wwPDB X-ray Structure Validation Summary Report (i)

Sep 20, 2023 – 03:18 AM EDT

PDB ID	:	5KKZ
Title	:	Rhodobacter sphaeroides bc1 with famoxadone
Authors	:	Xia, D.; Esser, L.; Zhou, F.; Tang, W.K.; Yu, C.A.
Deposited on	:	2016-06-23
Resolution	:	2.97 Å(reported)

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

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

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

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

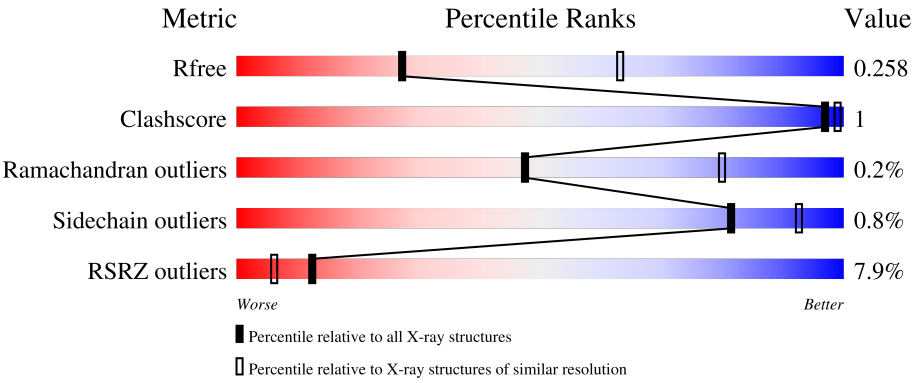
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	4% 92%
1	E	445	5% 92%
1	K	445	3% 91% 5%
1	O	445	6% 93%
2	B	272	8% 93% 6%

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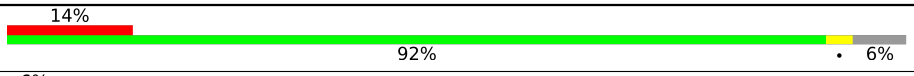
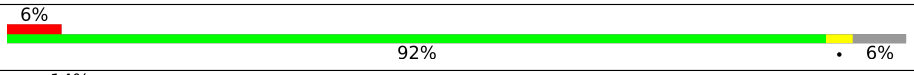
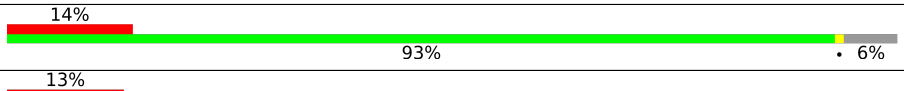
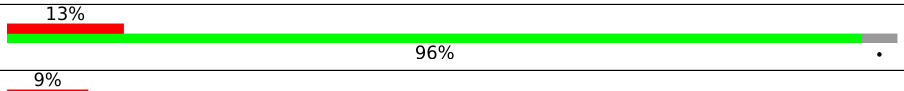
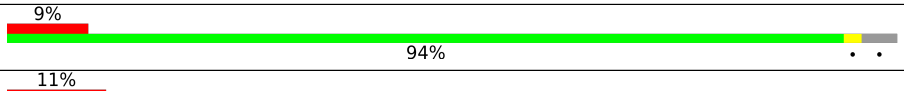
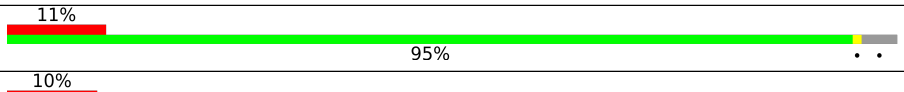
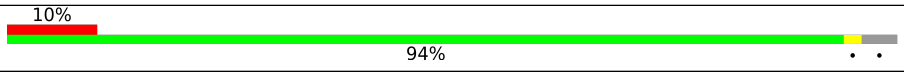
Mol	Chain	Length	Quality of chain
2	F	272	
2	L	272	
2	P	272	
3	C	187	
3	G	187	
3	M	187	
3	Q	187	

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 54985 atoms, of which 27067 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	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			
1	E	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			
1	K	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			
1	O	429	Total	C	H	N	O	S	0	0	0
			6857	2325	3412	548	557	15			

- 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			
2	P	256	Total	C	H	N	O	S	0	0	0
			3792	1240	1839	326	374	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	98	PRO	ALA	variant	UNP Q02760
B	264	GLY	-	expression tag	UNP Q02760
B	265	THR	-	expression tag	UNP Q02760
B	266	GLY	-	expression tag	UNP Q02760
B	267	HIS	-	expression tag	UNP Q02760
B	268	HIS	-	expression tag	UNP Q02760
B	269	HIS	-	expression tag	UNP Q02760
B	270	HIS	-	expression tag	UNP Q02760

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Chain	Residue	Modelled	Actual	Comment	Reference
B	271	HIS	-	expression tag	UNP Q02760
B	272	HIS	-	expression tag	UNP Q02760
F	98	PRO	ALA	variant	UNP Q02760
F	264	GLY	-	expression tag	UNP Q02760
F	265	THR	-	expression tag	UNP Q02760
F	266	GLY	-	expression tag	UNP Q02760
F	267	HIS	-	expression tag	UNP Q02760
F	268	HIS	-	expression tag	UNP Q02760
F	269	HIS	-	expression tag	UNP Q02760
F	270	HIS	-	expression tag	UNP Q02760
F	271	HIS	-	expression tag	UNP Q02760
F	272	HIS	-	expression tag	UNP Q02760
L	98	PRO	ALA	variant	UNP Q02760
L	264	GLY	-	expression tag	UNP Q02760
L	265	THR	-	expression tag	UNP Q02760
L	266	GLY	-	expression tag	UNP Q02760
L	267	HIS	-	expression tag	UNP Q02760
L	268	HIS	-	expression tag	UNP Q02760
L	269	HIS	-	expression tag	UNP Q02760
L	270	HIS	-	expression tag	UNP Q02760
L	271	HIS	-	expression tag	UNP Q02760
L	272	HIS	-	expression tag	UNP Q02760
P	98	PRO	ALA	variant	UNP Q02760
P	264	GLY	-	expression tag	UNP Q02760
P	265	THR	-	expression tag	UNP Q02760
P	266	GLY	-	expression tag	UNP Q02760
P	267	HIS	-	expression tag	UNP Q02760
P	268	HIS	-	expression tag	UNP Q02760
P	269	HIS	-	expression tag	UNP Q02760
P	270	HIS	-	expression tag	UNP Q02760
P	271	HIS	-	expression tag	UNP Q02760
P	272	HIS	-	expression tag	UNP Q02760

- 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
			2645	845	1304	237	253	6			
3	G	179	Total	C	H	N	O	S	0	0	0
			2645	845	1304	237	253	6			
3	M	179	Total	C	H	N	O	S	0	0	0
			2645	845	1304	237	253	6			

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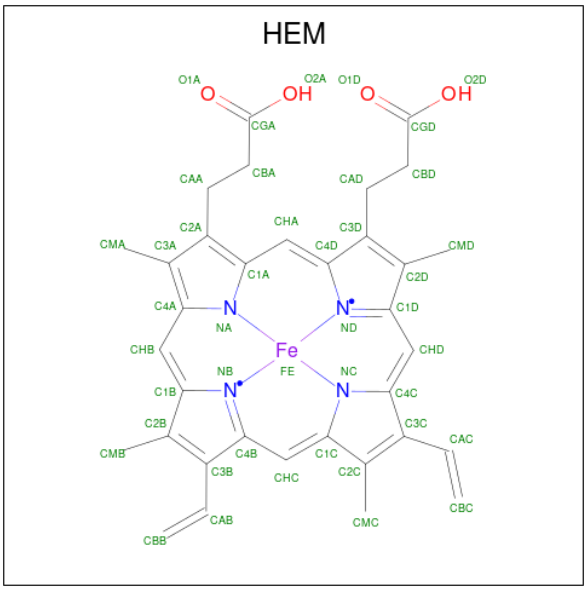
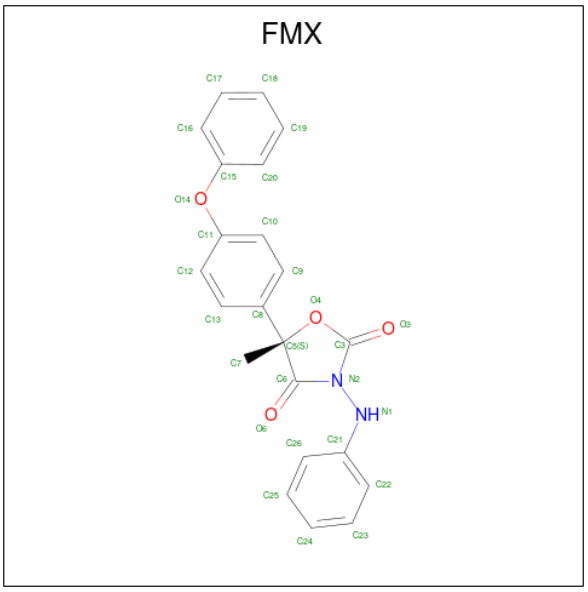
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	Q	179	2645	845	1304	237	253	6	0	0	0

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



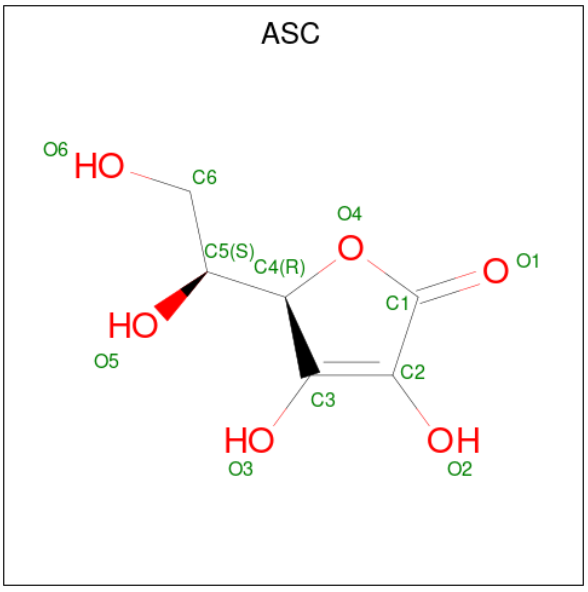
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
4	A	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
4	A	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
4	E	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
4	E	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O		
4	K	1	73	34	1	30	4	4	0	0
			Total	C	Fe	H	N	O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

- Molecule 5 is FAMOXADONE (three-letter code: FMX) (formula: $C_{22}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			46	22	18	2	4		
5	E	1	Total	C	H	N	O	0	0
			46	22	18	2	4		
5	K	1	Total	C	H	N	O	0	0
			46	22	18	2	4		
5	O	1	Total	C	H	N	O	0	0
			46	22	18	2	4		

- Molecule 6 is ASCORBIC ACID (three-letter code: ASC) (formula: $C_6H_8O_6$).

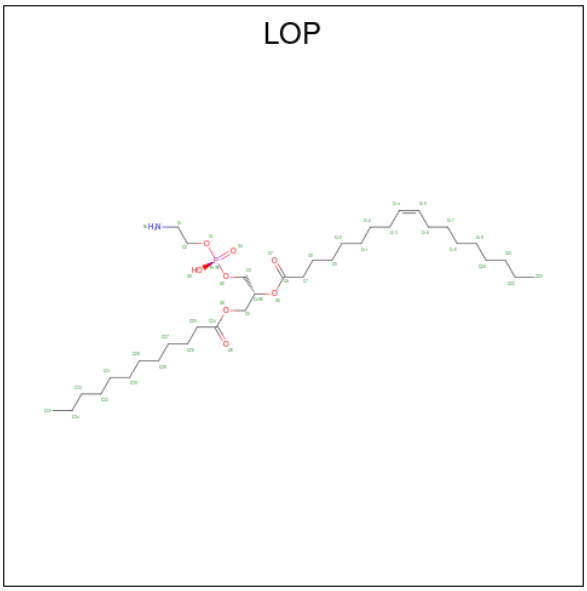


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 19 6 7 6	0	0
6	E	1	Total C H O 19 6 7 6	0	0
6	K	1	Total C H O 19 6 7 6	0	0
6	O	1	Total C H O 19 6 7 6	0	0

- Molecule 7 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

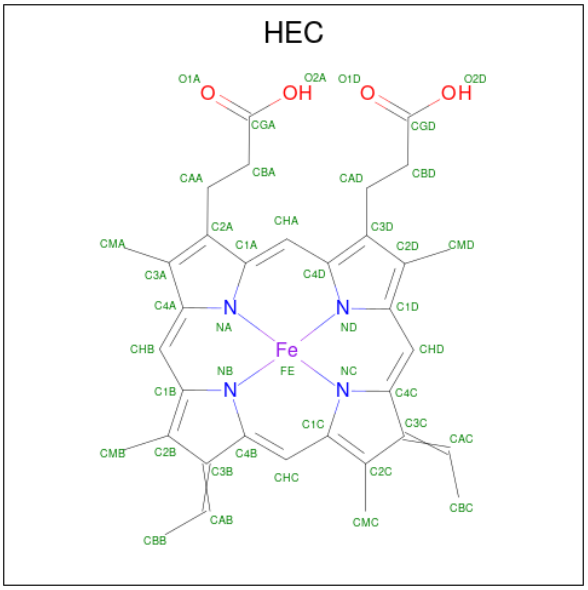
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Sr 1 1	0	0
7	B	1	Total Sr 1 1	0	0
7	F	1	Total Sr 1 1	0	0
7	K	1	Total Sr 1 1	0	0
7	L	1	Total Sr 1 1	0	0
7	P	1	Total Sr 1 1	0	0

- Molecule 8 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: $C_{35}H_{68}NO_8P$).



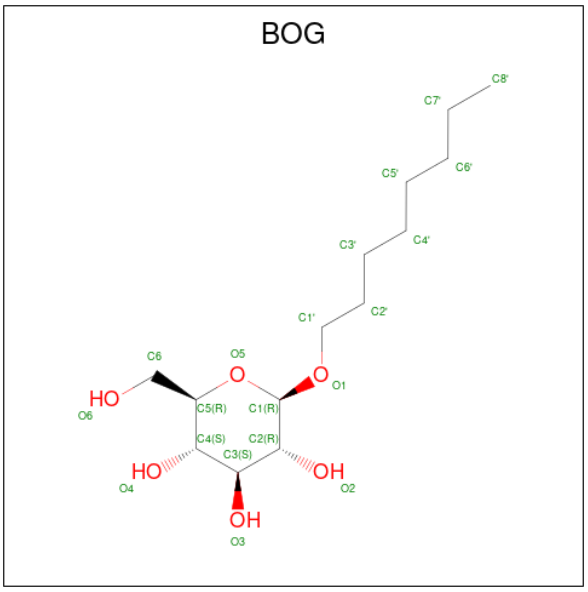
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	P	0	0
			112	35	67	1	8	1		
8	E	1	Total	C	H	N	O	P	0	0
			112	35	67	1	8	1		
8	K	1	Total	C	H	N	O	P	0	0
			112	35	67	1	8	1		
8	O	1	Total	C	H	N	O	P	0	0
			112	35	67	1	8	1		

- Molecule 9 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



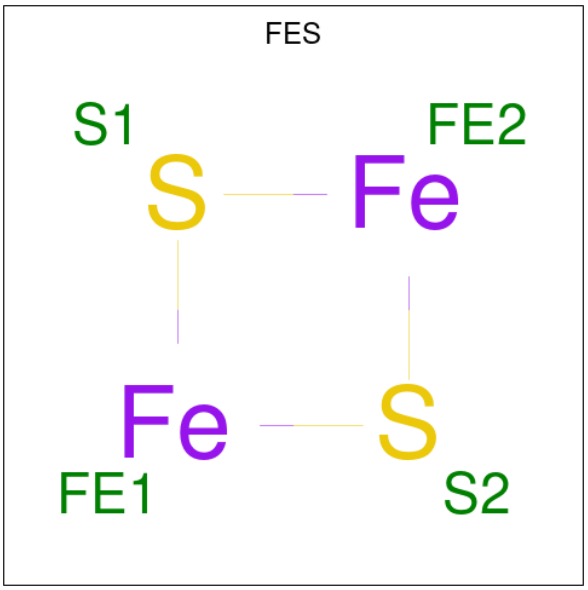
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
9	F	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
9	L	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
9	P	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 10 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			48	14	28	6		
10	F	1	Total	C	H	O	0	0
			47	14	27	6		
10	K	1	Total	C	H	O	0	0
			48	14	28	6		
10	P	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 11 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

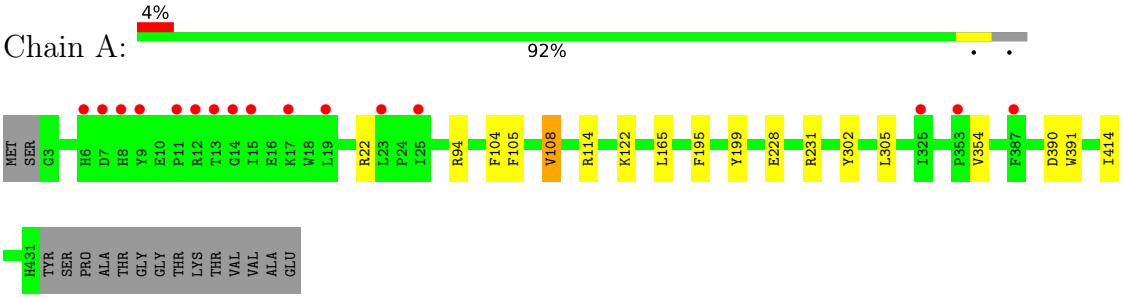
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total O 1 1	0	0
12	E	1	Total O 1 1	0	0
12	K	1	Total O 1 1	0	0
12	O	1	Total O 1 1	0	0

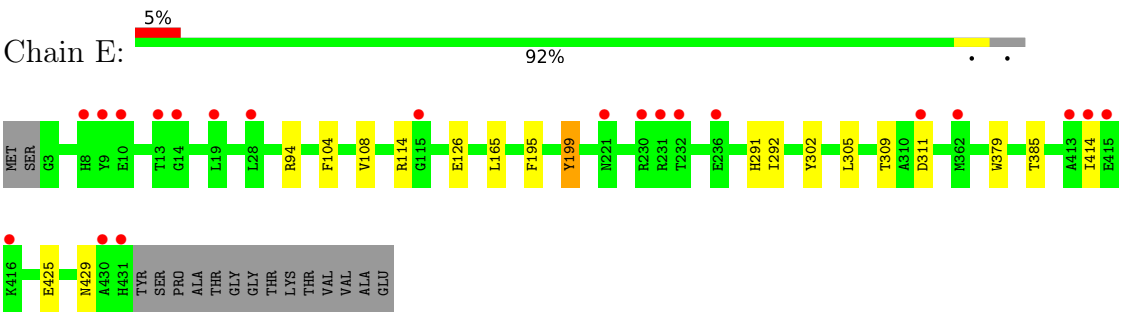
3 Residue-property plots (i)

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.

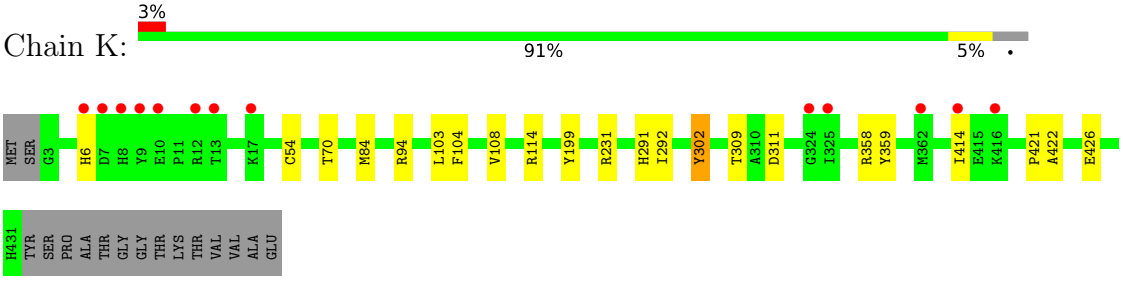
• Molecule 1: Cytochrome b



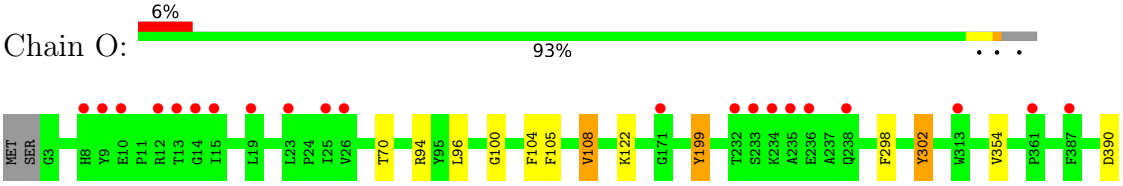
• Molecule 1: Cytochrome b

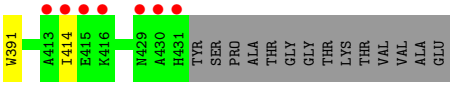


• Molecule 1: Cytochrome b



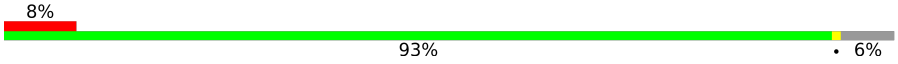
• Molecule 1: Cytochrome b





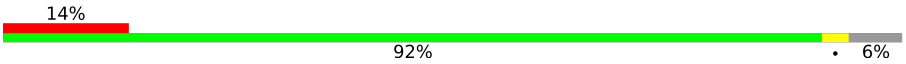
• Molecule 2: Cytochrome c1

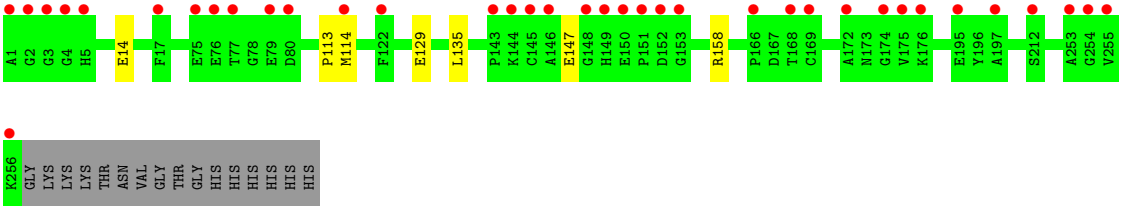
Chain B:



