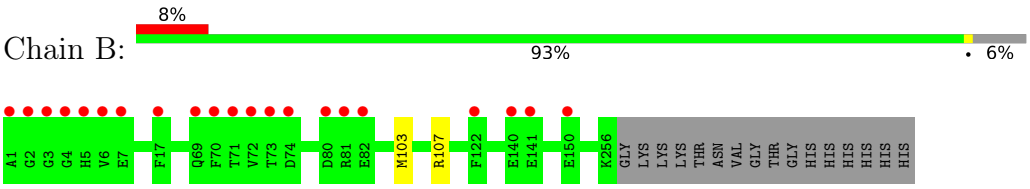
• Molecule 1: Cytochrome b



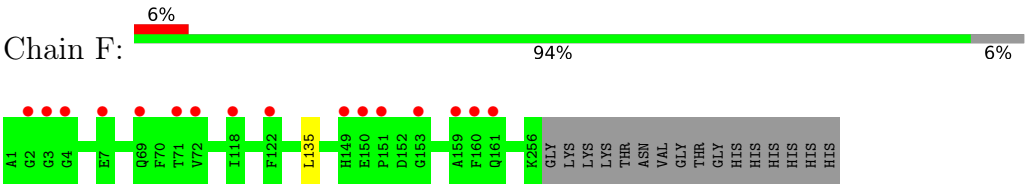
• Molecule 1: Cytochrome b



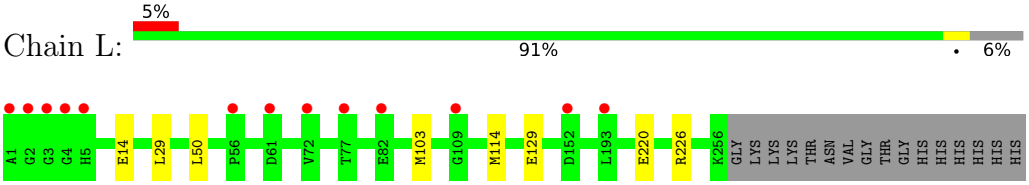
• Molecule 2: Cytochrome c1



• Molecule 2: Cytochrome c1

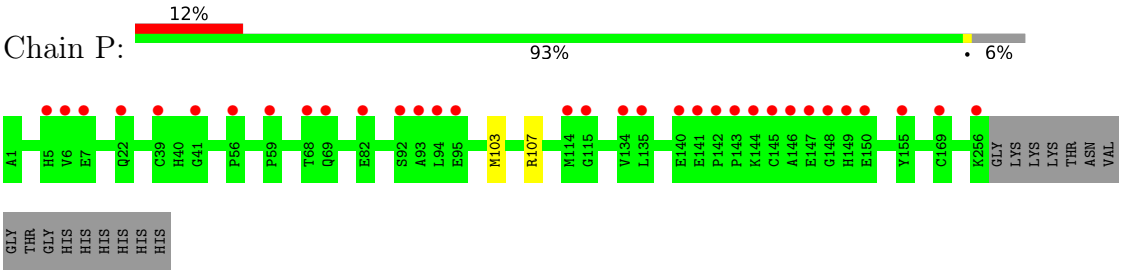


• Molecule 2: Cytochrome c1



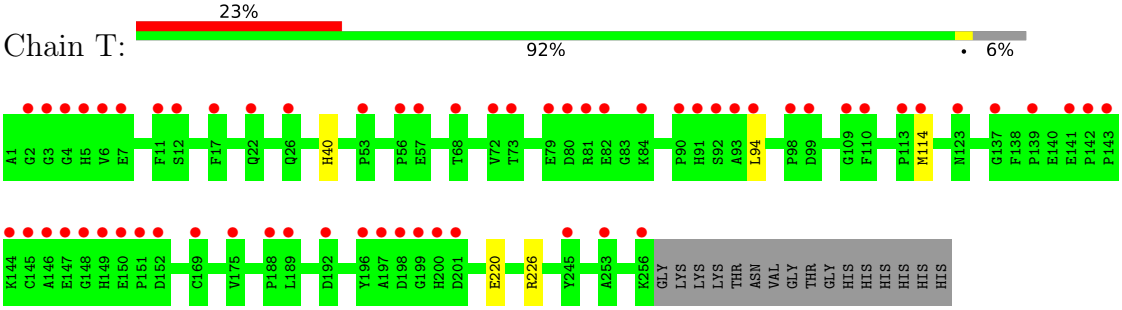
• Molecule 2: Cytochrome c1

Chain P:



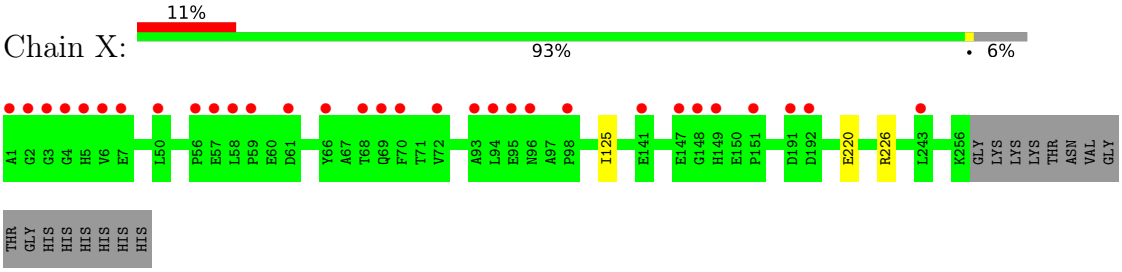
• Molecule 2: Cytochrome c1

Chain T:



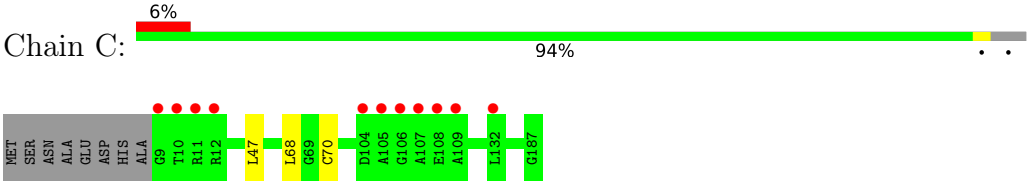
• Molecule 2: Cytochrome c1

Chain X:



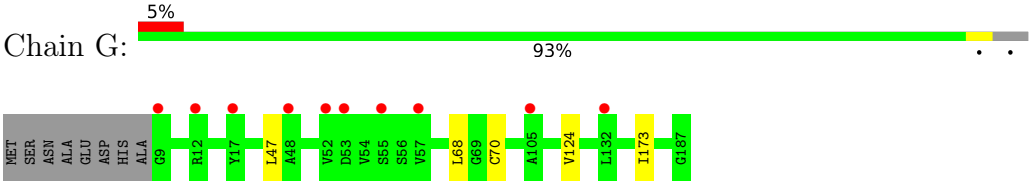
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain C:



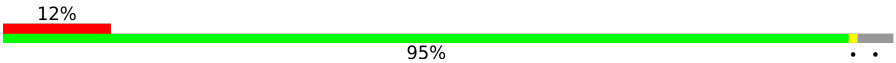
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

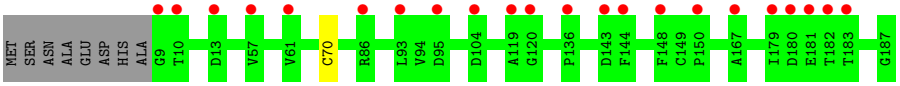
Chain G:



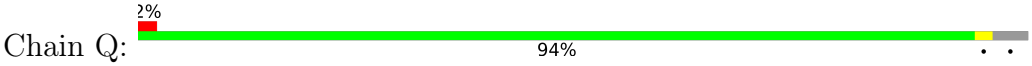
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

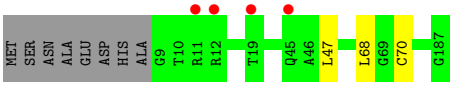
Chain M:



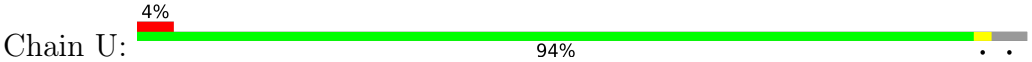


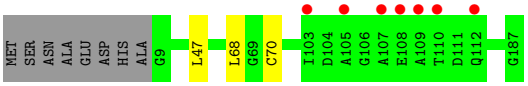
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



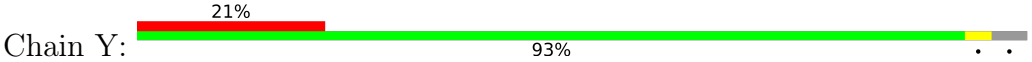


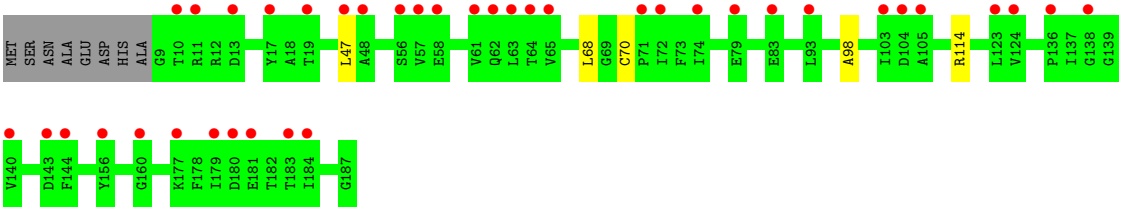
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit





• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit





4 Data and refinement statistics (i)

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 41.18 – 3.48	Depositor EDS
% Data completeness (in resolution range)	97.2 (28.91-3.60) 81.5 (41.18-3.48)	Depositor EDS
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 0.259 , 0.287	Depositor DCC
R_{free} test set	1200 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, HEM, SR, BOG, FES, SMA, 6PE

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	0.30	0/3566	0.51	0/4892
1	E	0.31	0/3566	0.51	0/4892
1	K	0.31	0/3566	0.51	0/4892
1	O	0.31	0/3566	0.50	0/4892
1	S	0.30	0/3566	0.50	0/4892
1	W	0.30	0/3566	0.50	0/4892
2	B	0.29	0/2010	0.49	0/2733
2	F	0.30	0/2010	0.49	0/2733
2	L	0.29	0/2010	0.49	0/2733
2	P	0.28	0/2010	0.49	0/2733
2	T	0.28	0/2010	0.49	0/2733
2	X	0.29	0/2010	0.49	0/2733
3	C	0.30	0/1368	0.56	0/1865
3	G	0.30	0/1368	0.56	0/1865
3	M	0.29	0/1368	0.56	0/1865
3	Q	0.30	0/1368	0.56	0/1865
3	U	0.29	0/1368	0.55	0/1865
3	Y	0.29	0/1368	0.55	0/1865
All	All	0.30	0/41664	0.51	0/56940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3436	3405	3419	13	0
1	E	3436	3405	3419	9	0
1	K	3436	3405	3419	17	0
1	O	3436	3405	3419	17	0
1	S	3436	3405	3419	14	0
1	W	3436	3405	3419	12	0
2	B	1953	1839	1848	2	0
2	F	1953	1839	1848	3	0
2	L	1953	1839	1848	5	0
2	P	1953	1839	1848	3	0
2	T	1953	1839	1848	4	0
2	X	1953	1839	1848	2	0
3	C	1338	1295	1298	1	0
3	G	1338	1295	1298	2	0
3	M	1338	1295	1298	0	0
3	Q	1338	1295	1298	1	0
3	U	1338	1295	1298	1	0
3	Y	1338	1295	1298	2	0
4	A	86	60	60	3	0
4	E	86	60	60	3	0
4	K	86	60	60	5	0
4	O	86	60	60	4	0
4	S	86	60	60	4	0
4	W	86	60	60	3	0
5	A	37	42	42	0	0
5	E	37	42	42	0	0
5	K	37	42	42	1	0
5	O	37	42	42	1	0
5	S	37	42	42	1	0
5	W	37	42	42	0	0
6	A	27	33	33	0	0
6	E	27	33	33	0	0
6	W	27	33	33	0	0
7	B	43	32	30	3	0
7	F	43	32	30	5	0
7	L	43	32	30	3	0
7	P	43	32	30	3	0
7	T	43	32	30	4	0
7	X	43	32	30	2	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	1	0	0	0	0
8	P	1	0	0	0	0
8	T	1	0	0	0	0
8	X	1	0	0	0	0
9	B	20	28	28	1	0
9	F	20	28	28	0	0
9	L	20	28	28	0	0
9	P	20	28	28	0	0
9	T	20	28	28	0	0
9	X	20	28	28	0	0
10	C	4	0	0	0	0
10	G	4	0	0	0	0
10	M	4	0	0	0	0
10	Q	4	0	0	0	0
10	U	4	0	0	0	0
10	Y	4	0	0	0	0
All	All	41589	40305	40449	125	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 2.

All (125) 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:S:71:PRO:O	1:S:192:ASN:ND2	2.22	0.73
2:F:135:LEU:HD21	7:F:1001:HEC:HMB2	1.71	0.72
1:W:71:PRO:O	1:W:192:ASN:ND2	2.23	0.71
1:O:71:PRO:O	1:O:192:ASN:ND2	2.23	0.71
4:A:1002:HEM:HBC2	4:A:1002:HEM:HHD	1.72	0.70
1:K:71:PRO:O	1:K:192:ASN:ND2	2.24	0.70
7:L:1001:HEC:HBC3	7:L:1001:HEC:HMC1	1.74	0.70
4:K:1002:HEM:HBC2	4:K:1002:HEM:HHD	1.73	0.70
7:B:1001:HEC:HBC3	7:B:1001:HEC:HMC1	1.75	0.68
7:P:1001:HEC:HMC1	7:P:1001:HEC:HBC3	1.74	0.68
7:F:1001:HEC:HMC1	7:F:1001:HEC:HBC3	1.76	0.68
4:W:1002:HEM:HBC2	4:W:1002:HEM:HHD	1.76	0.67
7:X:1001:HEC:HMC1	7:X:1001:HEC:HBC3	1.75	0.66
1:S:123:ALA:O	1:S:355:ARG:NH1	2.29	0.66
7:T:1001:HEC:HBC3	7:T:1001:HEC:HMC1	1.76	0.66
1:S:379:TRP:NE1	2:T:114:MET:O	2.31	0.64
1:E:71:PRO:O	1:E:192:ASN:ND2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PRO:O	1:A:192:ASN:ND2	2.32	0.62
7:L:1001:HEC:HBB3	7:L:1001:HEC:HMB1	1.83	0.60
1:A:130:ILE:HD11	1:A:348:TRP:HH2	1.66	0.60
1:E:130:ILE:HD11	1:E:348:TRP:HH2	1.67	0.59
1:A:64:VAL:HG11	1:A:93:LEU:HD13	1.85	0.58
7:X:1001:HEC:HMB1	7:X:1001:HEC:HBB3	1.85	0.58
2:L:103:MET:HG2	7:L:1001:HEC:HMA3	1.86	0.58
4:O:1002:HEM:HMC1	4:O:1002:HEM:HBC2	1.86	0.57
4:E:1002:HEM:HMC1	4:E:1002:HEM:HBC2	1.86	0.57
1:K:232:THR:OG1	1:K:236:GLU:OE2	2.22	0.57
7:B:1001:HEC:HBB3	7:B:1001:HEC:HMB1	1.87	0.56
7:T:1001:HEC:HBB3	7:T:1001:HEC:HMB1	1.86	0.56
7:F:1001:HEC:HMB1	7:F:1001:HEC:HBB3	1.87	0.56
2:P:103:MET:HG2	7:P:1001:HEC:HMA3	1.88	0.56
4:S:1002:HEM:HMC1	4:S:1002:HEM:HBC2	1.89	0.55
1:S:64:VAL:HG11	1:S:93:LEU:HD13	1.89	0.55
3:Q:47:LEU:HD22	3:Q:68:LEU:HD22	1.90	0.54
7:P:1001:HEC:HMB1	7:P:1001:HEC:HBB3	1.89	0.54
1:K:130:ILE:HD11	1:K:348:TRP:HH2	1.71	0.54
2:L:14:GLU:OE2	2:L:129:GLU:OE2	2.26	0.53
1:K:94:ARG:NH2	4:K:1002:HEM:O1A	2.43	0.52
1:W:130:ILE:HD11	1:W:348:TRP:HH2	1.75	0.52
1:S:47:TRP:CZ2	1:S:110:LEU:HD13	2.45	0.51
1:W:273:TYR:HA	2:X:125:ILE:HD11	1.93	0.51
1:E:232:THR:OG1	1:E:236:GLU:OE2	2.28	0.51
1:O:130:ILE:HD11	1:O:348:TRP:HH2	1.75	0.51
1:O:81:GLU:OE1	1:O:85:ARG:NE	2.45	0.50
1:E:64:VAL:HG11	1:E:93:LEU:HD13	1.92	0.50
1:O:306:ARG:NH2	1:O:383:GLN:O	2.44	0.50
2:B:103:MET:HG2	7:B:1001:HEC:HMA3	1.94	0.50
1:S:305:LEU:HD23	5:S:1003:SMA:H1	1.93	0.49
1:K:46:ILE:HD12	1:K:255:ALA:HB1	1.94	0.49
4:O:1001:HEM:HBB2	4:O:1001:HEM:HMB1	1.95	0.49
1:K:64:VAL:HG11	1:K:93:LEU:HD13	1.93	0.49
3:C:47:LEU:HD22	3:C:68:LEU:HD22	1.94	0.48
1:W:47:TRP:CZ2	1:W:110:LEU:HD13	2.48	0.48
3:Y:98:ALA:O	3:Y:114:ARG:NH1	2.46	0.48
4:W:1001:HEM:HBB2	4:W:1001:HEM:HMB1	1.96	0.47
1:O:354:VAL:HG21	1:O:417:PRO:CB	2.45	0.47
2:F:135:LEU:HD11	7:F:1001:HEC:HMB2	1.96	0.47
3:G:47:LEU:HD22	3:G:68:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:1001:HEM:HBB2	4:S:1001:HEM:HMB1	1.97	0.47
4:A:1001:HEM:HMB1	4:A:1001:HEM:HBB2	1.97	0.46
2:T:220:GLU:OE2	2:T:226:ARG:NH1	2.47	0.46
1:K:215:ALA:HA	1:O:23:LEU:HD13	1.97	0.46
1:E:47:TRP:CZ2	1:E:110:LEU:HD13	2.51	0.46
3:Y:47:LEU:HD22	3:Y:68:LEU:HD22	1.98	0.46
1:A:121:TYR:OH	1:A:350:ASP:OD2	2.32	0.46
1:A:269:PHE:O	9:B:1003:BOG:O6	2.33	0.45
1:K:390:ASP:OD1	1:K:391:TRP:N	2.49	0.45
1:S:199:TYR:CZ	4:S:1002:HEM:HBC1	2.50	0.45
1:O:281:ILE:HD11	2:P:107:ARG:HH12	1.82	0.45
2:T:40:HIS:CE1	7:T:1001:HEC:ND	2.83	0.45
2:T:94:LEU:HD23	7:T:1001:HEC:HMD3	1.98	0.45
4:K:1001:HEM:HBB2	4:K:1001:HEM:HMB1	1.99	0.45
1:W:46:ILE:HD12	1:W:255:ALA:HB1	1.97	0.44
1:E:390:ASP:OD1	1:E:391:TRP:N	2.50	0.44
1:A:390:ASP:OD1	1:A:391:TRP:N	2.50	0.44
4:E:1001:HEM:HMB1	4:E:1001:HEM:HBB2	1.98	0.44
2:F:135:LEU:HD21	7:F:1001:HEC:CMB	2.45	0.44
1:K:23:LEU:HD13	1:O:215:ALA:HA	1.99	0.44
1:O:47:TRP:CZ2	1:O:110:LEU:HD13	2.53	0.44
3:U:47:LEU:HD22	3:U:68:LEU:HD22	1.99	0.43
4:O:1001:HEM:HMC1	4:O:1001:HEM:HBC2	1.99	0.43
1:K:376:ILE:O	1:K:380:VAL:HG22	2.18	0.43
1:O:390:ASP:OD1	1:O:391:TRP:N	2.52	0.43
1:W:232:THR:OG1	1:W:236:GLU:OE2	2.34	0.43
1:K:379:TRP:NE1	2:L:114:MET:O	2.48	0.43
1:W:72:HIS:O	1:W:76:ALA:N	2.49	0.43
1:E:64:VAL:CG1	1:E:93:LEU:HD13	2.49	0.43
1:S:149:LEU:HD12	4:S:1002:HEM:C3D	2.54	0.43
1:S:390:ASP:OD1	1:S:391:TRP:N	2.52	0.43
1:K:64:VAL:CG1	1:K:93:LEU:HD13	2.49	0.42
1:A:64:VAL:CG1	1:A:93:LEU:HD13	2.49	0.42
1:A:72:HIS:O	1:A:76:ALA:N	2.49	0.42
1:A:46:ILE:HD12	1:A:255:ALA:HB1	2.01	0.42
1:O:281:ILE:HD11	2:P:107:ARG:NH1	2.34	0.42
1:S:376:ILE:O	1:S:380:VAL:HG22	2.20	0.42
1:W:108:VAL:HG12	1:W:112:ILE:HD12	2.00	0.42
1:E:149:LEU:HD12	4:E:1002:HEM:C4D	2.54	0.42
1:K:199:TYR:CE2	4:K:1002:HEM:HBC1	2.55	0.42
1:S:72:HIS:O	1:S:76:ALA:N	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:390:ASP:OD1	1:W:391:TRP:N	2.52	0.42
1:O:121:TYR:OH	1:O:350:ASP:OD2	2.36	0.41
1:S:64:VAL:CG1	1:S:93:LEU:HD13	2.50	0.41
1:K:306:ARG:NH2	1:K:383:GLN:O	2.46	0.41
1:K:354:VAL:HG21	1:K:417:PRO:CB	2.50	0.41
2:X:220:GLU:OE1	2:X:226:ARG:NH1	2.52	0.41
1:K:46:ILE:CD1	1:K:255:ALA:HB1	2.50	0.41
1:O:410:ILE:HG23	1:O:414:ILE:HD12	2.02	0.41
1:K:302:TYR:CE1	5:K:1003:SMA:H5	2.55	0.41
1:O:199:TYR:CZ	4:O:1002:HEM:HBC1	2.55	0.41
2:L:29:LEU:HD22	2:L:50:LEU:HD22	2.03	0.41
1:E:140:MET:HE1	1:E:340:ILE:HD13	2.03	0.41
1:A:81:GLU:OE1	1:A:85:ARG:NE	2.52	0.41
3:G:124:VAL:O	3:G:173:ILE:HG23	2.21	0.41
1:O:4:ILE:HG21	1:O:36:PRO:HG2	2.03	0.41
1:S:127:VAL:HG11	1:W:23:LEU:HD22	2.02	0.41
1:W:199:TYR:CE2	4:W:1002:HEM:HBC1	2.56	0.41
1:A:199:TYR:CE2	4:A:1002:HEM:HBC1	2.56	0.41
1:O:73:VAL:HG12	1:O:151:TRP:CE2	2.56	0.40
1:S:73:VAL:HG12	1:S:151:TRP:CE2	2.55	0.40
1:W:334:LEU:O	1:W:338:GLY:N	2.50	0.40
1:A:47:TRP:CZ2	1:A:110:LEU:HD13	2.55	0.40
1:A:281:ILE:HD11	2:B:107:ARG:HH12	1.86	0.40
4:K:1001:HEM:HMC1	4:K:1001:HEM:HBC2	2.04	0.40
2:L:220:GLU:OE2	2:L:226:ARG:NH1	2.51	0.40
1:O:161:VAL:HG11	5:O:1003:SMA:O4	2.22	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	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
1	E	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
1	K	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
1	O	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
1	S	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
1	W	426/445 (96%)	421 (99%)	5 (1%)	0	100	100
2	B	254/272 (93%)	247 (97%)	7 (3%)	0	100	100
2	F	254/272 (93%)	247 (97%)	7 (3%)	0	100	100
2	L	254/272 (93%)	247 (97%)	7 (3%)	0	100	100
2	P	254/272 (93%)	247 (97%)	7 (3%)	0	100	100
2	T	254/272 (93%)	247 (97%)	7 (3%)	0	100	100
2	X	254/272 (93%)	247 (97%)	7 (3%)	0	100	100
3	C	177/187 (95%)	171 (97%)	6 (3%)	0	100	100
3	G	177/187 (95%)	171 (97%)	6 (3%)	0	100	100
3	M	177/187 (95%)	171 (97%)	6 (3%)	0	100	100
3	Q	177/187 (95%)	171 (97%)	6 (3%)	0	100	100
3	U	177/187 (95%)	171 (97%)	6 (3%)	0	100	100
3	Y	177/187 (95%)	171 (97%)	6 (3%)	0	100	100
All	All	5142/5424 (95%)	5034 (98%)	108 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	354/367 (96%)	349 (99%)	5 (1%)	67	85
1	E	354/367 (96%)	350 (99%)	4 (1%)	73	88
1	K	354/367 (96%)	351 (99%)	3 (1%)	81	91

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	354/367 (96%)	349 (99%)	5 (1%)	67 85
1	S	354/367 (96%)	350 (99%)	4 (1%)	73 88
1	W	354/367 (96%)	349 (99%)	5 (1%)	67 85
2	B	203/216 (94%)	203 (100%)	0	100 100
2	F	203/216 (94%)	203 (100%)	0	100 100
2	L	203/216 (94%)	203 (100%)	0	100 100
2	P	203/216 (94%)	203 (100%)	0	100 100
2	T	203/216 (94%)	203 (100%)	0	100 100
2	X	203/216 (94%)	203 (100%)	0	100 100
3	C	138/144 (96%)	137 (99%)	1 (1%)	84 93
3	G	138/144 (96%)	137 (99%)	1 (1%)	84 93
3	M	138/144 (96%)	137 (99%)	1 (1%)	84 93
3	Q	138/144 (96%)	137 (99%)	1 (1%)	84 93
3	U	138/144 (96%)	137 (99%)	1 (1%)	84 93
3	Y	138/144 (96%)	137 (99%)	1 (1%)	84 93
All	All	4170/4362 (96%)	4138 (99%)	32 (1%)	81 91

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ARG
1	A	104	PHE
1	A	199	TYR
1	A	251	LYS
1	A	414	ILE
3	C	70	CYS
1	E	94	ARG
1	E	104	PHE
1	E	199	TYR
1	E	414	ILE
3	G	70	CYS
1	K	104	PHE
1	K	199	TYR
1	K	414	ILE
3	M	70	CYS
1	O	94	ARG
1	O	104	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	199	TYR
1	O	336	MET
1	O	414	ILE
3	Q	70	CYS
1	S	94	ARG
1	S	104	PHE
1	S	199	TYR
1	S	414	ILE
3	U	70	CYS
1	W	94	ARG
1	W	104	PHE
1	W	199	TYR
1	W	251	LYS
1	W	414	ILE
3	Y	70	CYS

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	192	ASN
1	K	192	ASN
1	O	192	ASN
1	W	192	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 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	S	1002	1	41,50,50	1.46	6 (14%)	45,82,82	1.25	5 (11%)
5	SMA	A	1003	-	38,38,38	1.75	2 (5%)	48,52,52	1.48	9 (18%)
4	HEM	S	1001	1	41,50,50	1.48	7 (17%)	45,82,82	1.48	7 (15%)
4	HEM	E	1001	1	41,50,50	1.46	7 (17%)	45,82,82	1.36	5 (11%)
9	BOG	T	1003	-	20,20,20	0.88	0	25,25,25	0.99	0
4	HEM	W	1001	1	41,50,50	1.45	5 (12%)	45,82,82	1.39	8 (17%)
6	6PE	E	1004	-	26,26,26	0.55	0	29,31,31	0.78	1 (3%)
9	BOG	P	1002	-	20,20,20	0.92	0	25,25,25	0.90	0
5	SMA	O	1003	-	38,38,38	1.79	4 (10%)	48,52,52	1.56	9 (18%)
4	HEM	K	1002	1	41,50,50	1.53	4 (9%)	45,82,82	1.37	6 (13%)
7	HEC	B	1001	2	32,50,50	2.10	4 (12%)	24,82,82	1.44	1 (4%)
10	FES	Q	1001	3	0,4,4	-	-	-		
4	HEM	E	1002	1	41,50,50	1.49	5 (12%)	45,82,82	1.48	7 (15%)
4	HEM	A	1002	1	41,50,50	1.50	6 (14%)	45,82,82	1.47	6 (13%)
4	HEM	K	1001	1	41,50,50	1.46	5 (12%)	45,82,82	1.47	8 (17%)
5	SMA	W	1003	-	38,38,38	1.72	4 (10%)	48,52,52	1.54	9 (18%)
5	SMA	K	1003	-	38,38,38	1.72	3 (7%)	48,52,52	1.50	7 (14%)
7	HEC	L	1001	2	32,50,50	2.16	4 (12%)	24,82,82	1.43	2 (8%)
9	BOG	L	1003	-	20,20,20	0.89	0	25,25,25	0.99	0
10	FES	U	1001	3	0,4,4	-	-	-		
5	SMA	E	1003	-	38,38,38	1.64	3 (7%)	48,52,52	1.62	10 (20%)
9	BOG	X	1003	-	20,20,20	0.92	0	25,25,25	0.93	0
10	FES	M	1001	3	0,4,4	-	-	-		
7	HEC	X	1001	2	32,50,50	2.11	3 (9%)	24,82,82	1.52	4 (16%)
5	SMA	S	1003	-	38,38,38	1.75	3 (7%)	48,52,52	1.56	9 (18%)
10	FES	G	1001	3	0,4,4	-	-	-		
7	HEC	T	1001	2	32,50,50	2.09	3 (9%)	24,82,82	1.51	3 (12%)
4	HEM	O	1002	1	41,50,50	1.47	5 (12%)	45,82,82	1.36	4 (8%)
6	6PE	A	1004	-	26,26,26	0.54	0	29,31,31	0.67	1 (3%)
10	FES	Y	1001	3	0,4,4	-	-	-		
9	BOG	B	1003	-	20,20,20	0.90	0	25,25,25	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	HEM	A	1001	1	41,50,50	1.47	5 (12%)	45,82,82	1.42	7 (15%)
4	HEM	W	1002	1	41,50,50	1.55	5 (12%)	45,82,82	1.33	6 (13%)
6	6PE	W	1004	-	26,26,26	0.55	0	29,31,31	0.70	0
7	HEC	F	1001	2	32,50,50	2.08	3 (9%)	24,82,82	1.56	3 (12%)
10	FES	C	1001	3	0,4,4	-	-	-		
7	HEC	P	1001	2	32,50,50	2.08	3 (9%)	24,82,82	1.55	6 (25%)
4	HEM	O	1001	1	41,50,50	1.47	6 (14%)	45,82,82	1.47	7 (15%)
9	BOG	F	1002	-	20,20,20	0.90	0	25,25,25	0.92	0

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FES	M	1001	3	-	-	0/1/1/1
7	HEC	X	1001	2	-	2/10/54/54	-
5	SMA	S	1003	-	-	5/34/34/34	0/2/2/2
10	FES	G	1001	3	-	-	0/1/1/1
7	HEC	T	1001	2	-	4/10/54/54	-
4	HEM	O	1002	1	-	2/12/54/54	-
6	6PE	A	1004	-	-	19/30/30/30	-
10	FES	Y	1001	3	-	-	0/1/1/1
9	BOG	B	1003	-	-	2/11/31/31	0/1/1/1
4	HEM	A	1001	1	-	2/12/54/54	-
4	HEM	W	1002	1	-	2/12/54/54	-
6	6PE	W	1004	-	-	12/30/30/30	-
7	HEC	F	1001	2	-	4/10/54/54	-
10	FES	C	1001	3	-	-	0/1/1/1
7	HEC	P	1001	2	-	2/10/54/54	-
4	HEM	O	1001	1	-	2/12/54/54	-
9	BOG	F	1002	-	-	2/11/31/31	0/1/1/1

