Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 04:30 PM EDT

PDB ID	:	5KLI
Title	:	Rhodobacter sphaeroides bc1 with stigmatellin and antimycin
Authors	:	Xia, D.; Esser, L.; Zhou, F.; Tang, W.K.; Yu, C.A.
Deposited on	:	2016-06-24
Resolution	:	3.00 Å(reported)

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

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

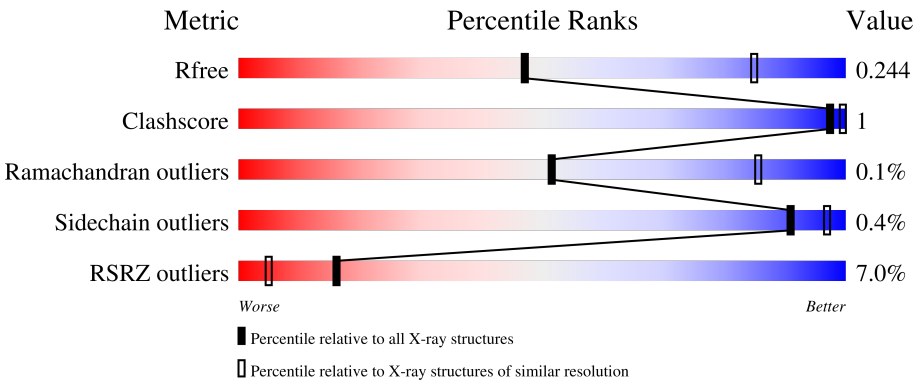
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% 94%
1	E	445	4% 94%
1	K	445	3% 93%
1	O	445	2% 94%
2	B	272	9% 93% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	272	9% 92% 6%
2	L	272	9% 92% 6%
2	P	272	12% 92% 6%
3	C	187	10% 95%
3	G	187	8% 95%
3	M	187	10% 96%
3	Q	187	6% 94%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 55093 atoms, of which 27155 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
			Total	C	H	N	O	S			
1	A	428	6841	2319	3406	545	556	15	0	0	0
1	E	428	6841	2319	3406	545	556	15	0	0	0
1	K	428	6841	2319	3406	545	556	15	0	0	0
1	O	428	6841	2319	3406	545	556	15	0	0	0

- Molecule 2 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	256	3792	1240	1839	326	374	13	0	0	0
2	F	256	3792	1240	1839	326	374	13	0	0	0
2	L	256	3791	1240	1838	326	374	13	0	0	0
2	P	256	3792	1240	1839	326	374	13	0	0	0

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

Continued on next page...

Continued from previous page...

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.

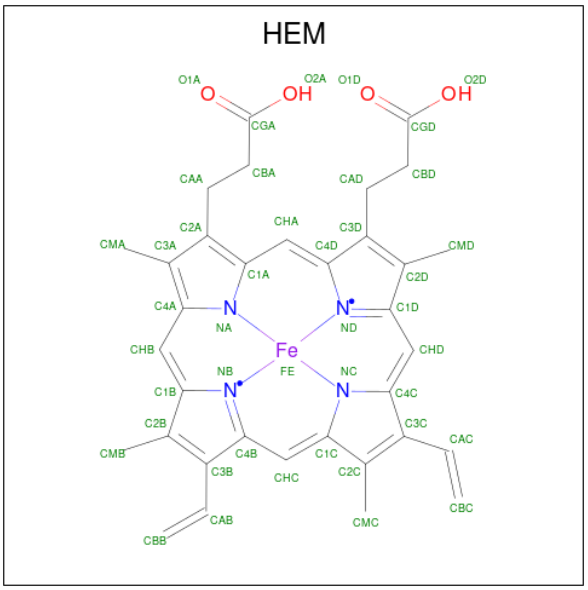
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	179	2645	845	1304	237	253	6	0	0	0
			Total	C	H	N	O	S			
3	G	179	2645	845	1304	237	253	6	0	0	0
			Total	C	H	N	O	S			
3	M	179	2645	845	1304	237	253	6	0	0	0

Continued on next page...

Continued from previous page...

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

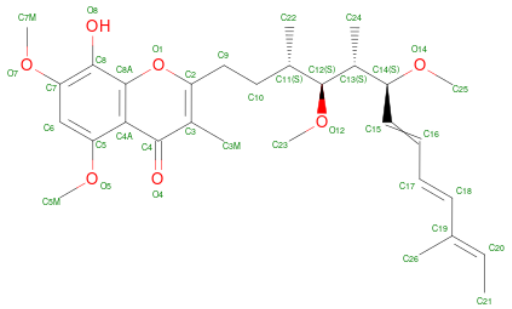
- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

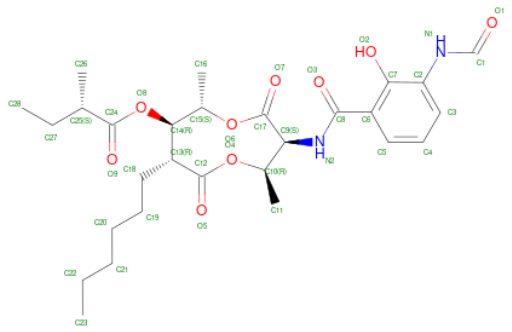
SMA



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

- Molecule 6 is (2R,3S,6S,7R,8R)-3-{[3-(FORMYLAMINO)-2-HYDROXYBENZOYL]AMINO}-8-HEXYL-2,6-DIMETHYL-4,9-DIOXO-1,5-DIOXONAN-7-YL (2S)-2-METHYLBUTANOATE (three-letter code: ANJ) (formula: $C_{28}H_{40}N_2O_9$).