• Molecule 2: Cytochrome c1

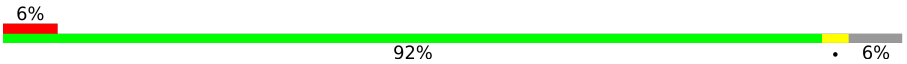
Chain F:

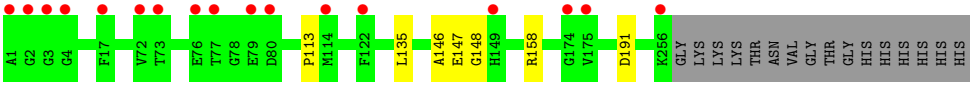




• Molecule 2: Cytochrome c1

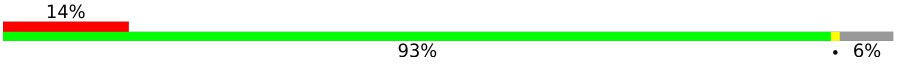
Chain L:

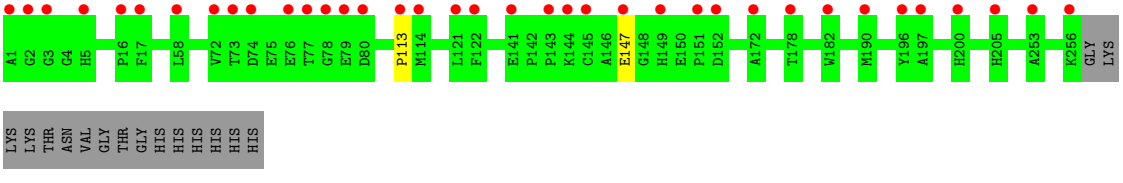




• Molecule 2: Cytochrome c1

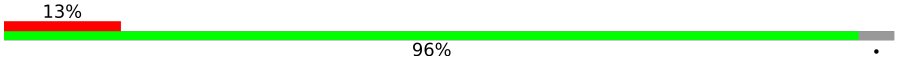
Chain P:

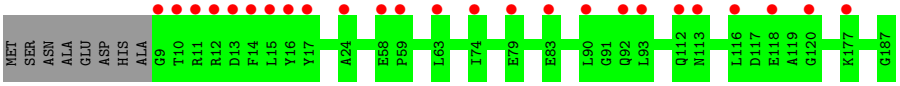




• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

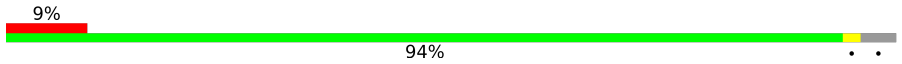
Chain C:

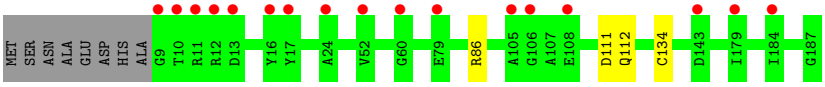




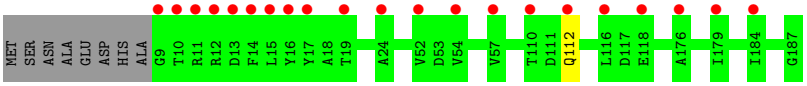
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain G:

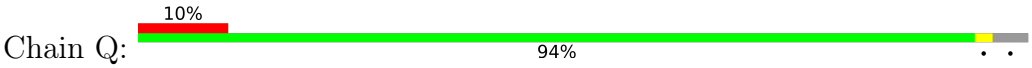


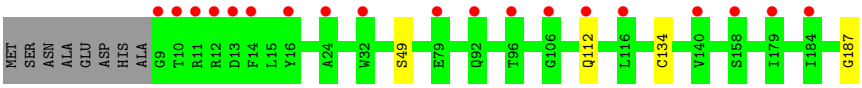


• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit



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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	120.77Å 128.28Å 128.28Å 63.92° 88.63° 63.38°	Depositor
Resolution (Å)	29.98 – 2.97 30.58 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.98-2.97) 77.1 (30.58-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.91 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.11rc1_2513: ???)	Depositor
R, R_{free}	0.215 , 0.258 0.219 , 0.258	Depositor DCC
R_{free} test set	1795 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.015 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	54985	wwPDB-VP
Average B, all atoms (Å^2)	78.0	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 63.55 % 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 9.4951e-06. 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BOG, HEM, ASC, SR, LOP, HEC, FMX, FES

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	0.65	1/3576 (0.0%)	0.72	4/4906 (0.1%)
1	E	0.58	0/3576	0.70	3/4906 (0.1%)
1	K	0.66	1/3576 (0.0%)	0.76	6/4906 (0.1%)
1	O	0.61	1/3576 (0.0%)	0.70	1/4906 (0.0%)
2	B	0.56	0/2010	0.70	1/2733 (0.0%)
2	F	0.51	0/2010	0.65	1/2733 (0.0%)
2	L	0.63	0/2010	0.72	2/2733 (0.1%)
2	P	0.46	0/2010	0.65	0/2733
3	C	0.46	0/1371	0.67	0/1868
3	G	0.49	1/1371 (0.1%)	0.67	0/1868
3	M	0.51	0/1371	0.68	0/1868
3	Q	0.47	1/1371 (0.1%)	0.66	0/1868
All	All	0.57	5/27828 (0.0%)	0.70	18/38028 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	134	CYS	CB-SG	-5.81	1.72	1.81
3	G	134	CYS	CB-SG	-5.63	1.72	1.81
1	K	70	THR	C-N	5.35	1.44	1.34
1	O	70	THR	C-N	5.20	1.44	1.34
1	A	228	GLU	CG-CD	5.12	1.59	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	302	TYR	CB-CG-CD1	-7.13	116.72	121.00
1	K	302	TYR	CB-CG-CD1	-7.02	116.79	121.00
1	A	302	TYR	CB-CG-CD1	-6.77	116.94	121.00
1	K	114	ARG	NE-CZ-NH2	-6.61	117.00	120.30
2	B	158	ARG	NE-CZ-NH1	6.01	123.31	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3445	3412	3427	7	0
1	E	3445	3412	3427	9	0
1	K	3445	3412	3427	8	0
1	O	3445	3412	3427	6	0
2	B	1953	1839	1848	1	0
2	F	1953	1839	1848	3	0
2	L	1953	1839	1848	2	0
2	P	1953	1839	1848	0	0
3	C	1341	1304	1307	0	0
3	G	1341	1304	1307	2	0
3	M	1341	1304	1307	1	0
3	Q	1341	1304	1307	2	0
4	A	86	60	60	3	0
4	E	86	60	60	1	0
4	K	86	60	60	3	0
4	O	86	60	60	3	0
5	A	28	18	18	0	0
5	E	28	18	18	0	0
5	K	28	18	18	0	0
5	O	28	18	18	0	0
6	A	12	7	7	0	0
6	E	12	7	7	1	0
6	K	12	7	7	2	0
6	O	12	7	7	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	P	1	0	0	0	0
8	A	45	67	67	0	0
8	E	45	67	67	0	0
8	K	45	67	67	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	45	67	67	0	0
9	B	43	32	30	1	0
9	F	43	32	30	3	0
9	L	43	32	30	2	0
9	P	43	32	30	2	0
10	B	20	28	28	0	0
10	F	20	27	28	0	0
10	K	20	28	28	0	0
10	P	20	28	28	0	0
11	C	4	0	0	0	0
11	G	4	0	0	0	0
11	M	4	0	0	0	0
11	Q	4	0	0	0	0
12	A	1	0	0	0	0
12	E	1	0	0	0	0
12	K	1	0	0	0	0
12	O	1	0	0	0	0
All	All	27918	27067	27168	51	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 1.

The worst 5 of 51 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:K:291:HIS:ND1	6:K:1004:ASC:O1	2.18	0.77
9:P:1001:HEC:HMC1	9:P:1001:HEC:HBC3	1.81	0.63
1:A:122:LYS:NZ	1:A:354:VAL:O	2.26	0.61
3:Q:49:SER:OG	3:Q:187:GLY:O	2.21	0.59
9:L:1001:HEC:HBB3	9:L:1001:HEC:HMB1	1.89	0.55

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	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
1	E	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
1	K	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
1	O	427/445 (96%)	422 (99%)	5 (1%)	0	100	100
2	B	254/272 (93%)	244 (96%)	9 (4%)	1 (0%)	34	70
2	F	254/272 (93%)	244 (96%)	8 (3%)	2 (1%)	19	55
2	L	254/272 (93%)	244 (96%)	8 (3%)	2 (1%)	19	55
2	P	254/272 (93%)	244 (96%)	8 (3%)	2 (1%)	19	55
3	C	177/187 (95%)	168 (95%)	9 (5%)	0	100	100
3	G	177/187 (95%)	169 (96%)	8 (4%)	0	100	100
3	M	177/187 (95%)	170 (96%)	7 (4%)	0	100	100
3	Q	177/187 (95%)	169 (96%)	8 (4%)	0	100	100
All	All	3432/3616 (95%)	3340 (97%)	85 (2%)	7 (0%)	47	80

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	113	PRO
2	B	113	PRO
2	L	113	PRO
2	P	147	GLU
2	F	147	GLU

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	354/366 (97%)	349 (99%)	5 (1%)	67	86
1	E	354/366 (97%)	348 (98%)	6 (2%)	60	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	354/366 (97%)	348 (98%)	6 (2%)	60 84
1	O	354/366 (97%)	349 (99%)	5 (1%)	67 86
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
3	C	138/144 (96%)	138 (100%)	0	100 100
3	G	138/144 (96%)	138 (100%)	0	100 100
3	M	138/144 (96%)	138 (100%)	0	100 100
3	Q	138/144 (96%)	138 (100%)	0	100 100
All	All	2780/2904 (96%)	2758 (99%)	22 (1%)	81 92

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	108	VAL
1	O	94	ARG
1	K	414	ILE
1	O	104	PHE
1	E	104	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	GLN
2	L	111	HIS
1	O	316	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 6 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HEM	K	1001	1	41,50,50	1.64	9 (21%)	45,82,82	1.64	9 (20%)
8	LOP	K	1006	-	44,44,44	1.11	2 (4%)	47,49,49	1.08	5 (10%)
5	FMX	A	1003	-	29,31,31	0.86	1 (3%)	34,44,44	1.63	7 (20%)
4	HEM	A	1001	1	41,50,50	1.71	9 (21%)	45,82,82	1.50	7 (15%)
6	ASC	K	1004	-	12,12,12	0.94	1 (8%)	17,17,17	2.35	7 (41%)
8	LOP	A	1006	-	44,44,44	0.99	1 (2%)	47,49,49	1.42	6 (12%)
4	HEM	K	1002	1	41,50,50	1.65	7 (17%)	45,82,82	1.64	11 (24%)
11	FES	Q	1001	3	0,4,4	-	-	-		
4	HEM	E	1001	1	41,50,50	1.58	4 (9%)	45,82,82	1.51	9 (20%)
6	ASC	O	1004	-	12,12,12	1.04	0	17,17,17	2.67	6 (35%)
8	LOP	E	1005	-	44,44,44	1.05	2 (4%)	47,49,49	1.29	6 (12%)
10	BOG	P	1003	-	20,20,20	1.01	1 (5%)	25,25,25	1.02	2 (8%)
9	HEC	B	1001	2	32,50,50	1.94	5 (15%)	24,82,82	1.85	5 (20%)
5	FMX	O	1003	-	29,31,31	0.99	2 (6%)	34,44,44	1.49	4 (11%)
11	FES	C	1001	3	0,4,4	-	-	-		
11	FES	G	1001	3	0,4,4	-	-	-		
4	HEM	A	1002	1	41,50,50	1.69	5 (12%)	45,82,82	1.50	7 (15%)
5	FMX	K	1003	-	29,31,31	0.80	1 (3%)	34,44,44	1.25	6 (17%)
9	HEC	L	1001	2	32,50,50	2.02	4 (12%)	24,82,82	2.32	5 (20%)
9	HEC	P	1001	2	32,50,50	2.09	4 (12%)	24,82,82	1.46	4 (16%)
4	HEM	O	1001	1	41,50,50	1.59	9 (21%)	45,82,82	1.85	13 (28%)
4	HEM	E	1002	1	41,50,50	1.63	7 (17%)	45,82,82	1.53	9 (20%)
8	LOP	O	1005	-	44,44,44	1.11	2 (4%)	47,49,49	1.16	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	HEC	F	1001	2	32,50,50	1.95	3 (9%)	24,82,82	2.00	7 (29%)
10	BOG	B	1003	-	20,20,20	1.02	1 (5%)	25,25,25	1.25	3 (12%)
6	ASC	A	1004	-	12,12,12	0.87	0	17,17,17	2.52	5 (29%)
4	HEM	O	1002	1	41,50,50	1.59	6 (14%)	45,82,82	1.64	9 (20%)
6	ASC	E	1004	-	12,12,12	0.90	0	17,17,17	2.43	8 (47%)
10	BOG	K	1007	-	20,20,20	1.12	2 (10%)	25,25,25	1.02	2 (8%)
10	BOG	F	1003	-	20,20,20	1.09	2 (10%)	25,25,25	1.19	3 (12%)
11	FES	M	1001	3	0,4,4	-	-	-		
5	FMX	E	1003	-	29,31,31	0.83	2 (6%)	34,44,44	1.10	3 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	K	1001	1	-	5/12/54/54	-
8	LOP	K	1006	-	-	24/48/48/48	-
5	FMX	A	1003	-	-	0/14/33/33	0/4/4/4
4	HEM	A	1001	1	-	5/12/54/54	-
6	ASC	K	1004	-	-	4/6/22/22	0/1/1/1
8	LOP	A	1006	-	-	24/48/48/48	-
4	HEM	K	1002	1	-	2/12/54/54	-
11	FES	Q	1001	3	-	-	0/1/1/1
4	HEM	E	1001	1	-	5/12/54/54	-
6	ASC	O	1004	-	-	4/6/22/22	0/1/1/1
8	LOP	E	1005	-	-	25/48/48/48	-
10	BOG	P	1003	-	-	6/11/31/31	0/1/1/1
9	HEC	B	1001	2	-	4/10/54/54	-
5	FMX	O	1003	-	-	0/14/33/33	0/4/4/4
11	FES	C	1001	3	-	-	0/1/1/1
11	FES	G	1001	3	-	-	0/1/1/1
4	HEM	A	1002	1	-	5/12/54/54	-
5	FMX	K	1003	-	-	0/14/33/33	0/4/4/4
9	HEC	L	1001	2	-	2/10/54/54	-
9	HEC	P	1001	2	-	2/10/54/54	-
4	HEM	O	1001	1	-	5/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	E	1002	1	-	2/12/54/54	-
8	LOP	O	1005	-	-	15/48/48/48	-
9	HEC	F	1001	2	-	2/10/54/54	-
10	BOG	B	1003	-	-	5/11/31/31	0/1/1/1
6	ASC	A	1004	-	-	2/6/22/22	0/1/1/1
4	HEM	O	1002	1	-	2/12/54/54	-
6	ASC	E	1004	-	-	4/6/22/22	0/1/1/1
10	BOG	K	1007	-	-	6/11/31/31	0/1/1/1
10	BOG	F	1003	-	-	4/11/31/31	0/1/1/1
11	FES	M	1001	3	-	-	0/1/1/1
5	FMX	E	1003	-	-	0/14/33/33	0/4/4/4

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	1001	HEC	C2B-C3B	-6.87	1.33	1.40
9	F	1001	HEC	C2B-C3B	-6.40	1.34	1.40
4	A	1002	HEM	C3C-C2C	-6.20	1.31	1.40
9	P	1001	HEC	C2B-C3B	-6.16	1.34	1.40
9	P	1001	HEC	C3C-C2C	-5.62	1.34	1.40

The worst 5 of 173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	O	1004	ASC	C4-O4-C1	-7.25	101.06	109.25
5	A	1003	FMX	O4-C3-O3	5.88	129.24	122.46
9	L	1001	HEC	CBD-CAD-C3D	-5.64	102.99	112.62
4	K	1001	HEM	CBA-CAA-C2A	-5.41	103.39	112.62
6	A	1004	ASC	O5-C5-C4	-5.39	100.15	110.77

There are no chirality outliers.

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	HEM	C1A-C2A-CAA-CBA
4	A	1002	HEM	C3A-C2A-CAA-CBA
4	O	1001	HEM	C2D-C3D-CAD-CBD
4	O	1001	HEM	C4D-C3D-CAD-CBD
6	E	1004	ASC	C3-C4-C5-C6

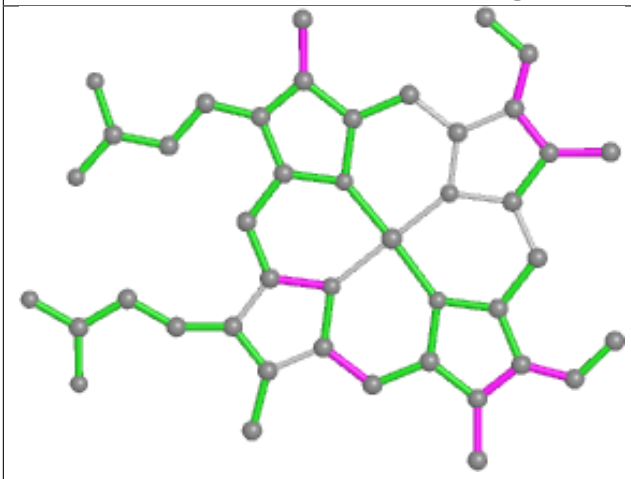
There are no ring outliers.

12 monomers are involved in 22 short contacts:

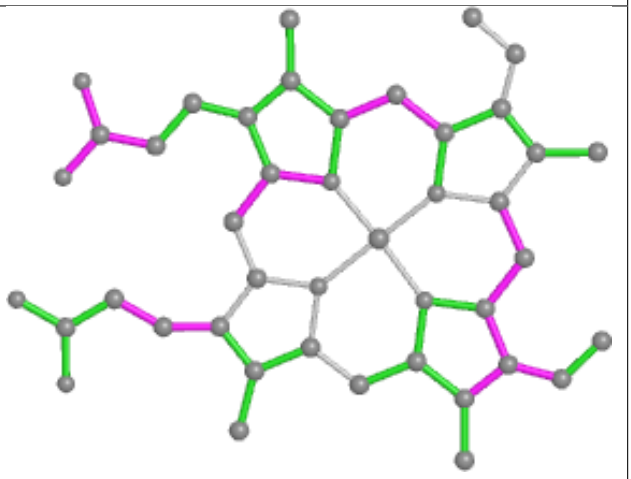
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1001	HEM	3	0
8	K	1006	LOP	1	0
4	A	1001	HEM	2	0
6	K	1004	ASC	2	0
4	E	1001	HEM	1	0
9	B	1001	HEC	1	0
4	A	1002	HEM	1	0
9	L	1001	HEC	2	0
9	P	1001	HEC	2	0
4	O	1001	HEM	3	0
9	F	1001	HEC	3	0
6	E	1004	ASC	1	0

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.