All (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
5	E	1003	SMA	C20-C19	7.46	1.39	1.33
7	L	1001	HEC	C2B-C3B	-6.45	1.34	1.40
7	P	1001	HEC	C2B-C3B	-6.23	1.34	1.40
7	X	1001	HEC	C2B-C3B	-6.12	1.34	1.40
7	T	1001	HEC	C2B-C3B	-5.97	1.34	1.40
7	B	1001	HEC	C2B-C3B	-5.97	1.34	1.40
7	F	1001	HEC	C2B-C3B	-5.94	1.34	1.40
7	L	1001	HEC	C3C-C2C	-5.56	1.34	1.40
7	T	1001	HEC	C3D-C2D	5.50	1.54	1.37
7	X	1001	HEC	C3C-C2C	-5.43	1.35	1.40
7	X	1001	HEC	C3D-C2D	5.39	1.53	1.37
7	P	1001	HEC	C3D-C2D	5.39	1.53	1.37
7	L	1001	HEC	C3D-C2D	5.38	1.53	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1001	HEC	C3D-C2D	5.38	1.53	1.37
7	F	1001	HEC	C3D-C2D	5.35	1.53	1.37
7	B	1001	HEC	C3C-C2C	-5.22	1.35	1.40
7	F	1001	HEC	C3C-C2C	-5.22	1.35	1.40
7	P	1001	HEC	C3C-C2C	-5.16	1.35	1.40
7	T	1001	HEC	C3C-C2C	-5.08	1.35	1.40
4	W	1002	HEM	C3C-C2C	-4.75	1.33	1.40
4	K	1002	HEM	C3C-C2C	-4.65	1.33	1.40
4	A	1002	HEM	C3C-C2C	-4.54	1.34	1.40
4	K	1002	HEM	C3C-CAC	4.07	1.56	1.47
4	O	1002	HEM	C3C-C2C	-3.90	1.35	1.40
4	W	1001	HEM	C3C-C2C	-3.89	1.35	1.40
4	S	1002	HEM	C3C-C2C	-3.88	1.35	1.40
4	O	1001	HEM	C3C-CAC	3.87	1.55	1.47
4	A	1001	HEM	C3C-CAC	3.87	1.55	1.47
4	S	1001	HEM	C3C-CAC	3.82	1.55	1.47
4	W	1002	HEM	C3C-CAC	3.82	1.55	1.47
4	K	1001	HEM	C3C-C2C	-3.79	1.35	1.40
4	E	1001	HEM	C3C-CAC	3.78	1.55	1.47
4	E	1002	HEM	C3C-C2C	-3.76	1.35	1.40
4	O	1001	HEM	C3C-C2C	-3.74	1.35	1.40
5	A	1003	SMA	C3-C2	3.66	1.41	1.34
4	A	1002	HEM	C3C-CAC	3.65	1.55	1.47
4	A	1001	HEM	C3C-C2C	-3.65	1.35	1.40
4	O	1002	HEM	C3C-CAC	3.63	1.55	1.47
4	E	1001	HEM	C3C-C2C	-3.59	1.35	1.40
4	S	1001	HEM	C3C-C2C	-3.58	1.35	1.40
4	E	1002	HEM	C3C-CAC	3.49	1.55	1.47
4	S	1002	HEM	C3C-CAC	3.48	1.54	1.47
4	K	1001	HEM	C3C-CAC	3.46	1.54	1.47
4	W	1001	HEM	C3C-CAC	3.36	1.54	1.47
5	K	1003	SMA	C3-C2	3.28	1.41	1.34
5	O	1003	SMA	C3-C2	3.25	1.41	1.34
5	S	1003	SMA	C3-C2	3.24	1.41	1.34
5	W	1003	SMA	C3-C2	3.19	1.40	1.34
4	S	1001	HEM	CAB-C3B	3.18	1.56	1.47
4	K	1001	HEM	CAB-C3B	3.12	1.55	1.47
4	W	1001	HEM	CAB-C3B	3.08	1.55	1.47
4	O	1001	HEM	CAB-C3B	3.03	1.55	1.47
5	E	1003	SMA	C3-C2	3.02	1.40	1.34
4	W	1002	HEM	CAB-C3B	3.01	1.55	1.47
4	E	1001	HEM	CAB-C3B	2.94	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1002	HEM	CAB-C3B	2.91	1.55	1.47
4	A	1001	HEM	CAB-C3B	2.91	1.55	1.47
4	O	1002	HEM	CAB-C3B	2.89	1.55	1.47
4	A	1002	HEM	CAB-C3B	2.88	1.55	1.47
4	S	1002	HEM	CAB-C3B	2.86	1.55	1.47
4	E	1002	HEM	FE-ND	2.80	2.10	1.96
4	K	1002	HEM	CAB-C3B	2.69	1.54	1.47
4	W	1001	HEM	CMB-C2B	2.45	1.56	1.50
4	K	1001	HEM	CMB-C2B	2.44	1.56	1.50
4	A	1001	HEM	CMB-C2B	2.32	1.55	1.50
4	O	1001	HEM	CMB-C2B	2.32	1.55	1.50
5	S	1003	SMA	C3-C4	-2.30	1.43	1.48
4	E	1001	HEM	FE-NB	2.26	2.08	1.96
5	O	1003	SMA	C3-C4	-2.24	1.43	1.48
4	A	1001	HEM	FE-NB	2.23	2.07	1.96
4	E	1001	HEM	CMB-C2B	2.22	1.55	1.50
4	S	1001	HEM	FE-NB	2.18	2.07	1.96
4	K	1001	HEM	FE-NB	2.16	2.07	1.96
4	E	1002	HEM	CMB-C2B	2.16	1.55	1.50
5	W	1003	SMA	C3-C4	-2.14	1.43	1.48
4	W	1002	HEM	CMB-C2B	2.13	1.55	1.50
4	K	1002	HEM	CMD-C2D	2.13	1.55	1.50
4	S	1001	HEM	CMB-C2B	2.13	1.55	1.50
5	E	1003	SMA	C3-C4	-2.13	1.43	1.48
4	S	1002	HEM	CMD-C2D	2.12	1.55	1.50
5	O	1003	SMA	C17-C18	2.11	1.40	1.34
7	L	1001	HEC	CAD-C3D	2.11	1.55	1.52
4	A	1002	HEM	CMB-C2B	2.10	1.55	1.50
4	O	1001	HEM	FE-NB	2.10	2.07	1.96
4	W	1002	HEM	CMD-C2D	2.09	1.55	1.50
4	E	1001	HEM	CAA-C2A	2.09	1.55	1.52
4	S	1002	HEM	CMB-C2B	2.08	1.55	1.50
4	A	1002	HEM	CMD-C2D	2.08	1.55	1.50
4	E	1001	HEM	CMD-C2D	2.08	1.55	1.50
4	S	1001	HEM	CMD-C2D	2.08	1.55	1.50
4	A	1002	HEM	CAA-C2A	2.07	1.55	1.52
5	K	1003	SMA	C3-C4	-2.07	1.43	1.48
4	S	1001	HEM	CAA-C2A	2.06	1.55	1.52
4	O	1002	HEM	CMB-C2B	2.06	1.55	1.50
7	B	1001	HEC	CAD-C3D	2.06	1.55	1.52
4	S	1002	HEM	FE-NB	2.06	2.07	1.96
4	O	1002	HEM	CMD-C2D	2.04	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	1001	HEM	CMD-C2D	2.03	1.55	1.50
5	W	1003	SMA	C7-C8	-2.03	1.37	1.40
4	W	1001	HEM	FE-NB	2.01	2.06	1.96

All (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
5	K	1003	SMA	C5M-O5-C5	-4.07	111.38	117.53
5	A	1003	SMA	O5-C5-C4A	4.06	121.50	115.85
5	E	1003	SMA	C5M-O5-C5	-4.01	111.47	117.53
5	O	1003	SMA	O7-C7-C8	3.96	118.54	114.54
5	A	1003	SMA	C5M-O5-C5	-3.96	111.56	117.53
5	K	1003	SMA	O5-C5-C4A	3.92	121.31	115.85
5	O	1003	SMA	O5-C5-C4A	3.91	121.30	115.85
5	O	1003	SMA	C5M-O5-C5	-3.77	111.83	117.53
7	F	1001	HEC	CMC-C2C-C1C	-3.74	122.71	128.46
7	B	1001	HEC	CMC-C2C-C1C	-3.66	122.85	128.46
5	E	1003	SMA	O5-C5-C6	-3.62	117.89	124.12
5	S	1003	SMA	C5M-O5-C5	-3.56	112.15	117.53
5	W	1003	SMA	O5-C5-C6	-3.51	118.08	124.12
4	O	1001	HEM	C4D-ND-C1D	3.46	108.64	105.07
5	S	1003	SMA	O5-C5-C6	-3.40	118.27	124.12
5	O	1003	SMA	O5-C5-C6	-3.40	118.28	124.12
4	A	1001	HEM	C4D-ND-C1D	3.39	108.57	105.07
4	K	1002	HEM	C4C-CHD-C1D	3.38	127.02	122.56
7	X	1001	HEC	CMC-C2C-C1C	-3.34	123.34	128.46
5	K	1003	SMA	O7-C7-C8	3.34	117.91	114.54
4	S	1001	HEM	C4D-ND-C1D	3.33	108.51	105.07
4	E	1001	HEM	CMC-C2C-C3C	3.32	130.88	124.68
4	E	1002	HEM	C4C-CHD-C1D	3.31	126.93	122.56
4	O	1002	HEM	C4C-CHD-C1D	3.28	126.88	122.56
5	A	1003	SMA	O5-C5-C6	-3.26	118.51	124.12
5	K	1003	SMA	O5-C5-C6	-3.22	118.57	124.12
5	E	1003	SMA	O7-C7-C8	3.21	117.78	114.54
7	L	1001	HEC	CMC-C2C-C1C	-3.20	123.54	128.46
4	S	1001	HEM	CMC-C2C-C3C	3.18	130.62	124.68
4	K	1001	HEM	C4D-ND-C1D	3.17	108.35	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	1001	HEC	CMC-C2C-C1C	-3.17	123.60	128.46
4	S	1001	HEM	C4B-CHC-C1C	3.15	126.72	122.56
4	W	1002	HEM	C4C-CHD-C1D	3.14	126.71	122.56
4	E	1002	HEM	C1B-NB-C4B	3.14	108.32	105.07
4	K	1001	HEM	C4B-CHC-C1C	3.13	126.69	122.56
5	O	1003	SMA	C22-C11-C10	3.12	115.26	110.36
5	W	1003	SMA	O7-C7-C8	3.12	117.69	114.54
4	A	1002	HEM	C4C-CHD-C1D	3.11	126.67	122.56
4	W	1001	HEM	C4D-ND-C1D	3.10	108.28	105.07
4	W	1002	HEM	C4B-CHC-C1C	3.05	126.59	122.56
5	A	1003	SMA	O7-C7-C8	3.04	117.61	114.54
4	O	1001	HEM	C4B-CHC-C1C	3.04	126.57	122.56
4	O	1001	HEM	CBA-CAA-C2A	-3.03	107.45	112.62
4	E	1001	HEM	C4D-ND-C1D	3.00	108.17	105.07
4	S	1001	HEM	C4C-CHD-C1D	3.00	126.51	122.56
7	P	1001	HEC	CMC-C2C-C1C	-2.96	123.91	128.46
4	S	1002	HEM	C4C-CHD-C1D	2.94	126.44	122.56
4	W	1001	HEM	CMC-C2C-C3C	2.93	130.16	124.68
4	A	1002	HEM	C4D-ND-C1D	2.88	108.05	105.07
5	E	1003	SMA	O1-C2-C9	2.88	116.70	110.58
4	A	1002	HEM	C1B-NB-C4B	2.86	108.03	105.07
4	A	1002	HEM	CHD-C1D-ND	2.84	127.51	124.43
4	O	1002	HEM	C1B-NB-C4B	2.83	108.00	105.07
5	S	1003	SMA	O1-C2-C9	2.81	116.55	110.58
4	A	1002	HEM	C4B-CHC-C1C	2.81	126.27	122.56
4	A	1001	HEM	C4B-CHC-C1C	2.80	126.26	122.56
4	E	1002	HEM	C4D-ND-C1D	2.78	107.94	105.07
4	E	1002	HEM	C4B-CHC-C1C	2.76	126.21	122.56
5	K	1003	SMA	O1-C2-C9	2.76	116.44	110.58
5	W	1003	SMA	O1-C2-C9	2.73	116.38	110.58
4	K	1002	HEM	C4B-CHC-C1C	2.71	126.13	122.56
4	W	1001	HEM	C4B-CHC-C1C	2.70	126.12	122.56
4	K	1002	HEM	C4D-ND-C1D	2.70	107.86	105.07
4	E	1001	HEM	C4B-CHC-C1C	2.67	126.08	122.56
4	K	1001	HEM	CBA-CAA-C2A	-2.62	108.14	112.62
4	K	1002	HEM	CBA-CAA-C2A	-2.62	108.14	112.62
5	E	1003	SMA	C22-C11-C10	2.62	114.47	110.36
4	W	1001	HEM	CBA-CAA-C2A	-2.61	108.17	112.62
4	A	1001	HEM	C4C-CHD-C1D	2.59	125.98	122.56
4	W	1002	HEM	C4D-ND-C1D	2.56	107.71	105.07
4	S	1001	HEM	C1B-NB-C4B	2.55	107.71	105.07
5	A	1003	SMA	O1-C2-C9	2.52	115.92	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	X	1001	HEC	C1D-C2D-C3D	-2.51	105.25	107.00
4	A	1001	HEM	CMC-C2C-C3C	2.51	129.37	124.68
4	O	1001	HEM	C1B-NB-C4B	2.51	107.66	105.07
5	W	1003	SMA	C22-C11-C12	-2.51	107.05	111.15
4	E	1002	HEM	CBA-CAA-C2A	-2.50	108.35	112.62
5	E	1003	SMA	C8A-O1-C2	2.49	123.19	119.35
4	O	1001	HEM	C4C-CHD-C1D	2.43	125.77	122.56
4	O	1002	HEM	C4D-ND-C1D	2.43	107.58	105.07
4	W	1002	HEM	C1B-NB-C4B	2.43	107.58	105.07
7	F	1001	HEC	C1D-C2D-C3D	-2.42	105.31	107.00
4	K	1001	HEM	C1B-NB-C4B	2.40	107.56	105.07
5	A	1003	SMA	C8A-O1-C2	2.38	123.02	119.35
5	S	1003	SMA	C8A-O1-C2	2.37	123.01	119.35
4	K	1001	HEM	CHA-C4D-ND	2.36	127.29	124.38
5	W	1003	SMA	C22-C11-C10	2.36	114.06	110.36
4	A	1001	HEM	CBA-CAA-C2A	-2.36	108.60	112.62
7	X	1001	HEC	CBD-CAD-C3D	-2.34	108.62	112.62
5	O	1003	SMA	O1-C2-C9	2.33	115.53	110.58
5	E	1003	SMA	C14-C15-C16	-2.33	121.06	125.61
4	S	1002	HEM	C4D-ND-C1D	2.32	107.47	105.07
5	W	1003	SMA	C8A-O1-C2	2.30	122.90	119.35
5	S	1003	SMA	C22-C11-C10	2.30	113.97	110.36
4	W	1001	HEM	C4C-CHD-C1D	2.30	125.59	122.56
7	T	1001	HEC	CBD-CAD-C3D	-2.29	108.71	112.62
4	K	1002	HEM	C1B-NB-C4B	2.29	107.44	105.07
5	K	1003	SMA	C8A-O1-C2	2.29	122.87	119.35
4	W	1001	HEM	C1B-NB-C4B	2.28	107.42	105.07
5	O	1003	SMA	C8A-O1-C2	2.28	122.86	119.35
4	E	1001	HEM	C4C-CHD-C1D	2.27	125.55	122.56
4	W	1001	HEM	C3D-C4D-ND	-2.27	107.64	110.17
5	W	1003	SMA	C14-C15-C16	-2.26	121.18	125.61
4	O	1002	HEM	C3B-C2B-C1B	2.26	108.16	106.49
5	E	1003	SMA	C22-C11-C12	-2.25	107.47	111.15
4	W	1002	HEM	CBA-CAA-C2A	-2.24	108.79	112.62
7	P	1001	HEC	CAA-CBA-CGA	-2.23	107.51	113.76
5	A	1003	SMA	C22-C11-C10	2.23	113.85	110.36
4	A	1001	HEM	C1B-NB-C4B	2.21	107.36	105.07
4	O	1001	HEM	C3D-C4D-ND	-2.21	107.71	110.17
4	O	1001	HEM	CMC-C2C-C3C	2.21	128.80	124.68
4	S	1002	HEM	C1B-NB-C4B	2.20	107.35	105.07
5	O	1003	SMA	C14-C15-C16	-2.20	121.30	125.61
4	S	1001	HEM	C3D-C4D-ND	-2.19	107.72	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	1001	HEC	CBD-CAD-C3D	-2.19	108.88	112.62
5	E	1003	SMA	C16-C17-C18	-2.19	119.20	124.67
4	E	1001	HEM	C1B-NB-C4B	2.19	107.33	105.07
4	W	1002	HEM	CHD-C1D-ND	2.19	126.81	124.43
5	S	1003	SMA	C14-C15-C16	-2.19	121.33	125.61
7	P	1001	HEC	CBA-CAA-C2A	-2.18	108.92	112.60
5	A	1003	SMA	C16-C17-C18	-2.18	119.22	124.67
7	P	1001	HEC	C1D-C2D-C3D	-2.18	105.48	107.00
5	O	1003	SMA	C22-C11-C12	-2.18	107.58	111.15
5	A	1003	SMA	C14-C15-C16	-2.17	121.35	125.61
4	S	1002	HEM	CMC-C2C-C3C	2.16	128.72	124.68
4	S	1002	HEM	CBA-CAA-C2A	-2.14	108.97	112.62
6	A	1004	6PE	O1-P1-O2	2.13	122.75	112.24
4	W	1001	HEM	CAD-CBD-CGD	-2.13	109.03	113.60
7	X	1001	HEC	CAA-CBA-CGA	-2.12	107.83	113.76
7	L	1001	HEC	C1D-C2D-C3D	-2.12	105.52	107.00
4	A	1001	HEM	C3D-C4D-ND	-2.11	107.82	110.17
5	K	1003	SMA	C16-C17-C18	-2.11	119.41	124.67
4	S	1001	HEM	C3B-C2B-C1B	2.10	108.05	106.49
5	S	1003	SMA	C16-C17-C18	-2.10	119.43	124.67
7	P	1001	HEC	CBD-CAD-C3D	-2.10	109.04	112.62
4	A	1002	HEM	C3D-C4D-ND	-2.08	107.85	110.17
4	K	1001	HEM	CMC-C2C-C3C	2.07	128.55	124.68
4	K	1001	HEM	C3D-C4D-ND	-2.03	107.91	110.17
4	K	1002	HEM	CHD-C1D-ND	2.03	126.63	124.43
6	E	1004	6PE	C2-O6-C10	2.03	122.78	117.79
4	K	1001	HEM	CAD-CBD-CGD	-2.02	109.25	113.60
7	P	1001	HEC	CMB-C2B-C1B	-2.02	125.36	128.46
4	E	1002	HEM	CMC-C2C-C3C	2.01	128.45	124.68
4	E	1002	HEM	C2C-C3C-C4C	2.01	108.30	106.90
7	T	1001	HEC	CBA-CAA-C2A	-2.01	109.22	112.60

There are no chirality outliers.

All (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
6	A	1004	6PE	O8-C16-C17-N1
6	E	1004	6PE	C1-O3-P1-O2
6	E	1004	6PE	C1-O3-P1-O8
6	E	1004	6PE	O6-C2-C3-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	W	1004	6PE	C1-O3-P1-O1
6	W	1004	6PE	C1-O3-P1-O2
6	W	1004	6PE	C1-O3-P1-O8
6	W	1004	6PE	O6-C2-C3-O4
9	L	1003	BOG	C4-C5-C6-O6
9	F	1002	BOG	C4-C5-C6-O6
9	L	1003	BOG	O5-C5-C6-O6
6	W	1004	6PE	C5-C4-O4-C3
9	F	1002	BOG	O5-C5-C6-O6
9	P	1002	BOG	C4-C5-C6-O6
5	E	1003	SMA	C6-C5-O5-C5M
5	A	1003	SMA	C6-C5-O5-C5M
5	K	1003	SMA	C6-C5-O5-C5M
5	O	1003	SMA	C6-C5-O5-C5M
5	S	1003	SMA	C6-C5-O5-C5M
5	W	1003	SMA	C6-C5-O5-C5M
9	P	1002	BOG	O5-C5-C6-O6
6	W	1004	6PE	O5-C4-O4-C3
6	A	1004	6PE	C5-C4-O4-C3
6	E	1004	6PE	C5-C4-O4-C3
5	E	1003	SMA	C4A-C5-O5-C5M
5	K	1003	SMA	C4A-C5-O5-C5M
5	O	1003	SMA	C4A-C5-O5-C5M
5	W	1003	SMA	C4A-C5-O5-C5M
5	A	1003	SMA	C4A-C5-O5-C5M
5	S	1003	SMA	C4A-C5-O5-C5M
6	A	1004	6PE	O5-C4-O4-C3
6	E	1004	6PE	O5-C4-O4-C3
6	A	1004	6PE	C16-O8-P1-O3
9	X	1003	BOG	C2'-C3'-C4'-C5'
5	K	1003	SMA	C8-C7-O7-C7M
5	A	1003	SMA	C8-C7-O7-C7M
5	W	1003	SMA	C8-C7-O7-C7M
5	S	1003	SMA	C8-C7-O7-C7M
5	O	1003	SMA	C8-C7-O7-C7M
9	X	1003	BOG	C4'-C5'-C6'-C7'
5	E	1003	SMA	C8-C7-O7-C7M
9	X	1003	BOG	O5-C1-O1-C1'
5	E	1003	SMA	C9-C10-C11-C22
5	W	1003	SMA	C9-C10-C11-C22
6	E	1004	6PE	O3-C1-C2-C3
5	K	1003	SMA	C6-C7-O7-C7M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	W	1003	SMA	C6-C7-O7-C7M
6	A	1004	6PE	C1-C2-C3-O4
6	E	1004	6PE	C1-C2-C3-O4
6	W	1004	6PE	C1-C2-C3-O4
5	A	1003	SMA	C6-C7-O7-C7M
5	O	1003	SMA	C6-C7-O7-C7M
5	S	1003	SMA	C6-C7-O7-C7M
6	W	1004	6PE	C11-C10-O6-C2
5	A	1003	SMA	C9-C10-C11-C22
5	E	1003	SMA	C6-C7-O7-C7M
6	A	1004	6PE	O6-C2-C3-O4
6	A	1004	6PE	C4-C5-C6-C7
6	W	1004	6PE	C10-C11-C12-C13
5	K	1003	SMA	C9-C10-C11-C22
6	A	1004	6PE	C10-C11-C12-C13
6	E	1004	6PE	C10-C11-C12-C13
9	P	1002	BOG	C4'-C5'-C6'-C7'
5	O	1003	SMA	C9-C10-C11-C22
5	S	1003	SMA	C9-C10-C11-C22
6	E	1004	6PE	O3-C1-C2-O6
6	W	1004	6PE	O7-C10-O6-C2
6	A	1004	6PE	C11-C10-O6-C2
9	X	1003	BOG	C2-C1-O1-C1'
6	A	1004	6PE	O7-C10-O6-C2
6	E	1004	6PE	O4-C4-C5-C6
6	E	1004	6PE	O8-C16-C17-N1
4	S	1001	HEM	CAA-CBA-CGA-O1A
4	A	1001	HEM	CAA-CBA-CGA-O1A
4	E	1001	HEM	CAA-CBA-CGA-O1A
4	O	1001	HEM	CAA-CBA-CGA-O1A
4	W	1001	HEM	CAA-CBA-CGA-O1A
4	K	1001	HEM	CAA-CBA-CGA-O1A
4	K	1002	HEM	CAD-CBD-CGD-O1D
4	S	1002	HEM	CAD-CBD-CGD-O1D
4	W	1002	HEM	CAD-CBD-CGD-O1D
9	B	1003	BOG	O5-C5-C6-O6
4	A	1002	HEM	CAD-CBD-CGD-O1D
4	K	1002	HEM	CAA-CBA-CGA-O1A
4	K	1002	HEM	CAA-CBA-CGA-O2A
4	A	1001	HEM	CAA-CBA-CGA-O2A
4	E	1001	HEM	CAA-CBA-CGA-O2A
4	W	1001	HEM	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	K	1001	HEM	CAA-CBA-CGA-O2A
4	O	1001	HEM	CAA-CBA-CGA-O2A
4	S	1001	HEM	CAA-CBA-CGA-O2A
4	O	1002	HEM	CAD-CBD-CGD-O1D
4	E	1002	HEM	CAD-CBD-CGD-O1D
7	T	1001	HEC	CAD-CBD-CGD-O2D
6	A	1004	6PE	O3-C1-C2-O6
7	L	1001	HEC	CAD-CBD-CGD-O2D
6	E	1004	6PE	C12-C13-C14-C15
7	F	1001	HEC	CAD-CBD-CGD-O2D
4	K	1002	HEM	CAD-CBD-CGD-O2D
4	O	1002	HEM	CAD-CBD-CGD-O2D
4	S	1002	HEM	CAD-CBD-CGD-O2D
4	W	1002	HEM	CAD-CBD-CGD-O2D
4	A	1002	HEM	CAD-CBD-CGD-O2D
4	E	1002	HEM	CAD-CBD-CGD-O2D
7	L	1001	HEC	CAA-CBA-CGA-O2A
7	P	1001	HEC	CAA-CBA-CGA-O2A
7	T	1001	HEC	CAA-CBA-CGA-O2A
7	B	1001	HEC	CAA-CBA-CGA-O2A
7	T	1001	HEC	CAD-CBD-CGD-O1D
7	X	1001	HEC	CAA-CBA-CGA-O2A
7	F	1001	HEC	CAA-CBA-CGA-O2A
6	W	1004	6PE	O6-C10-C11-C12
7	L	1001	HEC	CAD-CBD-CGD-O1D
7	T	1001	HEC	CAA-CBA-CGA-O1A
7	F	1001	HEC	CAD-CBD-CGD-O1D
6	A	1004	6PE	C5-C6-C7-C8
7	B	1001	HEC	CAA-CBA-CGA-O1A
7	L	1001	HEC	CAA-CBA-CGA-O1A
7	X	1001	HEC	CAA-CBA-CGA-O1A
7	F	1001	HEC	CAA-CBA-CGA-O1A
7	P	1001	HEC	CAA-CBA-CGA-O1A
6	A	1004	6PE	O6-C10-C11-C12
6	A	1004	6PE	O4-C4-C5-C6
6	A	1004	6PE	O5-C4-C5-C6
6	W	1004	6PE	O7-C10-C11-C12
6	A	1004	6PE	O3-C1-C2-C3
6	A	1004	6PE	O7-C10-C11-C12
9	B	1003	BOG	C4-C5-C6-O6
4	E	1002	HEM	C3D-CAD-CBD-CGD

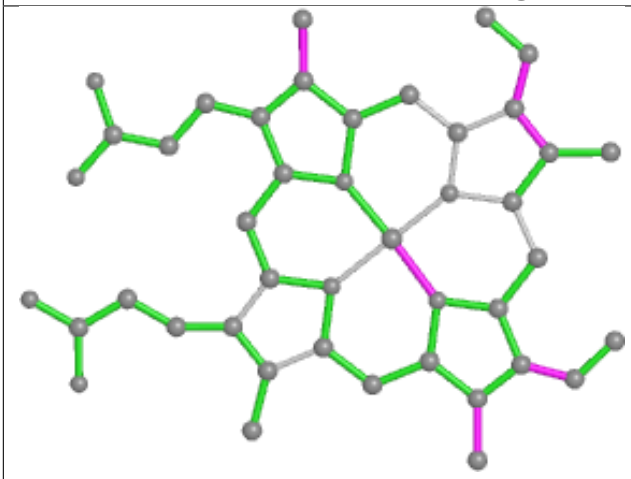
There are no ring outliers.

22 monomers are involved in 46 short contacts:

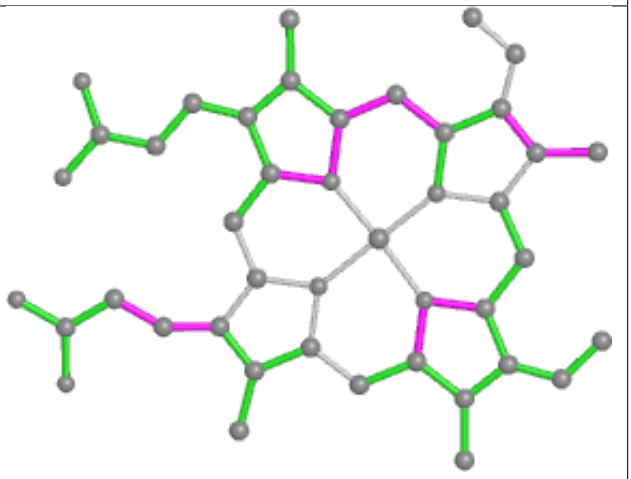
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1002	HEM	3	0
4	S	1001	HEM	1	0
4	E	1001	HEM	1	0
4	W	1001	HEM	1	0
5	O	1003	SMA	1	0
4	K	1002	HEM	3	0
7	B	1001	HEC	3	0
4	E	1002	HEM	2	0
4	A	1002	HEM	2	0
4	K	1001	HEM	2	0
5	K	1003	SMA	1	0
7	L	1001	HEC	3	0
7	X	1001	HEC	2	0
5	S	1003	SMA	1	0
7	T	1001	HEC	4	0
4	O	1002	HEM	2	0
9	B	1003	BOG	1	0
4	A	1001	HEM	1	0
4	W	1002	HEM	2	0
7	F	1001	HEC	5	0
7	P	1001	HEC	3	0
4	O	1001	HEM	2	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.