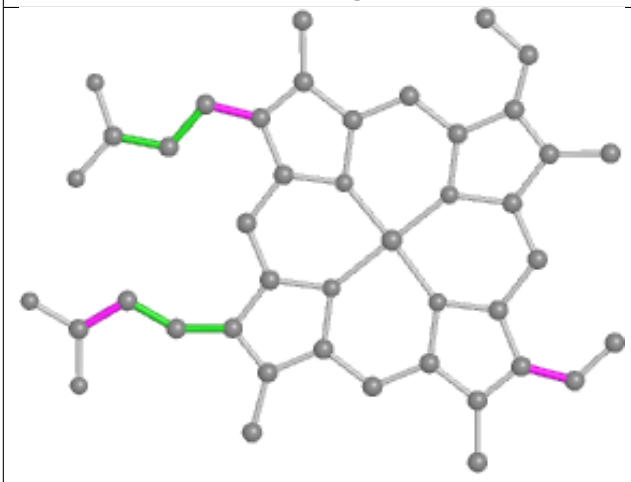
Ligand HEM K 1001



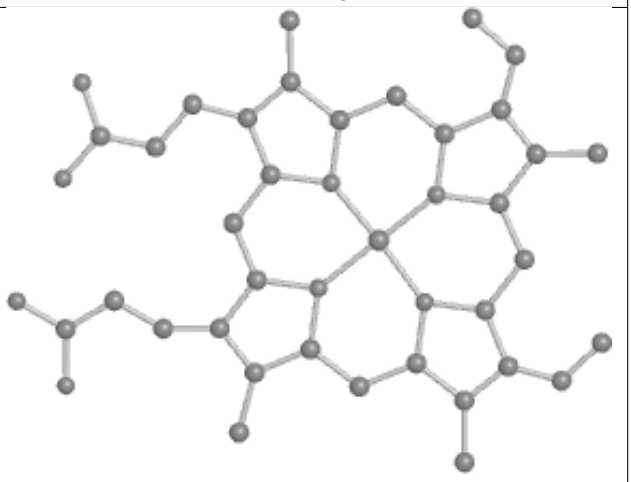
Bond lengths



Bond angles

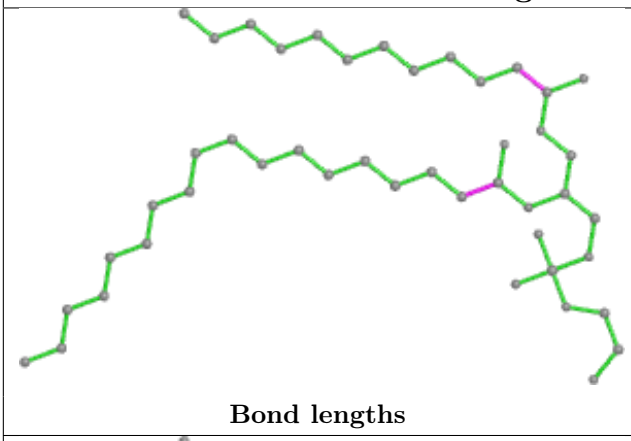


Torsions

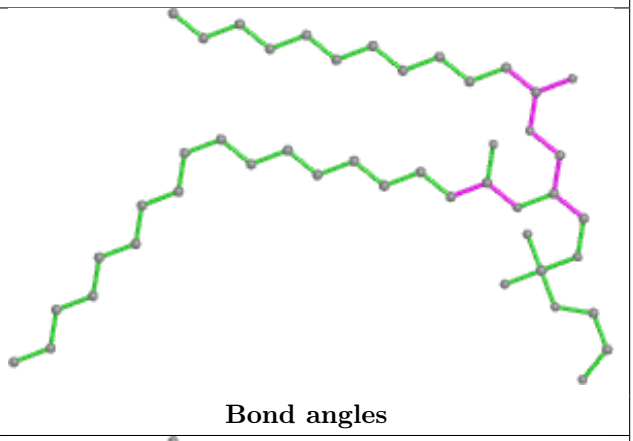


Rings

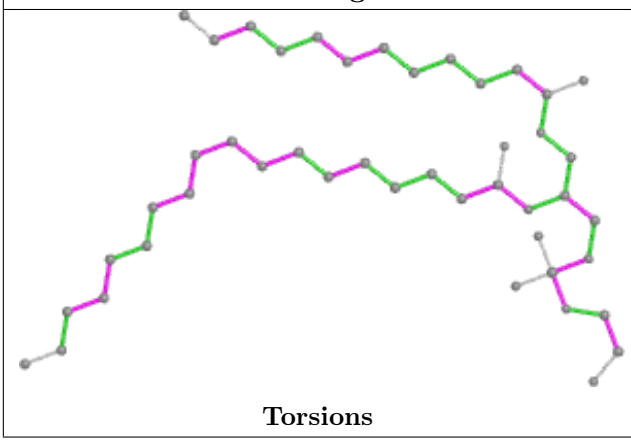
Ligand LOP K 1006



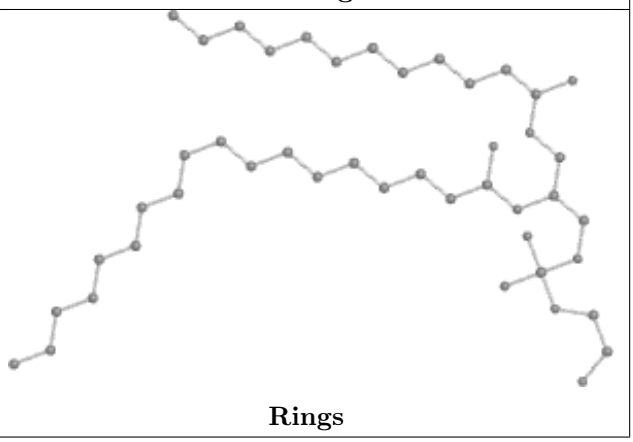
Bond lengths



Bond angles

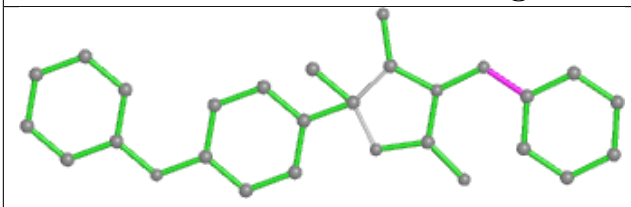


Torsions

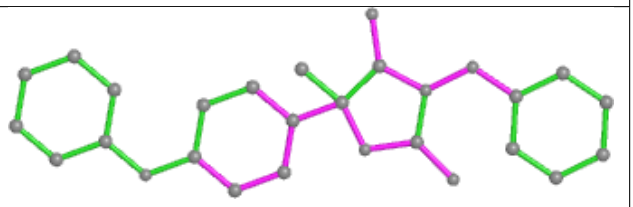


Rings

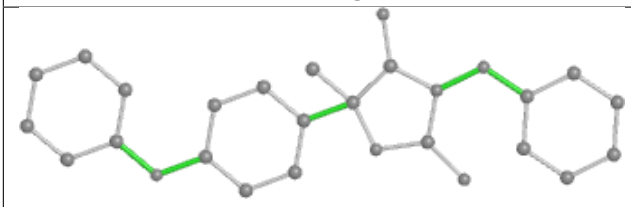
Ligand FMX A 1003



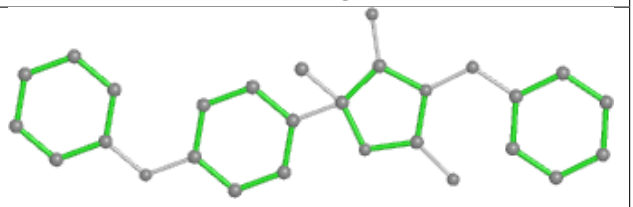
Bond lengths



Bond angles

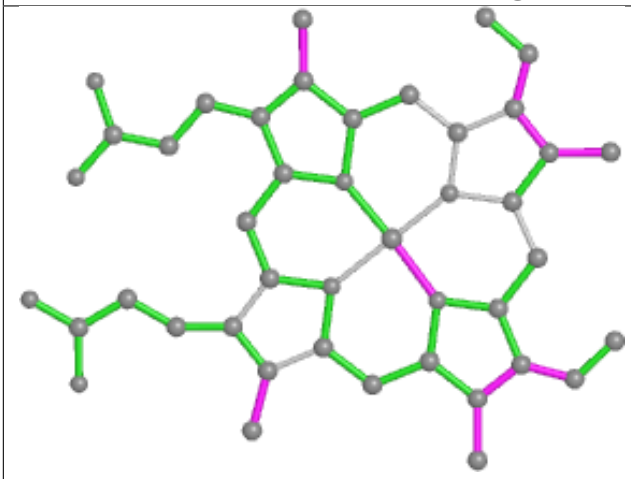


Torsions

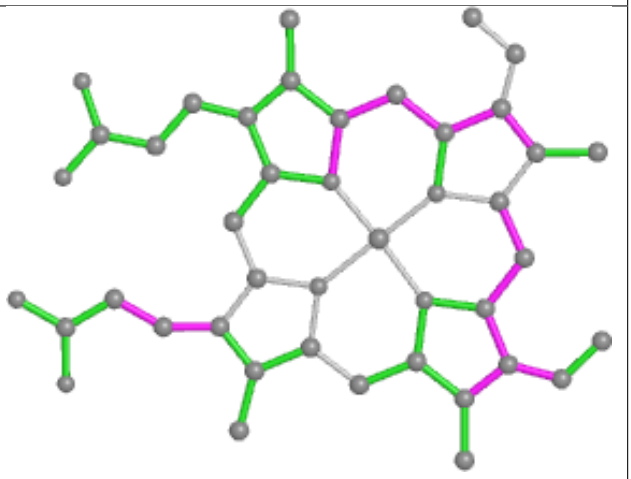


Rings

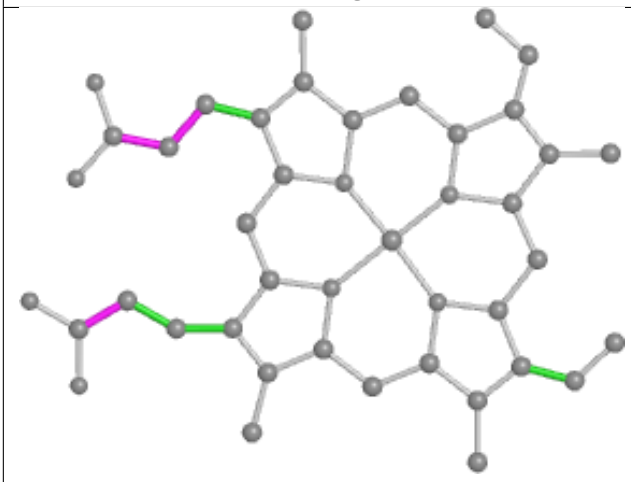
Ligand HEM A 1001



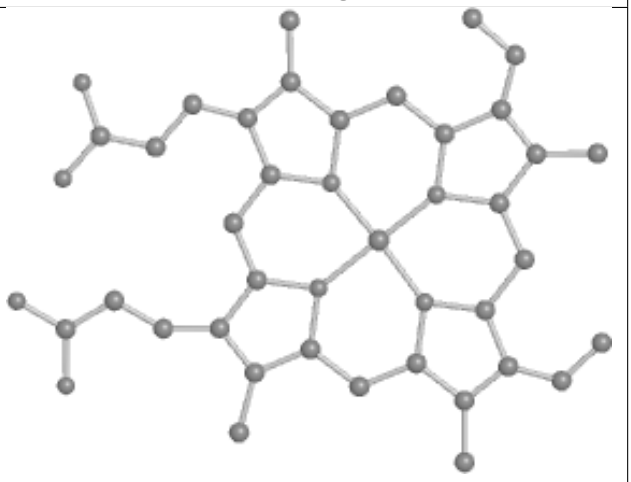
Bond lengths



Bond angles

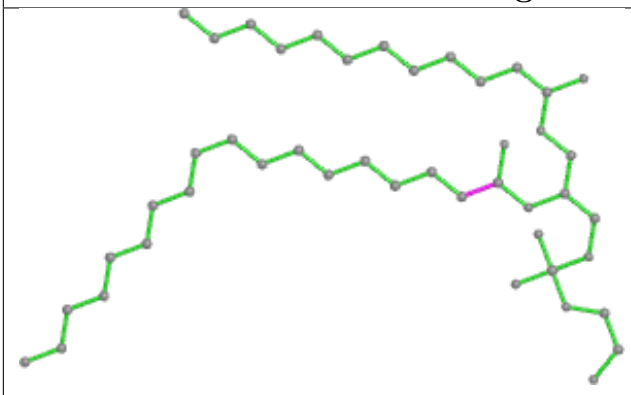


Torsions

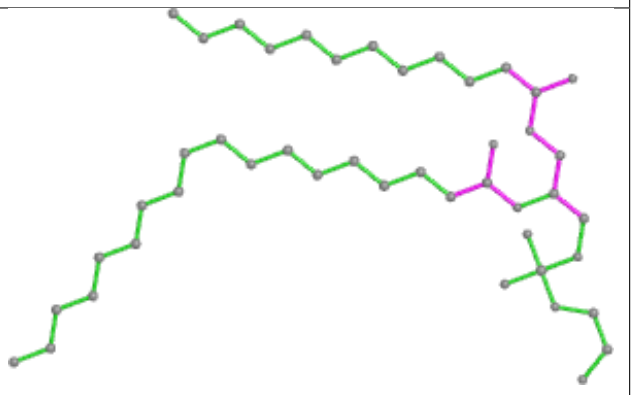


Rings

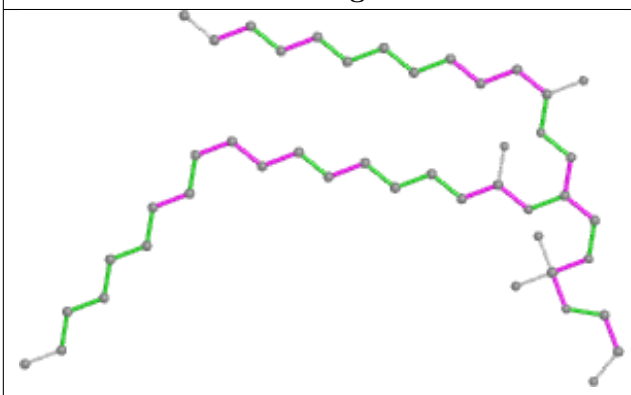
Ligand LOP A 1006



Bond lengths



Bond angles



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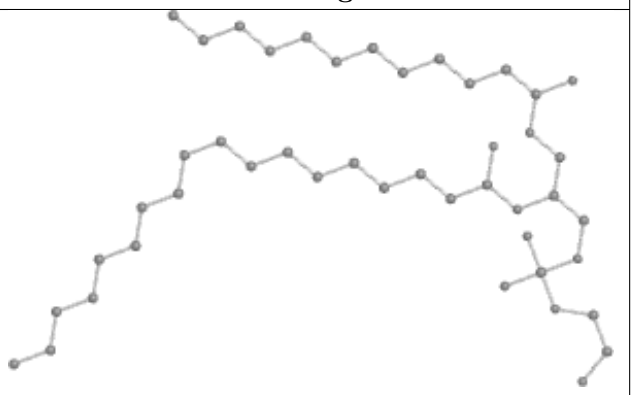
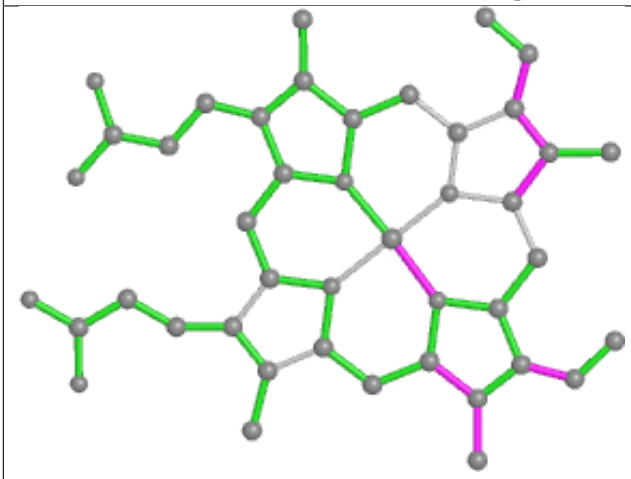


Rings

Ligand HEM K 1002



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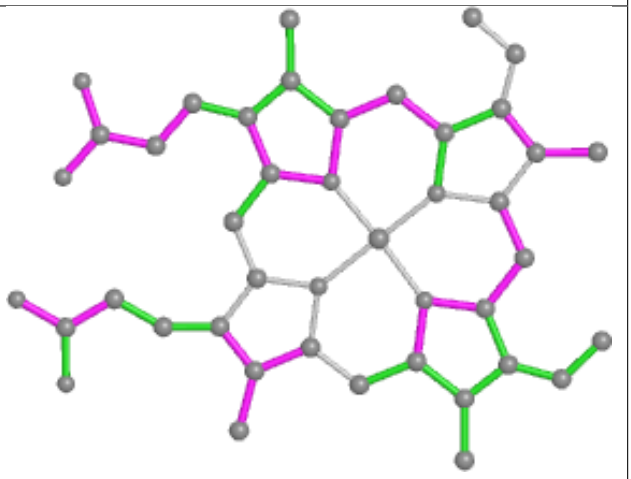
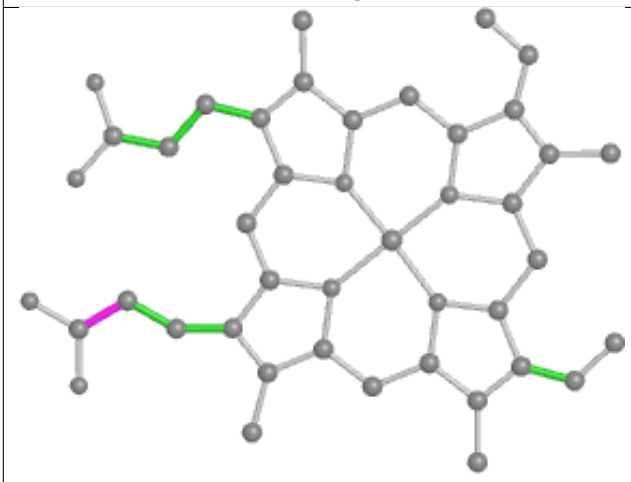
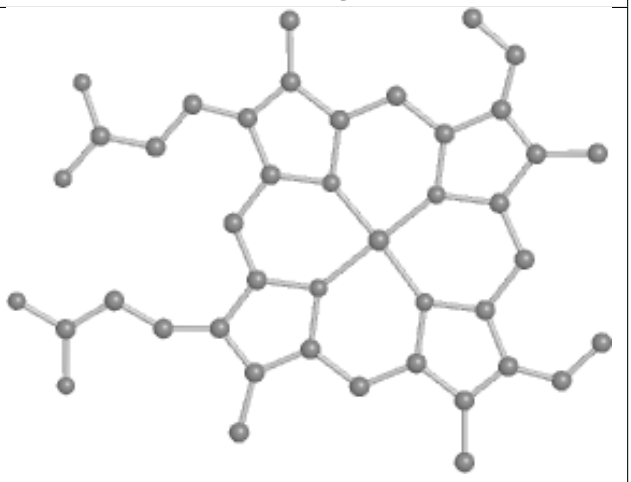


Bond angles

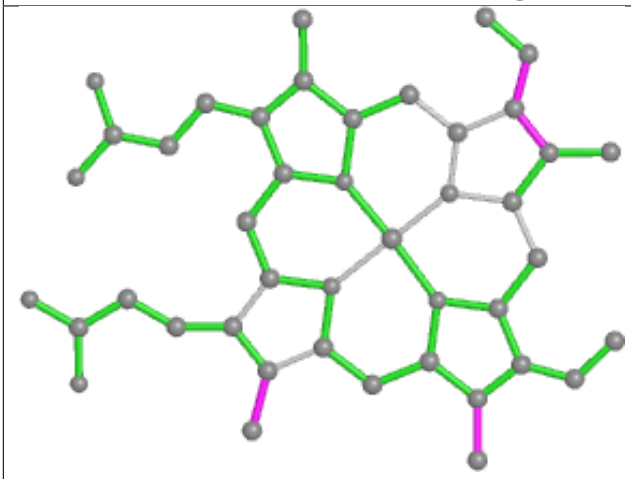


Torsions



Rings

Ligand HEM E 1001



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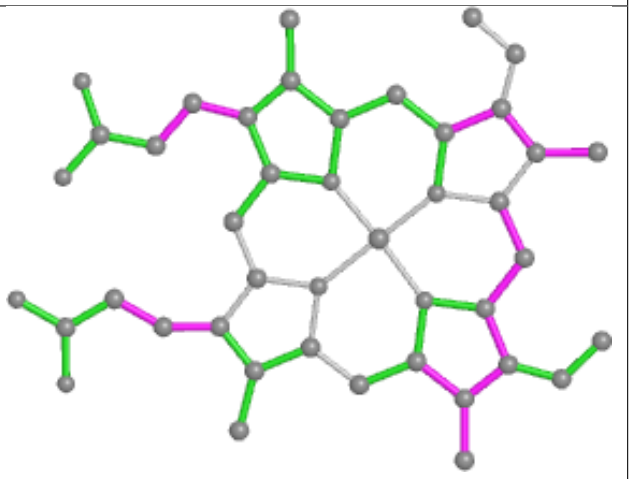
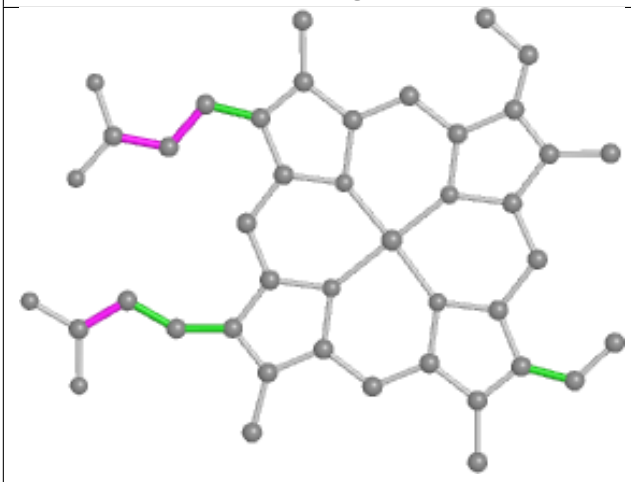


Bond angles



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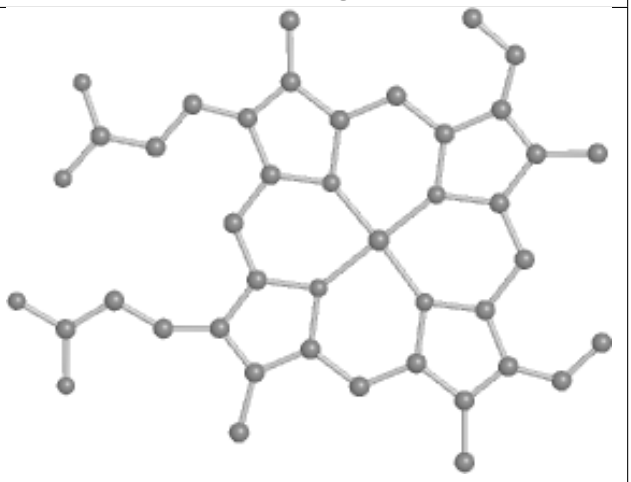
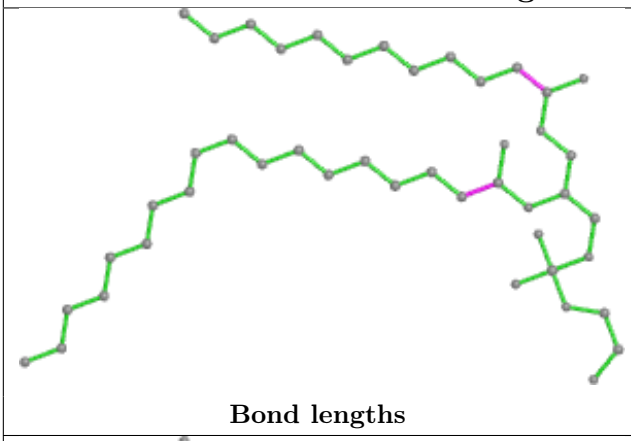


Rings

Ligand LOP E 1005



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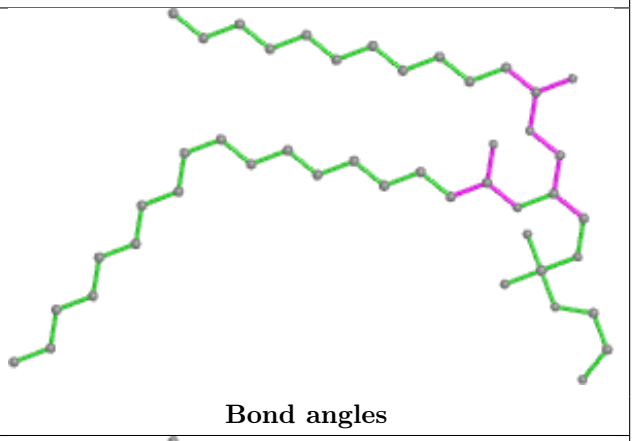

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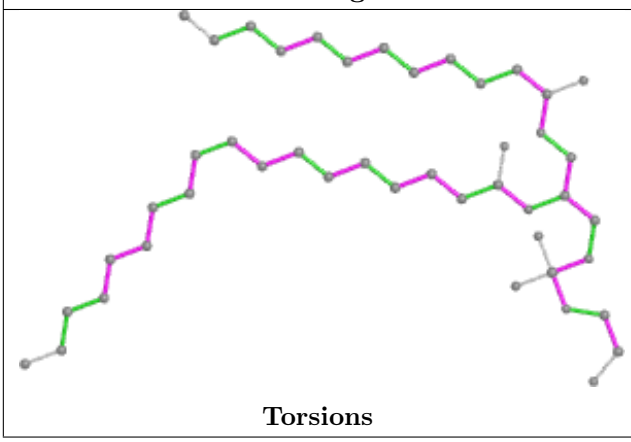

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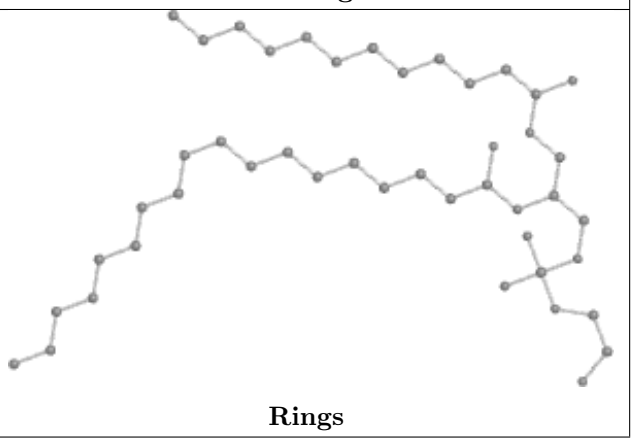
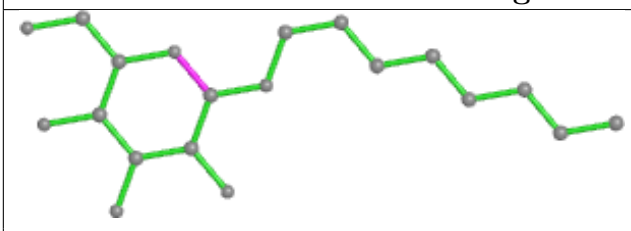
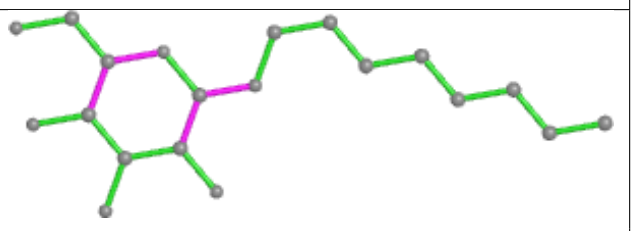


Rings

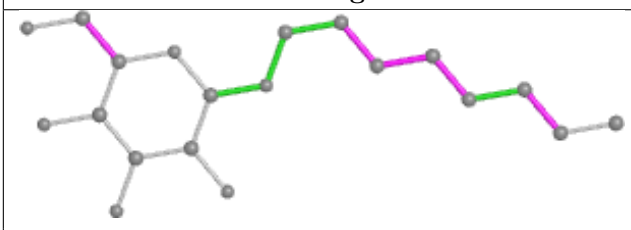
Ligand BOG P 1003



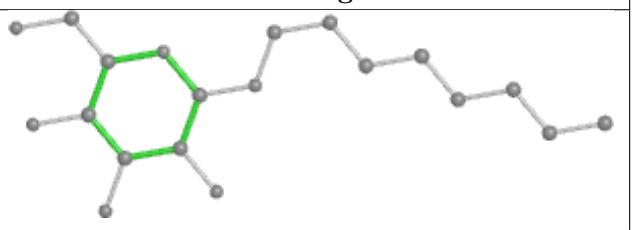
Bond lengths



Bond angles

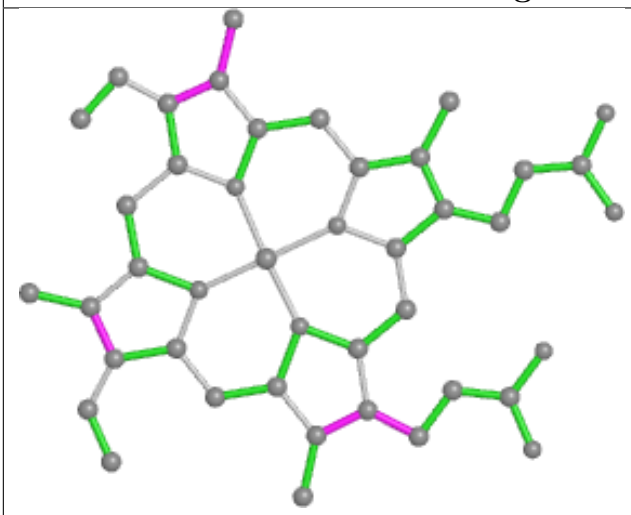


Torsions

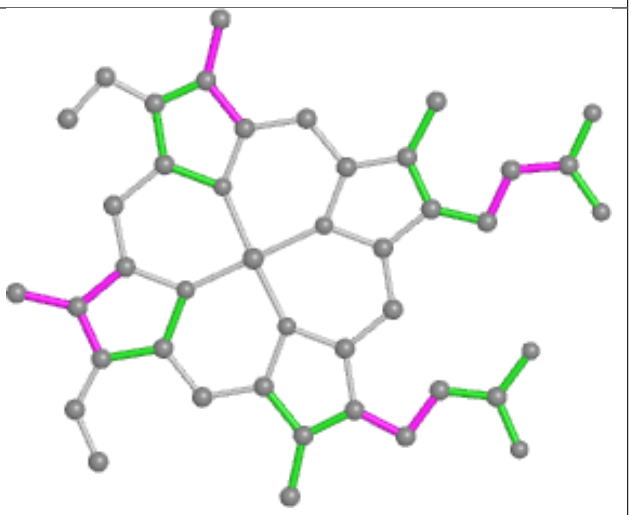


Rings

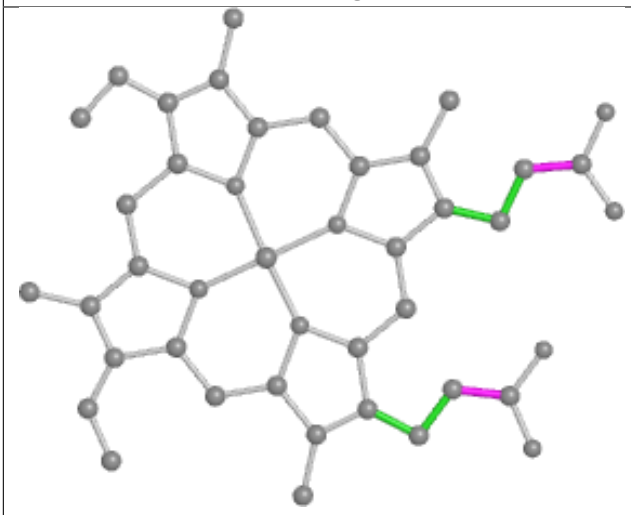
Ligand HEC B 1001



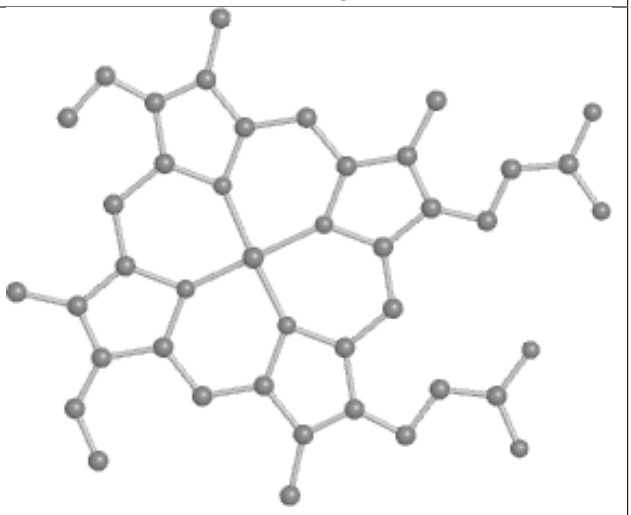
Bond lengths



Bond angles

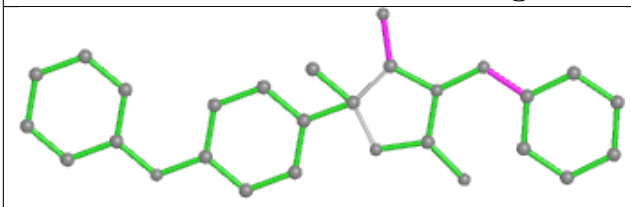


Torsions

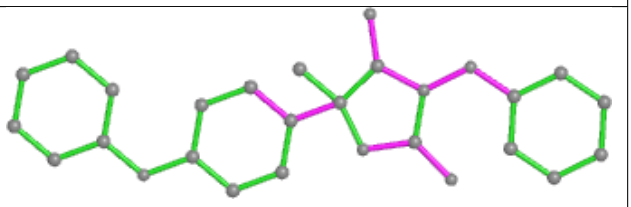


Rings

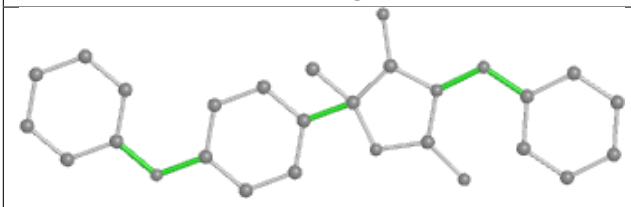
Ligand FMX O 1003



Bond lengths



Bond angles



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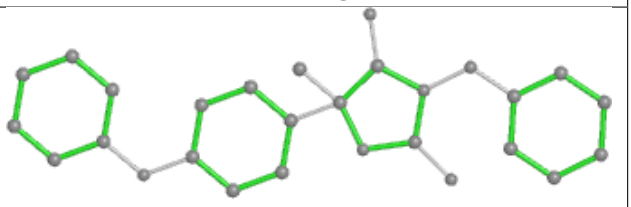
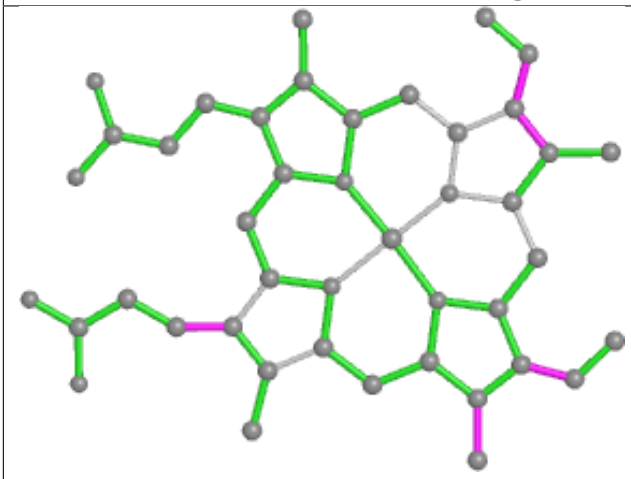
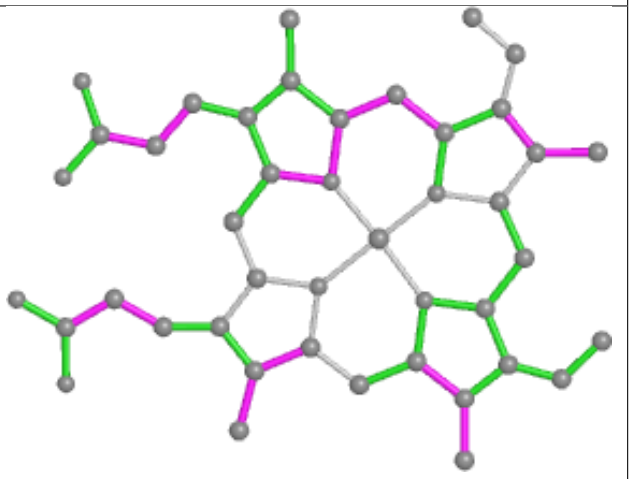