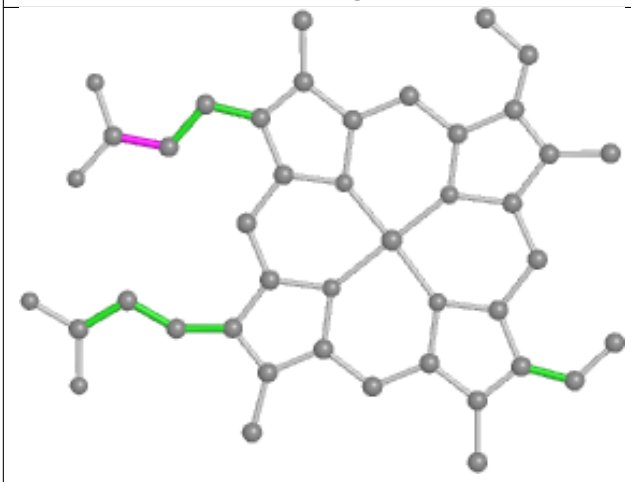
Ligand HEM S 1002



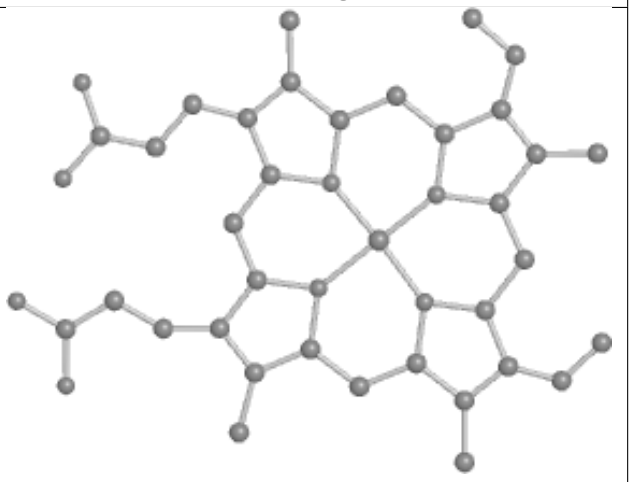
Bond lengths



Bond angles

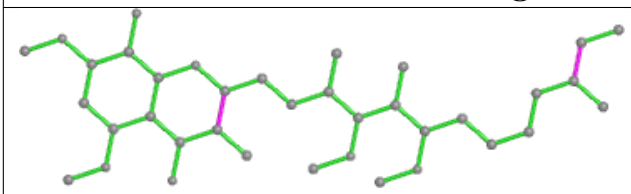


Torsions

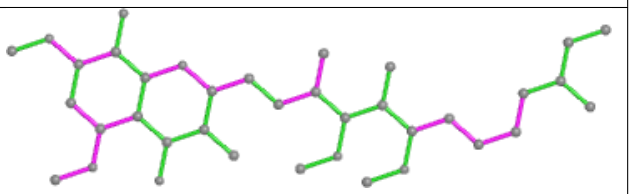


Rings

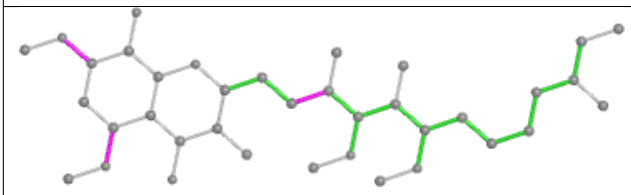
Ligand SMA A 1003



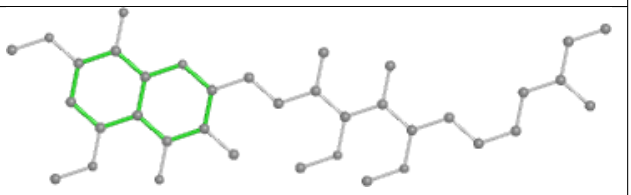
Bond lengths



Bond angles

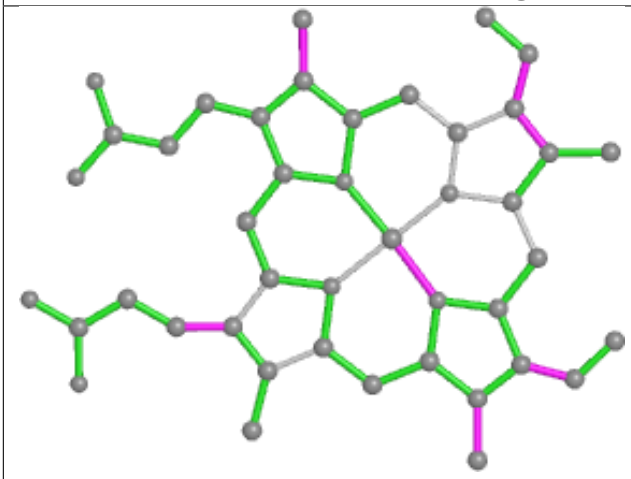


Torsions

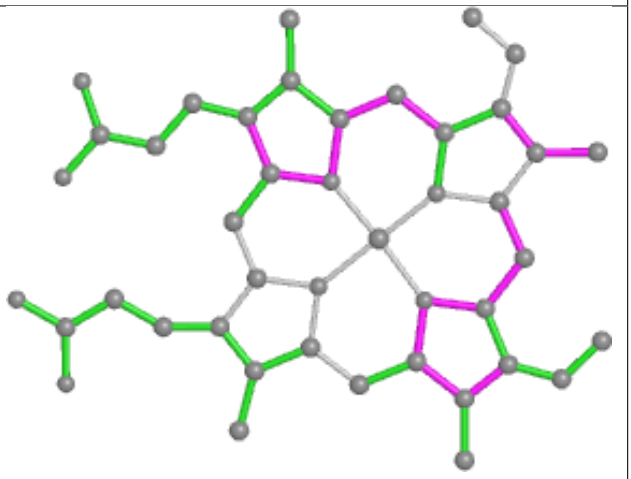


Rings

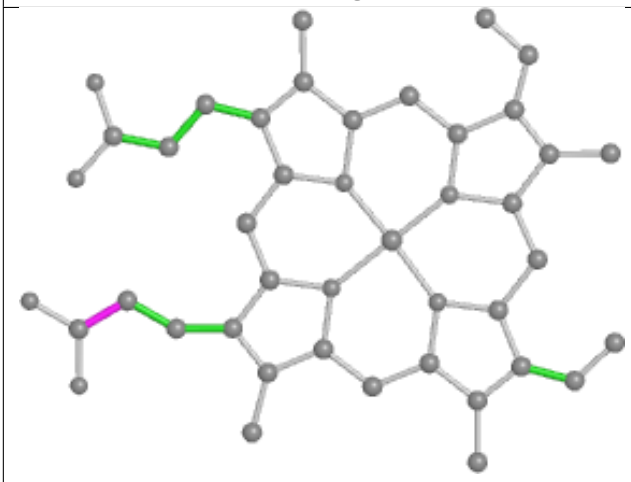
Ligand HEM S 1001



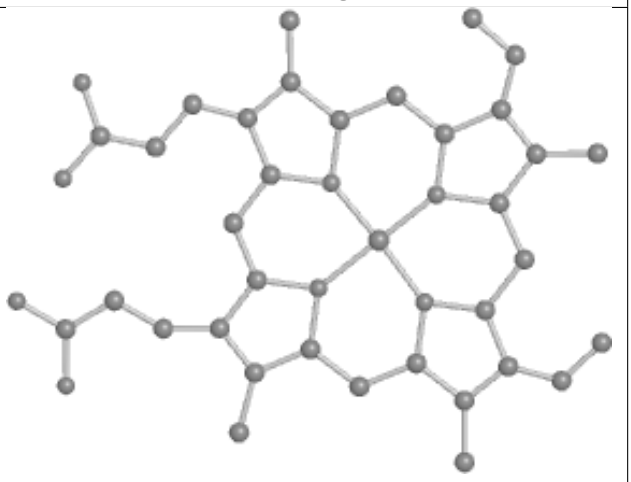
Bond lengths



Bond angles

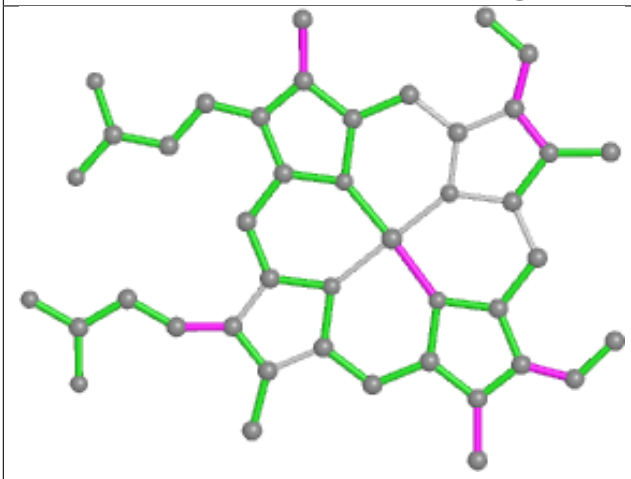


Torsions

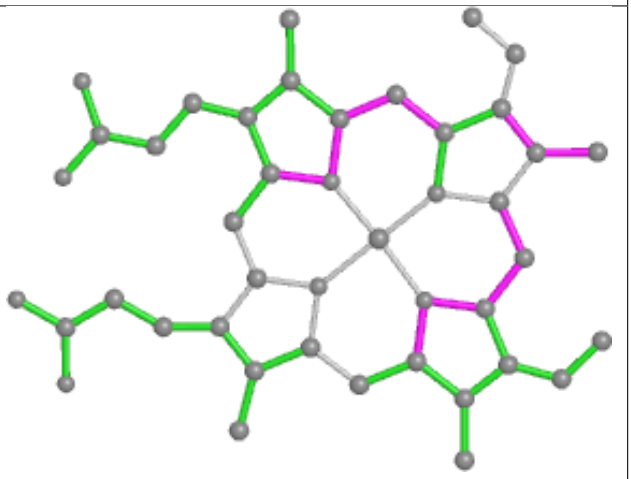


Rings

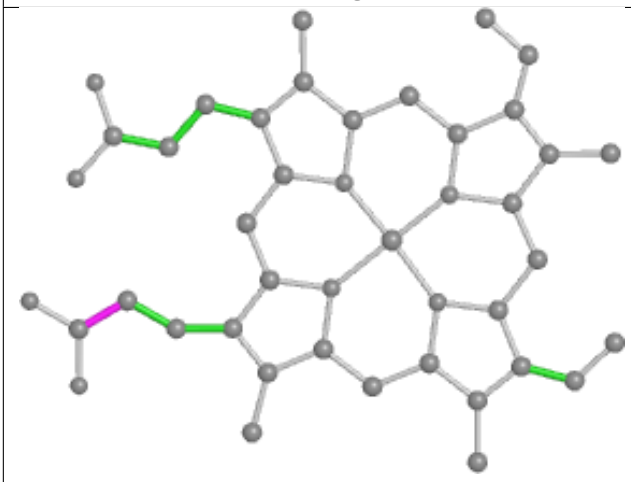
Ligand HEM E 1001



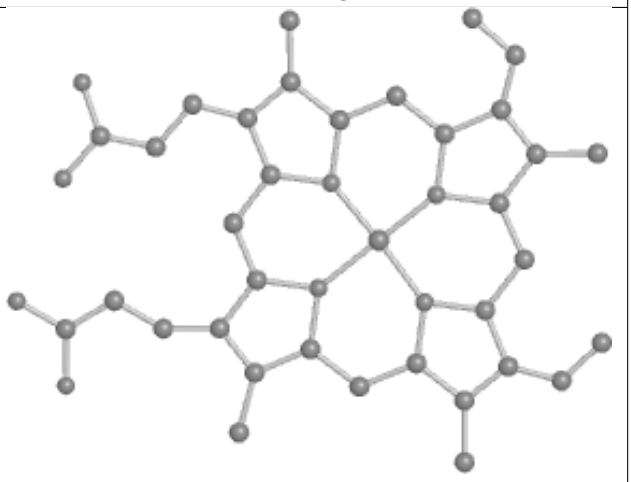
Bond lengths



Bond angles

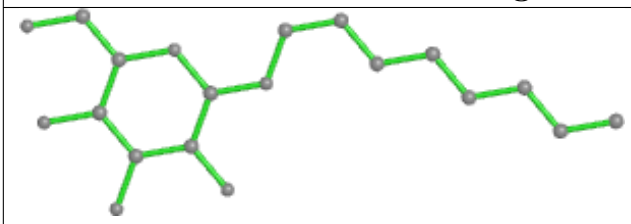


Torsions

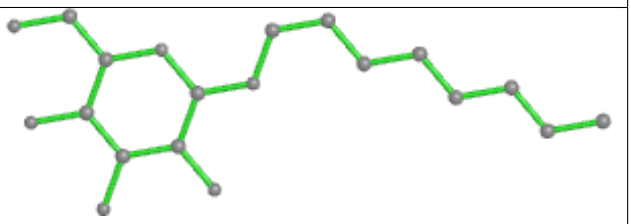


Rings

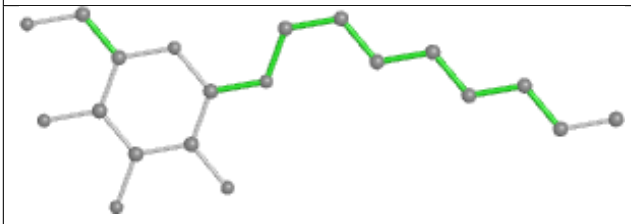
Ligand BOG T 1003



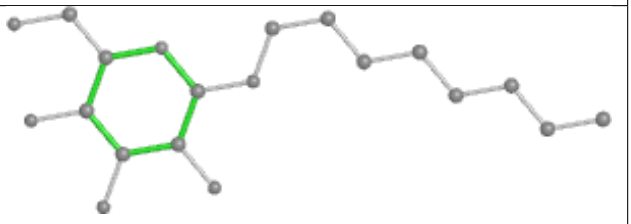
Bond lengths



Bond angles

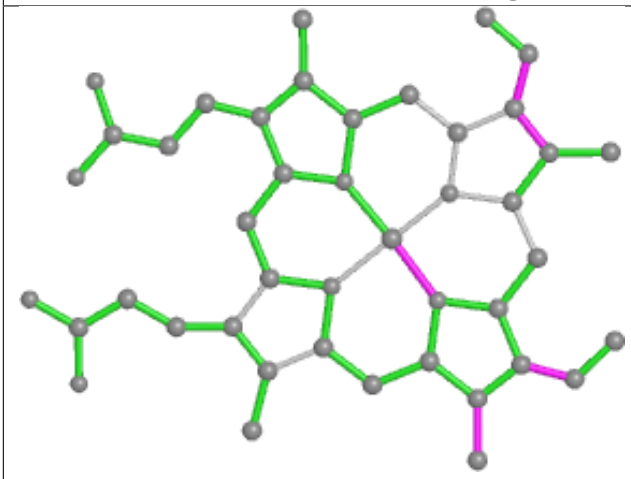


Torsions

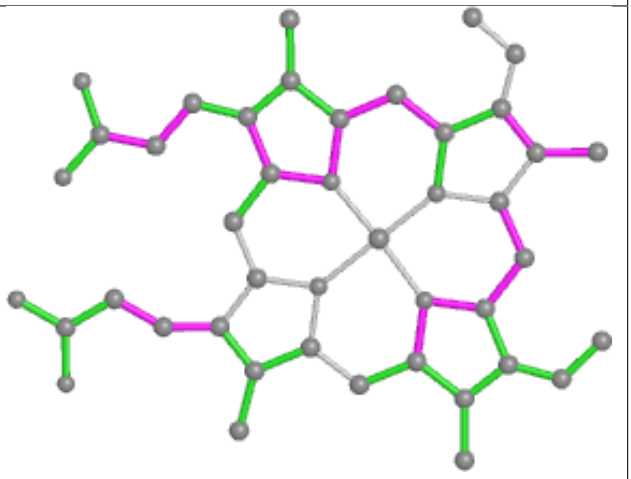


Rings

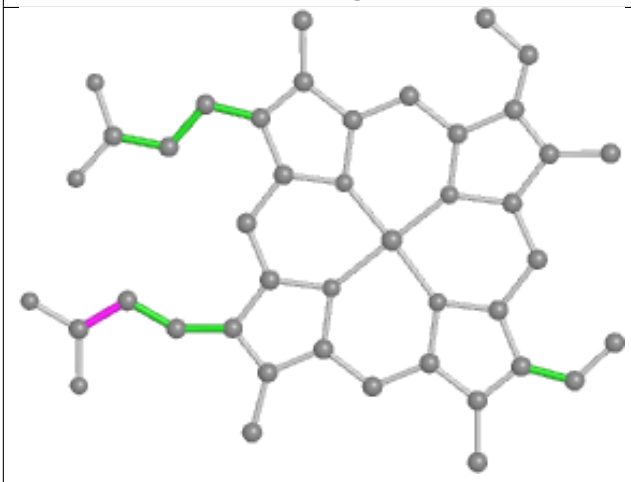
Ligand HEM W 1001



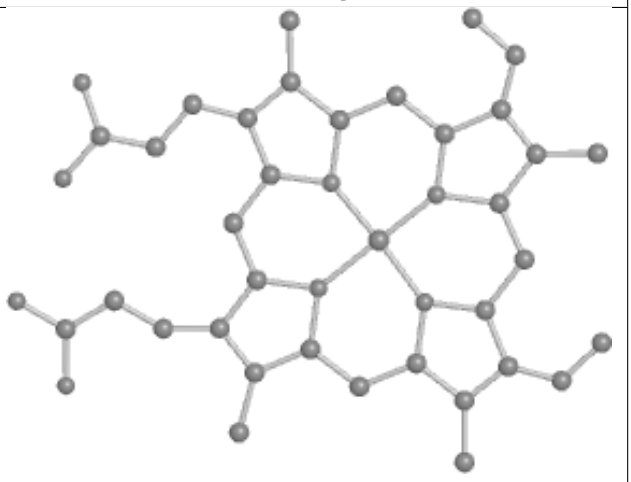
Bond lengths



Bond angles

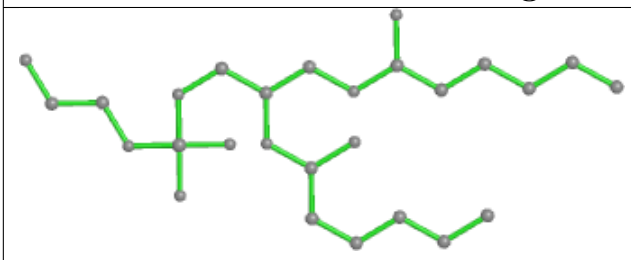


Torsions

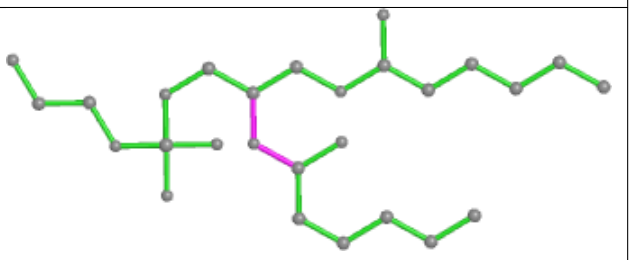


Rings

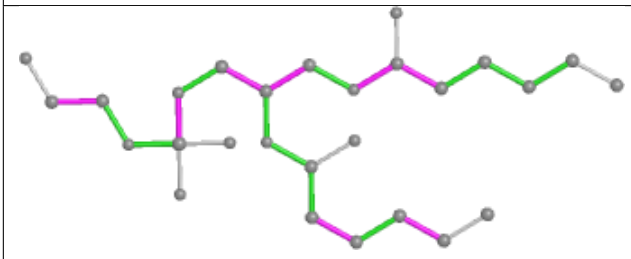
Ligand 6PE E 1004



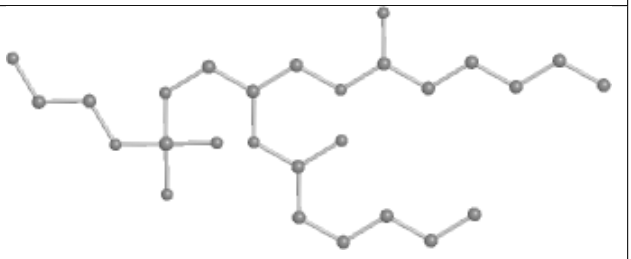
Bond lengths



Bond angles

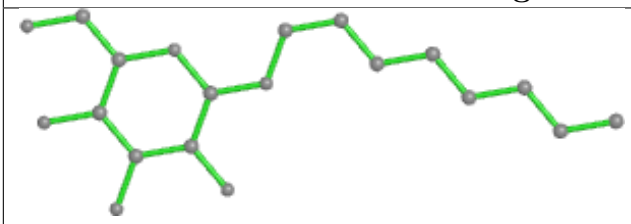


Torsions

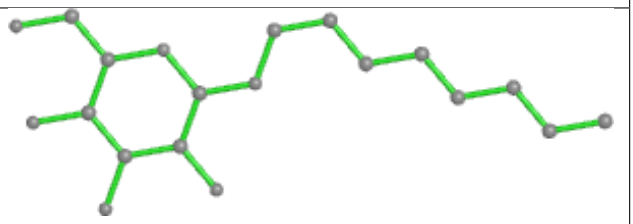


Rings

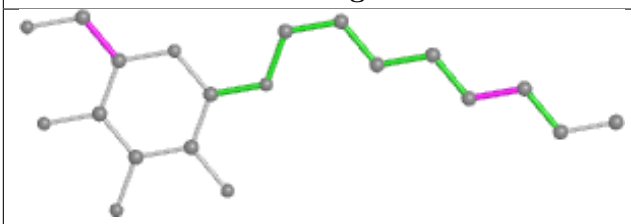
Ligand BOG P 1002



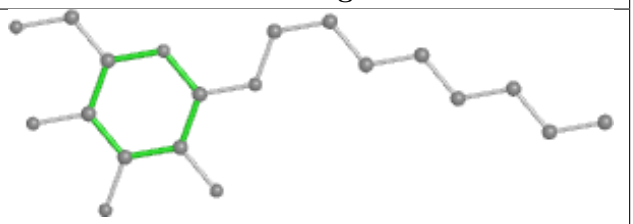
Bond lengths



Bond angles

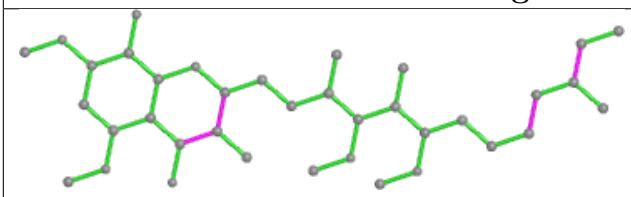


Torsions

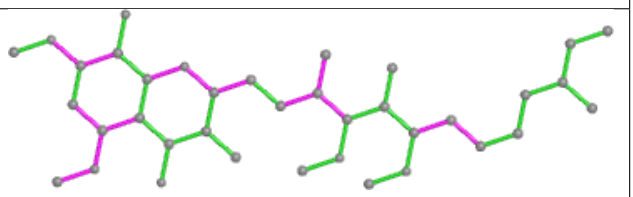


Rings

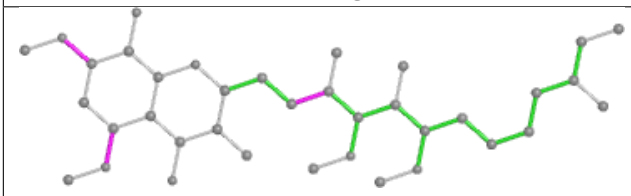
Ligand SMA O 1003



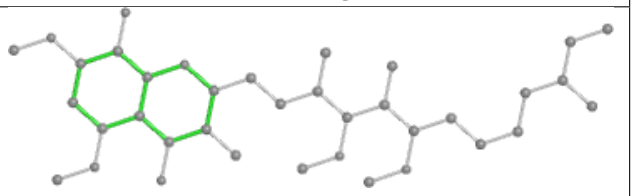
Bond lengths



Bond angles

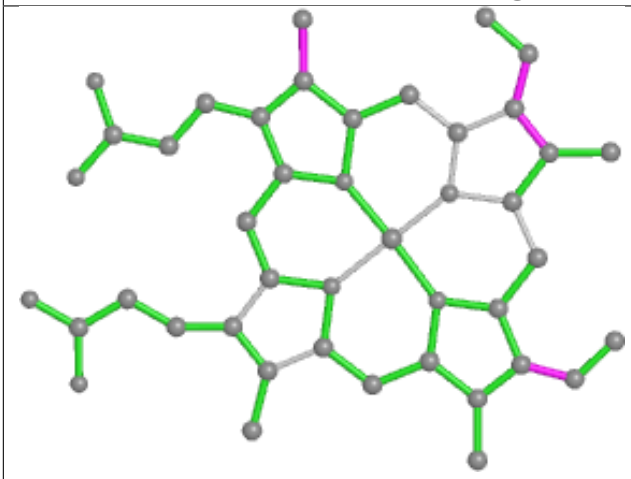


Torsions

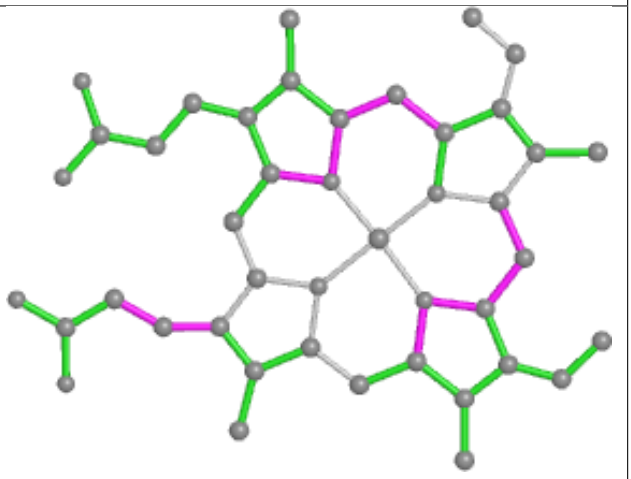


Rings

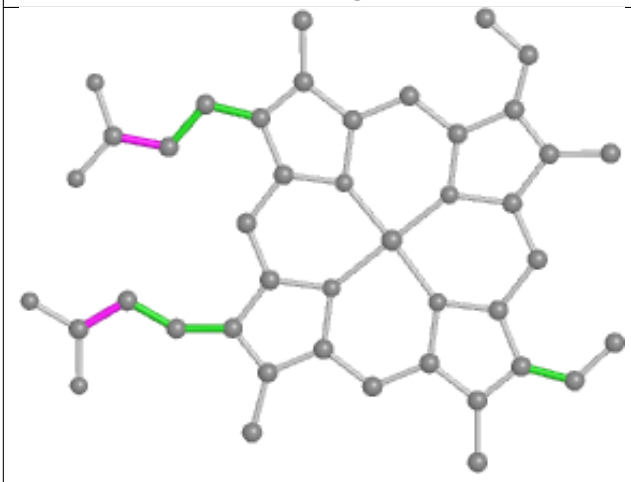
Ligand HEM K 1002



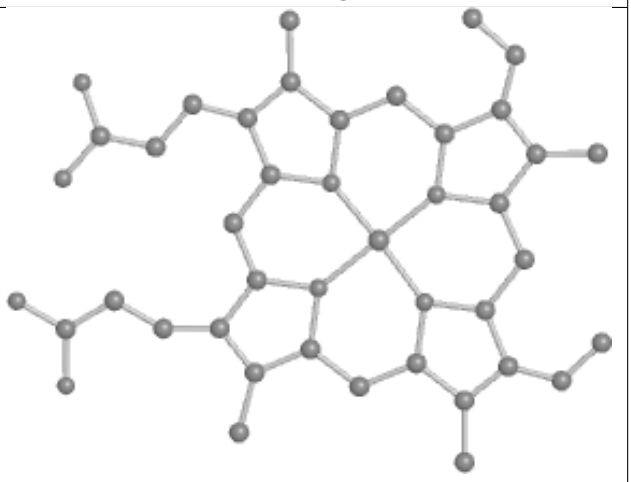
Bond lengths



Bond angles

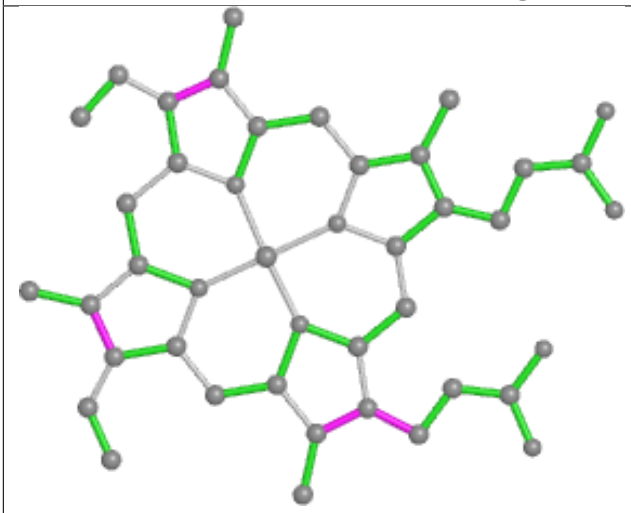


Torsions

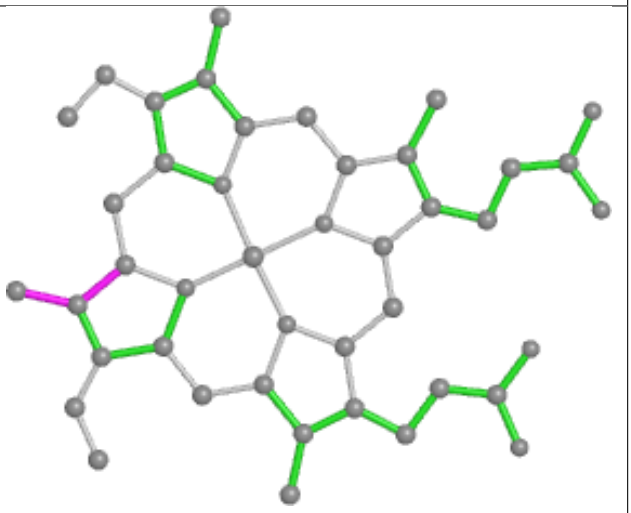


Rings

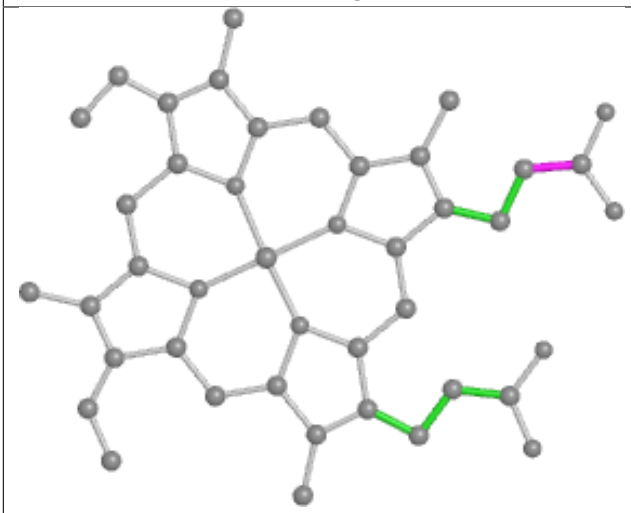
Ligand HEC B 1001



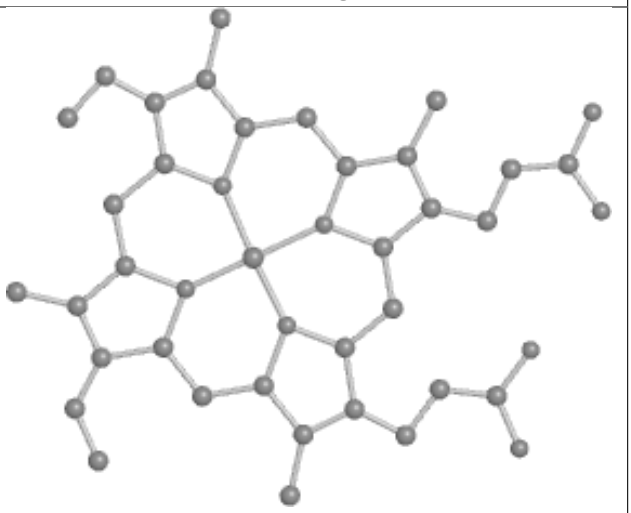
Bond lengths



Bond angles

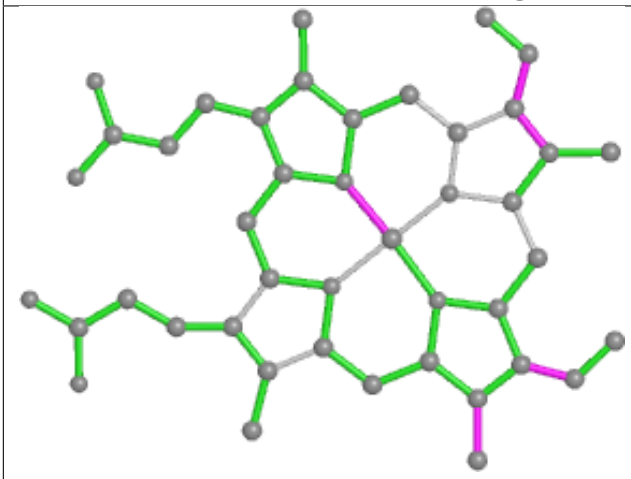


Torsions

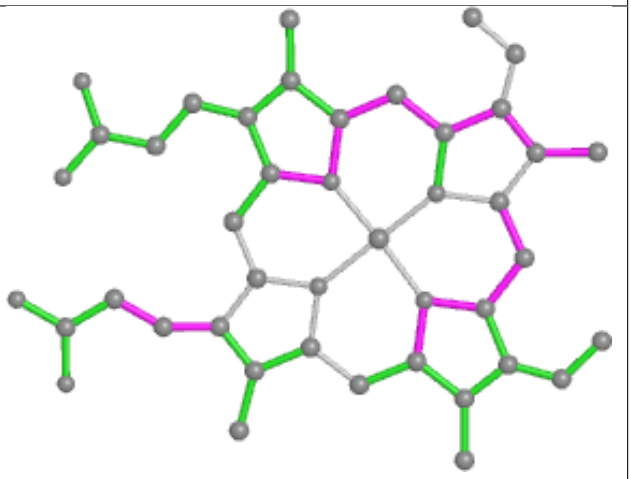


Rings

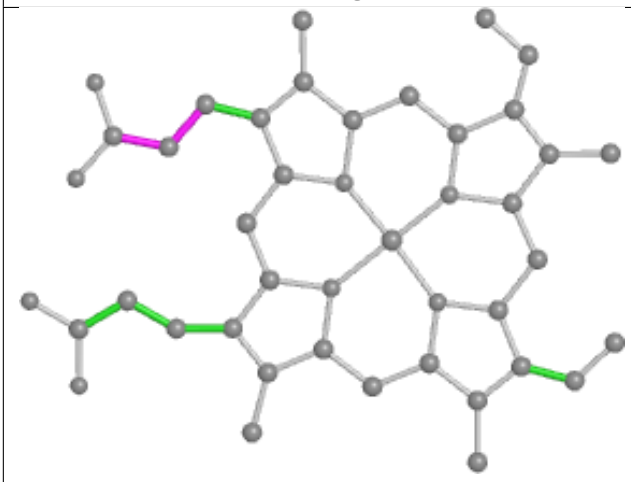
Ligand HEM E 1002



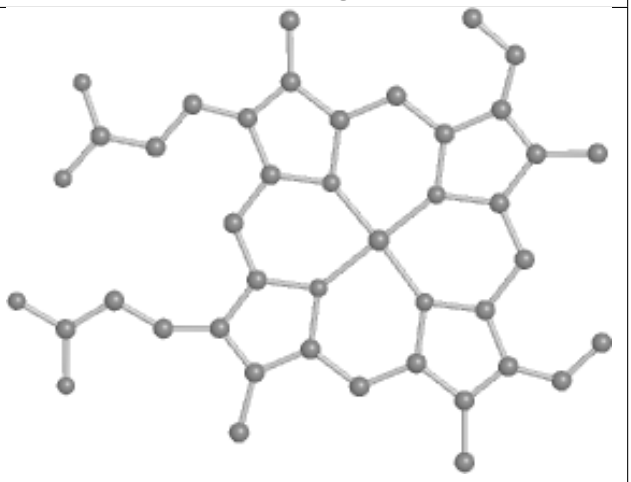
Bond lengths



Bond angles

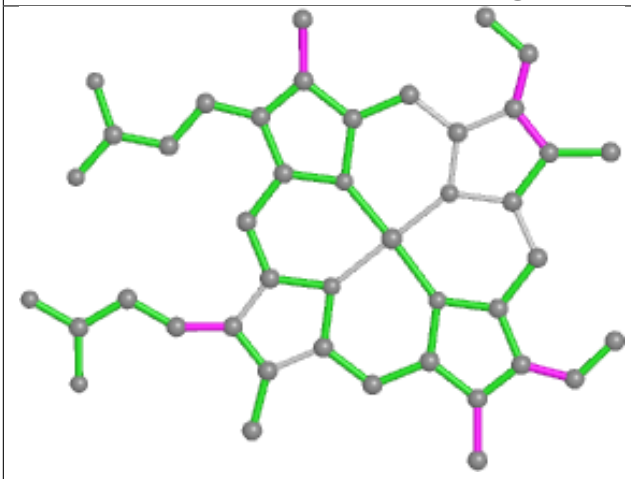


Torsions

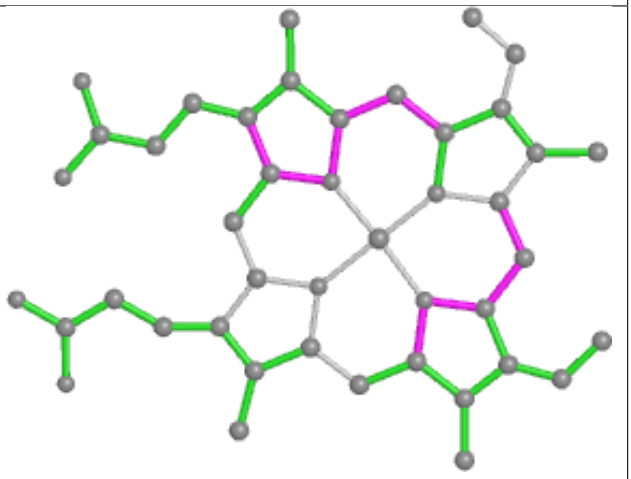


Rings

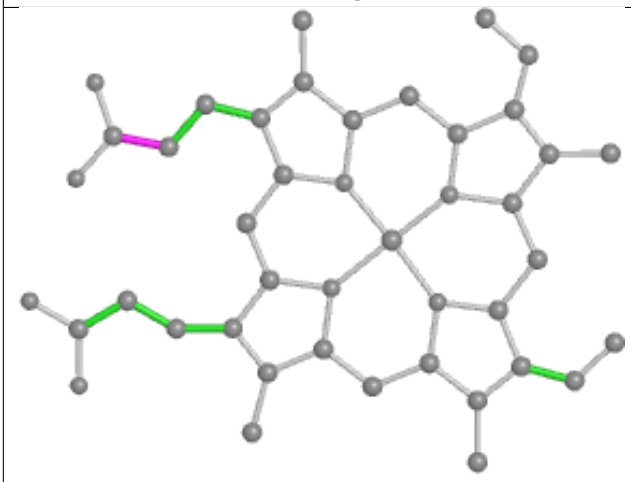
Ligand HEM A 1002



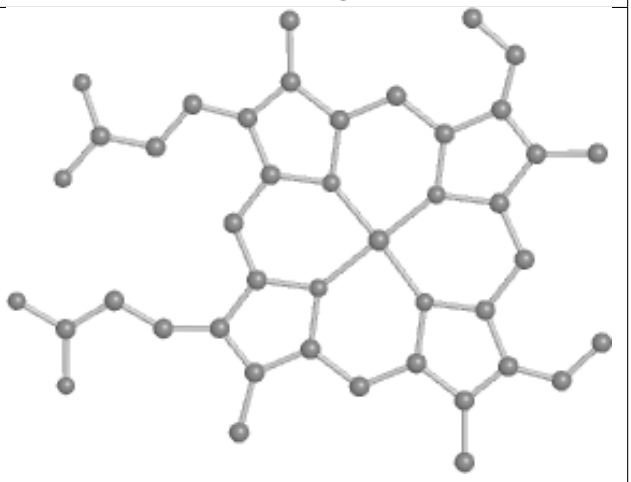
Bond lengths



Bond angles

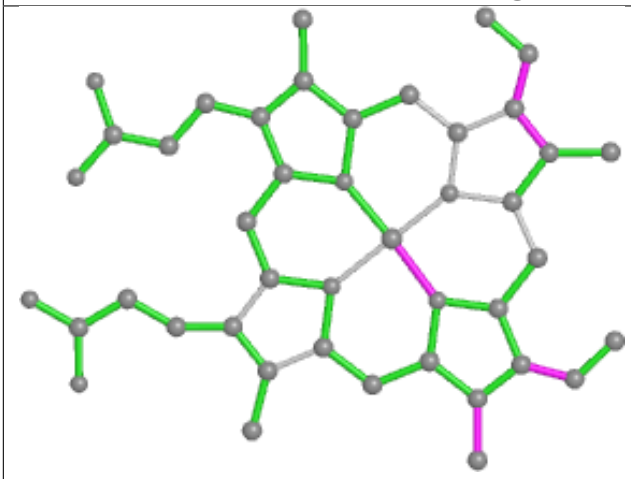


Torsions

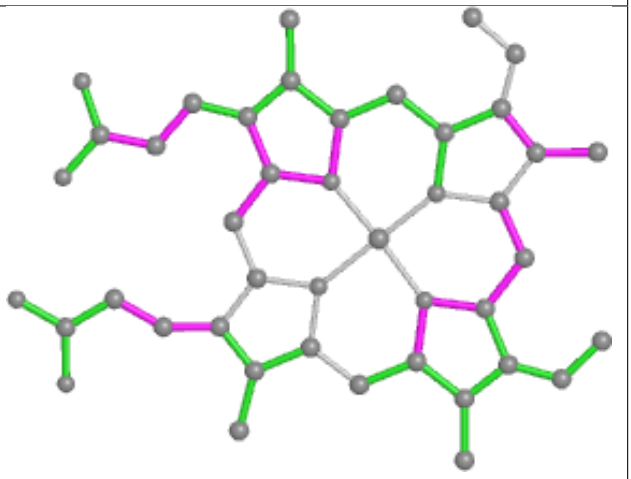


Rings

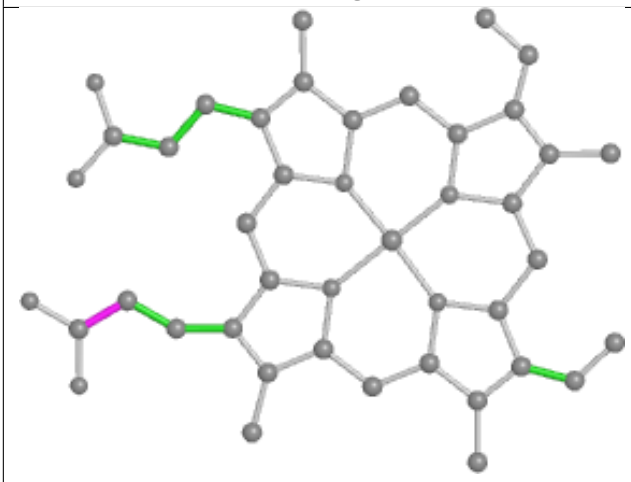
Ligand HEM K 1001



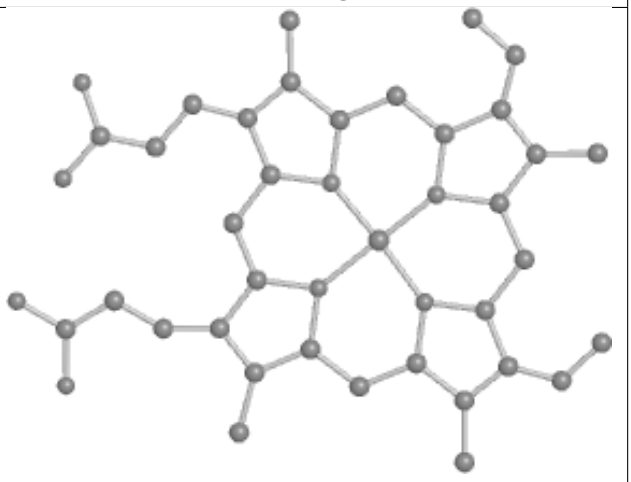
Bond lengths



Bond angles

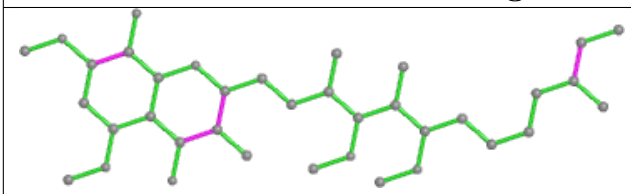


Torsions

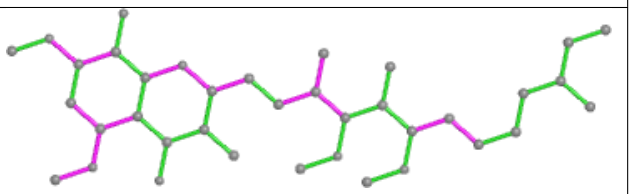


Rings

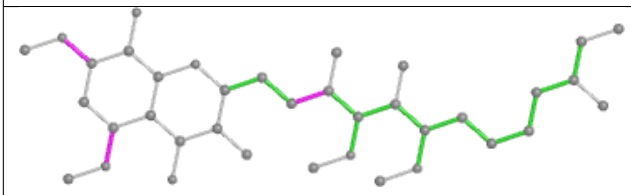
Ligand SMA W 1003



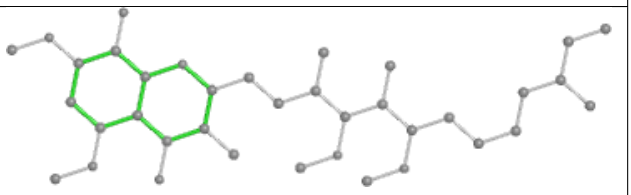
Bond lengths



Bond angles

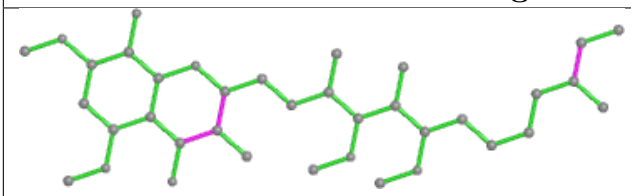


Torsions

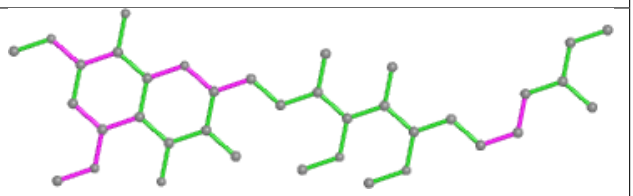


Rings

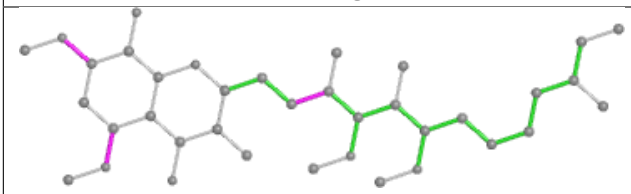
Ligand SMA K 1003



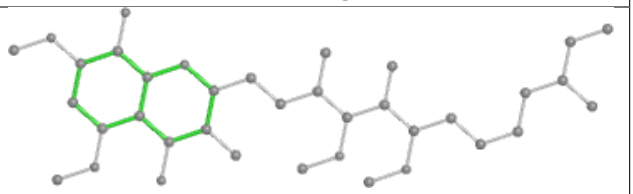
Bond lengths



Bond angles

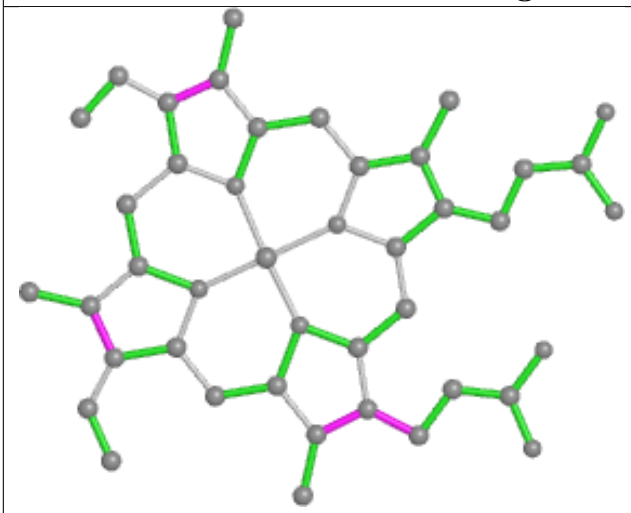


Torsions

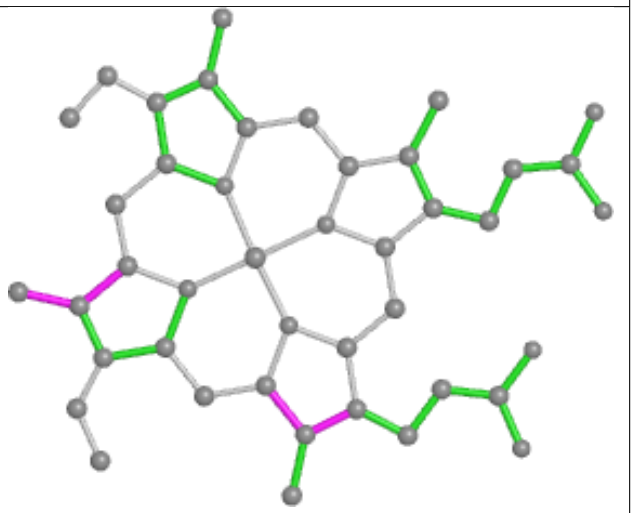


Rings

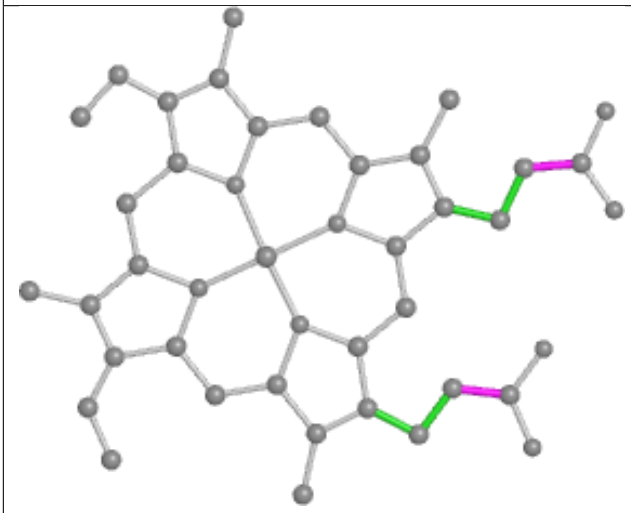
Ligand HEC L 1001



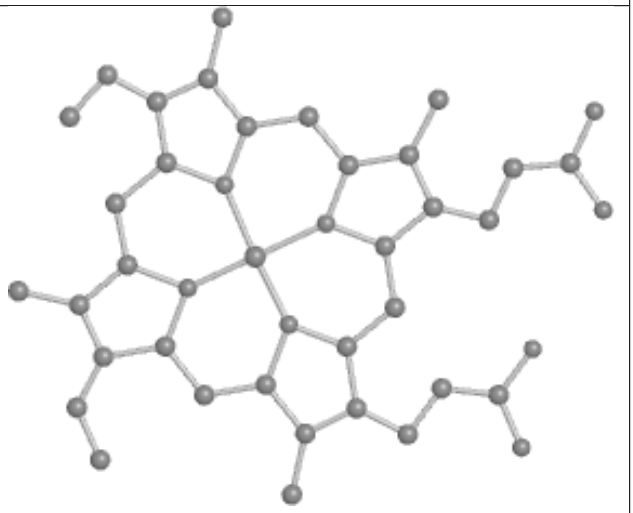
Bond lengths



Bond angles

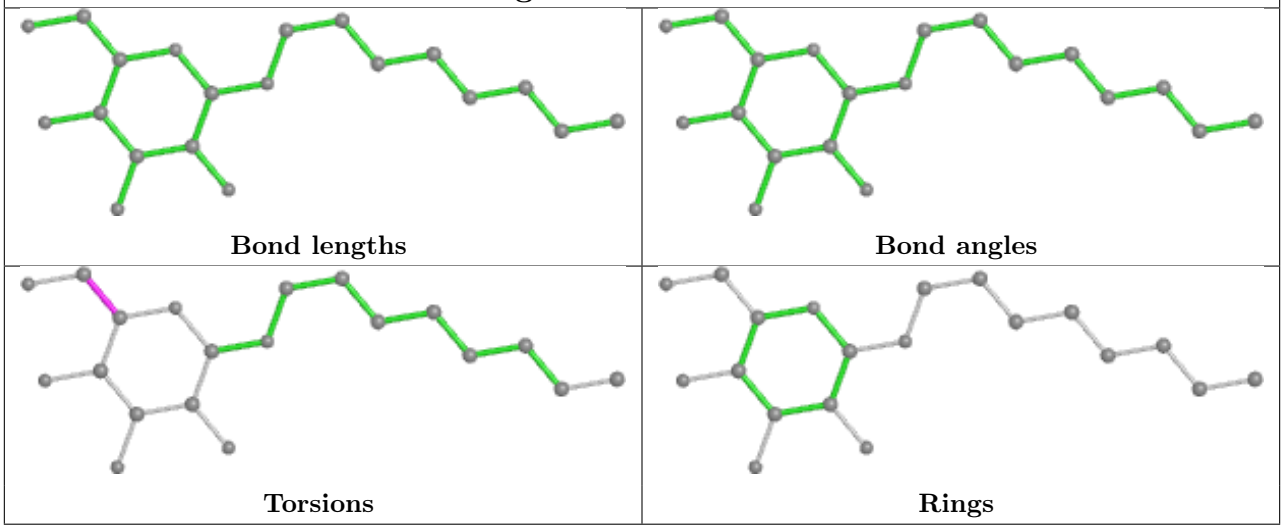


Torsions

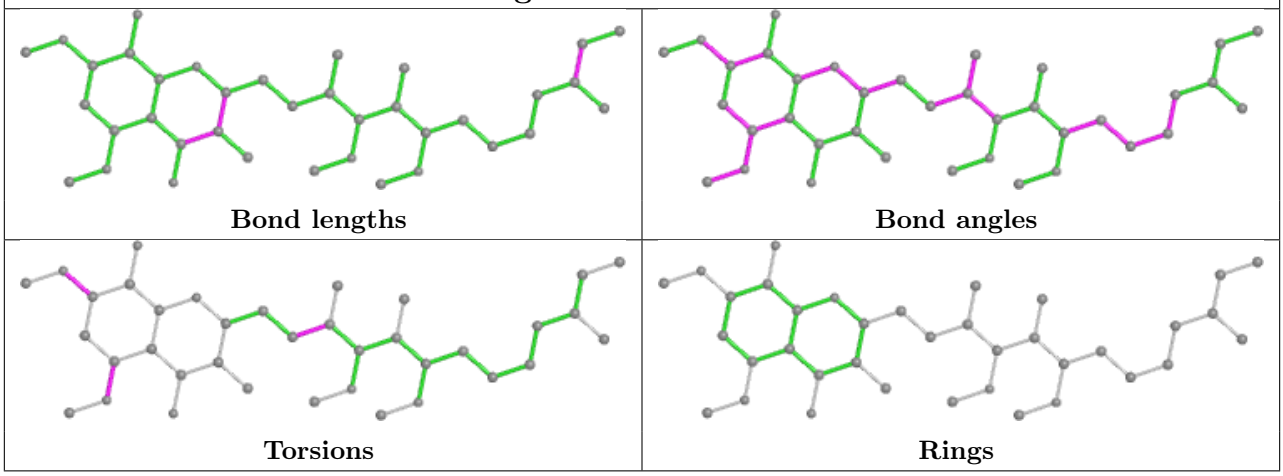


Rings

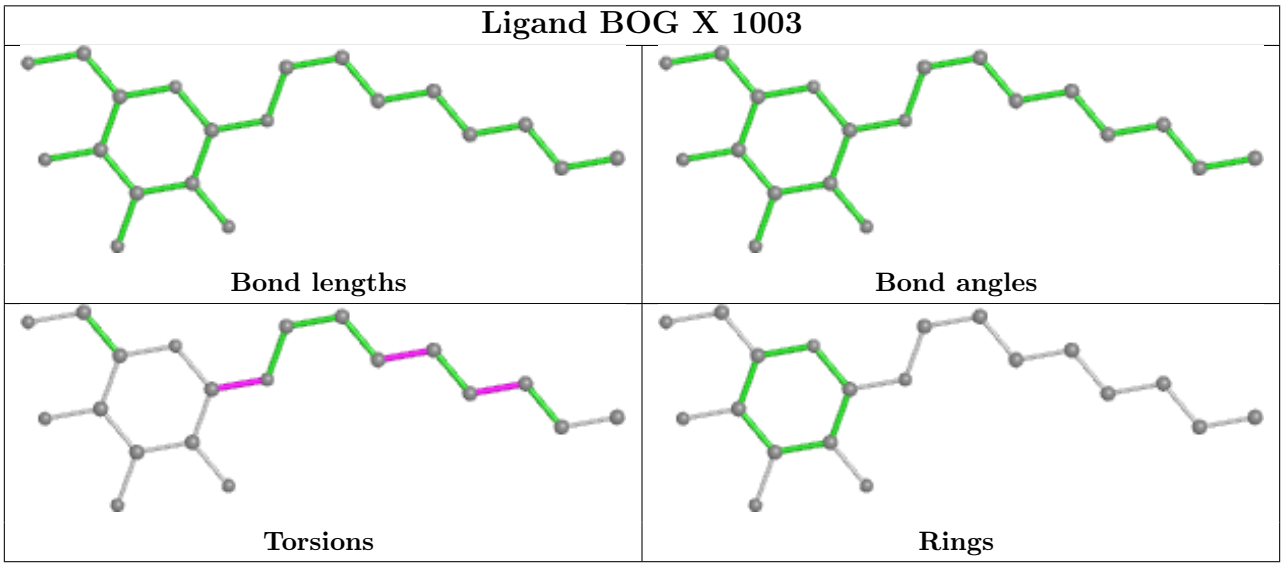
Ligand BOG L 1003



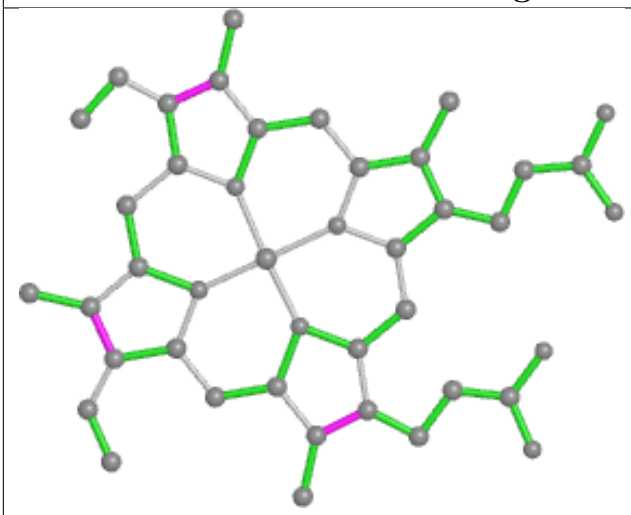
Ligand SMA E 1003



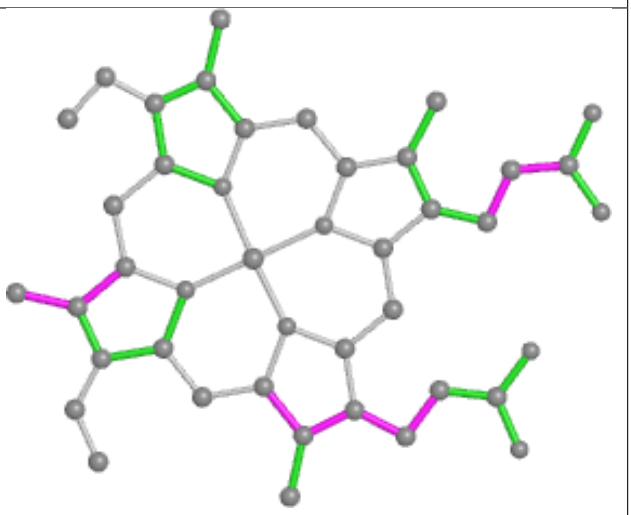
Ligand BOG X 1003



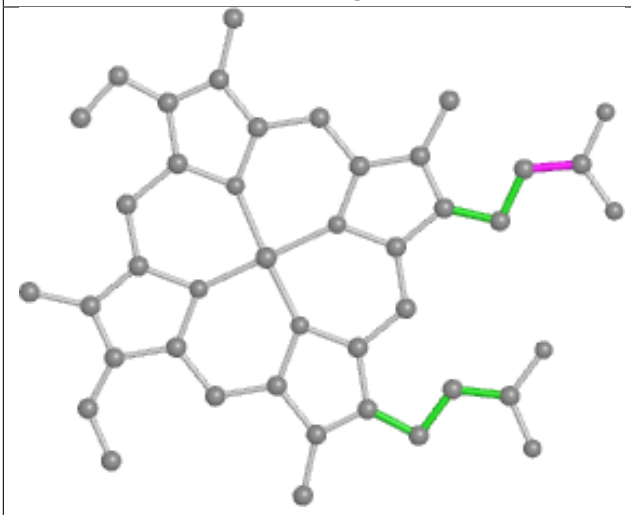
Ligand HEC X 1001



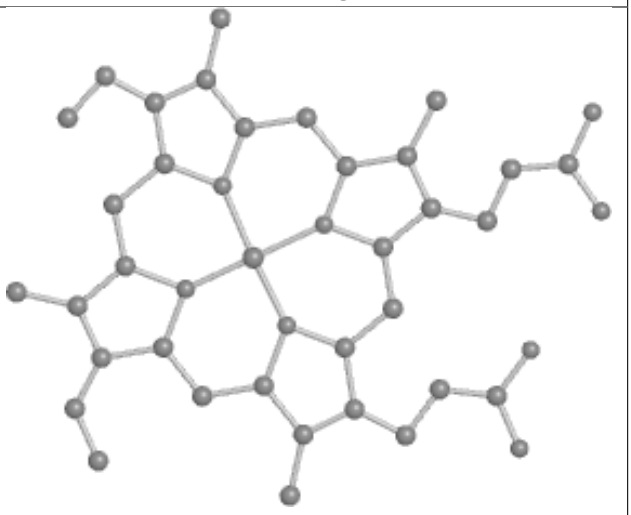
Bond lengths



Bond angles

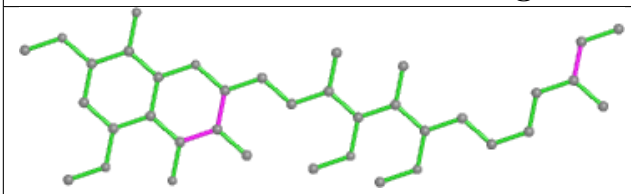


Torsions

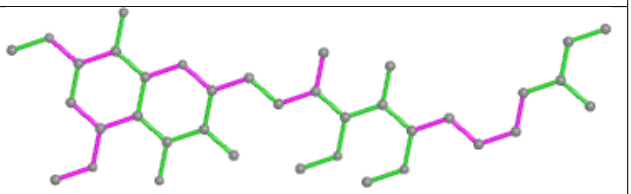


Rings