Rings

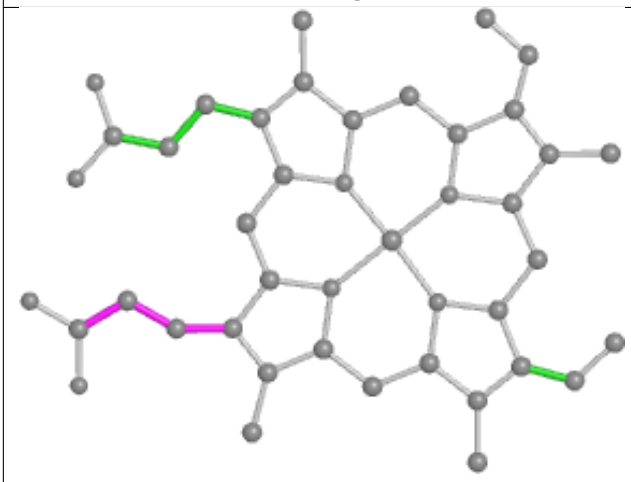
Ligand HEM A 1002



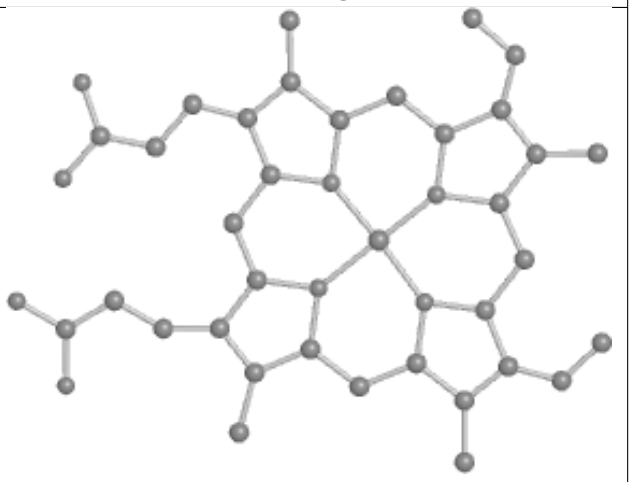
Bond lengths



Bond angles

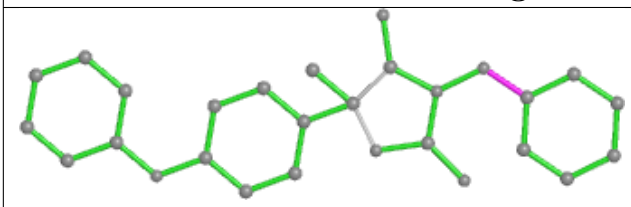


Torsions

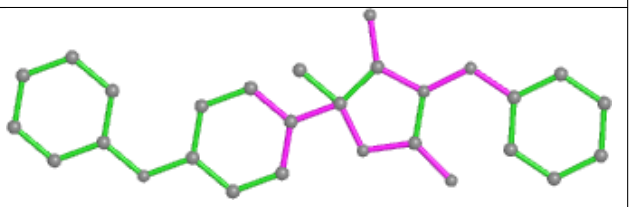


Rings

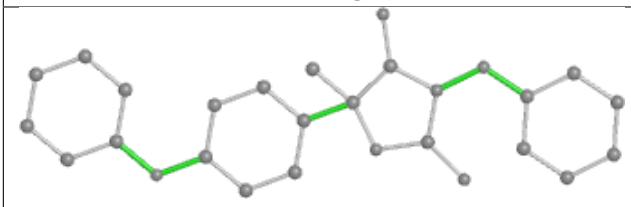
Ligand FMX K 1003



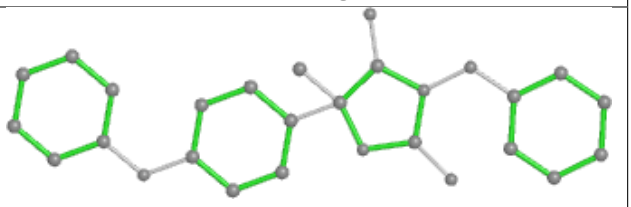
Bond lengths



Bond angles

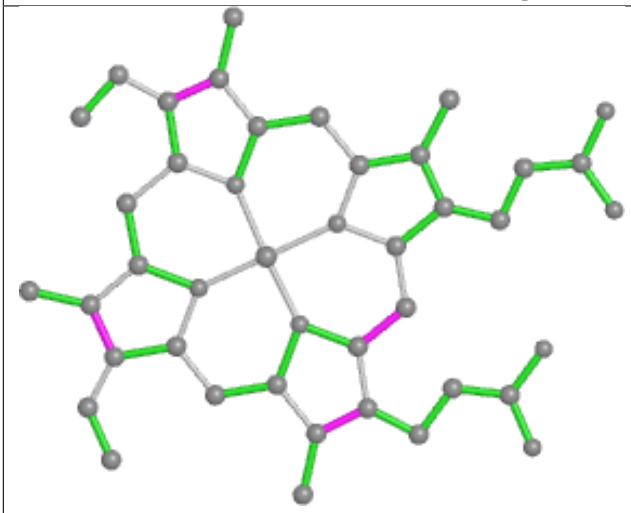


Torsions

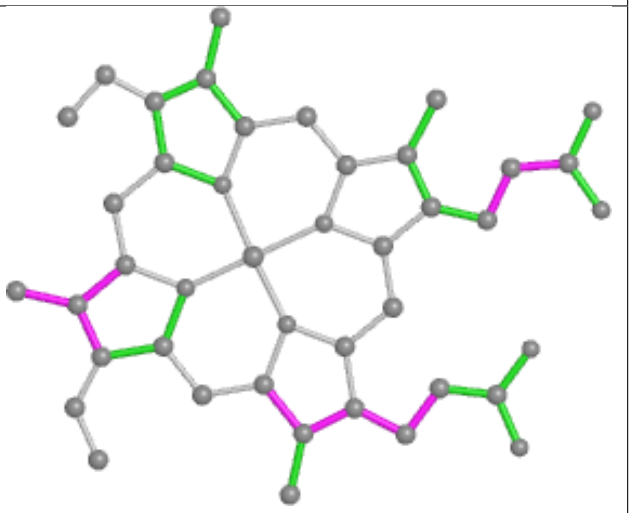


Rings

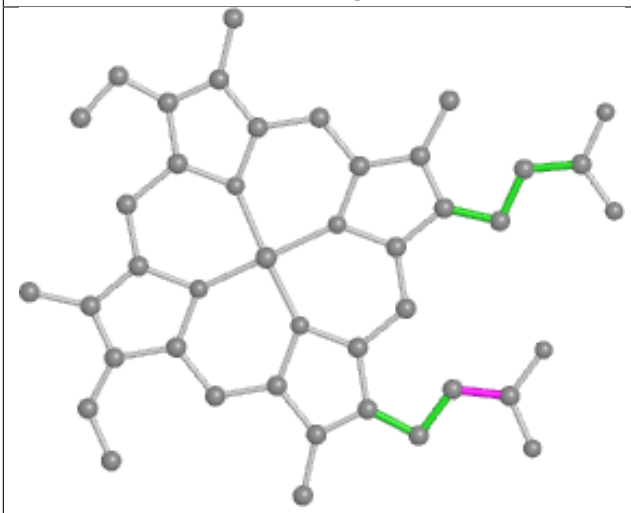
Ligand HEC L 1001



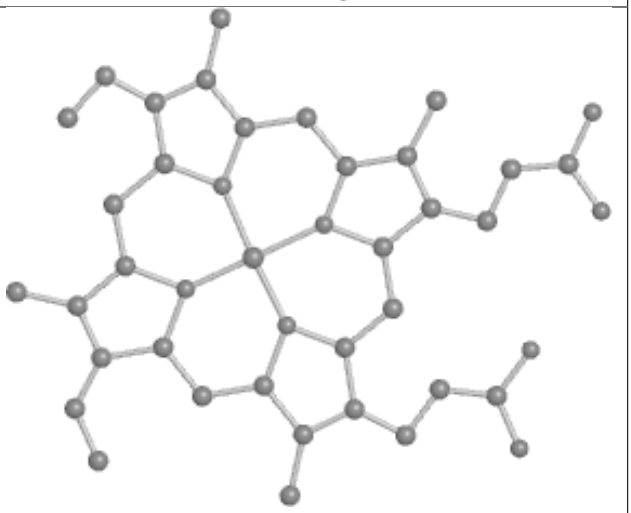
Bond lengths



Bond angles

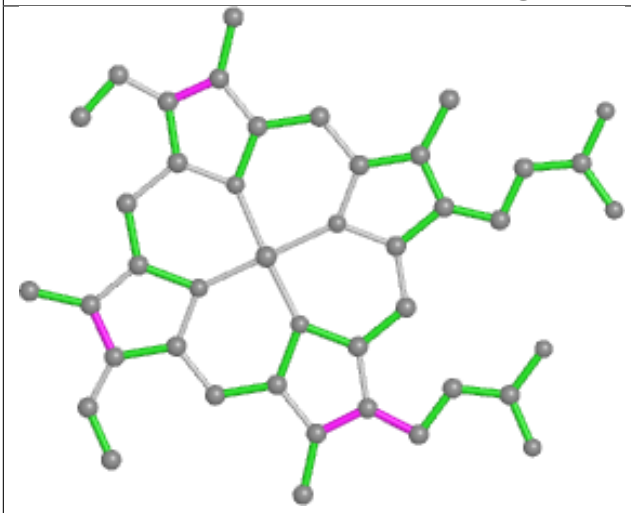


Torsions

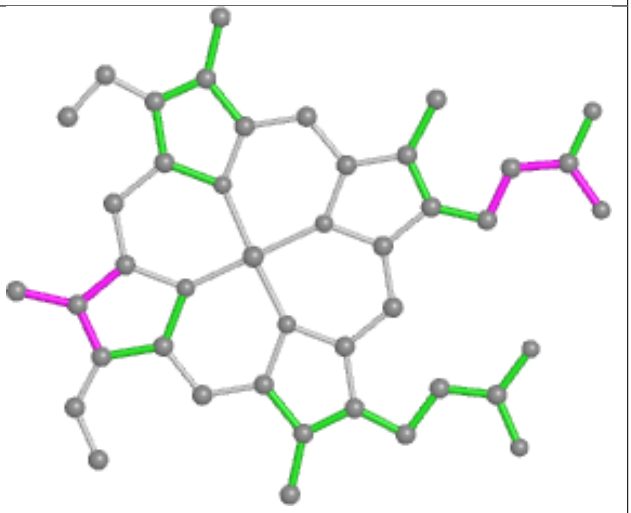


Rings

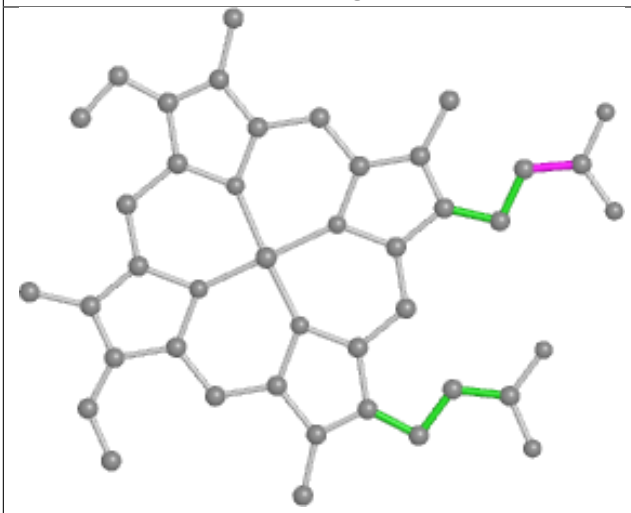
Ligand HEC P 1001



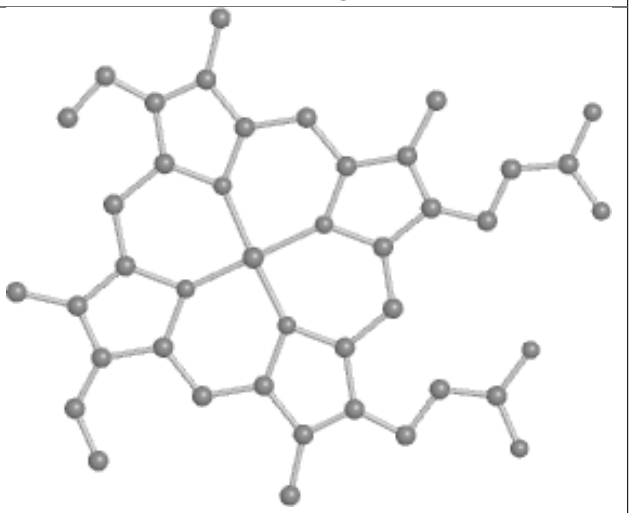
Bond lengths



Bond angles

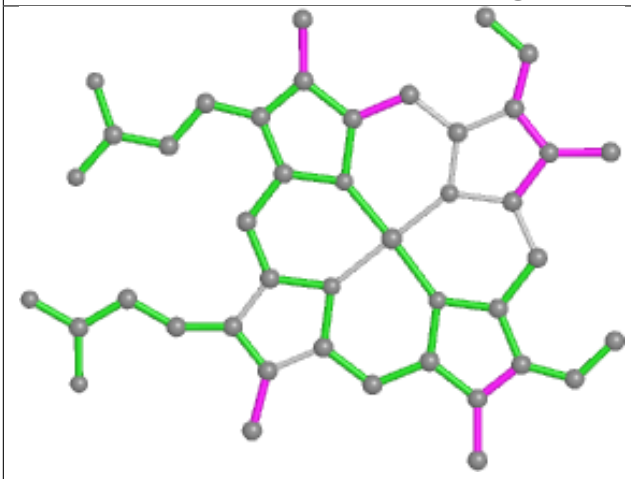


Torsions

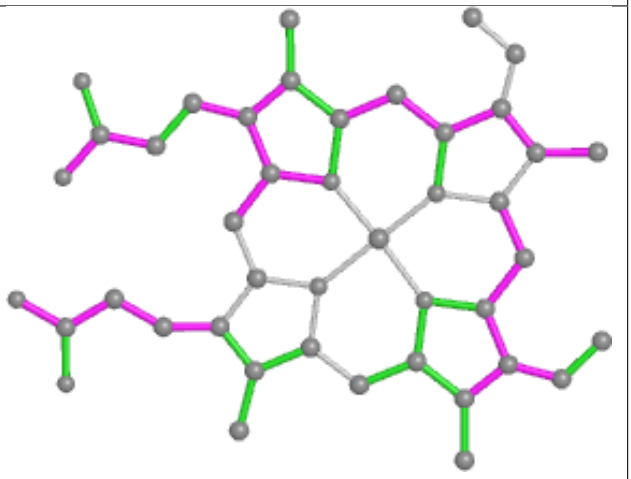


Rings

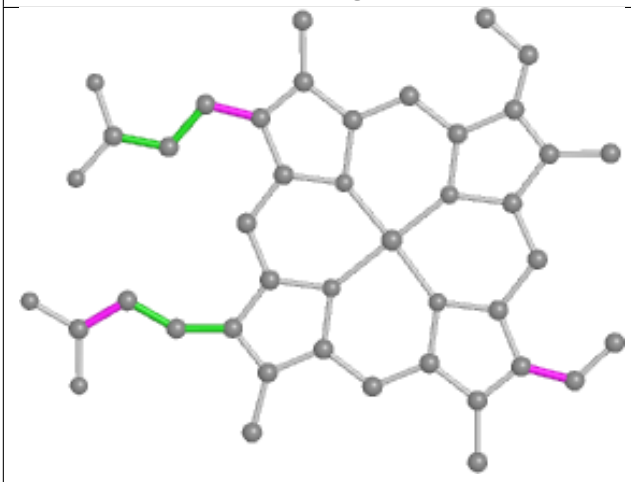
Ligand HEM O 1001



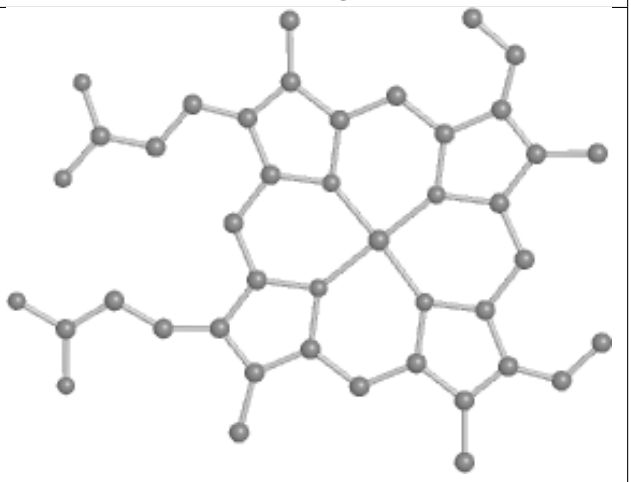
Bond lengths



Bond angles

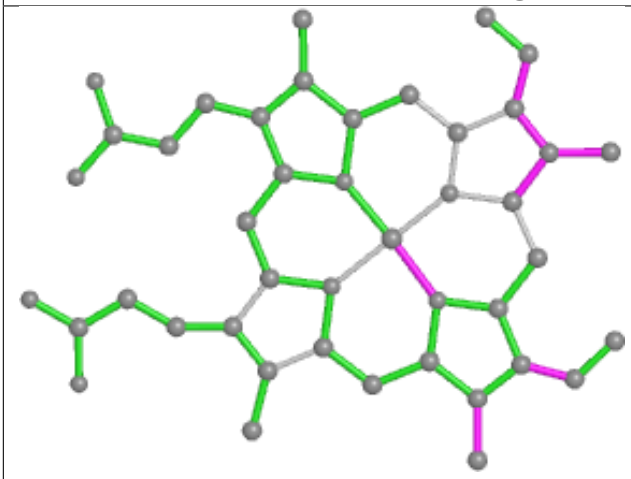


Torsions

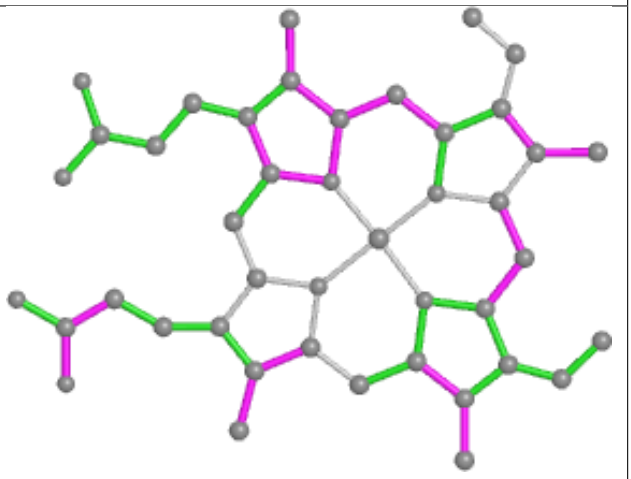


Rings

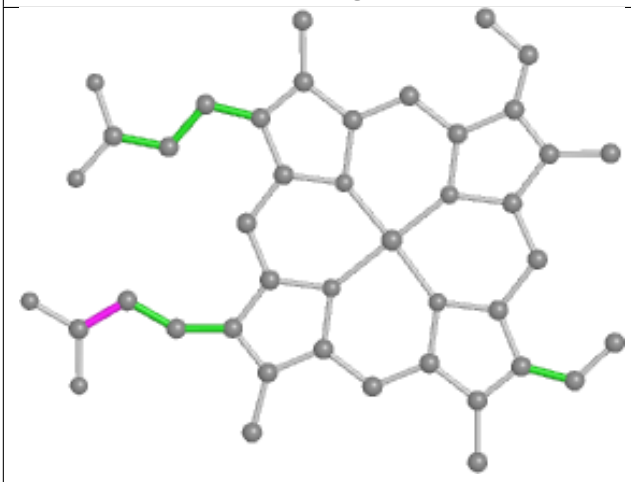
Ligand HEM E 1002



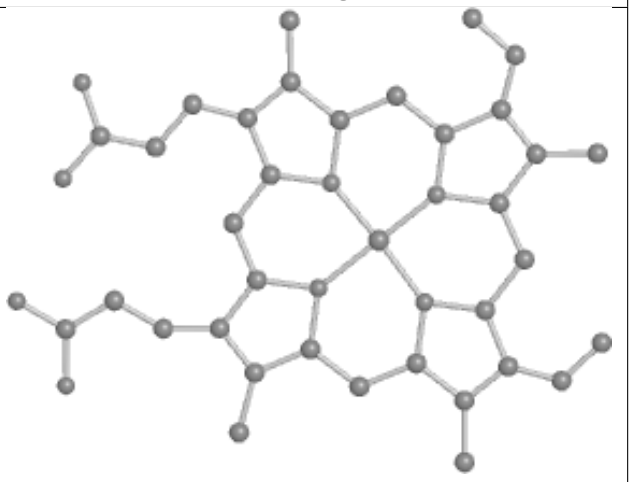
Bond lengths



Bond angles

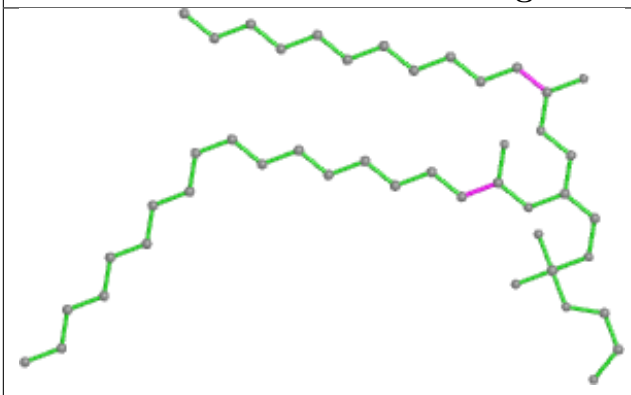


Torsions

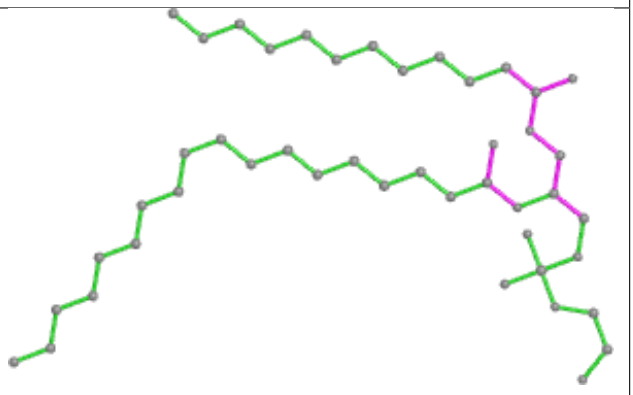


Rings

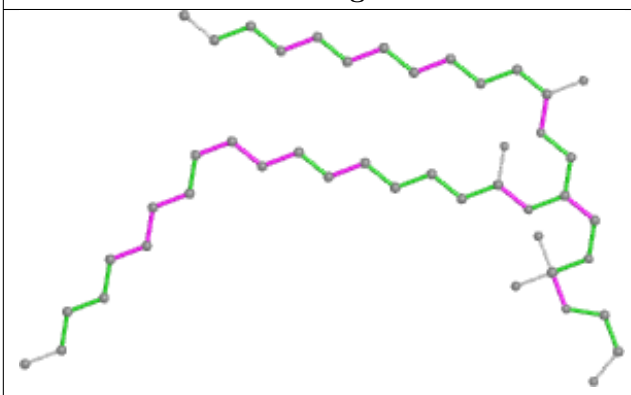
Ligand LOP O 1005



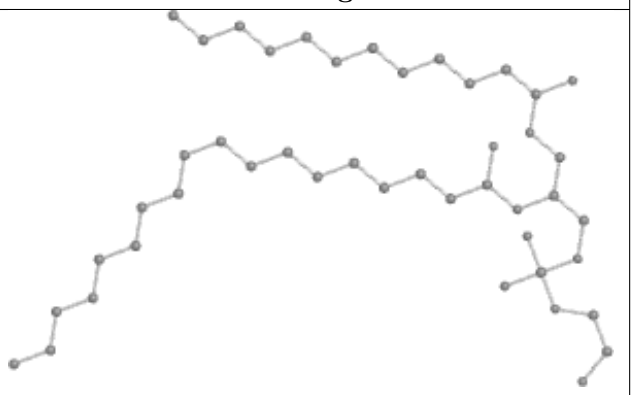
Bond lengths



Bond angles

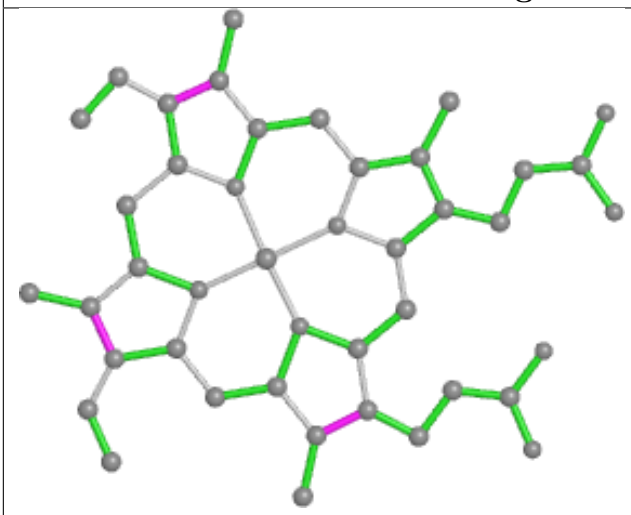


Torsions

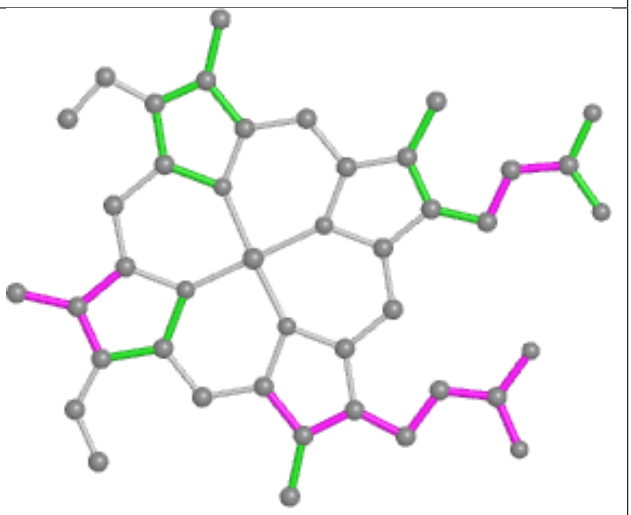


Rings

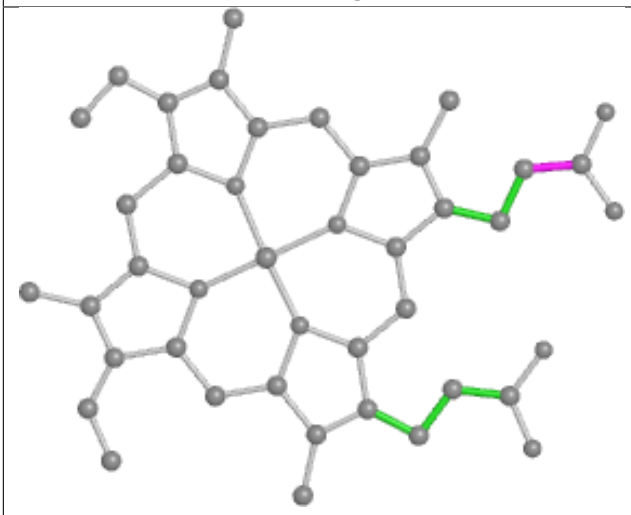
Ligand HEC F 1001



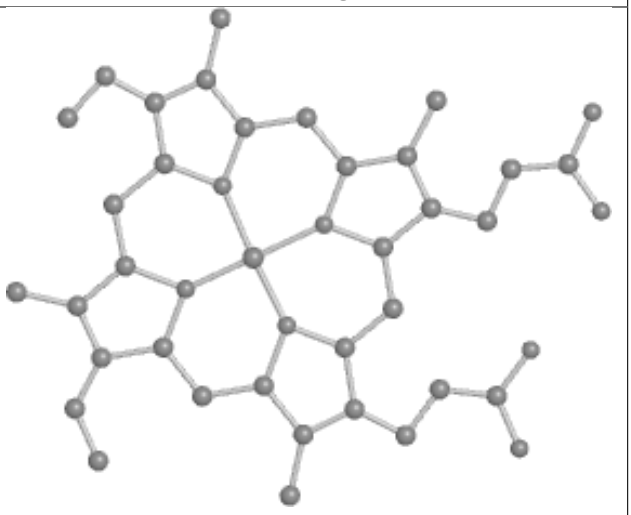
Bond lengths



Bond angles

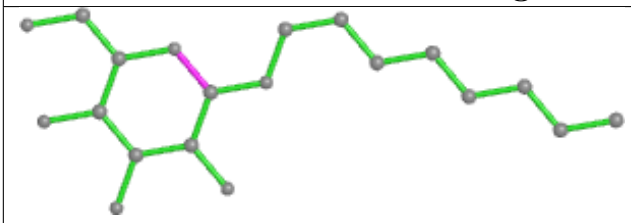


Torsions

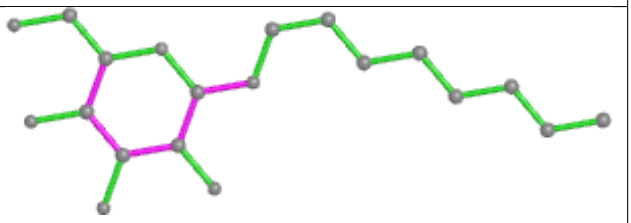


Rings

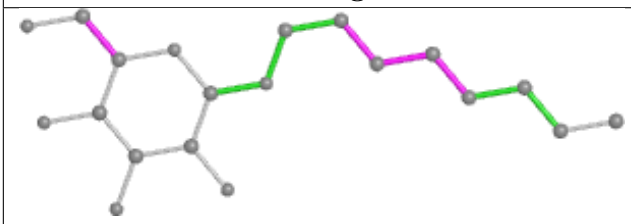
Ligand BOG B 1003



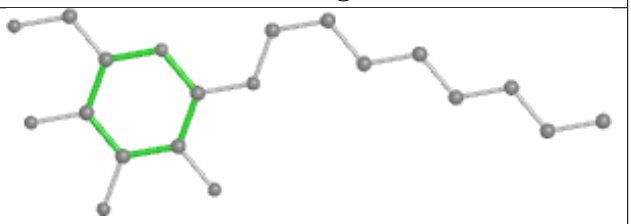
Bond lengths



Bond angles

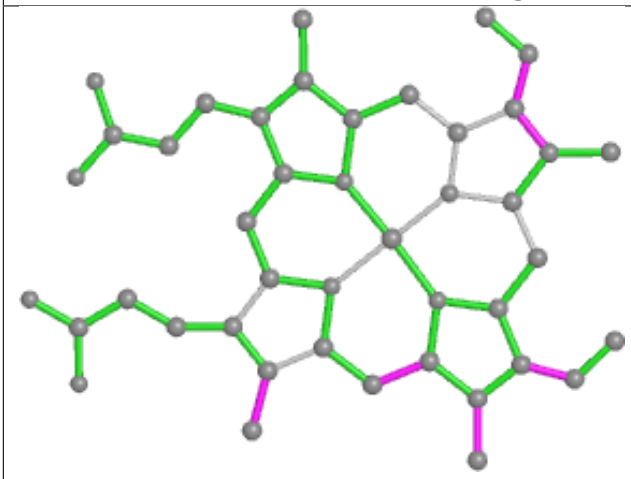


Torsions

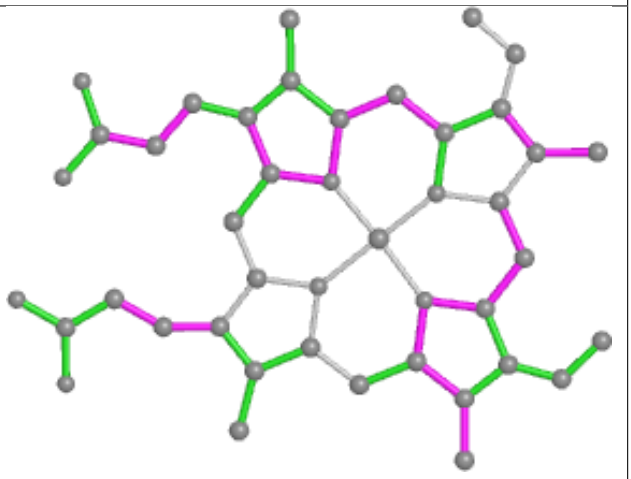


Rings

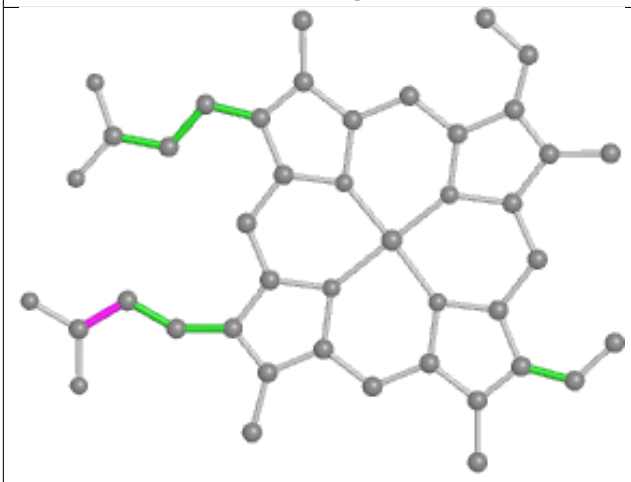
Ligand HEM O 1002



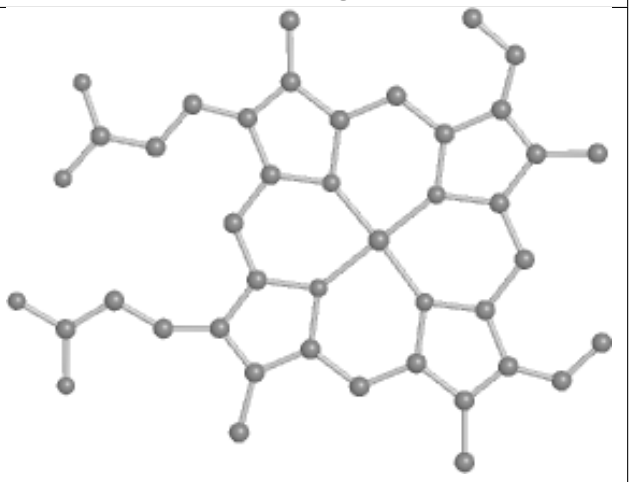
Bond lengths



Bond angles

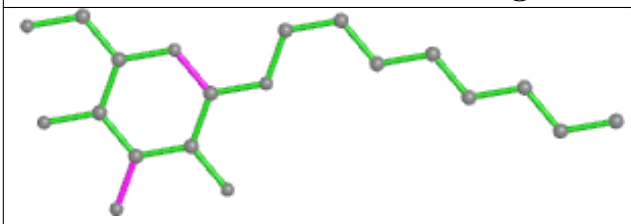


Torsions

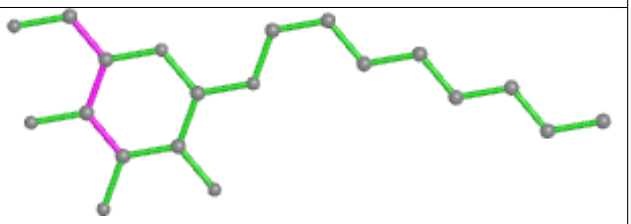


Rings

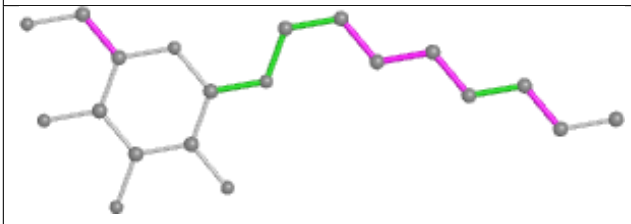
Ligand BOG K 1007



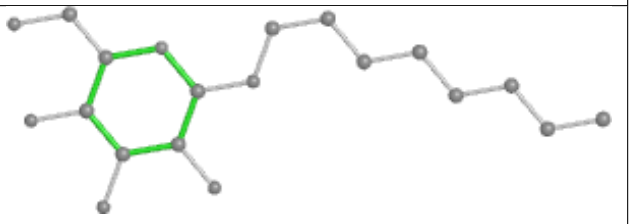
Bond lengths



Bond angles

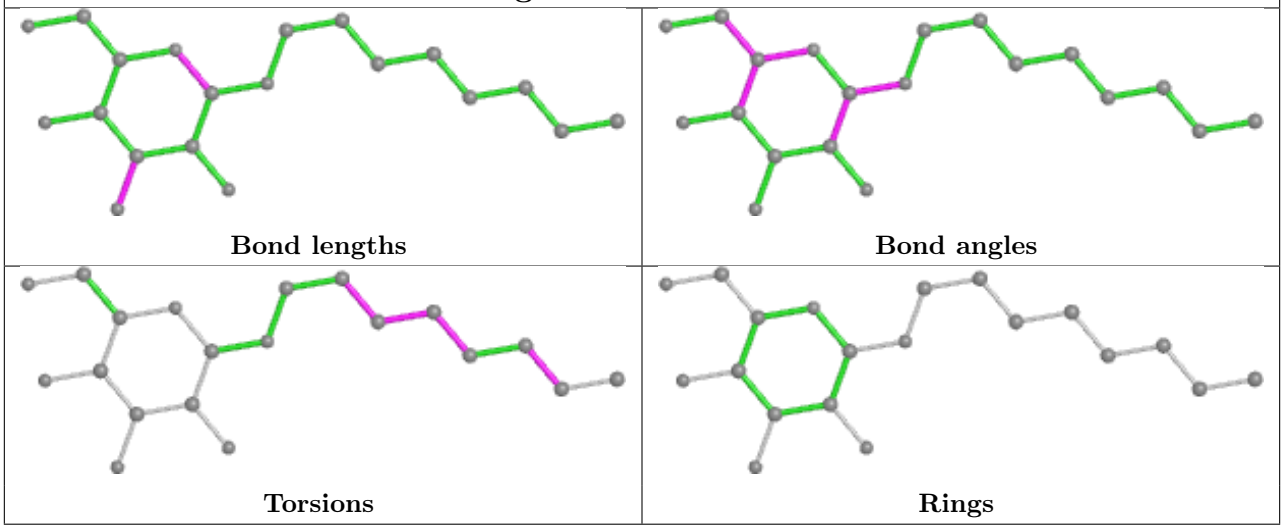


Torsions

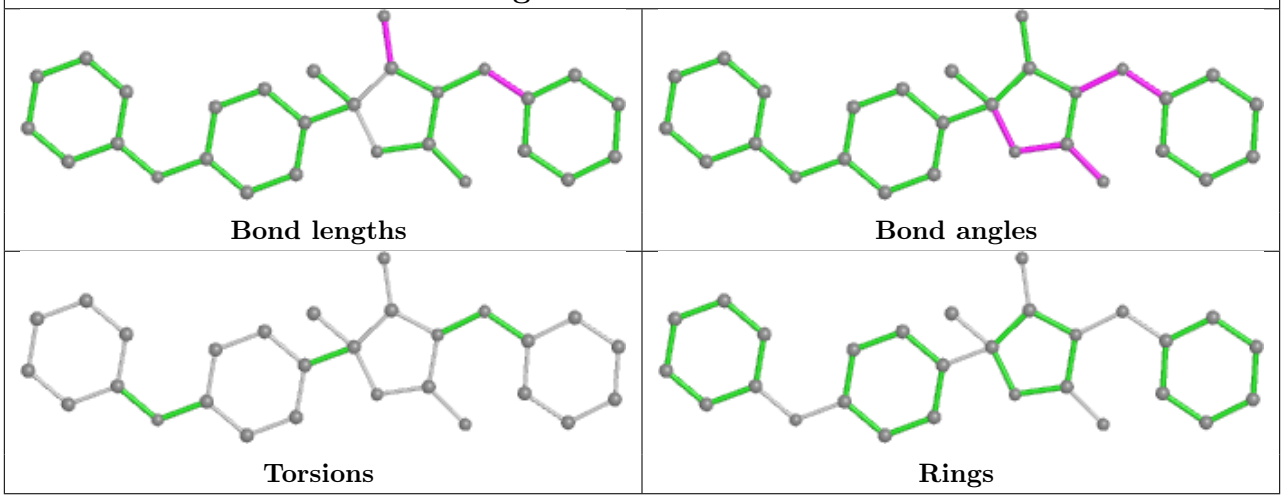


Rings

Ligand BOG F 1003



Ligand FMX E 1003



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	429/445 (96%)	0.14	16 (3%) 41 25	50, 60, 93, 184	0
1	E	429/445 (96%)	0.19	21 (4%) 29 17	34, 62, 102, 156	0
1	K	429/445 (96%)	-0.08	13 (3%) 50 31	20, 50, 89, 150	0
1	O	429/445 (96%)	0.13	28 (6%) 18 10	27, 62, 96, 168	0
2	B	256/272 (94%)	0.22	21 (8%) 11 5	48, 68, 113, 174	0
2	F	256/272 (94%)	0.56	37 (14%) 2 1	45, 77, 132, 164	0
2	L	256/272 (94%)	0.20	17 (6%) 18 9	36, 61, 113, 145	0
2	P	256/272 (94%)	0.64	37 (14%) 2 1	42, 82, 124, 169	0
3	C	179/187 (95%)	0.93	25 (13%) 2 1	61, 97, 150, 212	0
3	G	179/187 (95%)	0.47	17 (9%) 8 4	46, 86, 131, 168	0
3	M	179/187 (95%)	0.64	21 (11%) 4 2	41, 84, 126, 154	0
3	Q	179/187 (95%)	0.63	19 (10%) 6 3	54, 95, 139, 167	0
All	All	3456/3616 (95%)	0.31	272 (7%) 12 6	20, 68, 120, 212	0

The worst 5 of 272 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	9	GLY	10.9
3	C	10	THR	10.1
2	F	2	GLY	9.4
3	C	9	GLY	8.8
2	L	2	GLY	8.6

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

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
10	BOG	P	1003	20/20	0.79	0.31	50,67,85,90	0
8	LOP	E	1005	45/45	0.81	0.30	71,92,108,113	0
10	BOG	B	1003	20/20	0.84	0.34	50,63,70,73	0
8	LOP	O	1005	45/45	0.84	0.26	51,84,107,118	0
10	BOG	F	1003	20/20	0.87	0.31	48,65,80,81	0
8	LOP	A	1006	45/45	0.88	0.27	56,76,90,94	0
8	LOP	K	1006	45/45	0.89	0.23	49,71,92,103	0
10	BOG	K	1007	20/20	0.90	0.29	39,60,75,75	0
6	ASC	O	1004	12/12	0.90	0.22	25,43,59,63	0
7	SR	A	1005	1/1	0.91	0.04	148,148,148,148	0
6	ASC	K	1004	12/12	0.93	0.16	39,48,57,60	0
6	ASC	E	1004	12/12	0.94	0.18	52,56,71,76	0
4	HEM	A	1001	43/43	0.94	0.30	51,52,62,62	0
5	FMX	E	1003	28/28	0.94	0.20	53,67,77,79	0
5	FMX	K	1003	28/28	0.95	0.20	47,58,69,78	0
5	FMX	O	1003	28/28	0.95	0.19	52,64,75,81	0
6	ASC	A	1004	12/12	0.95	0.16	35,46,56,62	0
4	HEM	E	1001	43/43	0.95	0.26	46,52,69,82	0
9	HEC	P	1001	43/43	0.95	0.21	63,71,89,95	0
4	HEM	E	1002	43/43	0.95	0.32	53,64,77,77	0
5	FMX	A	1003	28/28	0.95	0.19	52,62,72,77	0
4	HEM	A	1002	43/43	0.95	0.28	54,58,70,70	0
7	SR	F	1002	1/1	0.95	0.05	111,111,111,111	0
4	HEM	K	1002	43/43	0.96	0.23	30,49,74,78	0
9	HEC	B	1001	43/43	0.96	0.19	53,57,69,70	0
9	HEC	F	1001	43/43	0.96	0.20	61,69,82,90	0
9	HEC	L	1001	43/43	0.96	0.19	34,52,66,72	0
7	SR	K	1005	1/1	0.96	0.03	110,110,110,110	0
7	SR	P	1002	1/1	0.96	0.06	109,109,109,109	0
4	HEM	O	1001	43/43	0.96	0.24	33,50,66,72	0
4	HEM	O	1002	43/43	0.96	0.28	46,56,70,73	0
4	HEM	K	1001	43/43	0.96	0.26	40,49,65,71	0

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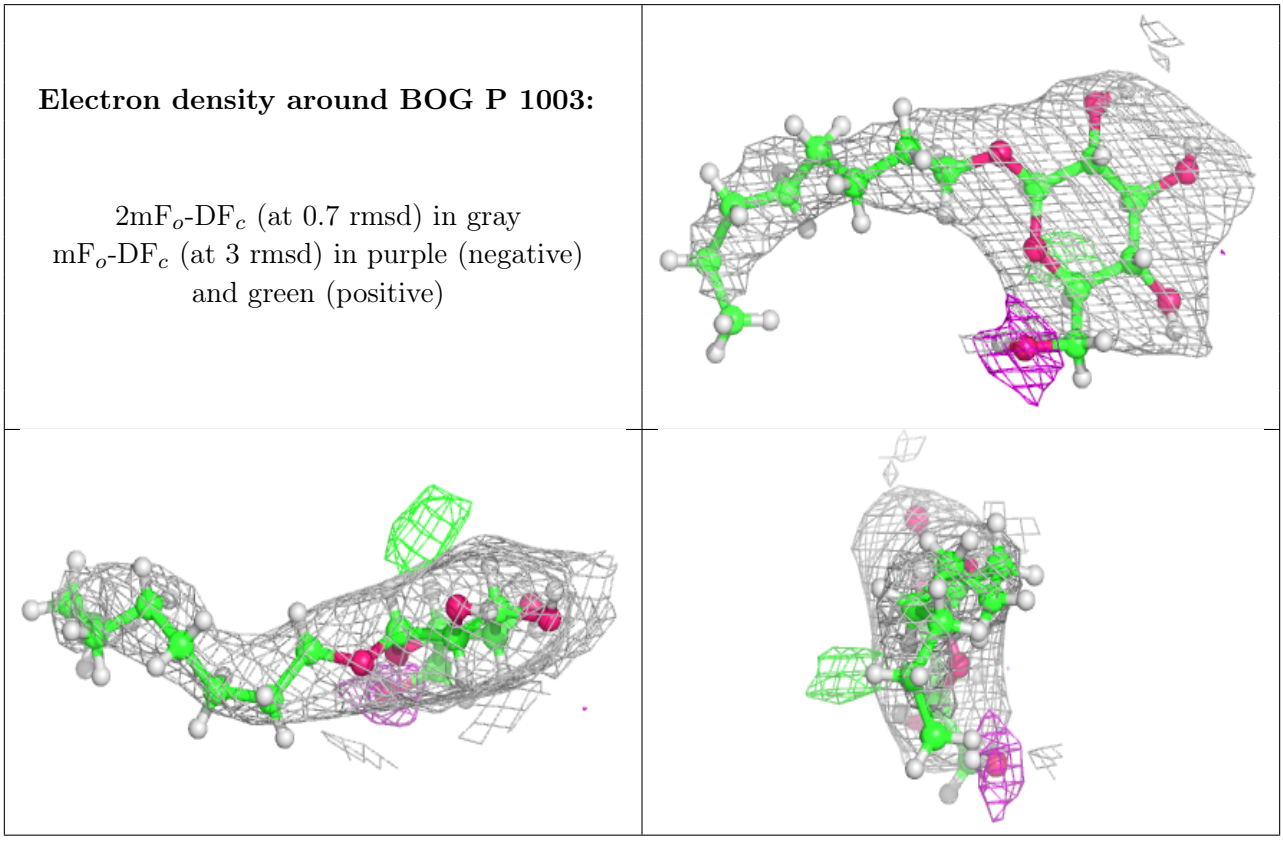
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	FES	M	1001	4/4	0.96	0.17	64,65,65,65	0
7	SR	B	1002	1/1	0.97	0.07	96,96,96,96	0
11	FES	C	1001	4/4	0.99	0.23	82,82,83,87	0
11	FES	G	1001	4/4	0.99	0.22	59,63,65,65	0
7	SR	L	1002	1/1	0.99	0.06	88,88,88,88	0
11	FES	Q	1001	4/4	0.99	0.24	67,70,72,73	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.

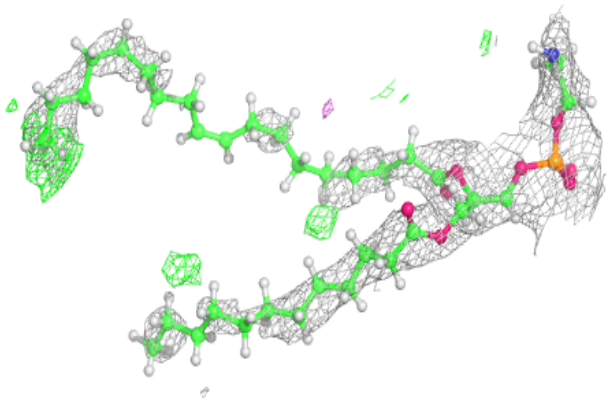
Electron density around BOG P 1003:

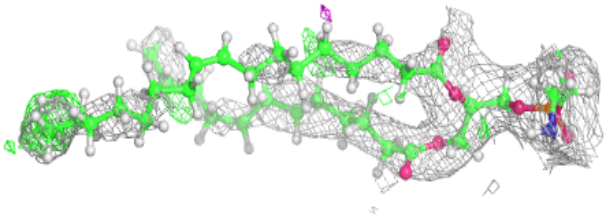
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

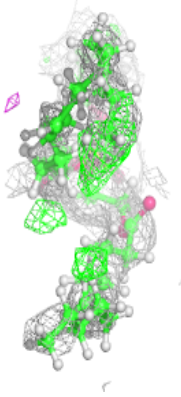


Electron density around LOP E 1005:

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

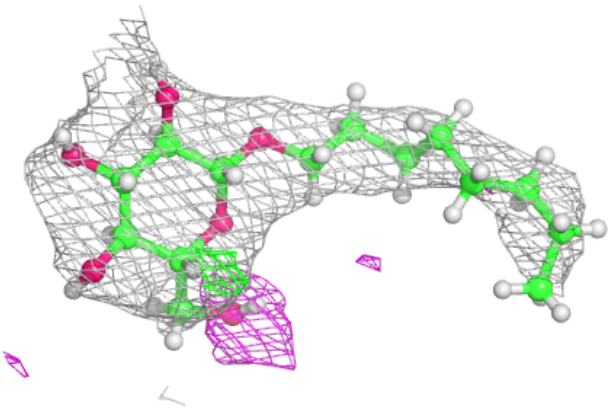


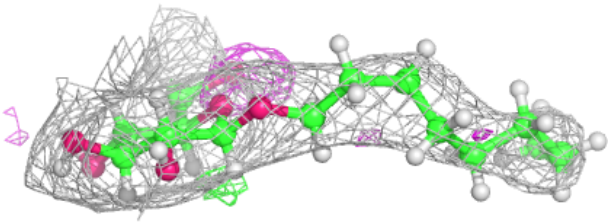


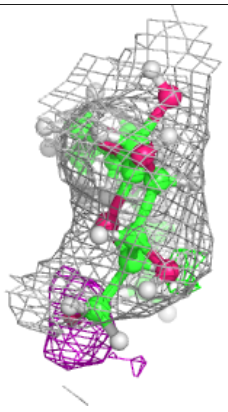


Electron density around BOG B 1003:

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

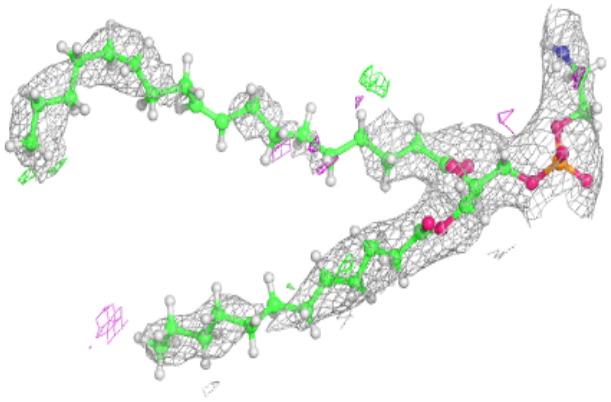


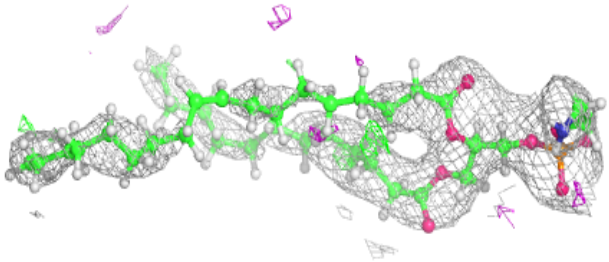


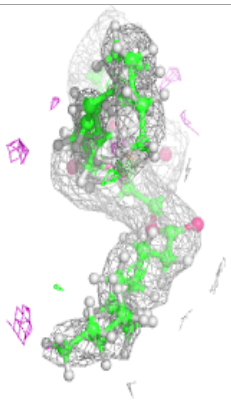


Electron density around LOP O 1005:

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

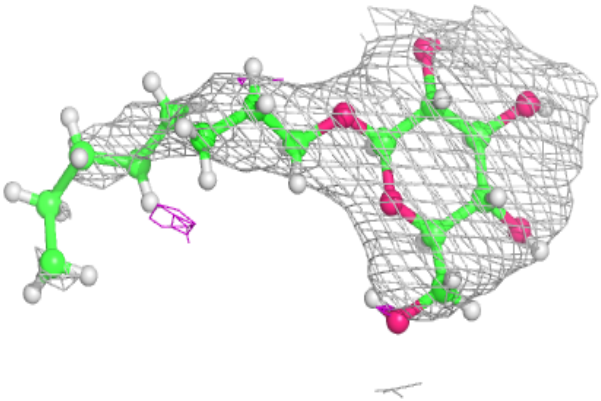


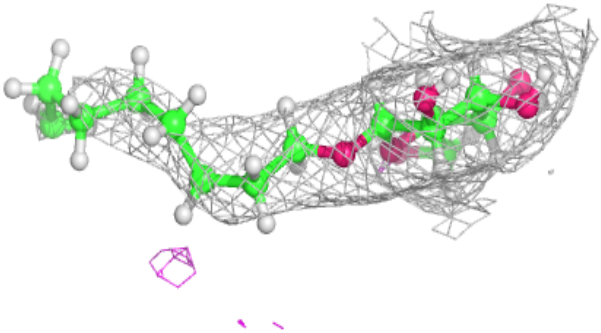


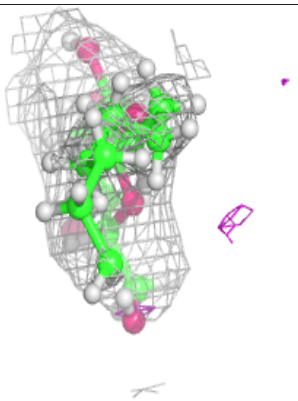


Electron density around BOG F 1003:

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

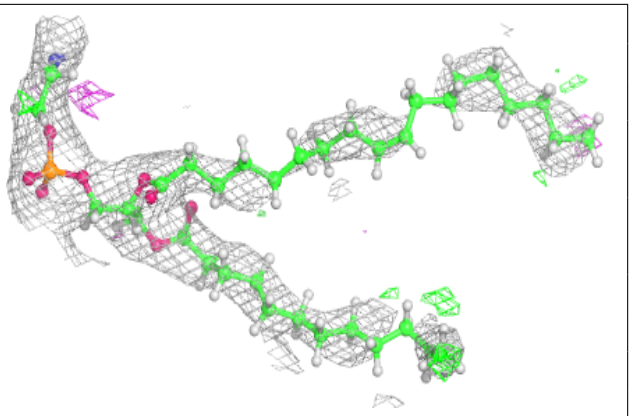


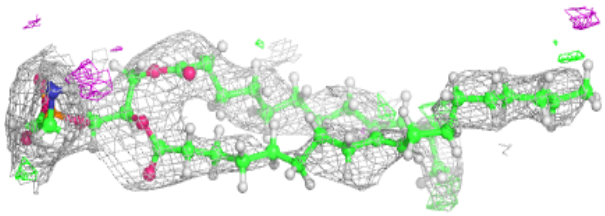




Electron density around LOP A 1006:

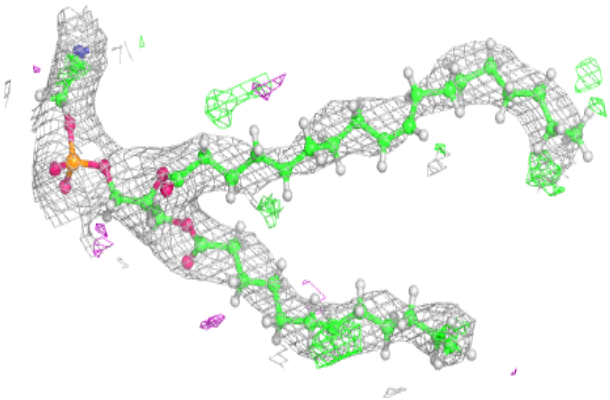
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

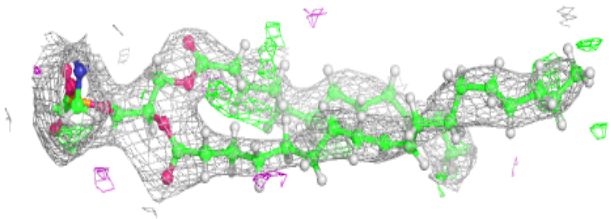


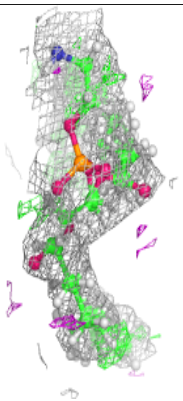


Electron density around LOP K 1006:

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

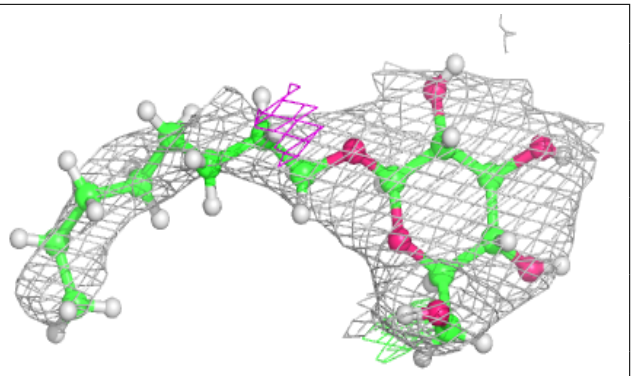


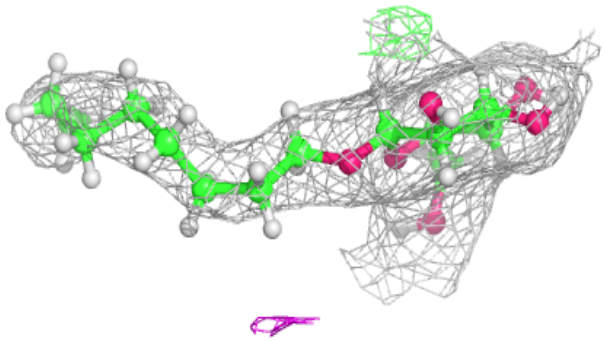


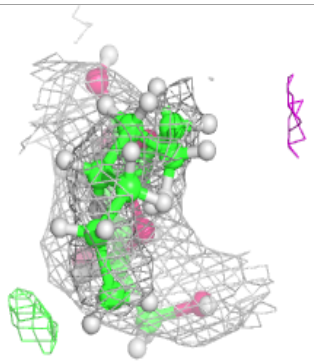


Electron density around BOG K 1007:

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

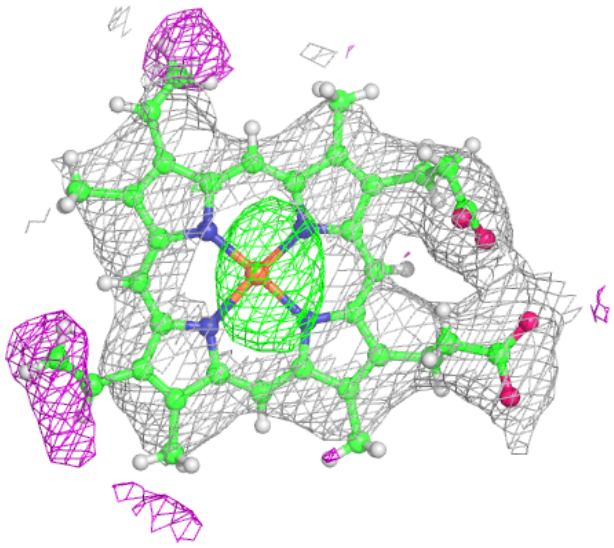


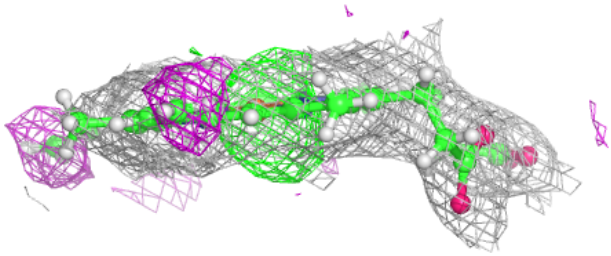


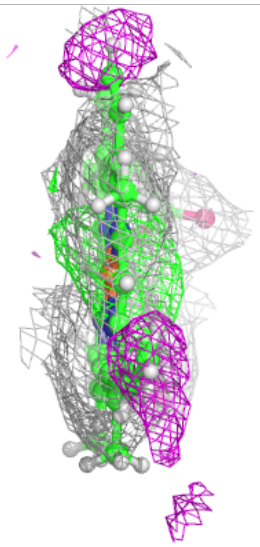


Electron density around HEM A 1001:

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

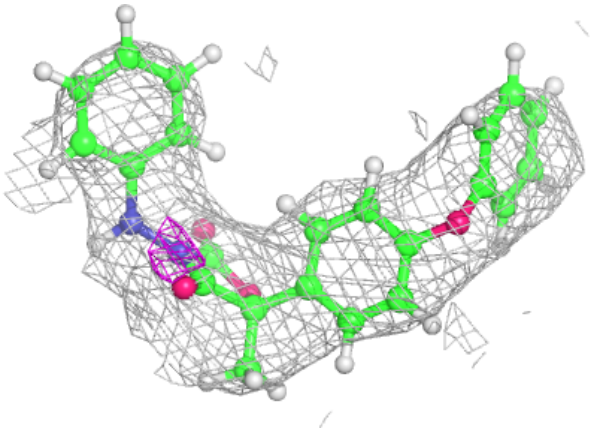


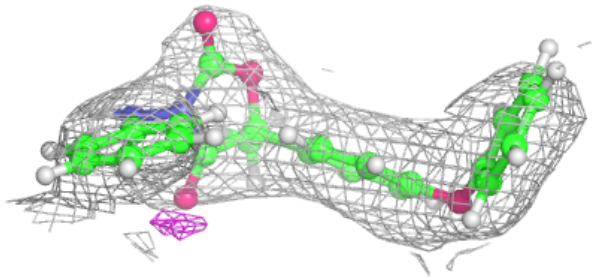


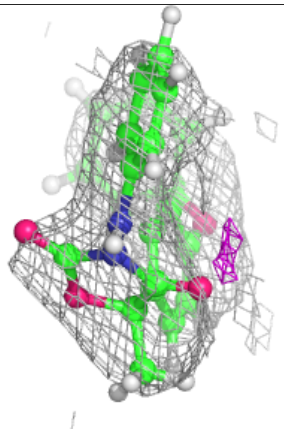


Electron density around FMX E 1003:

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

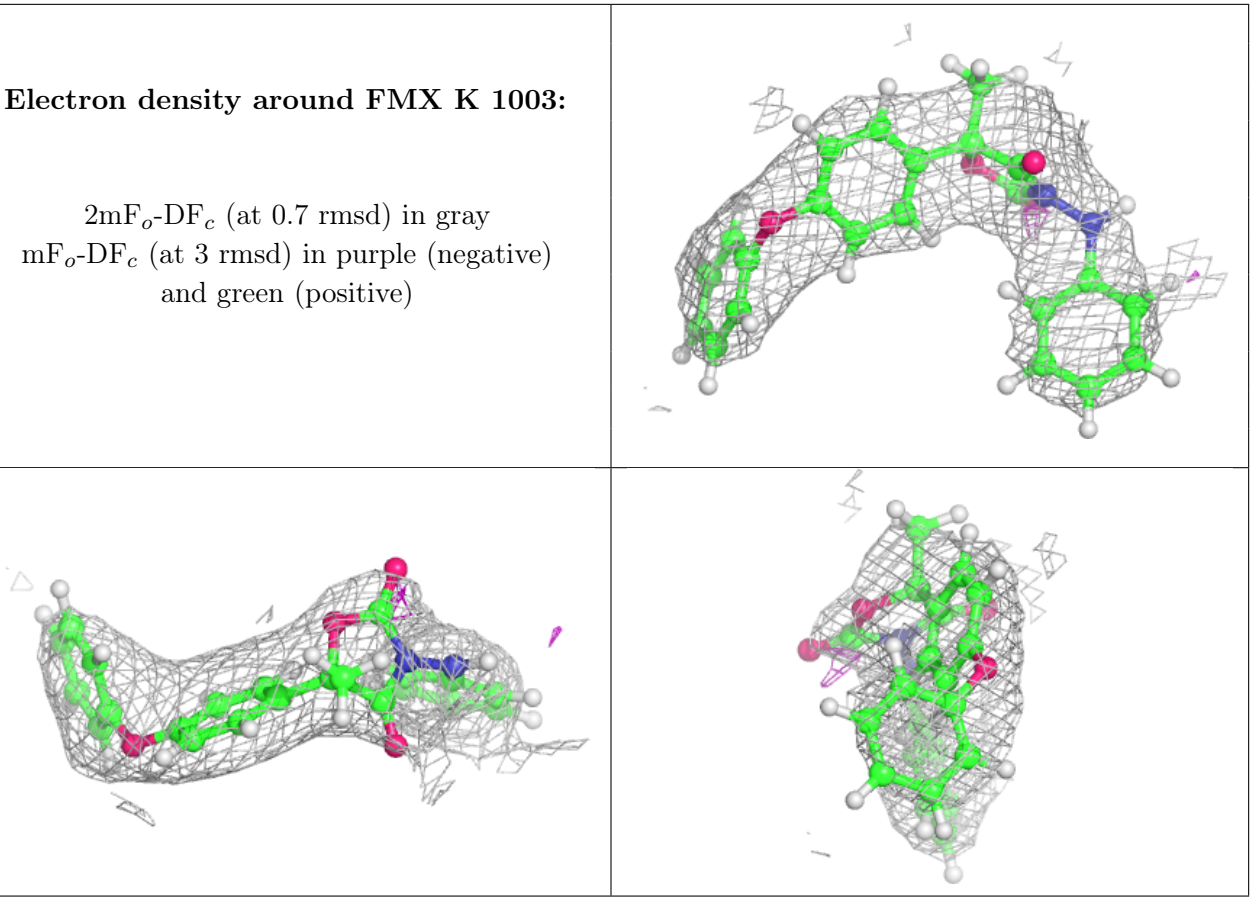






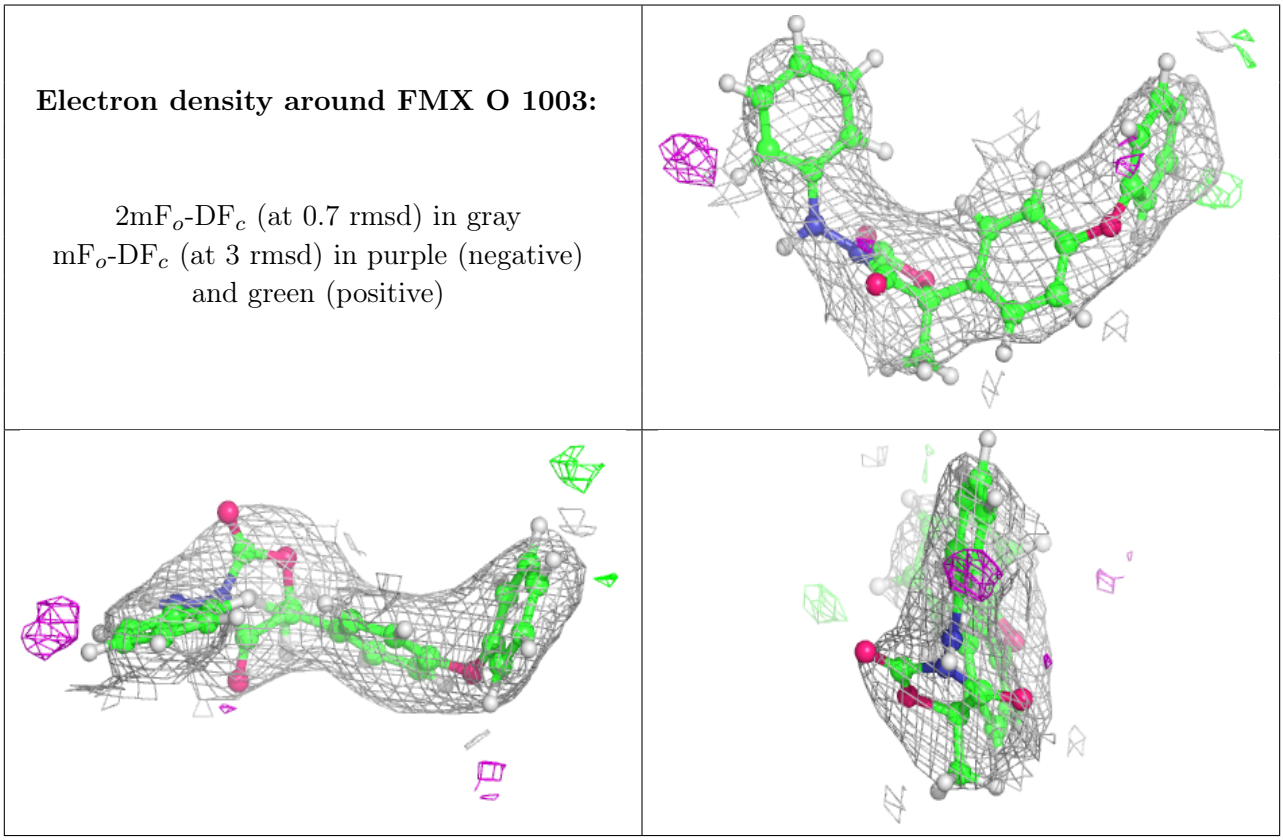
Electron density around FMX K 1003:

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



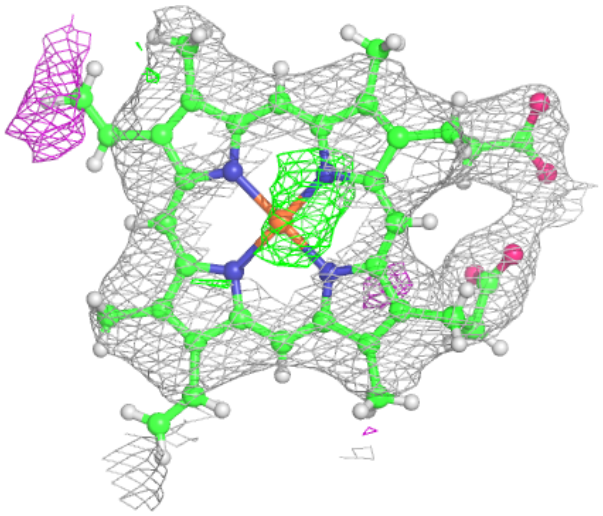
Electron density around FMX O 1003:

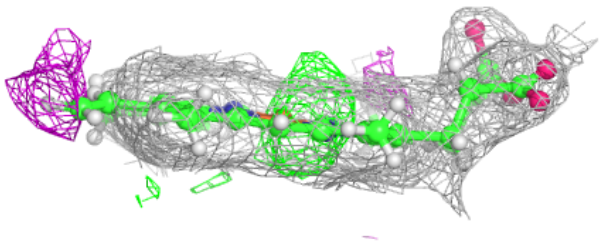
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

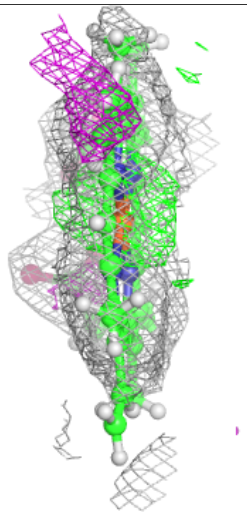


Electron density around HEM E 1001:

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

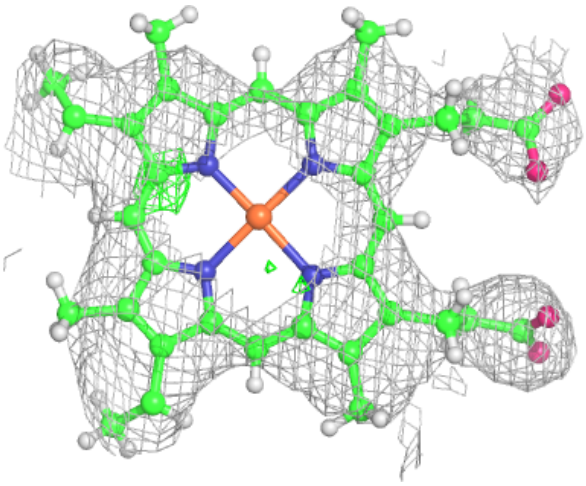


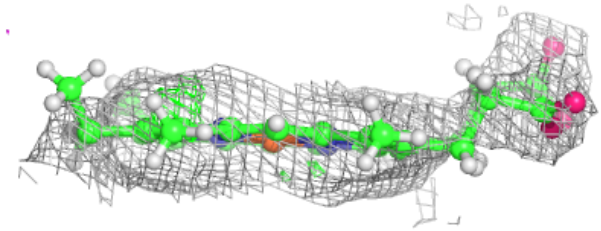


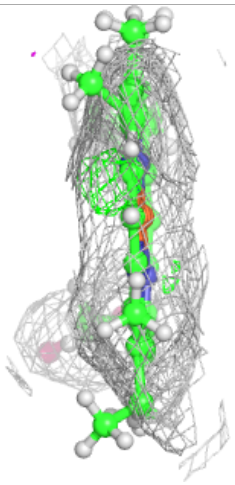


Electron density around HEC P 1001:

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

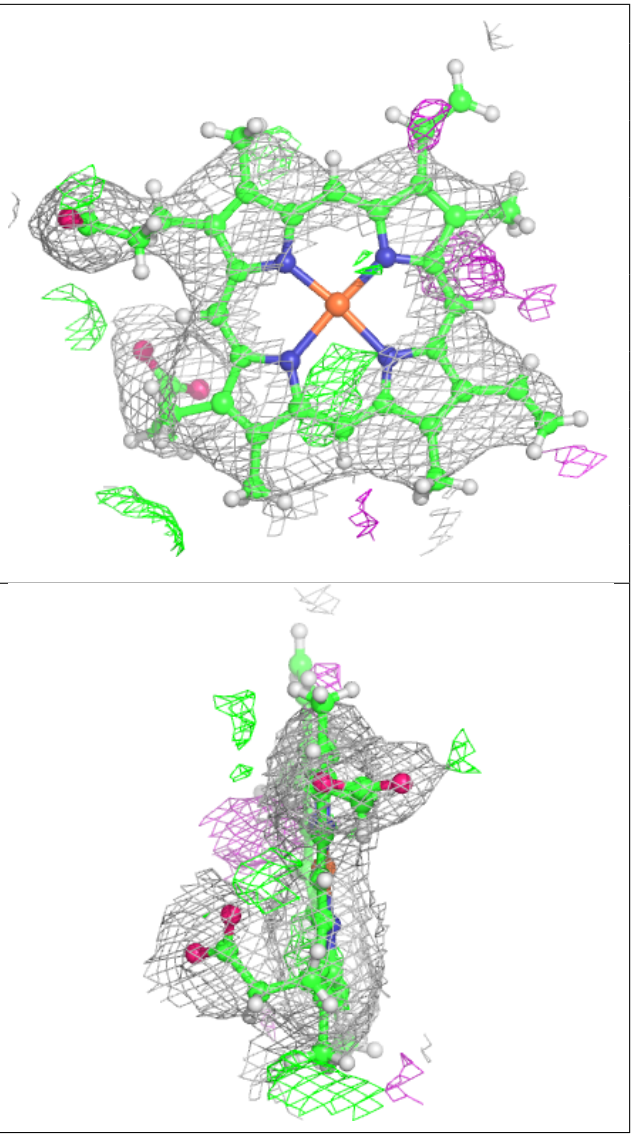






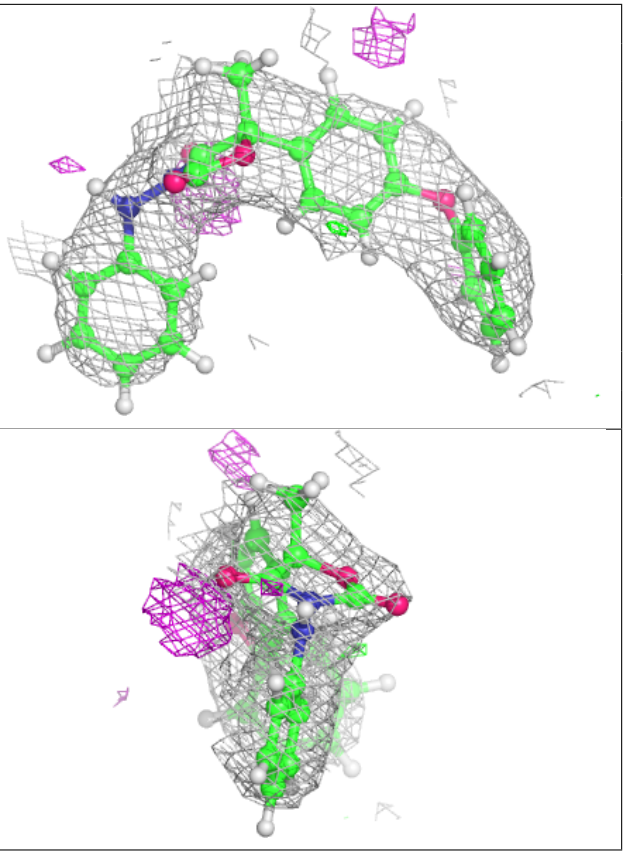
Electron density around HEM E 1002:

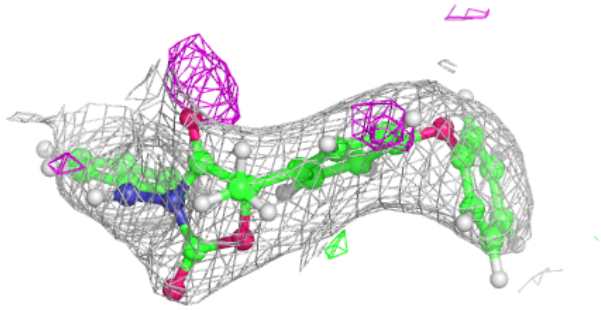
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FMX A 1003:

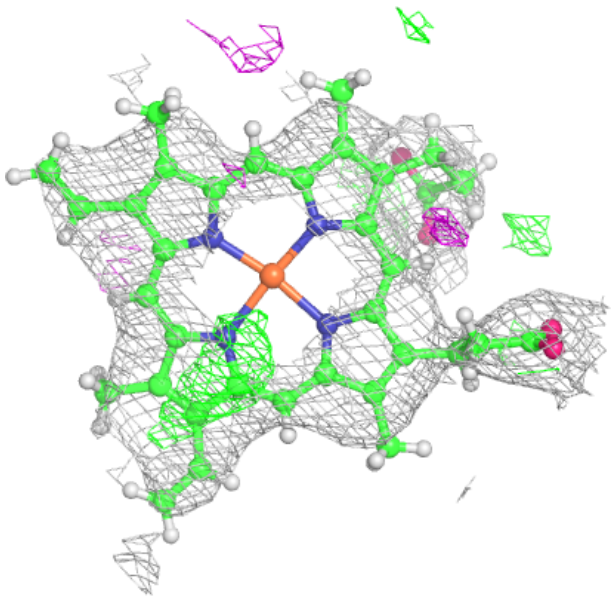
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

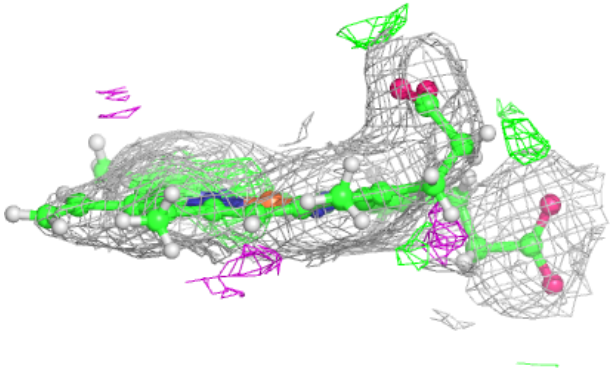


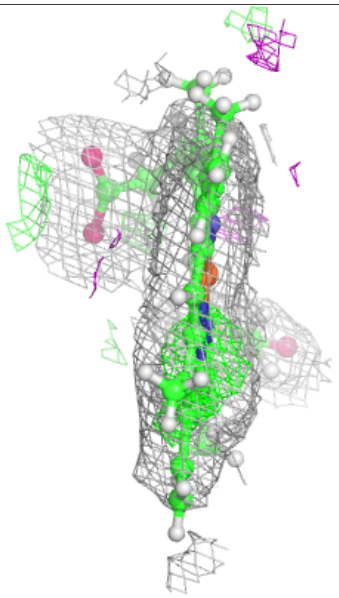


Electron density around HEM A 1002:

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

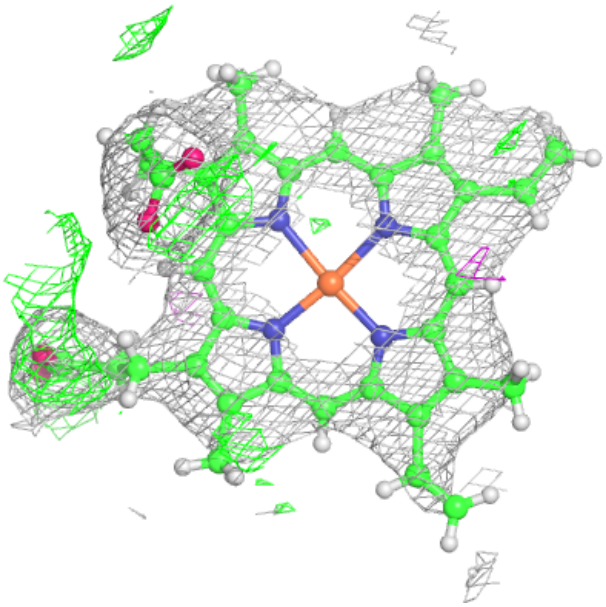


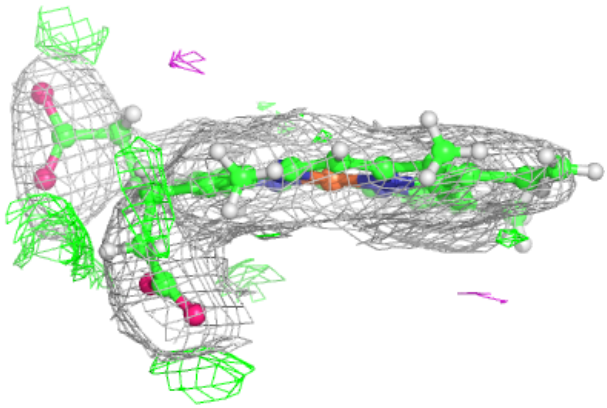


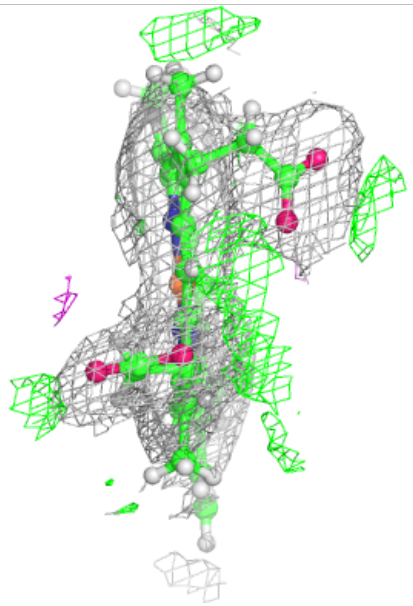


Electron density around HEM K 1002:

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

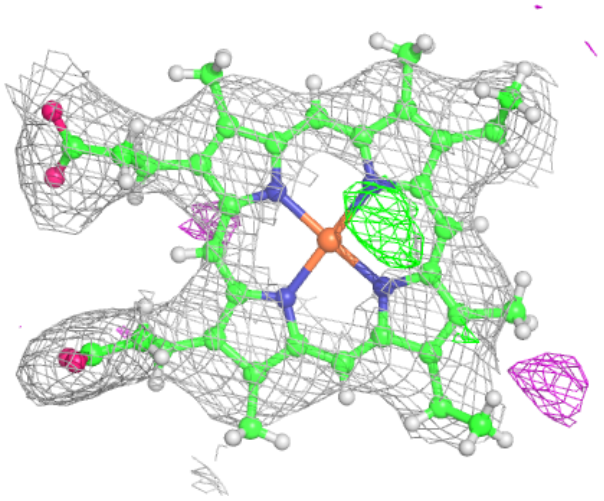


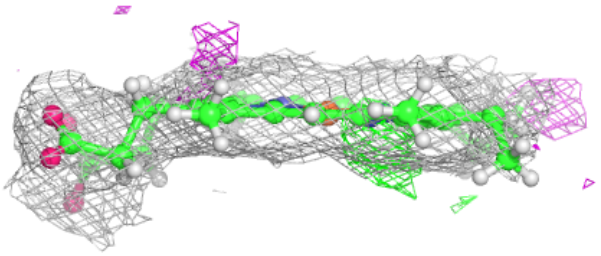


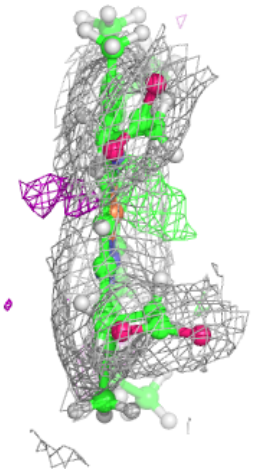


Electron density around HEC B 1001:

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

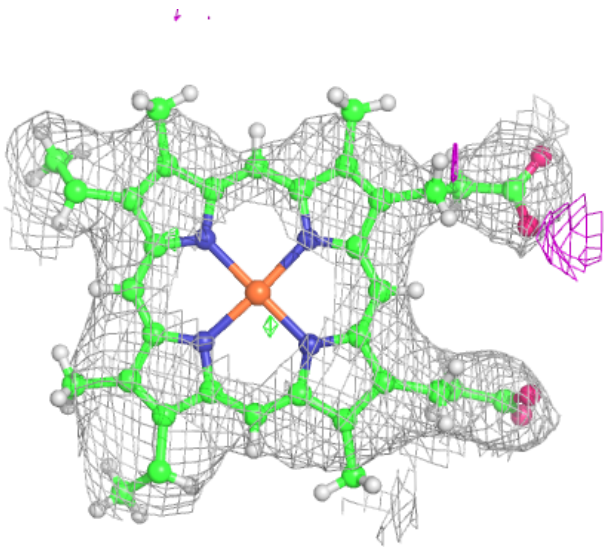


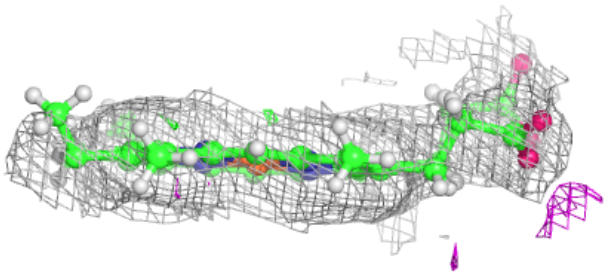


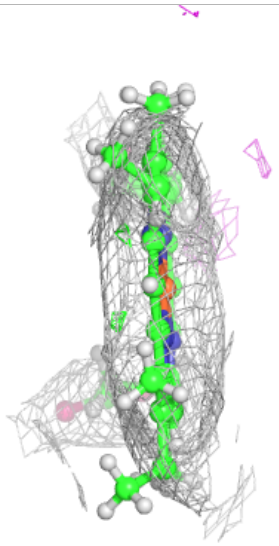


Electron density around HEC F 1001:

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

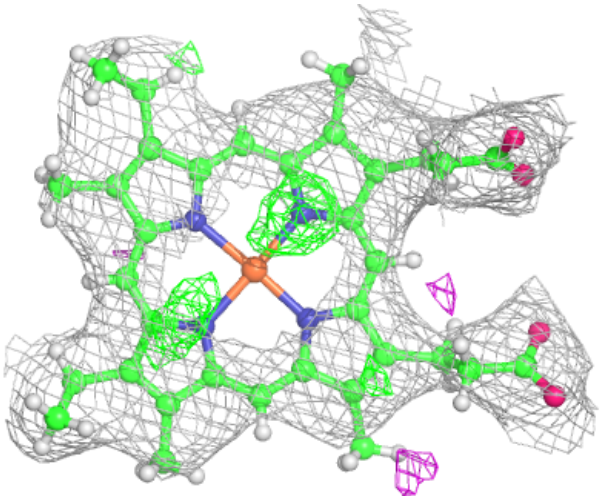


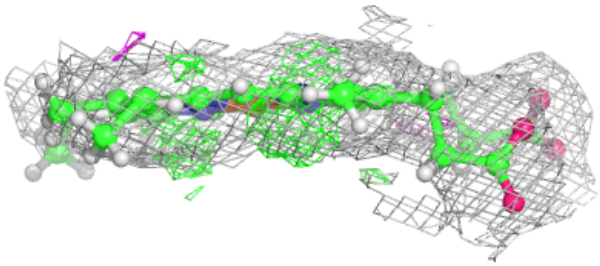


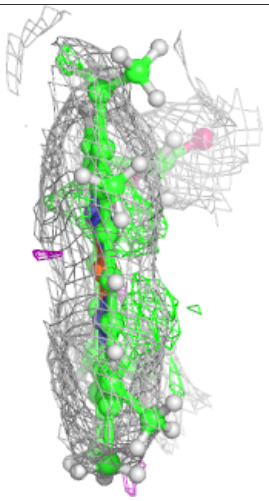


Electron density around HEC L 1001:

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

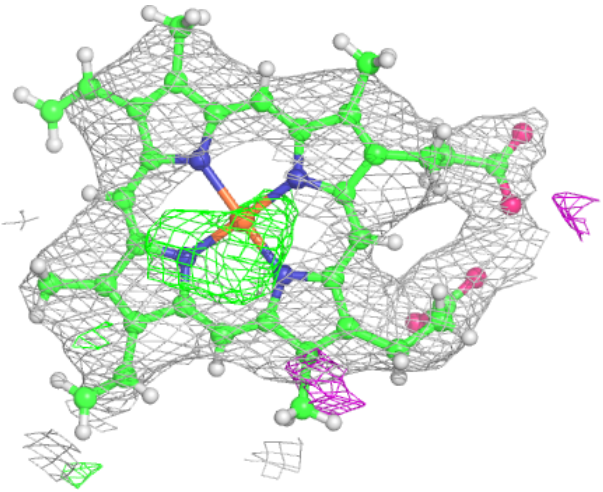


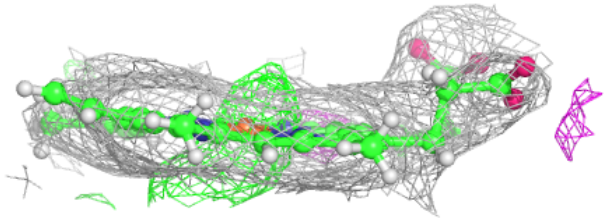


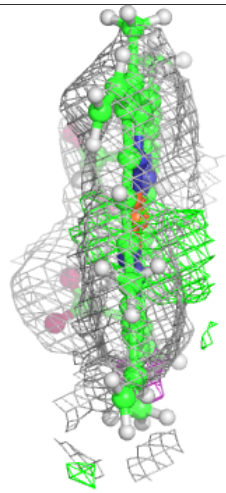


Electron density around HEM O 1001:

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

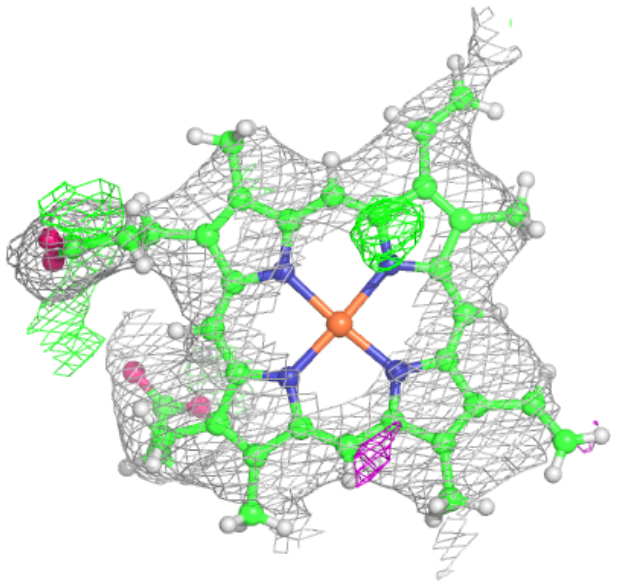


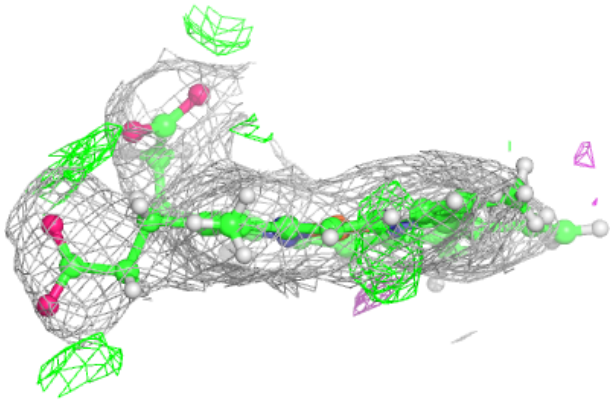


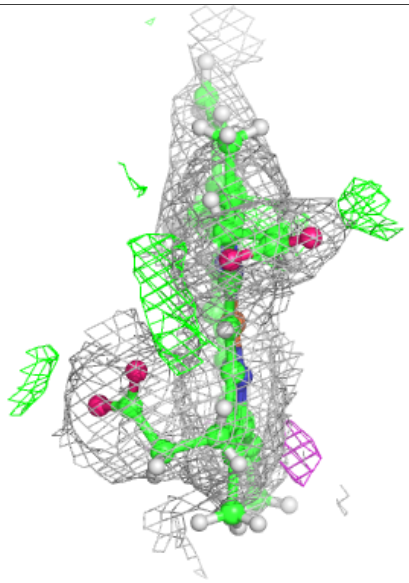


Electron density around HEM O 1002:

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

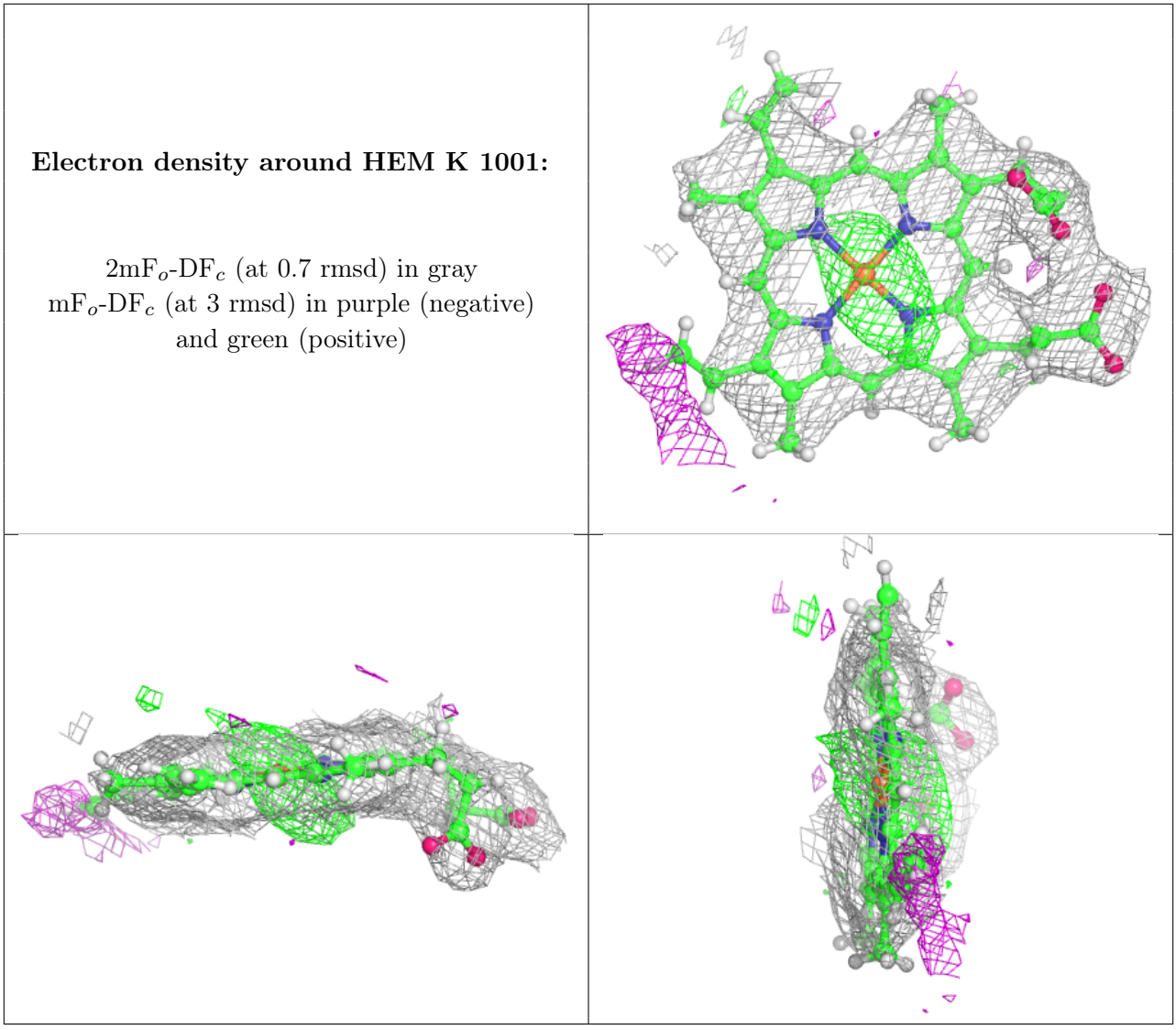






Electron density around HEM K 1001:

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



6.5 Other polymers (i)

There are no such residues in this entry.