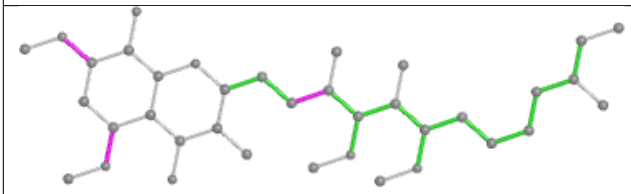
Ligand SMA S 1003



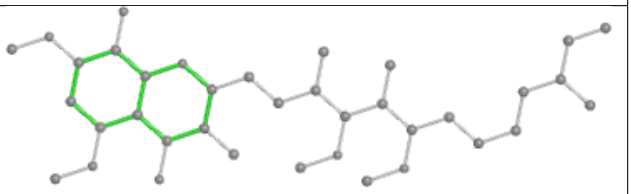
Bond lengths



Bond angles

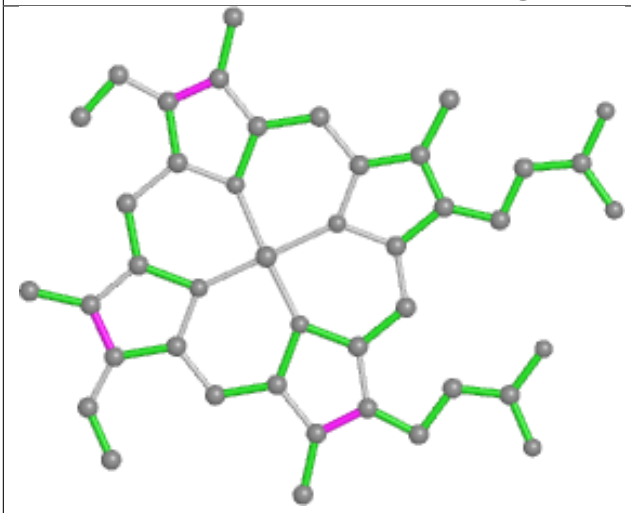


Torsions

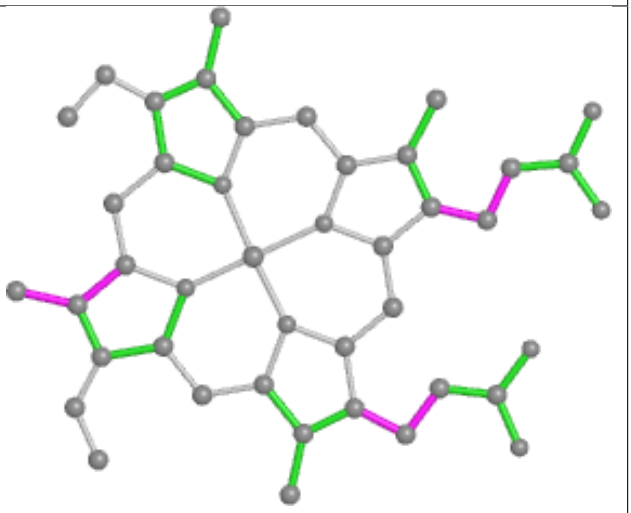


Rings

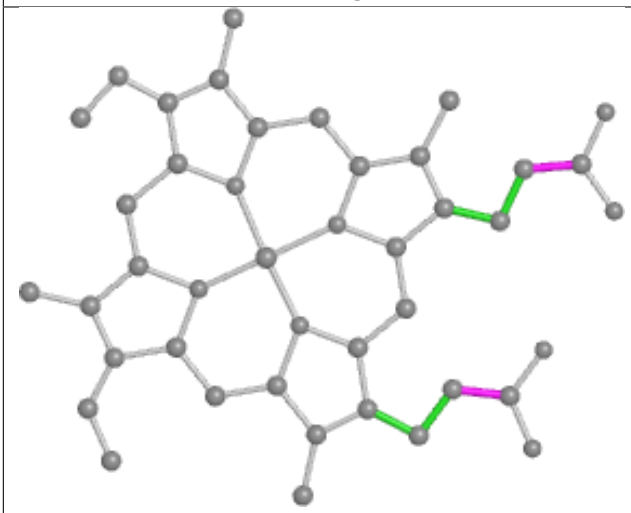
Ligand HEC T 1001



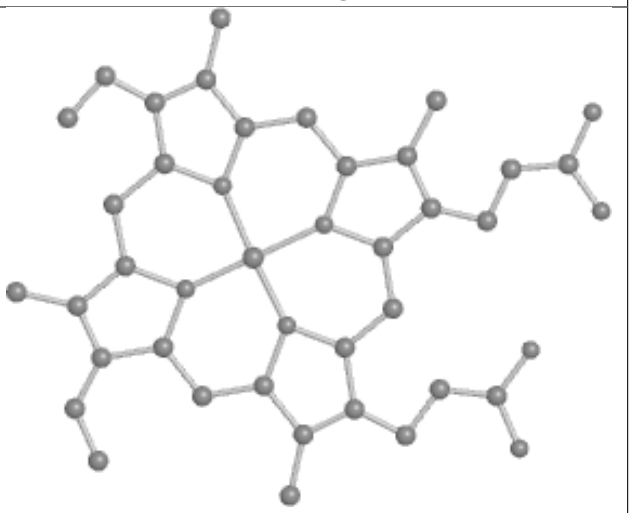
Bond lengths



Bond angles

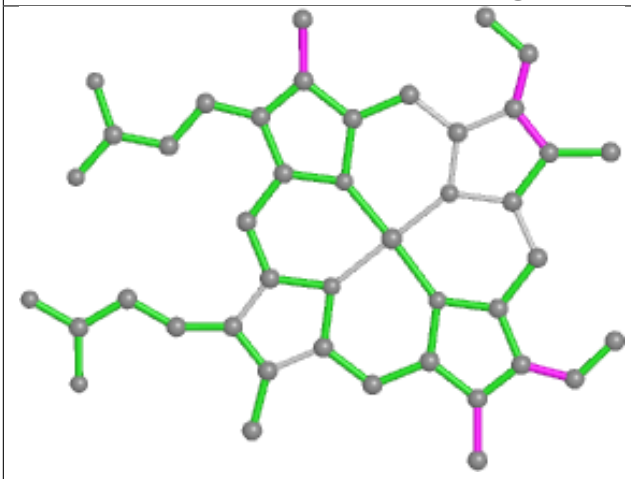


Torsions

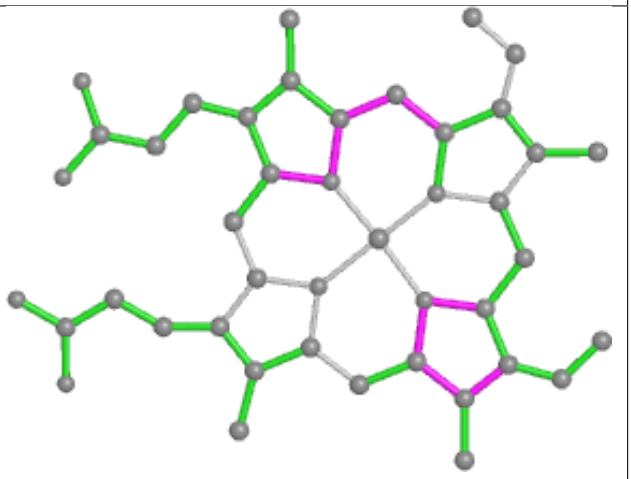


Rings

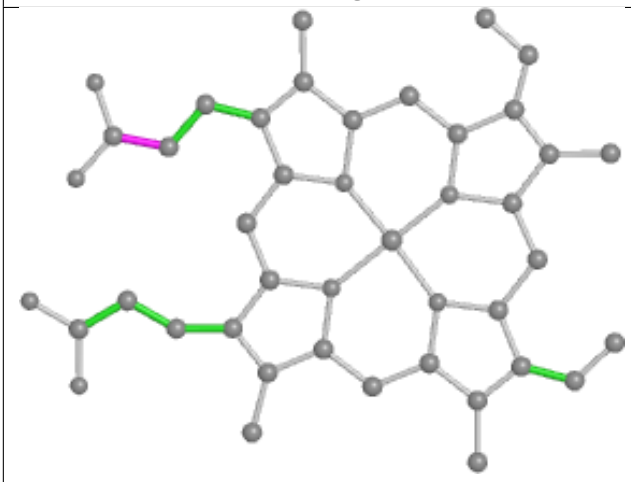
Ligand HEM O 1002



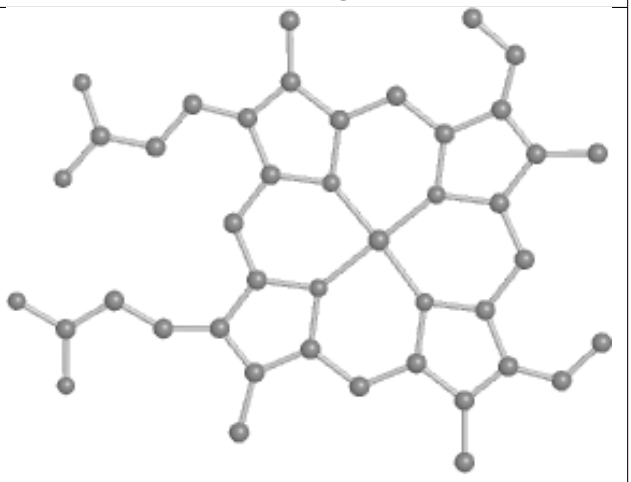
Bond lengths



Bond angles

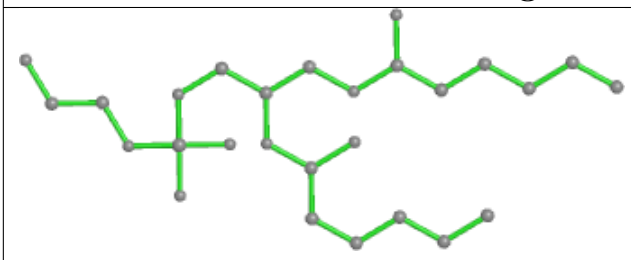


Torsions

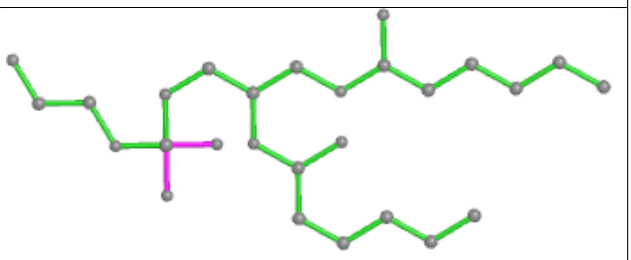


Rings

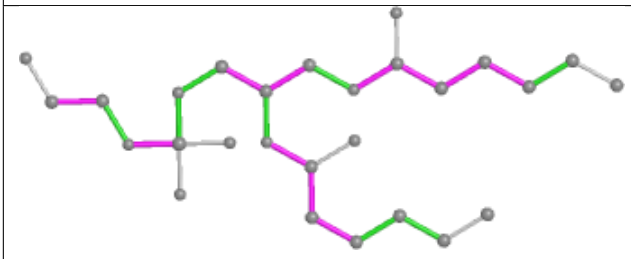
Ligand 6PE A 1004



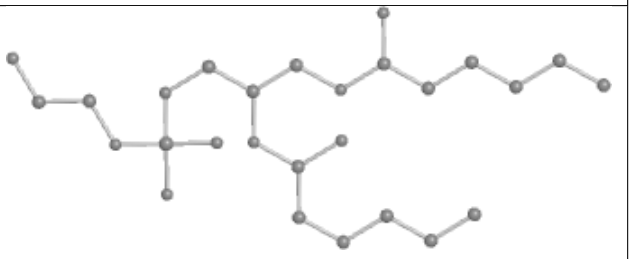
Bond lengths



Bond angles

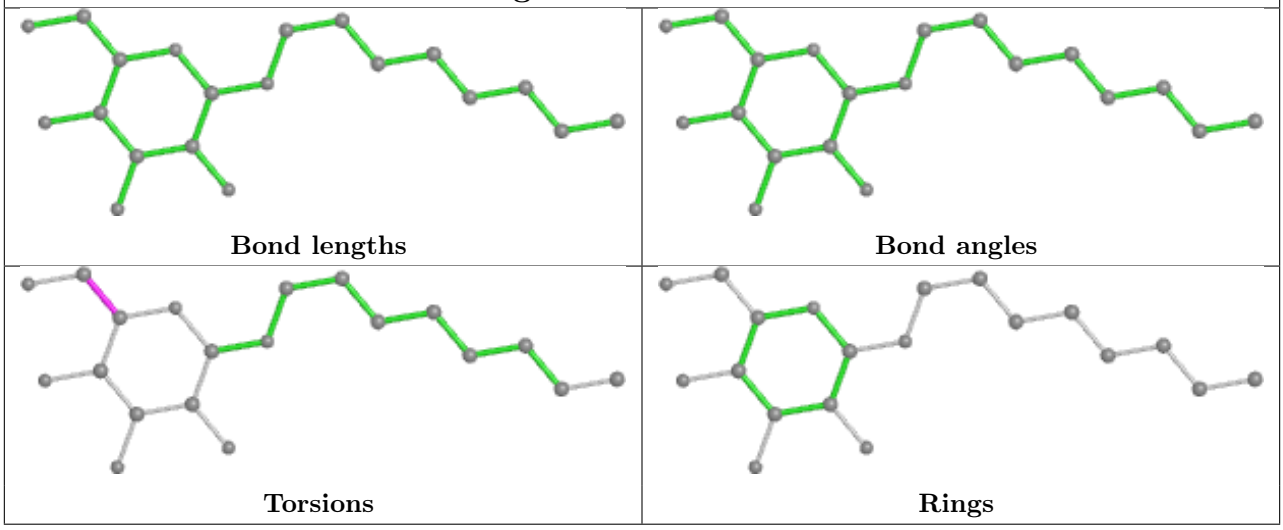


Torsions

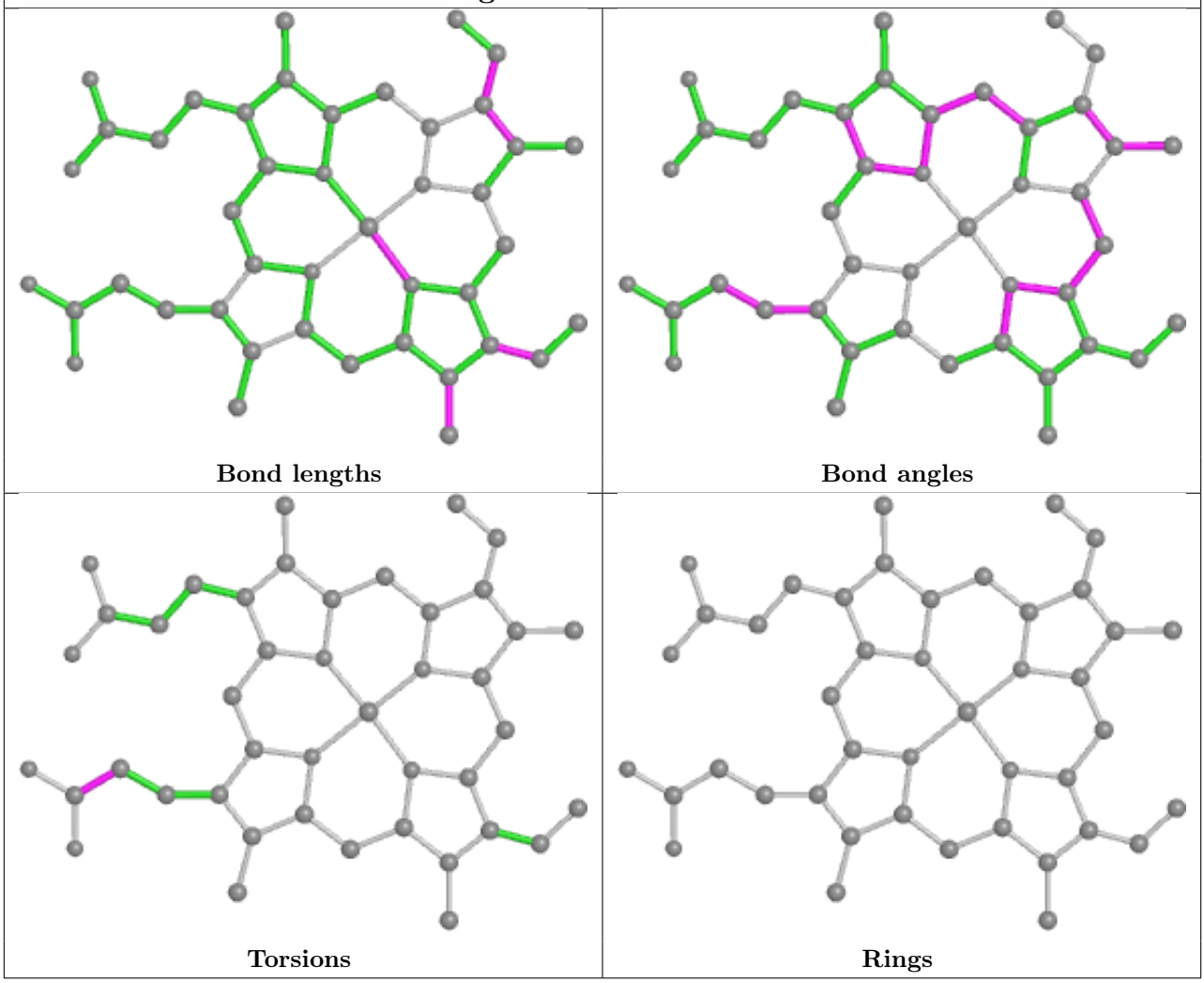


Rings

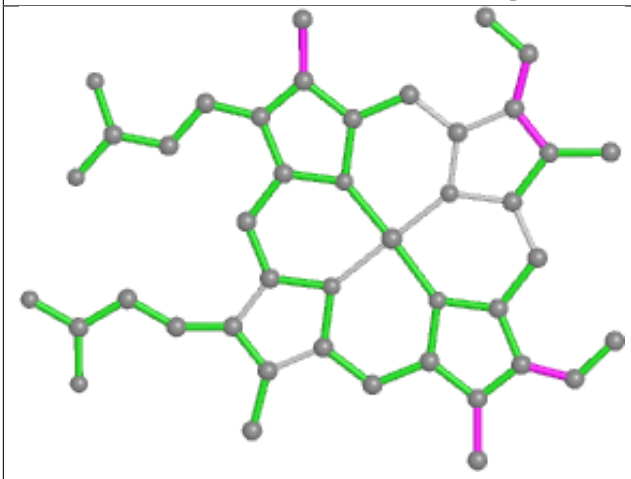
Ligand BOG B 1003



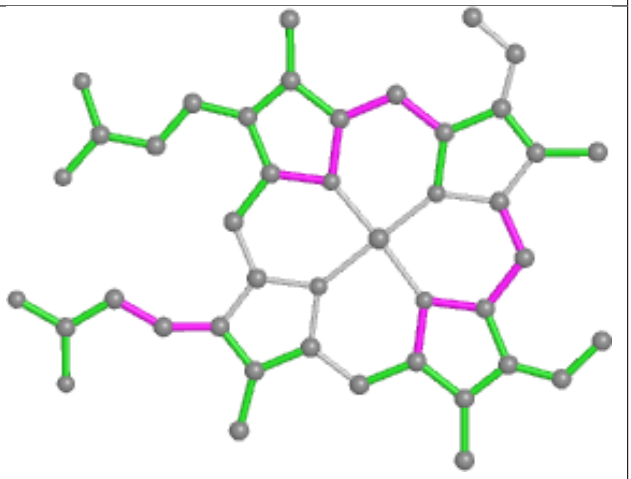
Ligand HEM A 1001



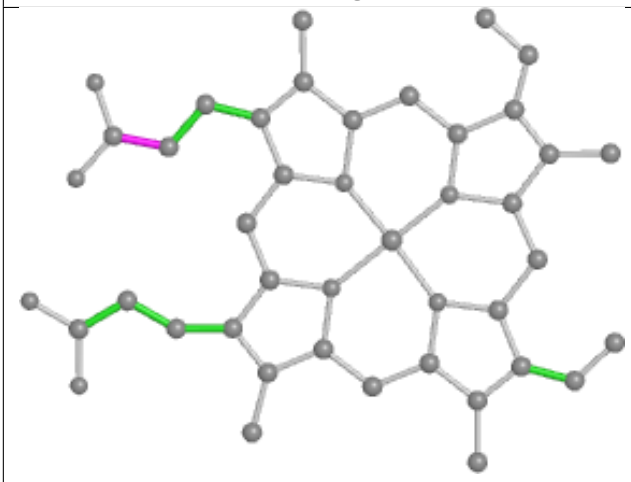
Ligand HEM W 1002



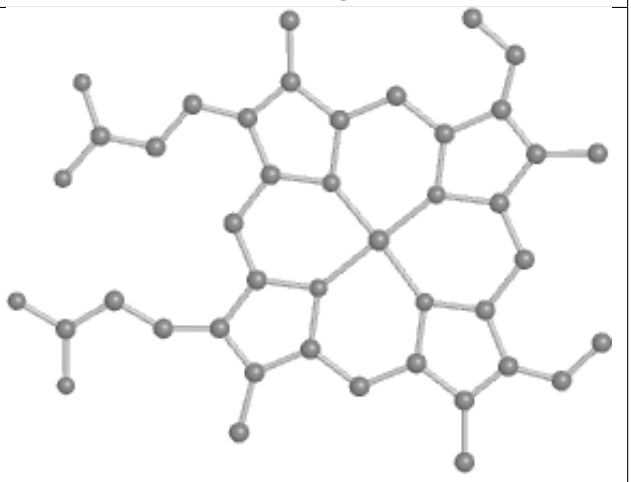
Bond lengths



Bond angles

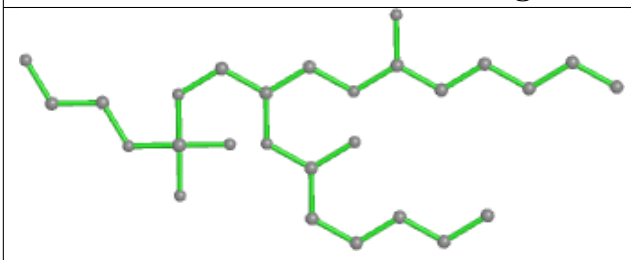


Torsions

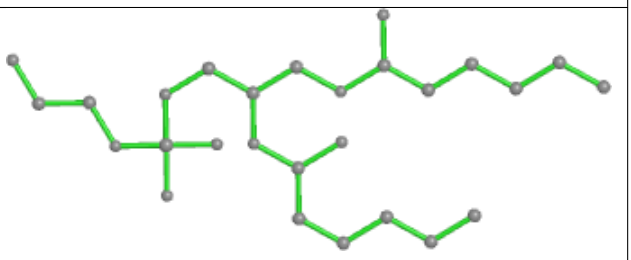


Rings

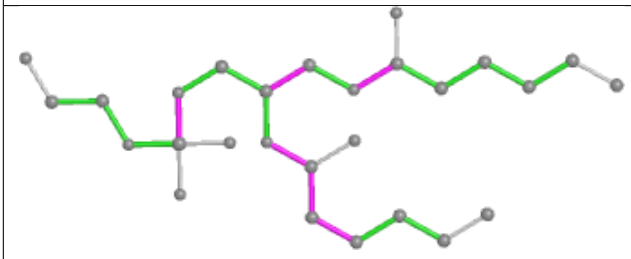
Ligand 6PE W 1004



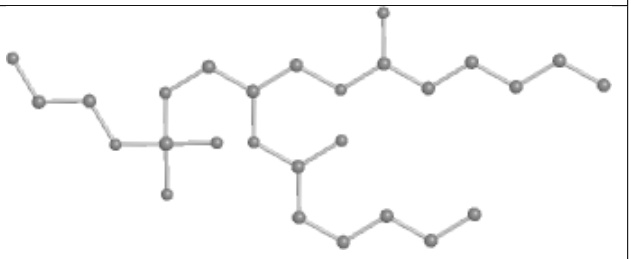
Bond lengths



Bond angles

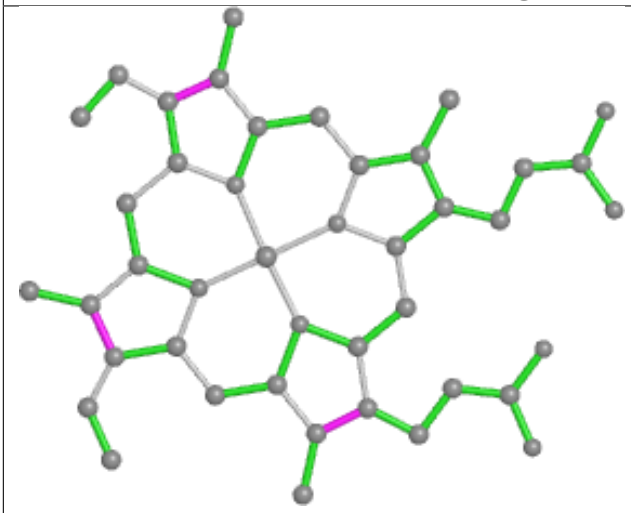


Torsions

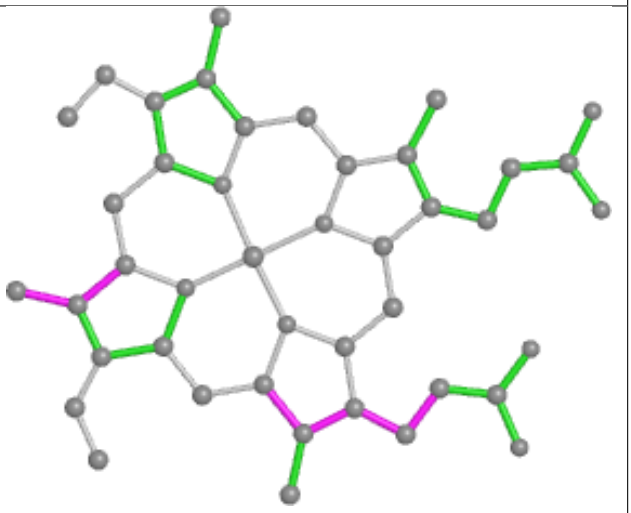


Rings

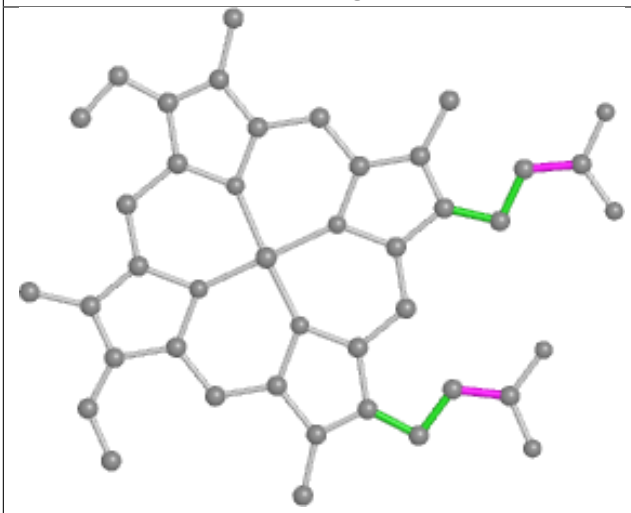
Ligand HEC F 1001



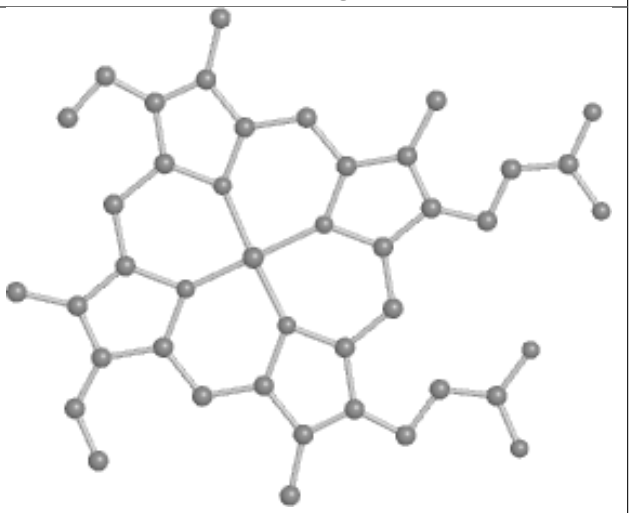
Bond lengths



Bond angles

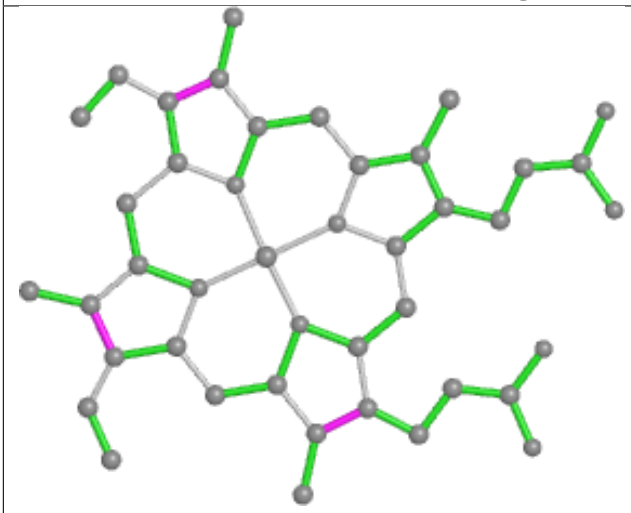


Torsions

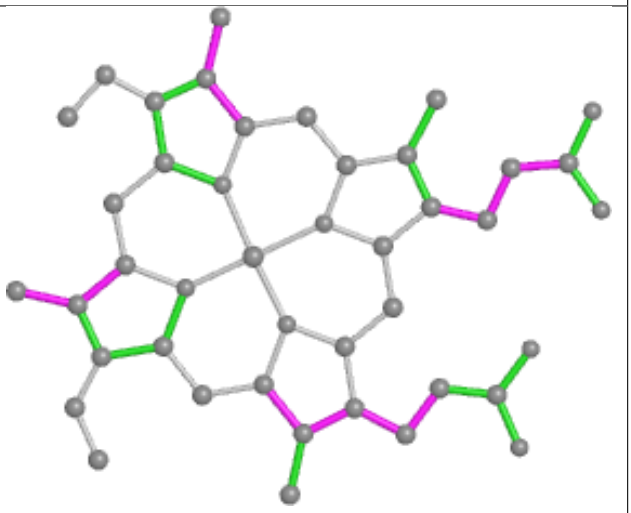


Rings

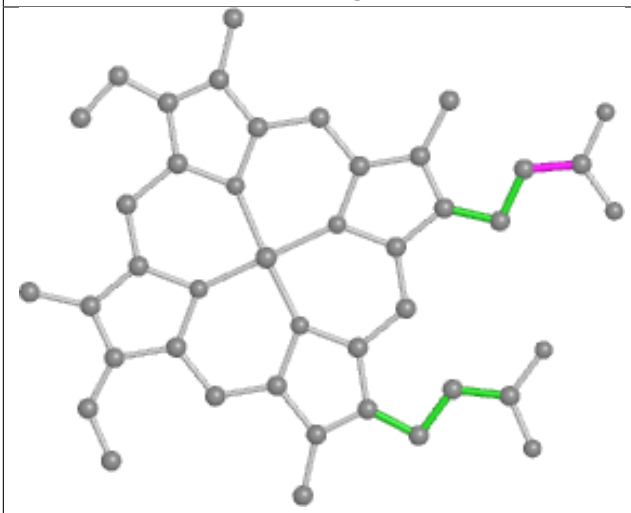
Ligand HEC P 1001



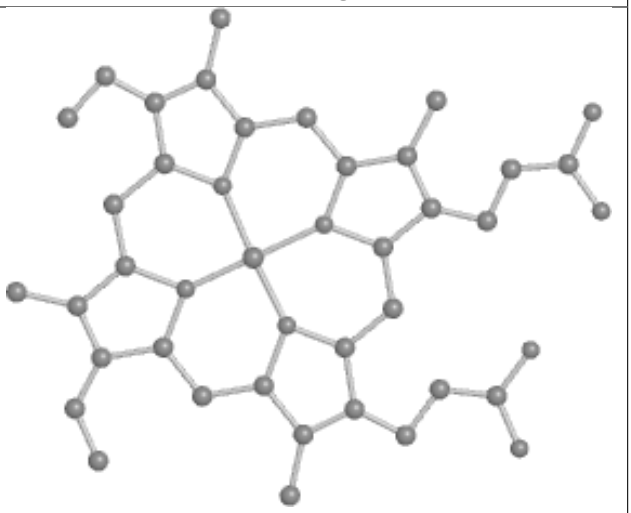
Bond lengths



Bond angles

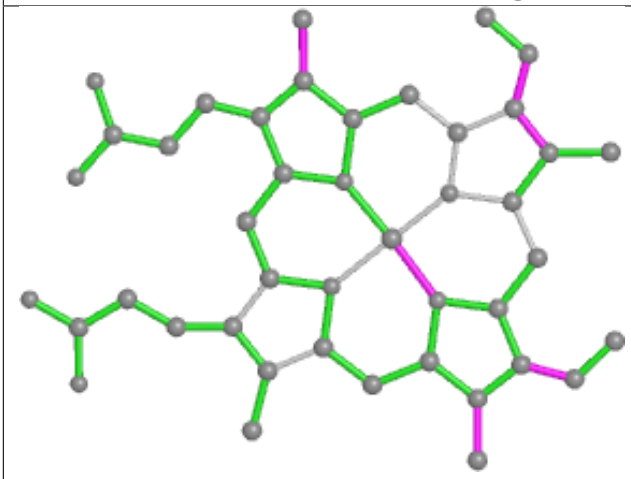


Torsions

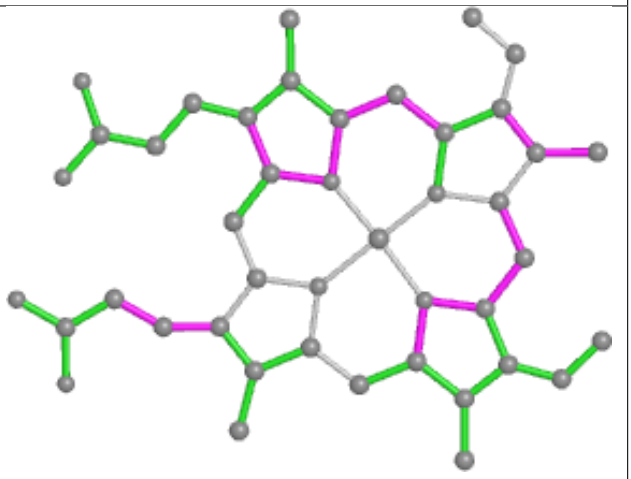


Rings

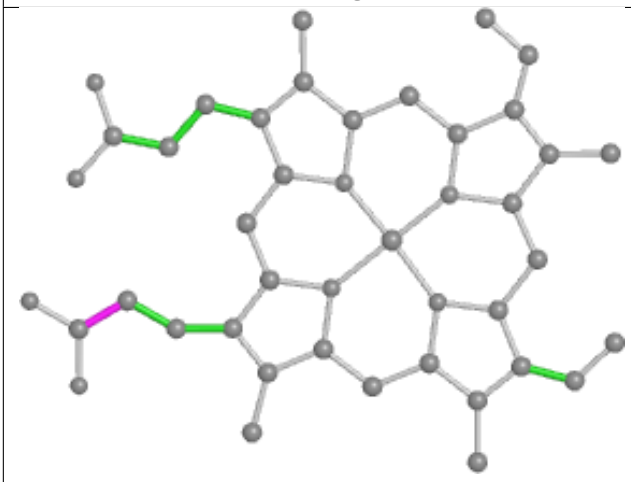
Ligand HEM O 1001



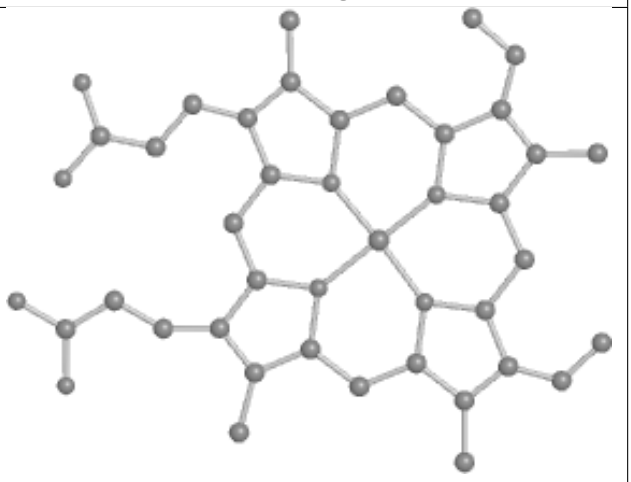
Bond lengths



Bond angles

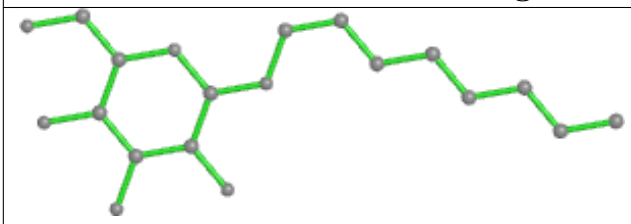


Torsions

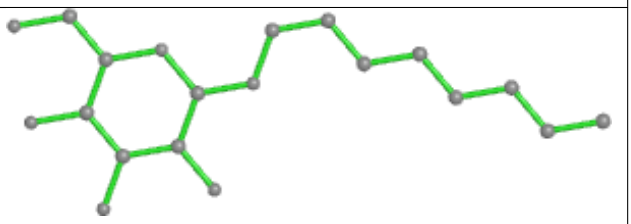


Rings

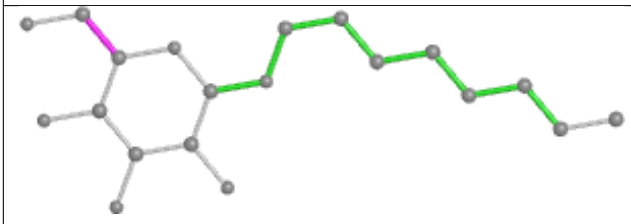
Ligand BOG F 1002



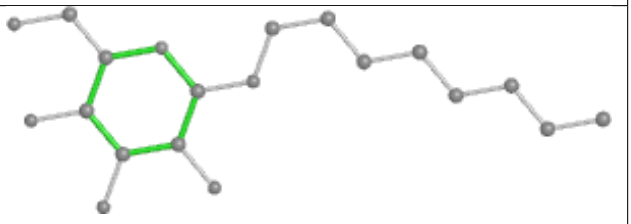
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	428/445 (96%)	-0.00	6 (1%) 75 61	76, 102, 148, 174	0
1	E	428/445 (96%)	0.13	16 (3%) 41 27	75, 100, 145, 179	0
1	K	428/445 (96%)	0.06	20 (4%) 31 19	78, 101, 188, 237	0
1	O	428/445 (96%)	0.48	38 (8%) 9 5	84, 132, 178, 210	0
1	S	428/445 (96%)	0.55	36 (8%) 11 7	92, 161, 203, 232	0
1	W	428/445 (96%)	0.12	16 (3%) 41 27	84, 109, 179, 201	0
2	B	256/272 (94%)	0.37	21 (8%) 11 7	103, 136, 159, 182	0
2	F	256/272 (94%)	0.23	16 (6%) 20 11	101, 136, 159, 174	0
2	L	256/272 (94%)	0.19	13 (5%) 28 17	104, 129, 158, 172	0
2	P	256/272 (94%)	0.44	33 (12%) 3 2	116, 154, 184, 196	0
2	T	256/272 (94%)	1.07	62 (24%) 0 0	133, 186, 236, 255	0
2	X	256/272 (94%)	0.57	31 (12%) 4 3	114, 158, 197, 230	0
3	C	179/187 (95%)	-0.04	11 (6%) 21 12	86, 113, 162, 220	0
3	G	179/187 (95%)	0.15	10 (5%) 24 14	88, 126, 169, 206	0
3	M	179/187 (95%)	0.53	22 (12%) 4 3	125, 145, 179, 201	0
3	Q	179/187 (95%)	-0.10	4 (2%) 62 45	75, 110, 153, 193	0
3	U	179/187 (95%)	0.08	7 (3%) 39 25	96, 133, 179, 202	0
3	Y	179/187 (95%)	0.99	39 (21%) 0 0	135, 195, 228, 255	0
All	All	5178/5424 (95%)	0.31	401 (7%) 13 8	75, 132, 198, 255	0

All (401) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	9	GLY	12.2
2	T	150	GLU	11.3
2	X	2	GLY	11.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	183	GLY	10.9
2	X	58	LEU	9.9
3	Y	123	LEU	9.0
2	B	4	GLY	8.5
2	P	147	GLU	7.9
2	X	5	HIS	7.5
2	F	3	GLY	7.2
2	P	7	GLU	7.0
2	T	149	HIS	7.0
2	X	4	GLY	6.8
1	O	36	PRO	6.6
3	M	10	THR	6.3
2	B	2	GLY	6.3
1	K	247	TYR	6.3
2	X	3	GLY	6.3
2	F	2	GLY	6.2
1	S	182	GLY	6.1
2	B	3	GLY	6.0
2	X	7	GLU	5.9
1	S	232	THR	5.9
1	S	414	ILE	5.8
1	O	428	PHE	5.8
1	O	35	ILE	5.8
1	E	11	PRO	5.7
1	S	413	ALA	5.7
2	T	143	PRO	5.6
1	S	5	PRO	5.5
2	T	199	GLY	5.4
2	T	146	ALA	5.4
2	X	6	VAL	5.1
3	Y	136	PRO	5.1
2	T	93	ALA	5.0
2	X	61	ASP	5.0
2	X	149	HIS	4.9
2	P	150	GLU	4.9
2	X	192	ASP	4.9
1	W	351	THR	4.8
1	S	386	THR	4.8
3	M	181	GLU	4.8
1	W	23	LEU	4.8
1	S	385	THR	4.8
1	O	33	ILE	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	34	MET	4.7
2	X	70	PHE	4.7
2	T	148	GLY	4.7
3	Y	13	ASP	4.6
2	T	7	GLU	4.5
2	F	71	THR	4.5
2	T	147	GLU	4.5
2	X	59	PRO	4.5
2	B	1	ALA	4.5
1	O	244	PHE	4.5
3	Y	62	GLN	4.5
3	Y	56	SER	4.4
1	E	12	ARG	4.4
2	L	4	GLY	4.3
2	T	188	PRO	4.3
1	S	348	TRP	4.3
2	T	137	GLY	4.3
1	W	350	ASP	4.3
2	P	146	ALA	4.2
3	Y	10	THR	4.2
2	P	5	HIS	4.2
2	B	122	PHE	4.2
3	Y	74	ILE	4.2
2	X	94	LEU	4.2
1	K	427	ASP	4.2
1	O	355	ARG	4.1
1	S	410	ILE	4.1
1	O	8	HIS	4.1
3	C	104	ASP	4.1
2	L	3	GLY	4.1
2	T	57	GLU	4.1
2	B	140	GLU	4.0
2	L	5	HIS	4.0
2	T	80	ASP	4.0
3	C	10	THR	3.9
1	K	425	GLU	3.9
1	E	350	ASP	3.9
2	T	144	LYS	3.9
2	L	2	GLY	3.9
3	M	179	ILE	3.9
2	P	6	VAL	3.9
2	X	96	ASN	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	110	PHE	3.9
3	C	105	ALA	3.9
1	S	411	LEU	3.8
3	Y	143	ASP	3.8
2	T	3	GLY	3.8
1	O	5	PRO	3.8
3	Y	181	GLU	3.8
1	K	417	PRO	3.8
2	T	109	GLY	3.8
3	Y	79	GLU	3.8
1	W	241	THR	3.7
2	P	149	HIS	3.7
2	F	153	GLY	3.7
2	T	256	LYS	3.7
3	U	108	GLU	3.7
1	O	37	THR	3.7
1	S	415	GLU	3.7
2	P	94	LEU	3.7
1	O	11	PRO	3.6
2	L	109	GLY	3.6
3	U	105	ALA	3.6
2	P	145	CYS	3.6
3	M	120	GLY	3.6
1	K	229	VAL	3.6
1	O	9	TYR	3.6
1	O	6	HIS	3.5
2	T	197	ALA	3.5
3	Y	183	THR	3.5
1	K	34	MET	3.5
2	L	56	PRO	3.5
2	T	175	VAL	3.5
3	M	180	ASP	3.5
2	L	1	ALA	3.5
1	S	387	PHE	3.5
1	S	428	PHE	3.5
1	S	231	ARG	3.5
3	Y	17	TYR	3.5
3	Y	57	VAL	3.5
1	O	414	ILE	3.5
1	S	315	VAL	3.4
3	Y	65	VAL	3.4
3	G	53	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	351	THR	3.4
3	Y	160	GLY	3.4
1	O	413	ALA	3.4
1	S	119	GLY	3.4
3	Y	64	THR	3.4
1	S	430	ALA	3.4
1	E	10	GLU	3.3
3	Y	63	LEU	3.3
2	T	151	PRO	3.3
2	B	141	GLU	3.3
2	T	56	PRO	3.3
1	S	419	ALA	3.3
2	B	6	VAL	3.3
1	A	12	ARG	3.3
1	W	12	ARG	3.2
2	T	201	ASP	3.2
3	C	108	GLU	3.2
3	Y	156	TYR	3.2
2	X	69	GLN	3.2
2	X	147	GLU	3.2
2	T	152	ASP	3.2
1	O	354	VAL	3.2
2	L	72	VAL	3.2
2	T	22	GLN	3.2
3	M	95	ASP	3.2
3	Y	71	PRO	3.2
3	Y	83	GLU	3.2
3	M	148	PHE	3.2
1	A	11	PRO	3.1
2	B	80	ASP	3.1
3	C	9	GLY	3.1
2	P	59	PRO	3.1
1	S	349	LEU	3.1
1	E	8	HIS	3.1
3	Y	61	VAL	3.1
2	P	41	GLY	3.1
1	K	246	PRO	3.1
1	S	429	ASN	3.1
3	C	107	ALA	3.1
2	T	4	GLY	3.1
2	B	5	HIS	3.0
2	P	68	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	256	LYS	3.0
2	X	72	VAL	3.0
3	M	86	ARG	3.0
3	Y	48	ALA	3.0
2	P	82	GLU	3.0
3	Y	180	ASP	3.0
1	O	31	ASP	3.0
2	F	72	VAL	3.0
3	Y	72	ILE	3.0
3	Y	138	GLY	3.0
1	K	9	TYR	3.0
2	P	148	GLY	3.0
3	U	103	ILE	3.0
2	T	5	HIS	2.9
2	X	148	GLY	2.9
1	O	4	ILE	2.9
2	F	151	PRO	2.9
3	Y	144	PHE	2.9
1	K	245	TRP	2.9
2	B	81	ARG	2.9
2	T	114	MET	2.9
1	O	410	ILE	2.9
1	E	349	LEU	2.9
2	T	12	SER	2.9
2	T	142	PRO	2.9
2	X	50	LEU	2.9
1	O	385	THR	2.8
3	Y	103	ILE	2.8
2	X	191	ASP	2.8
1	K	430	ALA	2.8
1	W	412	GLY	2.8
1	O	122	LYS	2.8
1	W	9	TYR	2.8
2	X	95	GLU	2.8
2	B	72	VAL	2.8
2	T	245	TYR	2.8
2	T	253	ALA	2.8
2	T	79	GLU	2.8
3	Y	124	VAL	2.8
1	S	35	ILE	2.8
2	T	139	PRO	2.8
2	P	114	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	77	THR	2.8
3	G	9	GLY	2.8
2	B	74	ASP	2.8
1	S	184	PRO	2.7
2	F	7	GLU	2.7
3	G	12	ARG	2.7
2	P	155	TYR	2.7
2	B	150	GLU	2.7
1	O	248	PHE	2.7
1	W	39	ARG	2.7
2	P	143	PRO	2.7
3	G	55	SER	2.7
3	C	12	ARG	2.7
1	E	235	ALA	2.7
2	F	149	HIS	2.7
3	M	119	ALA	2.7
2	L	61	ASP	2.7
2	B	69	GLN	2.7
2	T	141	GLU	2.7
2	P	92	SER	2.7
1	W	222	ASN	2.7
2	T	94	LEU	2.7
1	O	316	GLN	2.7
2	P	93	ALA	2.7
1	K	23	LEU	2.7
1	S	313	TRP	2.7
1	K	30	TYR	2.7
2	T	145	CYS	2.7
3	Y	11	ARG	2.7
3	G	105	ALA	2.7
2	X	56	PRO	2.6
3	Y	104	ASP	2.6
3	Y	177	LYS	2.6
2	T	198	ASP	2.6
1	O	386	THR	2.6
2	F	159	ALA	2.6
1	S	11	PRO	2.6
1	A	93	LEU	2.6
2	L	193	LEU	2.6
1	K	228	GLU	2.6
1	S	416	LYS	2.6
1	O	10	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	200	HIS	2.6
2	X	1	ALA	2.6
2	F	161	GLN	2.6
2	T	98	PRO	2.5
2	F	122	PHE	2.5
1	S	356	SER	2.5
2	T	2	GLY	2.5
3	M	104	ASP	2.5
2	T	90	PRO	2.5
2	F	69	GLN	2.5
1	K	357	GLY	2.5
1	E	93	LEU	2.5
3	U	109	ALA	2.5
1	S	233	SER	2.5
2	T	53	PRO	2.5
2	B	7	GLU	2.5
3	Y	93	LEU	2.5
3	M	182	THR	2.5
1	S	318	ALA	2.5
3	C	11	ARG	2.5
1	A	20	HIS	2.5
2	B	73	THR	2.5
1	A	10	GLU	2.4
1	K	39	ARG	2.4
1	E	13	THR	2.4
3	M	93	LEU	2.4
2	T	11	PHE	2.4
3	Y	140	VAL	2.4
3	M	144	PHE	2.4
2	T	192	ASP	2.4
2	X	93	ALA	2.4
1	O	12	ARG	2.4
2	P	95	GLU	2.4
3	G	52	VAL	2.4
1	S	326	ILE	2.4
2	L	152	ASP	2.4
3	U	107	ALA	2.4
1	W	40	ASN	2.4
2	P	142	PRO	2.4
1	O	348	TRP	2.4
2	T	6	VAL	2.4
3	C	132	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	412	GLY	2.4
3	Y	184	ILE	2.3
1	W	124	PRO	2.3
1	W	27	ALA	2.3
2	P	169	CYS	2.3
3	G	132	LEU	2.3
1	K	428	PHE	2.3
2	P	144	LYS	2.3
1	O	168	ALA	2.3
1	E	102	SER	2.3
1	S	127	VAL	2.3
3	U	110	THR	2.3
2	X	57	GLU	2.3
2	X	68	THR	2.3
3	G	17	TYR	2.3
1	W	34	MET	2.3
3	Q	45	GLN	2.3
2	P	140	GLU	2.3
1	O	231	ARG	2.3
2	T	82	GLU	2.3
1	W	6	HIS	2.3
3	C	109	ALA	2.3
1	O	121	TYR	2.3
2	P	141	GLU	2.3
2	B	71	THR	2.3
1	E	190	THR	2.3
2	B	70	PHE	2.3
1	O	171	GLY	2.3
2	T	113	PRO	2.2
2	F	4	GLY	2.2
2	T	123	ASN	2.2
1	E	246	PRO	2.2
3	M	150	PRO	2.2
1	O	365	ILE	2.2
1	O	48	GLY	2.2
2	X	141	GLU	2.2
1	A	357	GLY	2.2
3	C	106	GLY	2.2
2	L	82	GLU	2.2
2	T	68	THR	2.2
2	X	98	PRO	2.2
1	K	14	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	61	VAL	2.2
2	T	81	ARG	2.2
1	S	236	GLU	2.2
2	B	82	GLU	2.2
3	Y	58	GLU	2.2
1	S	12	ARG	2.2
1	O	241	THR	2.2
1	E	186	VAL	2.2
1	W	30	TYR	2.2
3	Q	11	ARG	2.2
2	P	56	PRO	2.2
2	P	115	GLY	2.2
1	S	221	ASN	2.2
2	T	91	HIS	2.1
3	M	57	VAL	2.1
3	Q	12	ARG	2.1
2	F	160	PHE	2.1
3	Y	179	ILE	2.1
1	K	13	THR	2.1
3	M	183	THR	2.1
3	Q	19	THR	2.1
2	T	196	TYR	2.1
2	T	73	THR	2.1
2	P	69	GLN	2.1
2	P	39	CYS	2.1
2	T	99	ASP	2.1
2	T	189	LEU	2.1
2	B	17	PHE	2.1
2	T	72	VAL	2.1
3	Y	47	LEU	2.1
3	Y	105	ALA	2.1
2	X	151	PRO	2.1
2	P	22	GLN	2.1
2	T	26	GLN	2.1
2	X	66	TYR	2.1
2	P	135	LEU	2.1
1	K	429	ASN	2.1
1	O	349	LEU	2.1
1	S	171	GLY	2.1
2	F	150	GLU	2.1
3	Y	19	THR	2.1
3	U	112	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	T	92	SER	2.1
2	P	134	VAL	2.1
3	G	57	VAL	2.1
1	E	236	GLU	2.1
1	K	12	ARG	2.0
1	W	427	ASP	2.0
2	T	17	PHE	2.0
2	T	84	LYS	2.0
2	X	243	LEU	2.0
3	M	143	ASP	2.0
1	O	40	ASN	2.0
2	F	118	ILE	2.0
3	M	136	PRO	2.0
3	M	13	ASP	2.0
3	M	167	ALA	2.0
1	S	311	ASP	2.0
2	T	169	CYS	2.0
3	G	48	ALA	2.0
1	O	30	TYR	2.0
1	O	119	GLY	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SR	T	1002	1/1	0.50	0.17	205,205,205,205	0
9	BOG	T	1003	20/20	0.61	0.52	152,185,198,205	0
5	SMA	S	1003	37/37	0.69	0.58	131,165,195,201	0

Continued on next page...

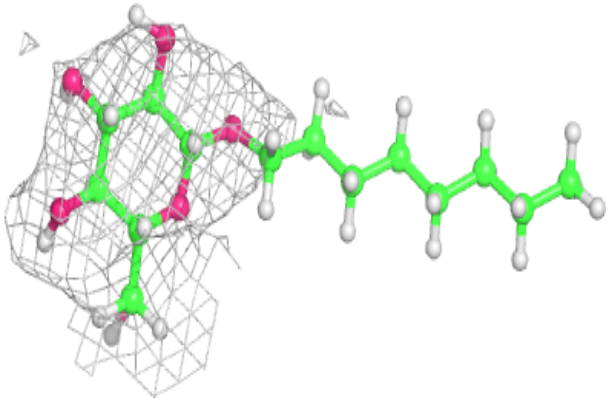
Continued from previous page...

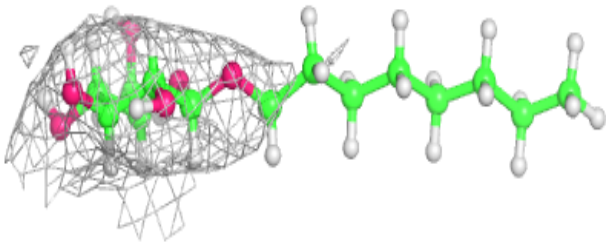
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SR	X	1002	1/1	0.74	0.08	184,184,184,184	0
9	BOG	X	1003	20/20	0.76	0.23	122,153,182,186	0
9	BOG	F	1002	20/20	0.77	0.47	120,147,163,164	0
9	BOG	B	1003	20/20	0.78	0.43	120,145,158,167	0
6	6PE	W	1004	27/27	0.78	0.60	105,134,161,162	0
8	SR	P	1003	1/1	0.80	0.07	184,184,184,184	0
5	SMA	O	1003	37/37	0.81	0.45	89,121,154,155	0
6	6PE	A	1004	27/27	0.81	0.48	97,130,156,160	0
9	BOG	P	1002	20/20	0.82	0.22	126,154,177,178	0
7	HEC	T	1001	43/43	0.86	0.30	167,189,231,232	0
9	BOG	L	1003	20/20	0.87	0.34	117,142,165,166	0
8	SR	B	1002	1/1	0.87	0.12	165,165,165,165	0
5	SMA	A	1003	37/37	0.88	0.39	82,103,130,131	0
7	HEC	P	1001	43/43	0.89	0.32	138,143,169,171	0
6	6PE	E	1004	27/27	0.89	0.32	93,121,171,173	0
4	HEM	O	1001	43/43	0.90	0.39	114,139,189,190	0
5	SMA	K	1003	37/37	0.90	0.36	79,98,114,127	0
5	SMA	W	1003	37/37	0.90	0.34	84,107,129,130	0
7	HEC	X	1001	43/43	0.91	0.38	124,166,212,215	0
4	HEM	E	1001	43/43	0.91	0.34	76,96,120,127	0
8	SR	F	1003	1/1	0.91	0.06	164,164,164,164	0
7	HEC	L	1001	43/43	0.91	0.33	90,109,137,153	0
4	HEM	S	1001	43/43	0.91	0.37	129,164,207,210	0
4	HEM	K	1001	43/43	0.91	0.36	95,118,147,151	0
4	HEM	E	1002	43/43	0.93	0.37	74,99,132,136	0
5	SMA	E	1003	37/37	0.93	0.29	72,94,117,122	0
4	HEM	O	1002	43/43	0.93	0.39	76,93,120,125	0
4	HEM	A	1002	43/43	0.93	0.36	72,93,116,118	0
7	HEC	F	1001	43/43	0.94	0.34	132,134,159,161	0
4	HEM	W	1001	43/43	0.94	0.35	78,112,142,152	0
4	HEM	A	1001	43/43	0.95	0.27	75,104,130,142	0
7	HEC	B	1001	43/43	0.95	0.27	114,124,150,155	0
4	HEM	K	1002	43/43	0.95	0.33	84,104,130,132	0
4	HEM	W	1002	43/43	0.96	0.37	81,99,133,144	0
4	HEM	S	1002	43/43	0.96	0.36	94,114,137,151	0
8	SR	L	1002	1/1	0.96	0.12	162,162,162,162	0
10	FES	Y	1001	4/4	0.97	0.20	154,156,162,163	0
10	FES	G	1001	4/4	0.99	0.19	85,87,88,88	0
10	FES	M	1001	4/4	0.99	0.20	127,127,129,129	0
10	FES	Q	1001	4/4	0.99	0.24	68,71,71,81	0
10	FES	U	1001	4/4	0.99	0.21	95,95,97,100	0
10	FES	C	1001	4/4	0.99	0.19	91,93,96,96	0

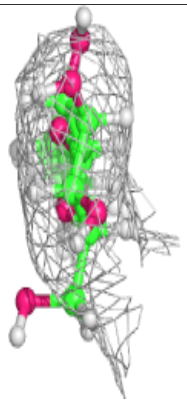
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG T 1003:

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

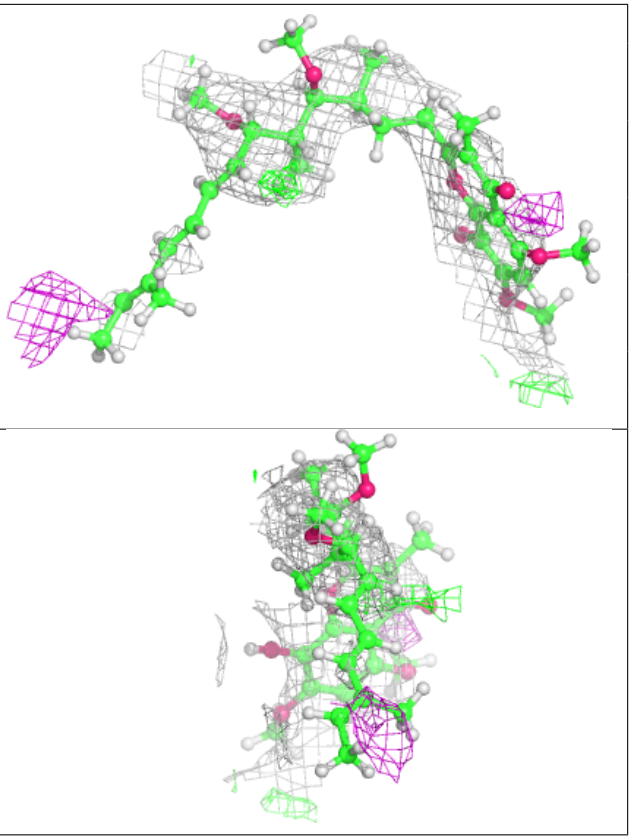






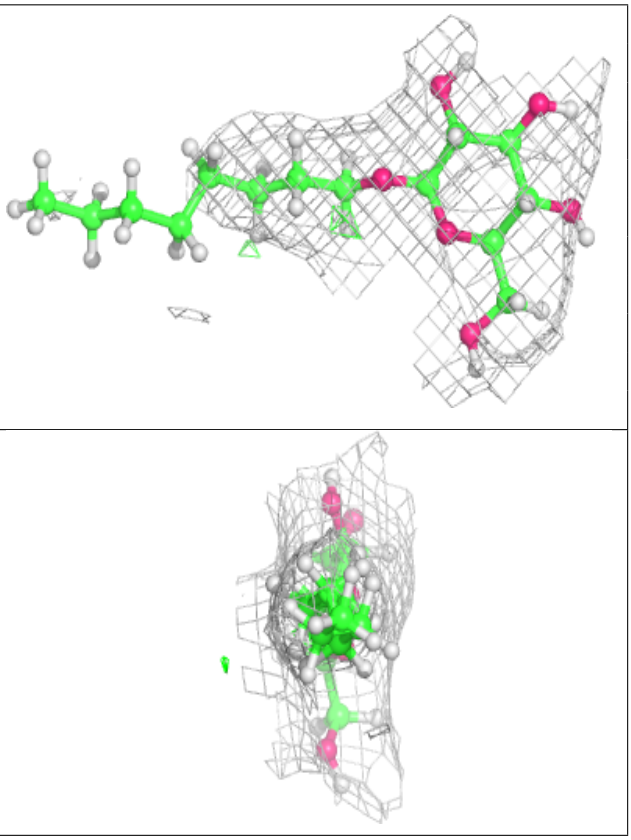
Electron density around SMA S 1003:

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



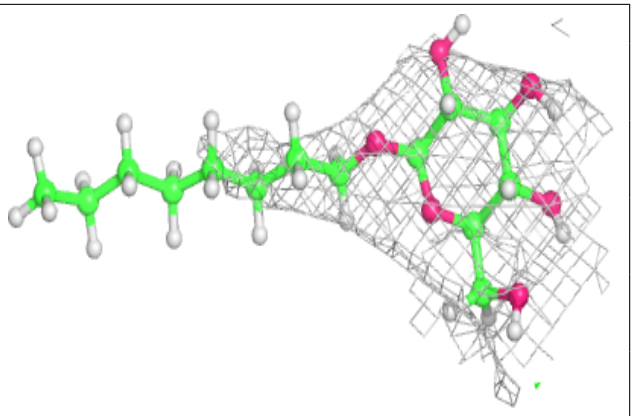
Electron density around BOG X 1003:

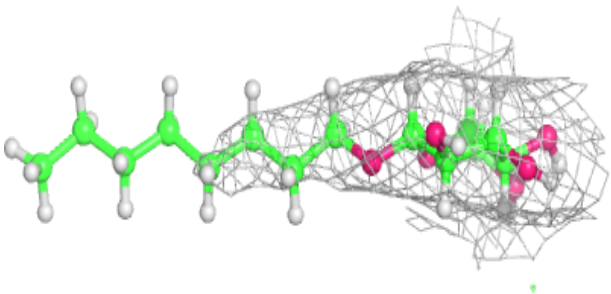
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

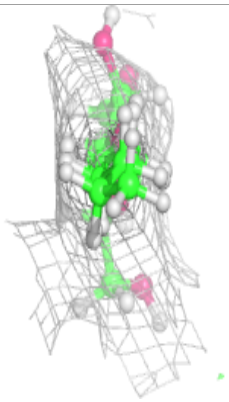


Electron density around BOG F 1002:

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

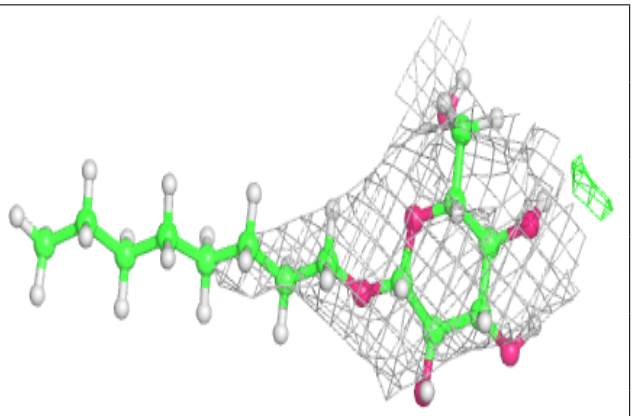


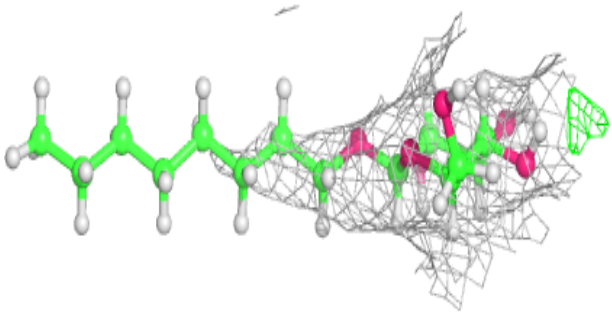


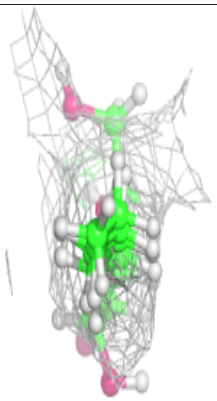


Electron density around BOG B 1003:

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

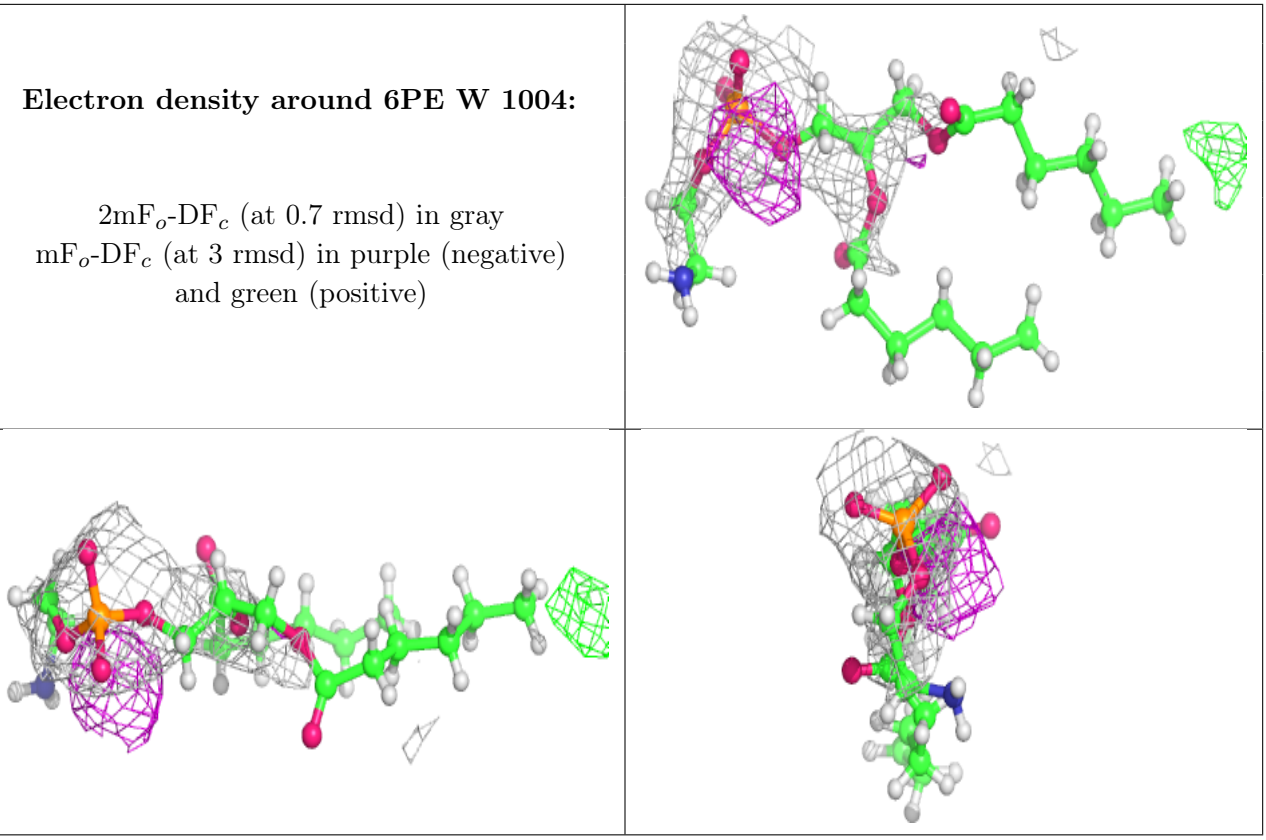






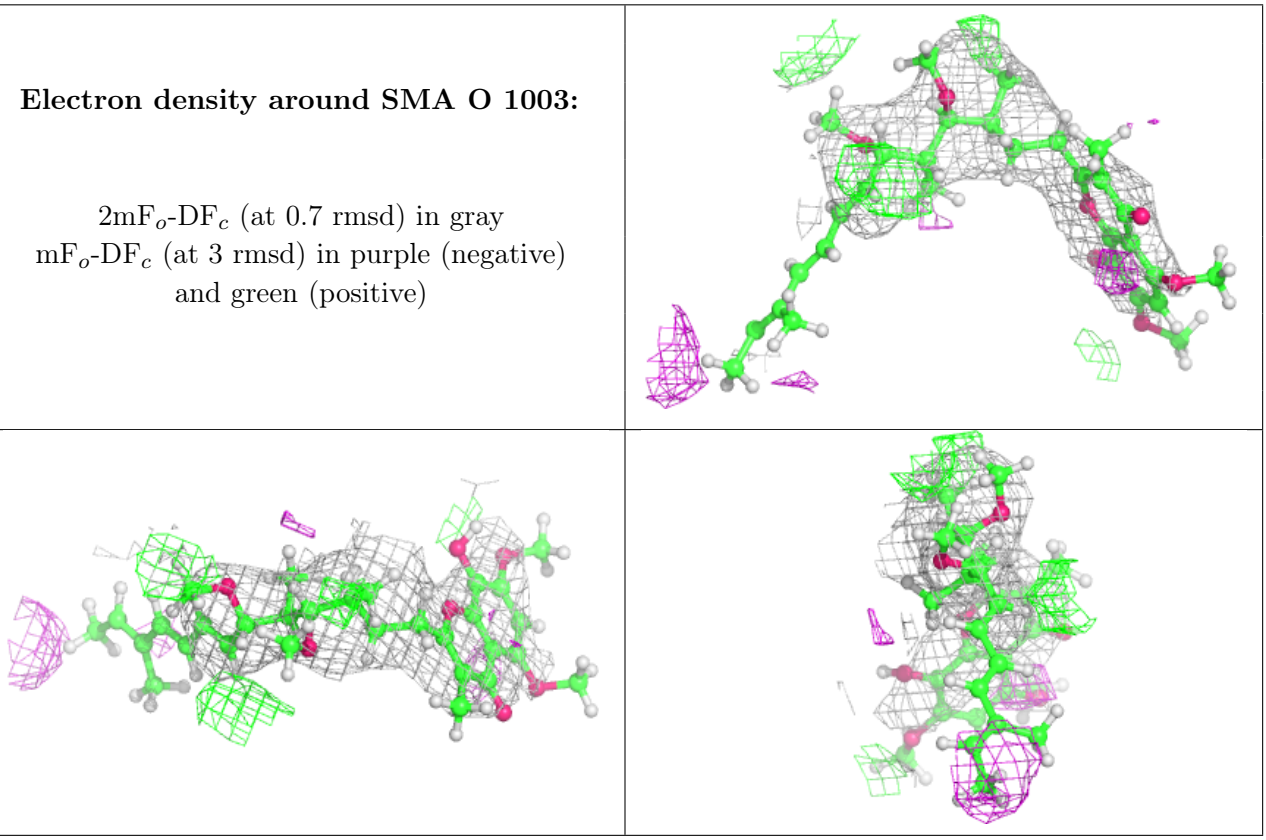
Electron density around 6PE W 1004:

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



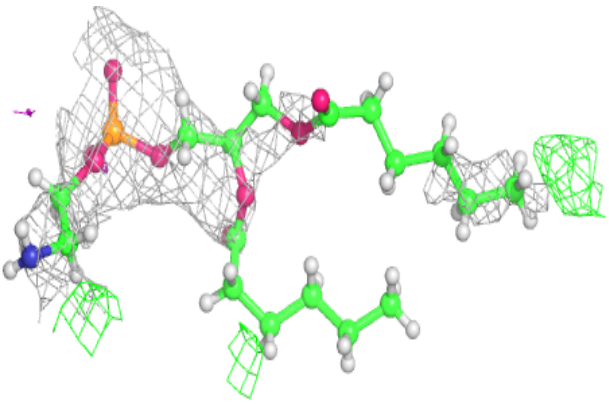
Electron density around SMA O 1003:

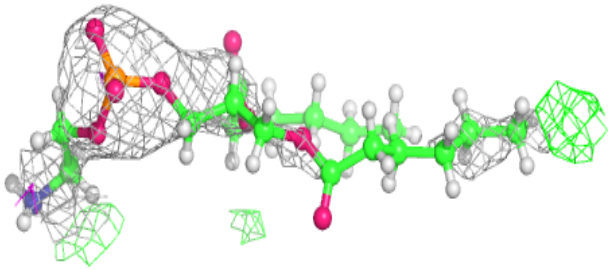
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

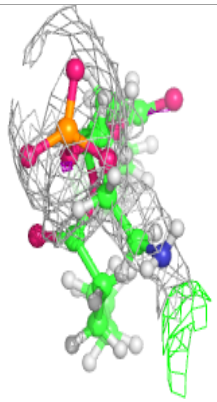


Electron density around 6PE A 1004:

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

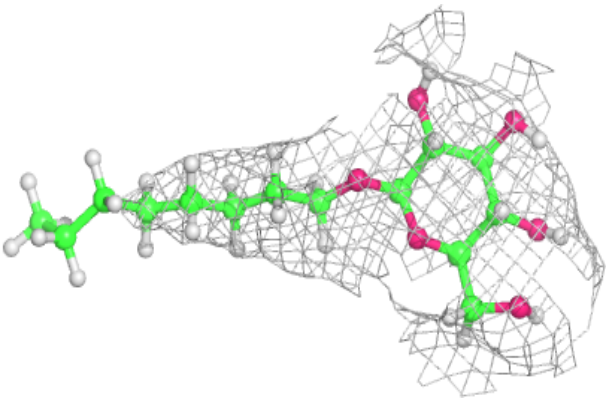


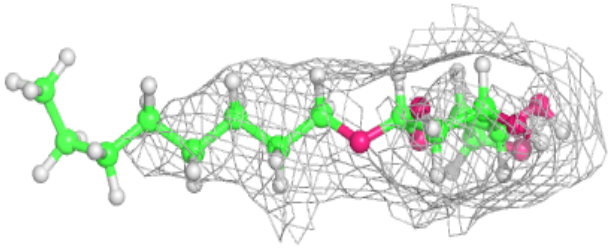


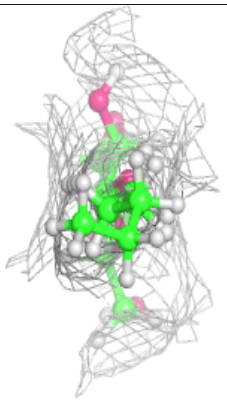


Electron density around BOG P 1002:

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

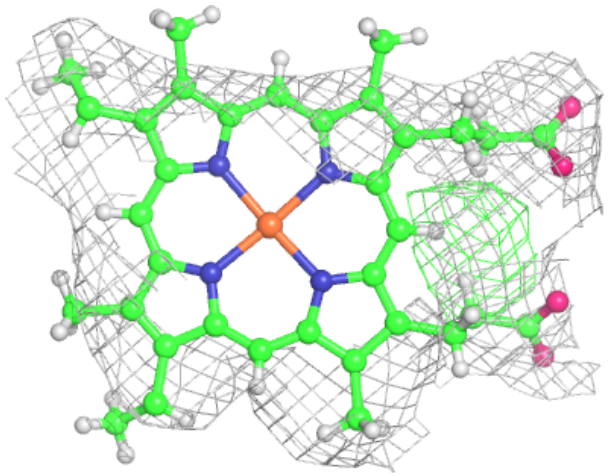


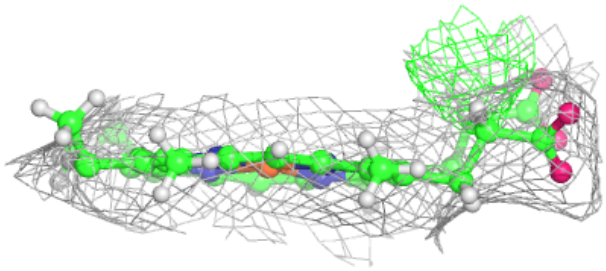


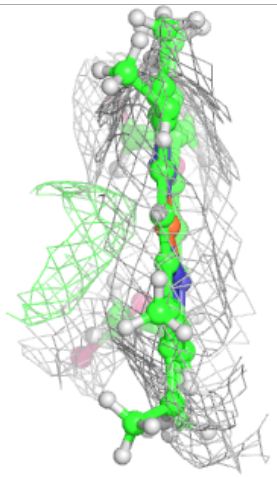


Electron density around HEC T 1001:

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

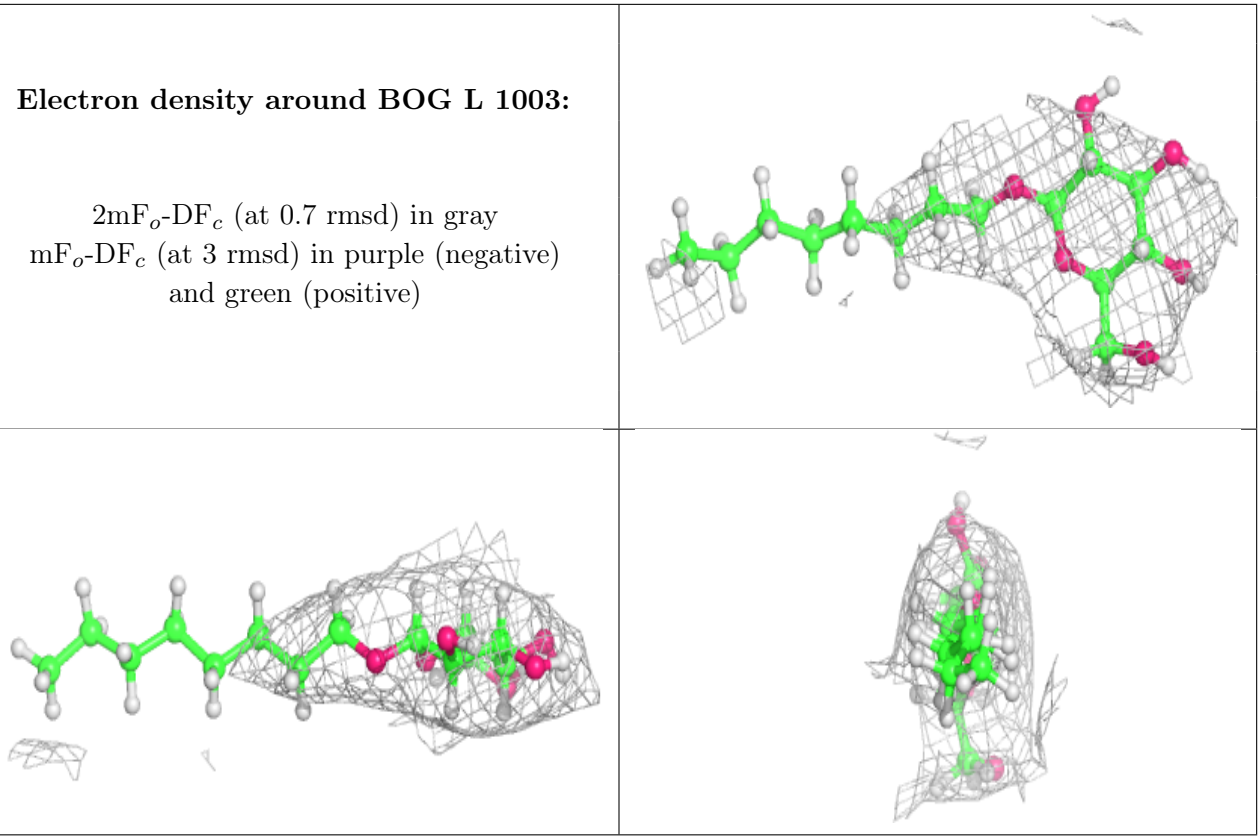






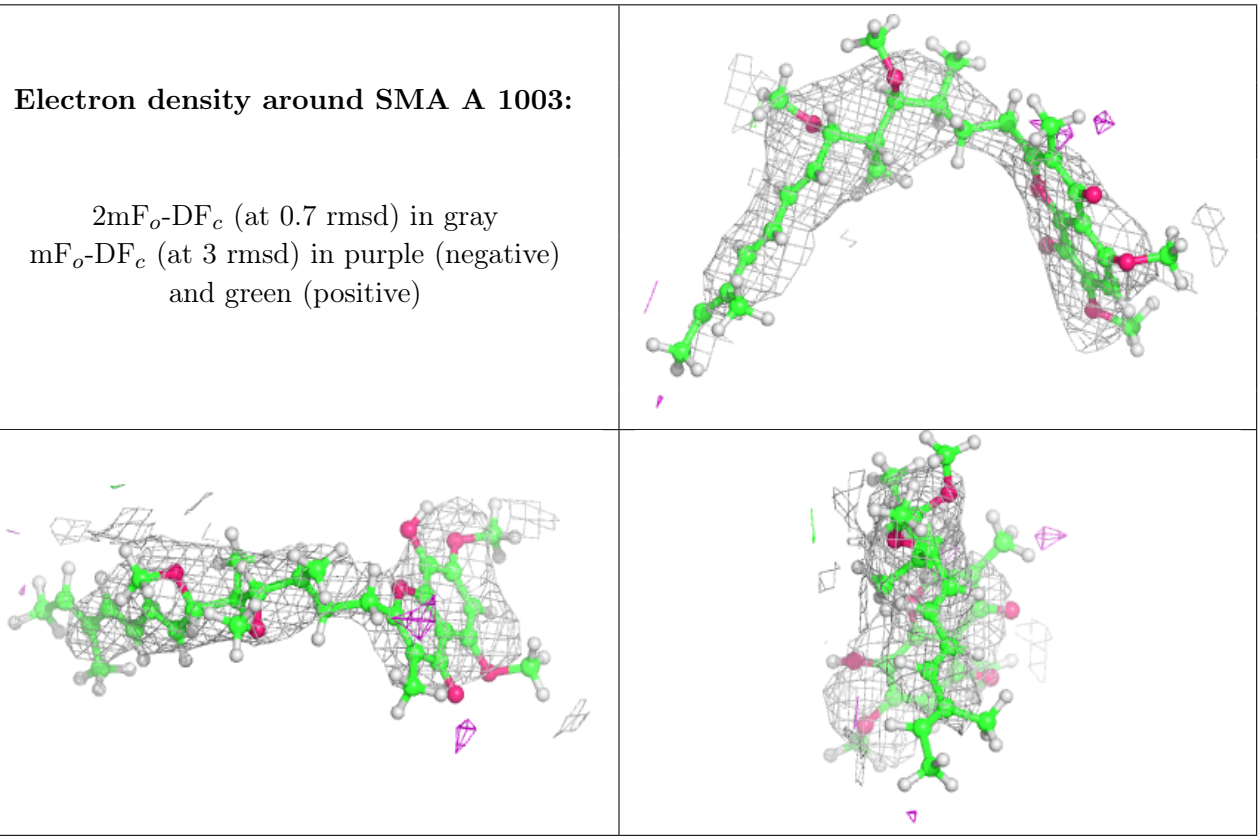
Electron density around BOG L 1003:

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



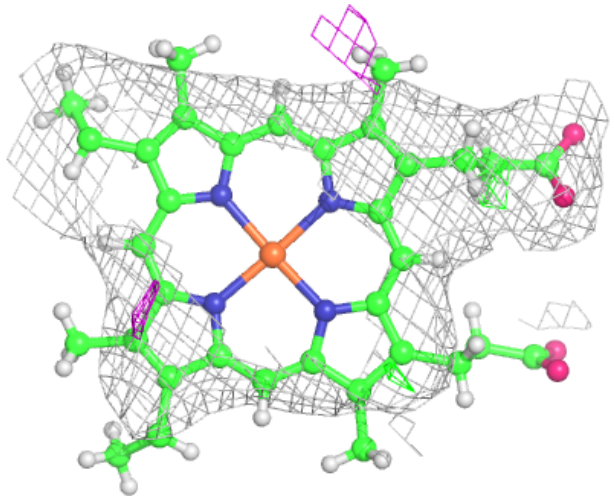
Electron density around SMA A 1003:

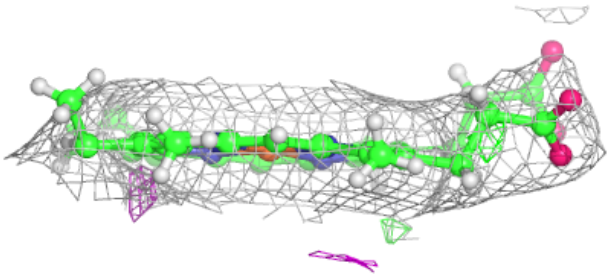
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

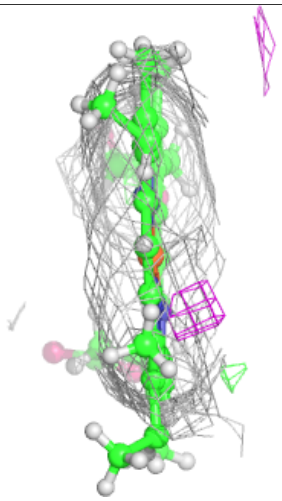


Electron density around HEC P 1001:

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

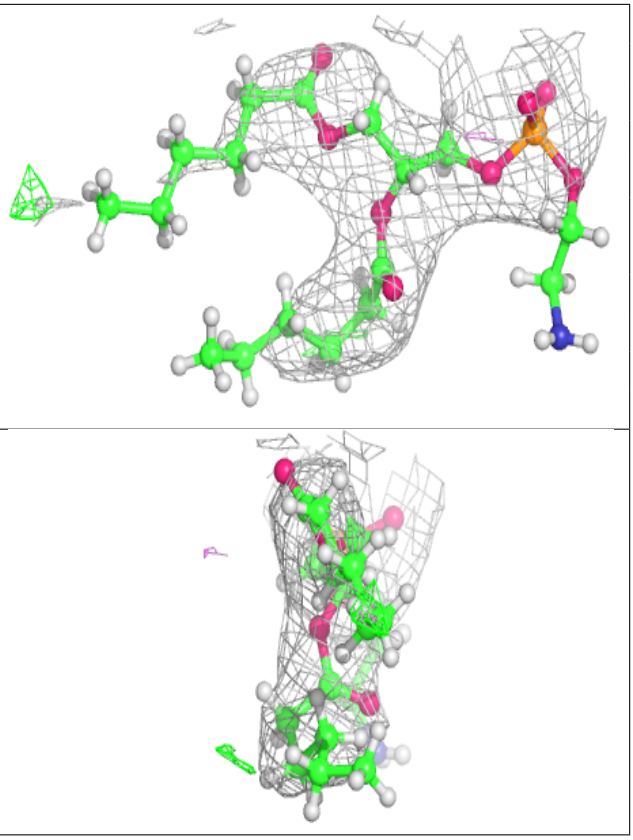


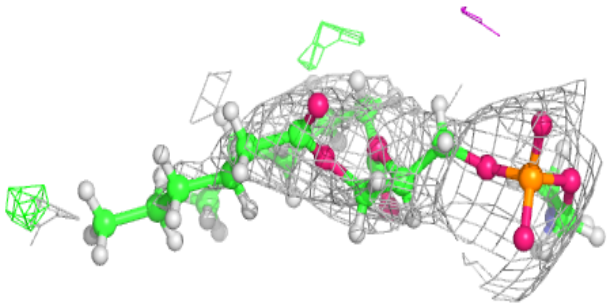




Electron density around 6PE E 1004:

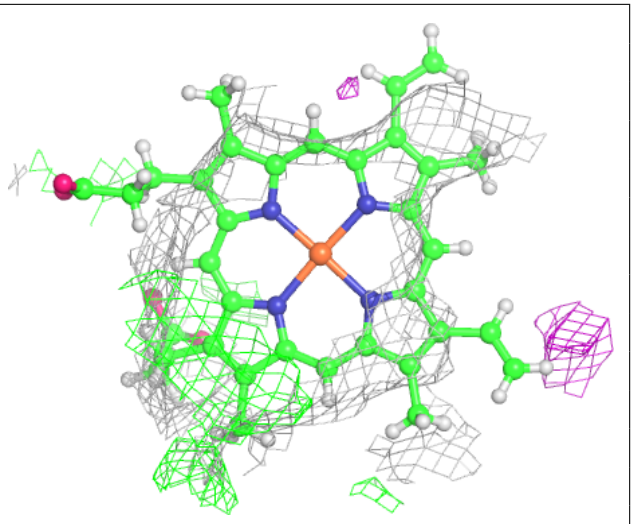
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

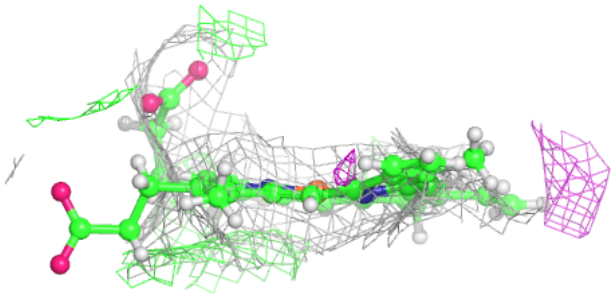


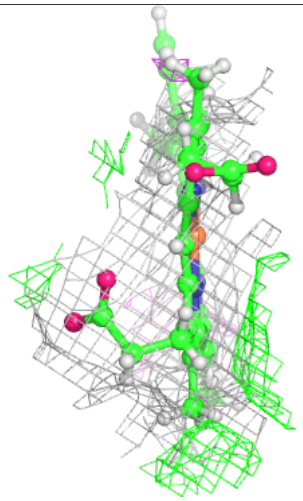


Electron density around HEM O 1001:

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

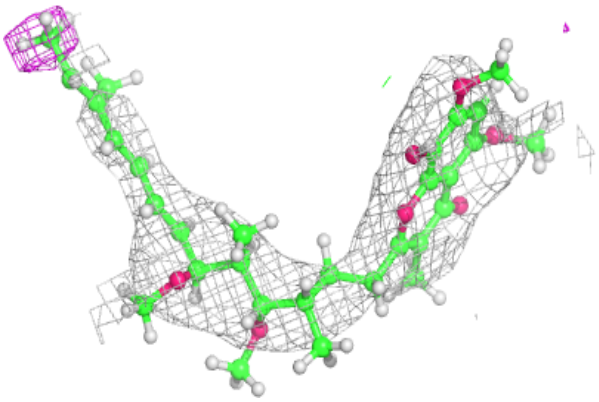


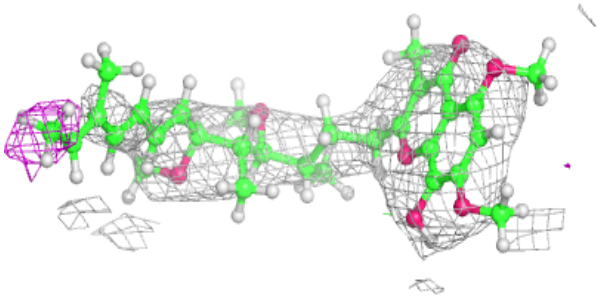


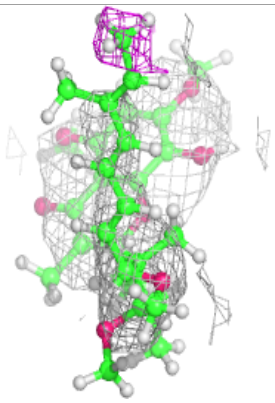


Electron density around SMA K 1003:

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

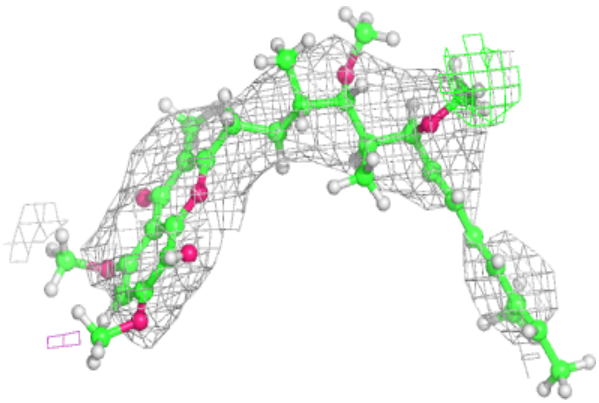


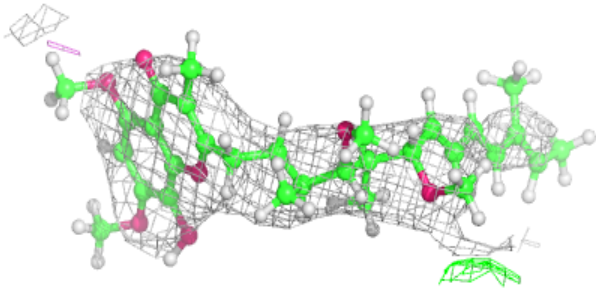


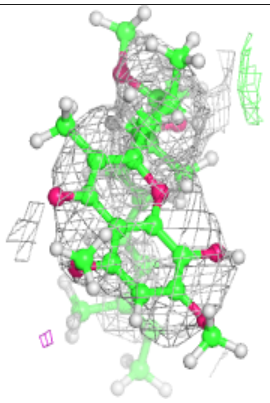


Electron density around SMA W 1003:

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

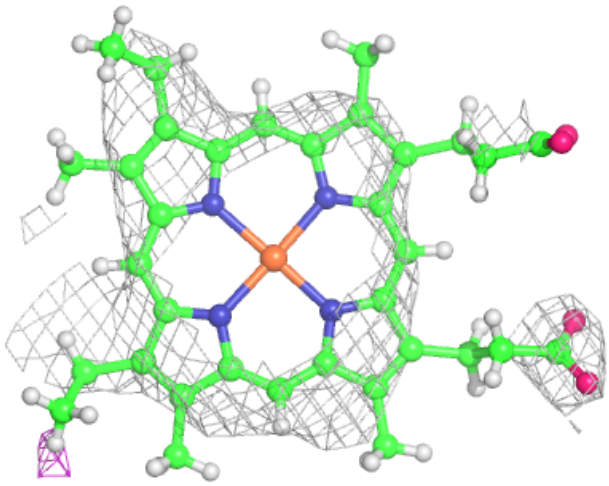


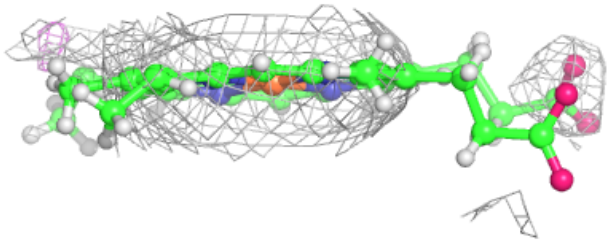


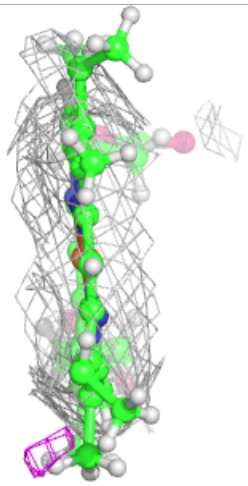


Electron density around HEC X 1001:

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

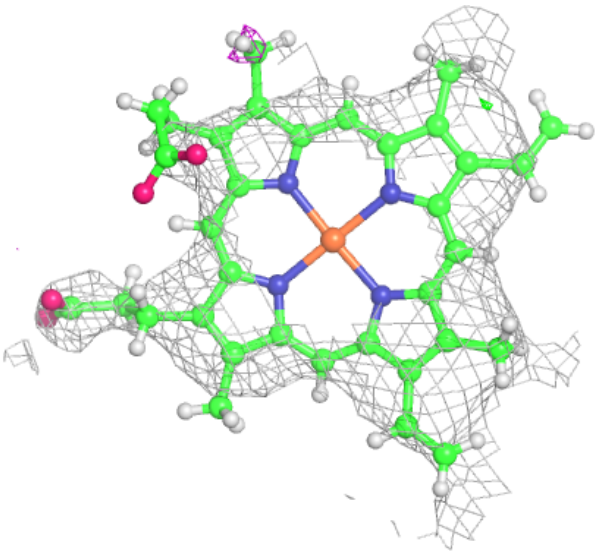


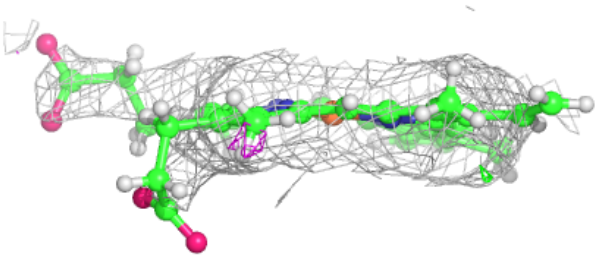


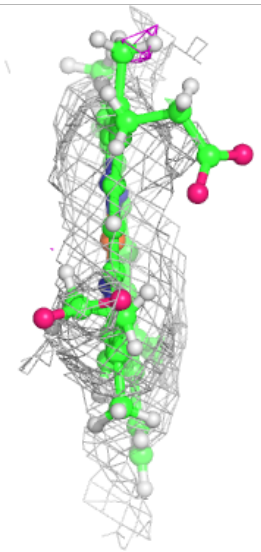


Electron density around HEM E 1001:

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

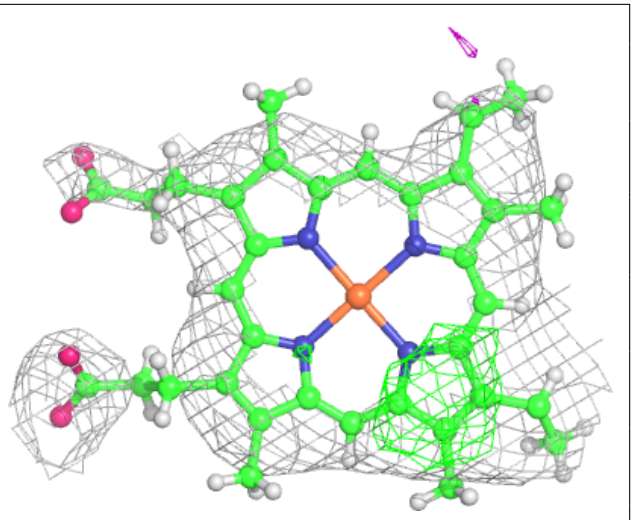


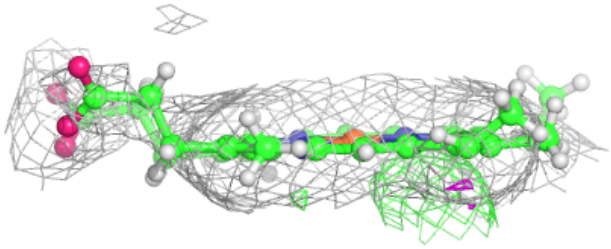


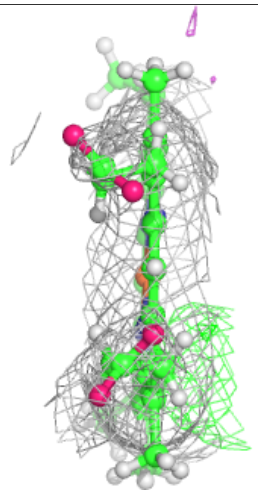


Electron density around HEC L 1001:

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

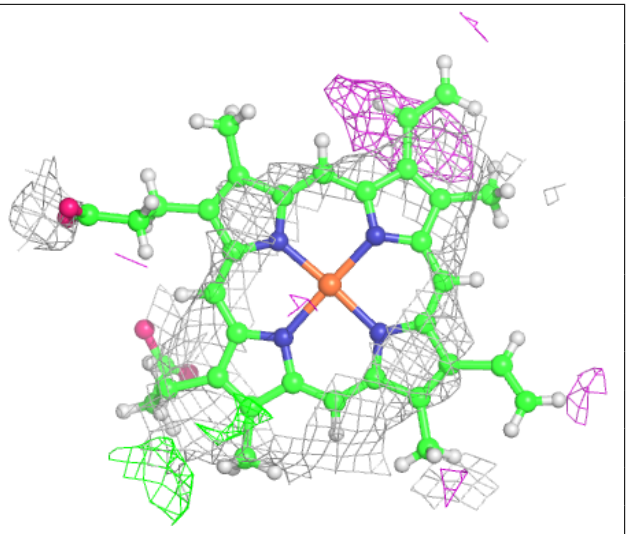


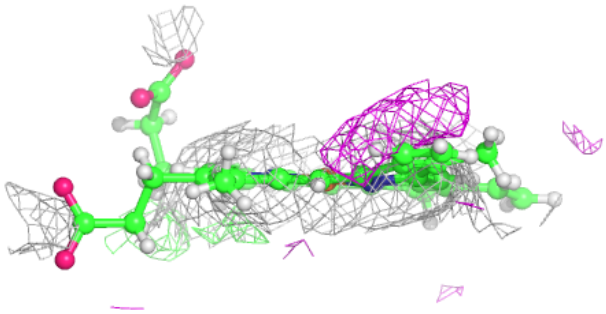


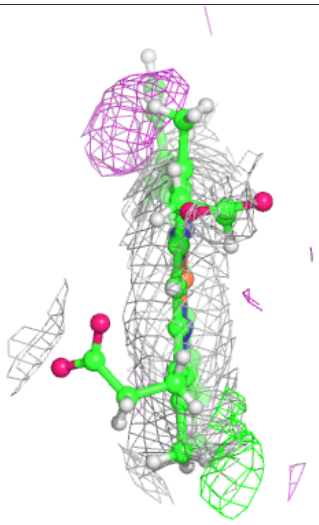


Electron density around HEM S 1001:

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

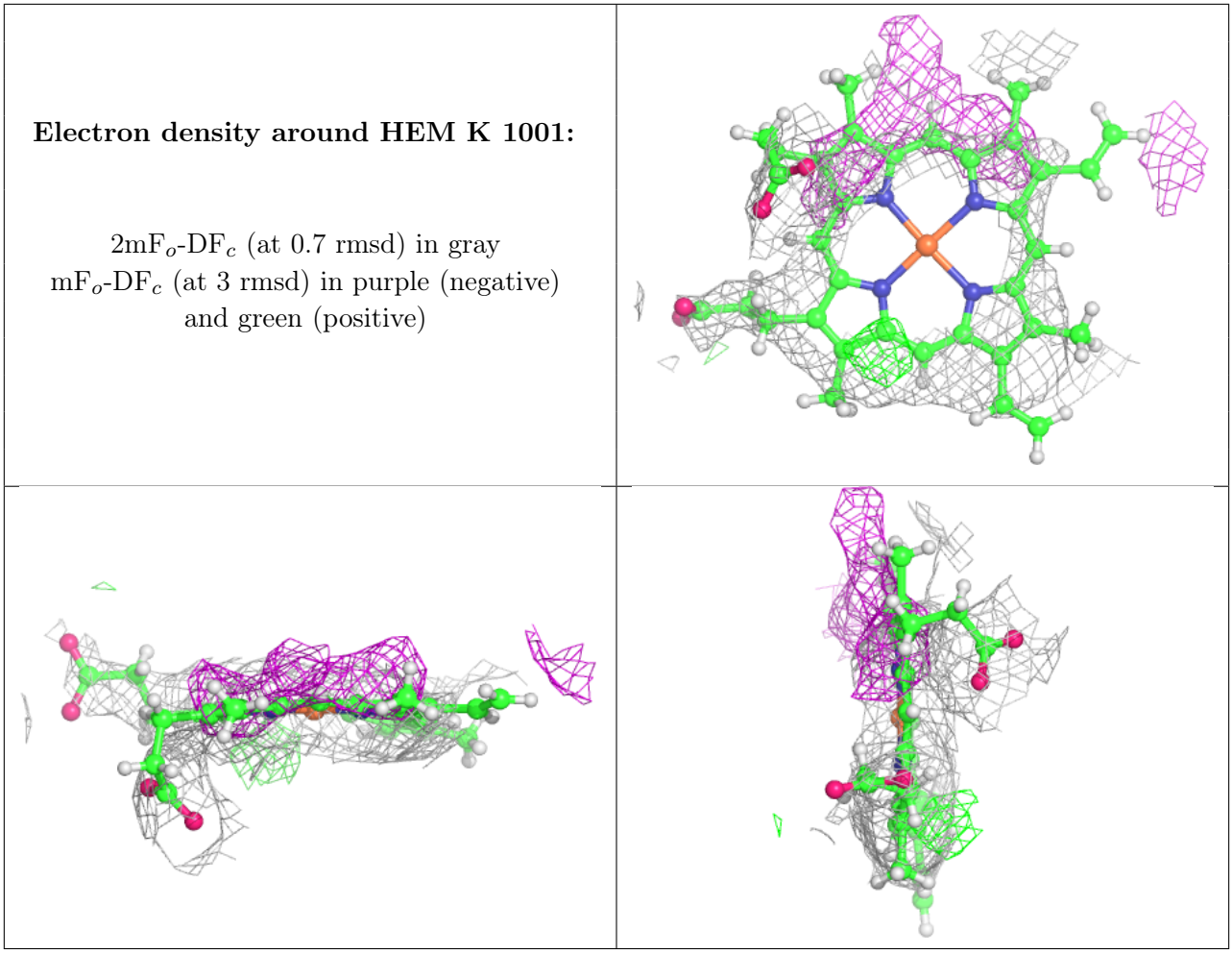






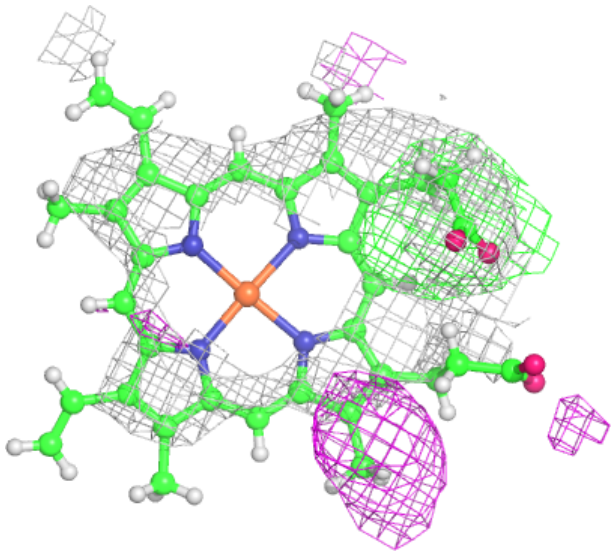
Electron density around HEM K 1001:

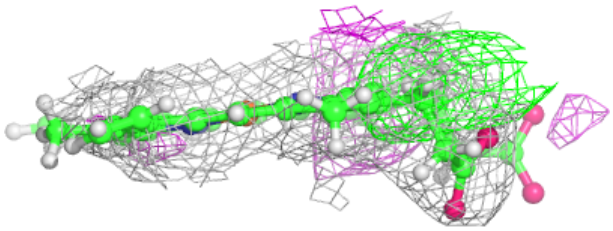
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

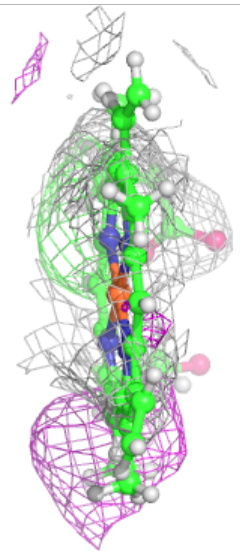


Electron density around HEM E 1002:

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

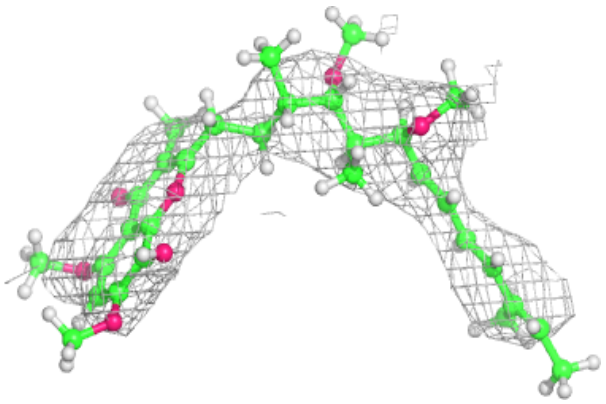


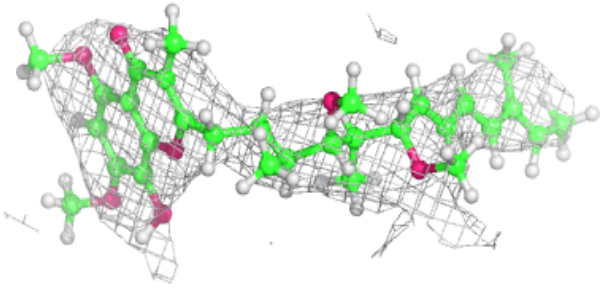


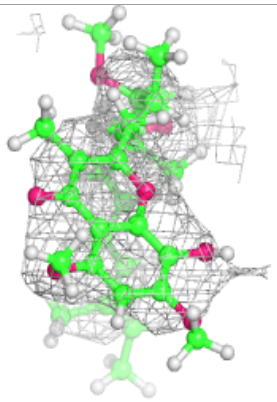


Electron density around SMA E 1003:

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

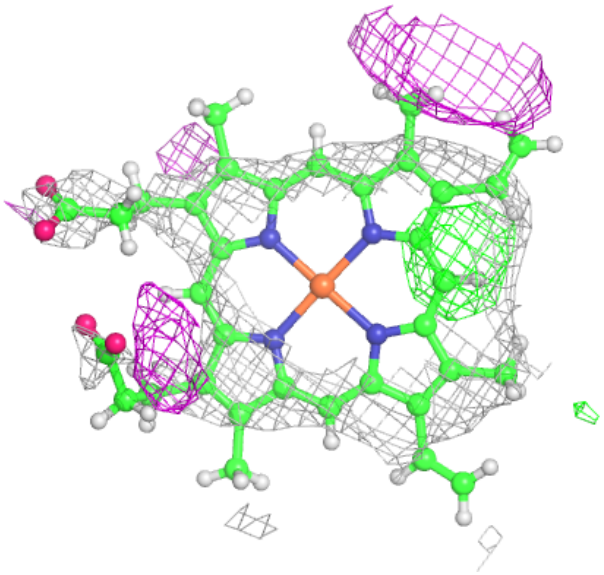


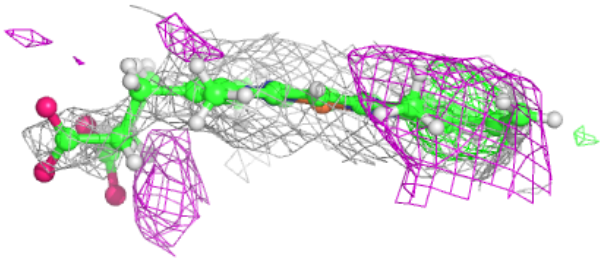


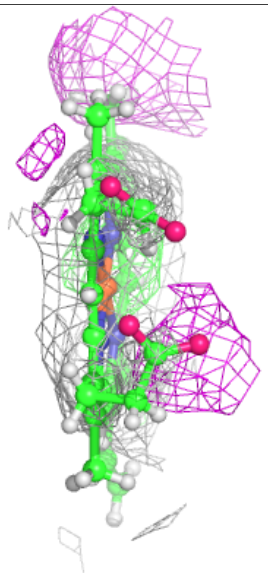


Electron density around HEM O 1002:

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

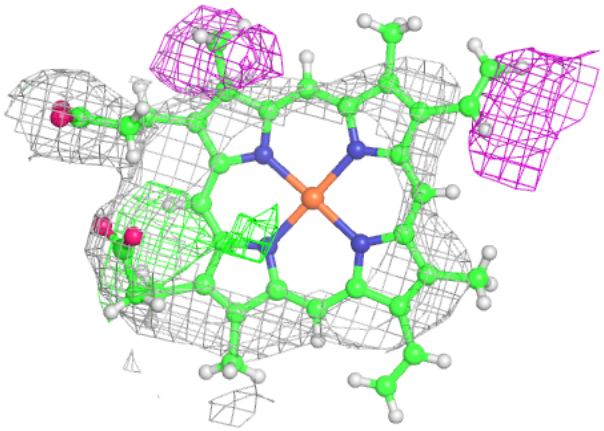


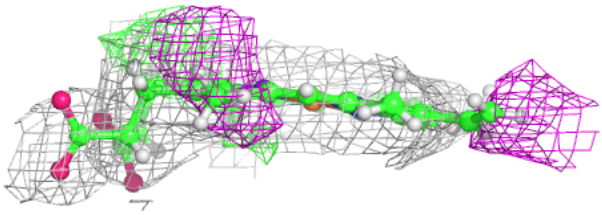


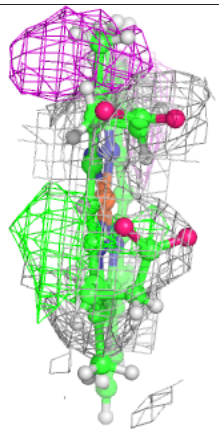


Electron density around HEM A 1002:

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

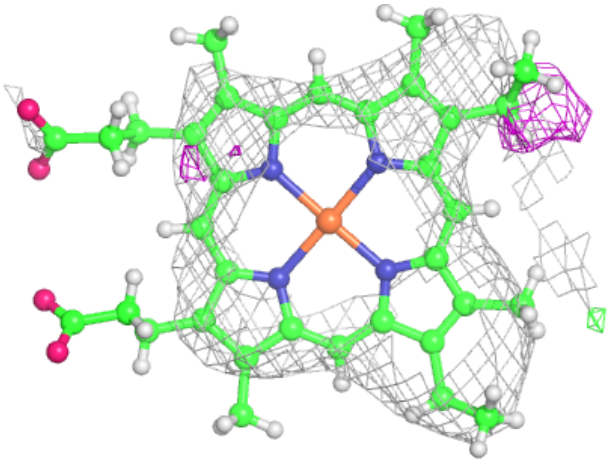


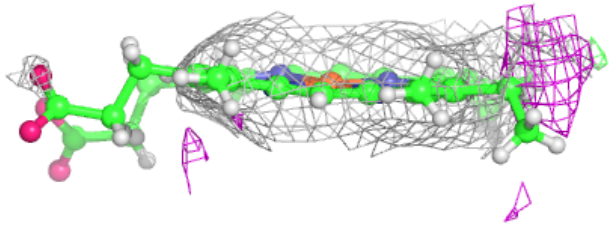


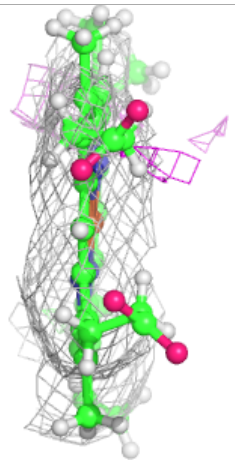


Electron density around HEC F 1001:

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

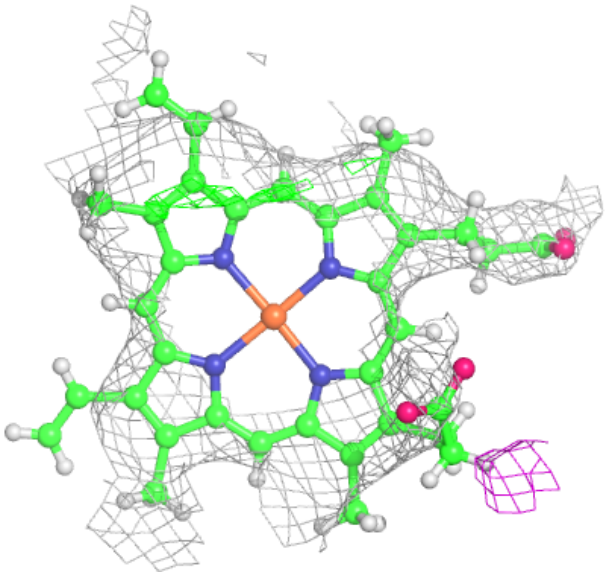


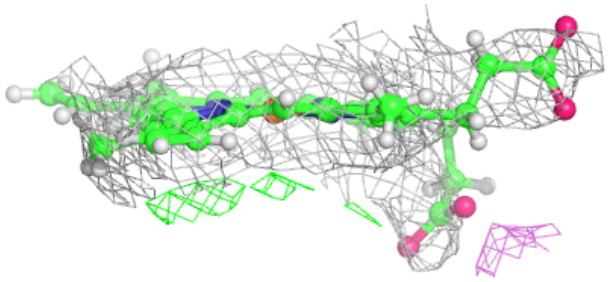


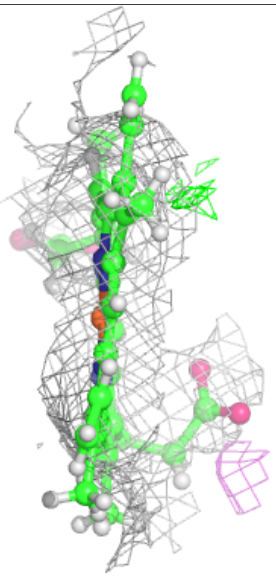


Electron density around HEM W 1001:

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

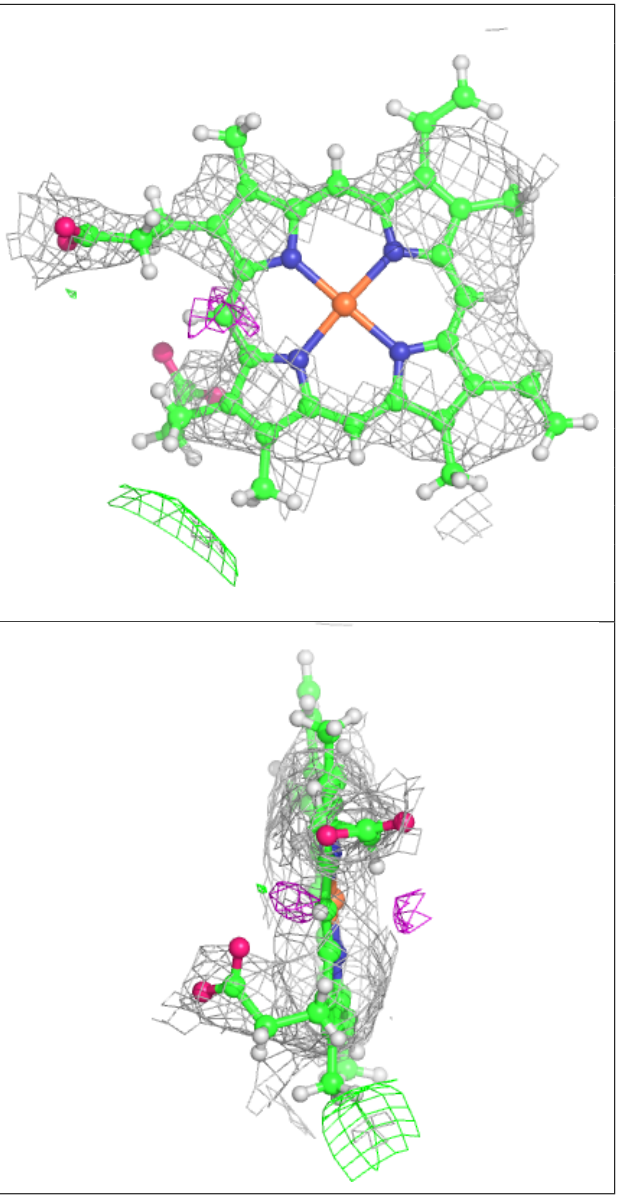






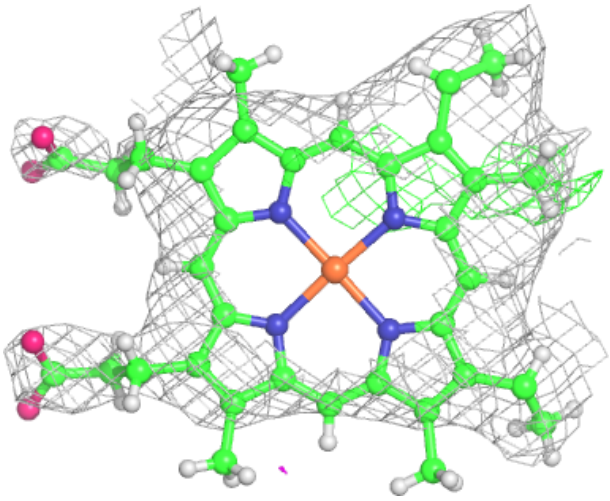
Electron density around HEM A 1001:

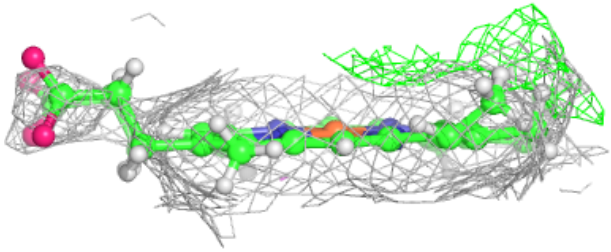
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

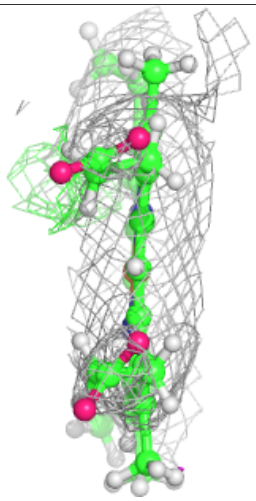


Electron density around HEC B 1001:

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

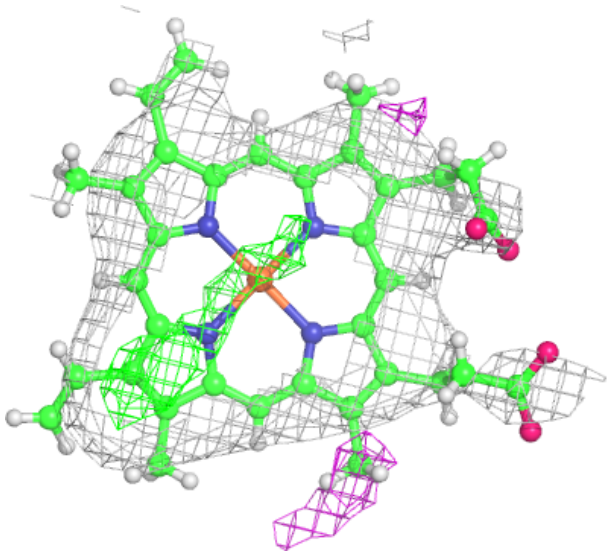


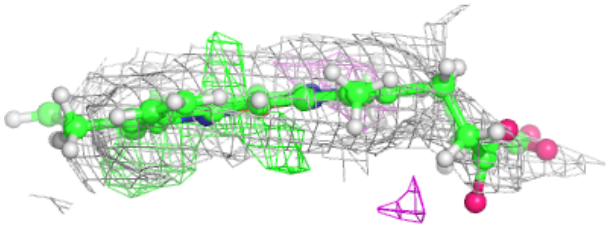


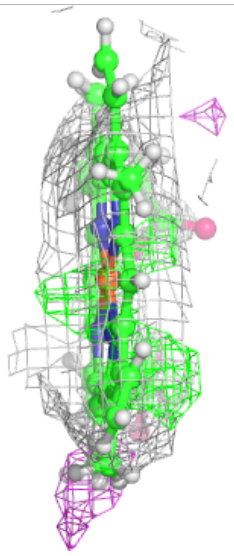


Electron density around HEM K 1002:

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

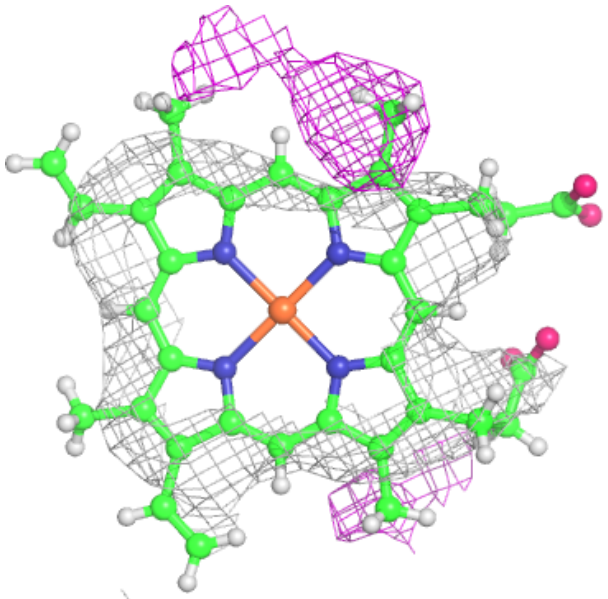


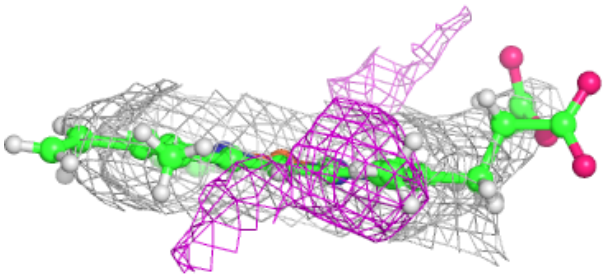


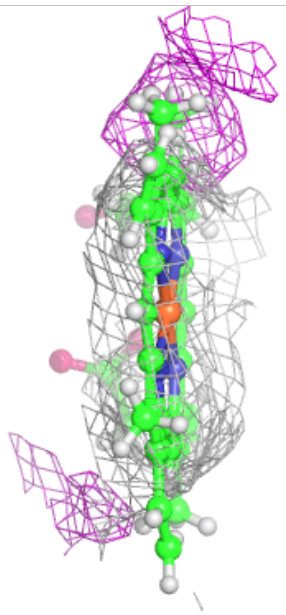


Electron density around HEM W 1002:

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

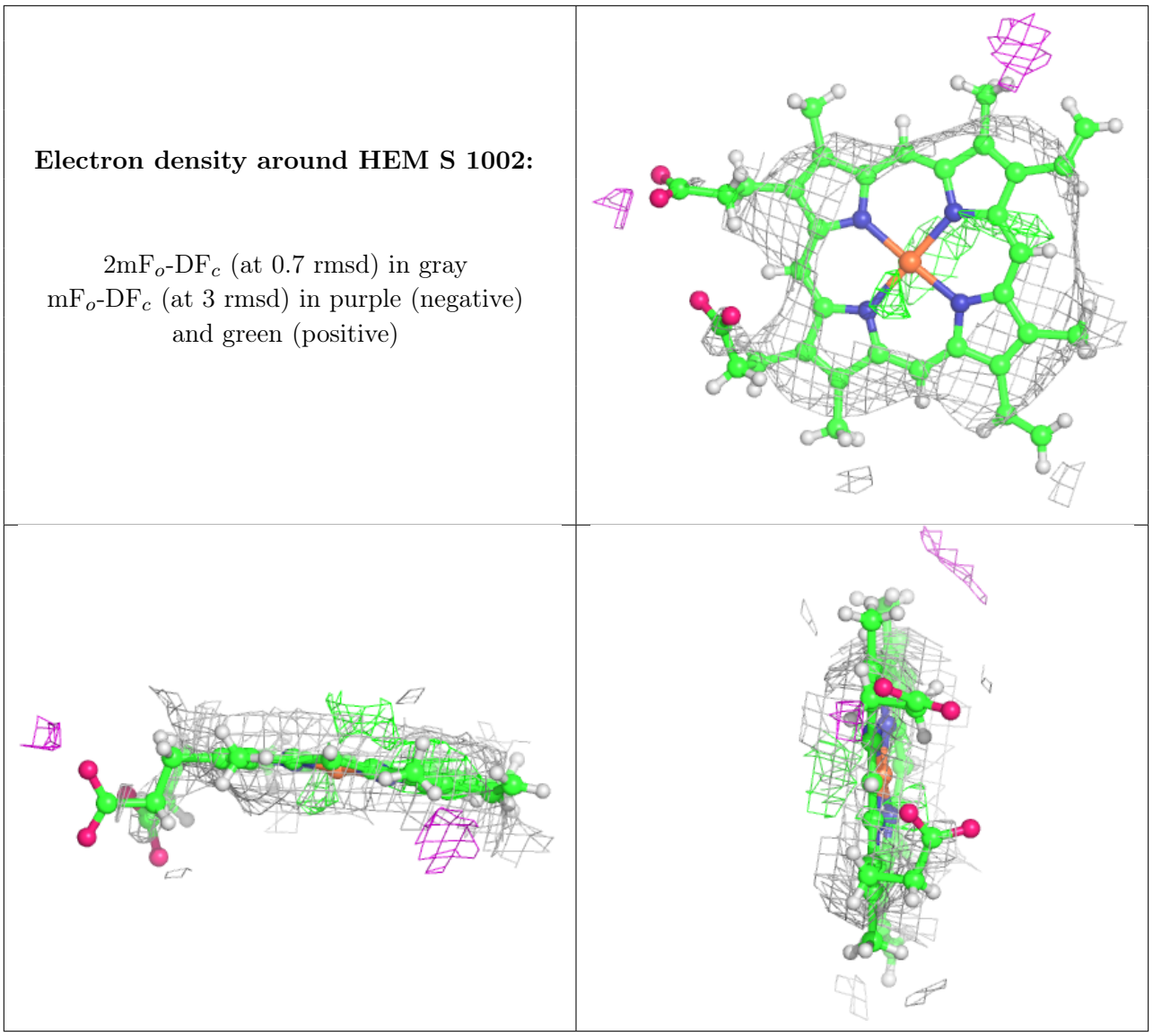






Electron density around HEM S 1002:

$2mF_o$-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.