ANJ

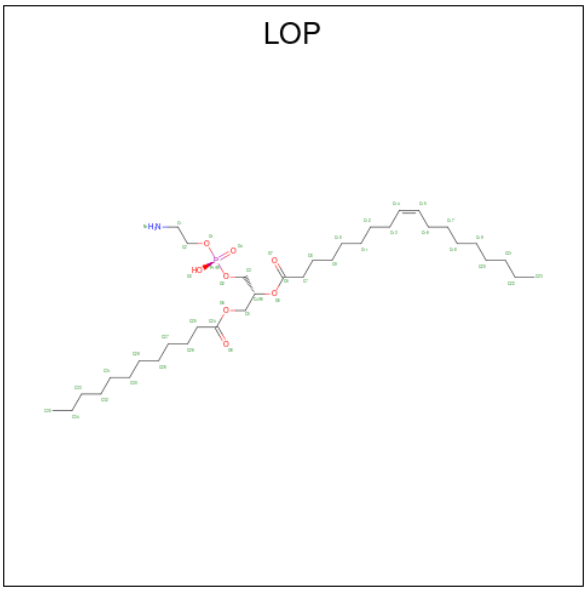


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
6	A	1	78	28	39	2	9	0	0
6	E	1	78	28	39	2	9	0	0
6	K	1	78	28	39	2	9	0	0
6	O	1	78	28	39	2	9	0	0

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

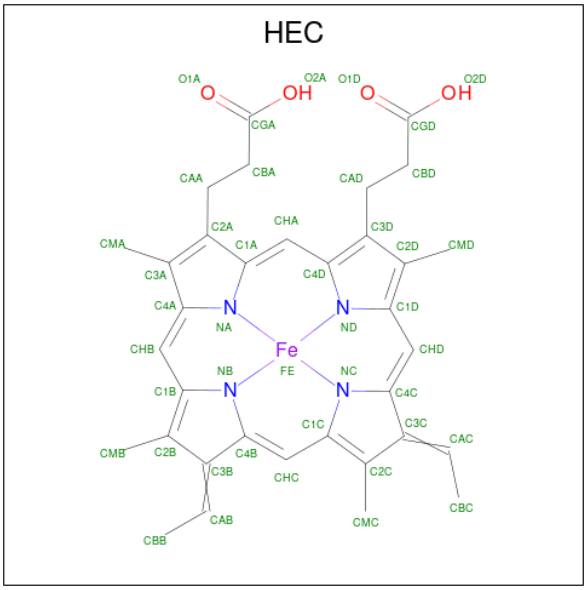
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
7	A	1	1	1	0	0
7	B	1	1	1	0	0
7	F	1	1	1	0	0
7	K	1	1	1	0	0
7	L	1	1	1	0	0
7	P	1	1	1	0	0

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



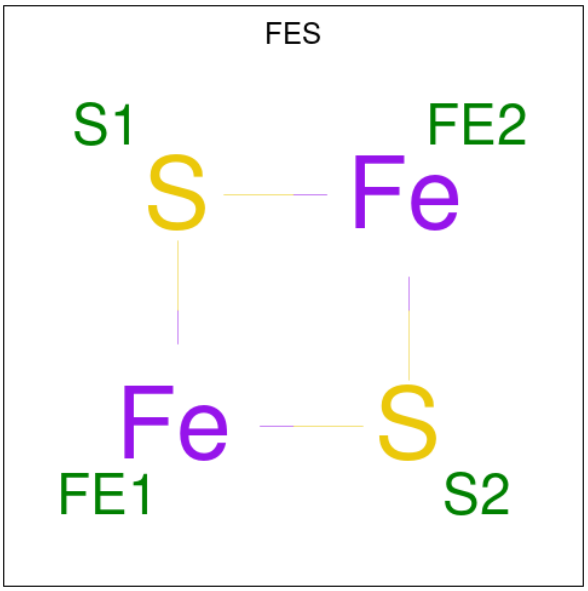
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
8	A	1	112	35	67	1	8	1	0	0
8	E	1	112	35	67	1	8	1	0	0
8	K	1	112	35	67	1	8	1	0	0
8	O	1	112	35	67	1	8	1	0	0

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



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

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



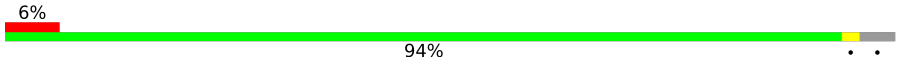
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	C	1	4	2	2	0	0
10	G	1	4	2	2	0	0
10	M	1	4	2	2	0	0
10	Q	1	4	2	2	0	0

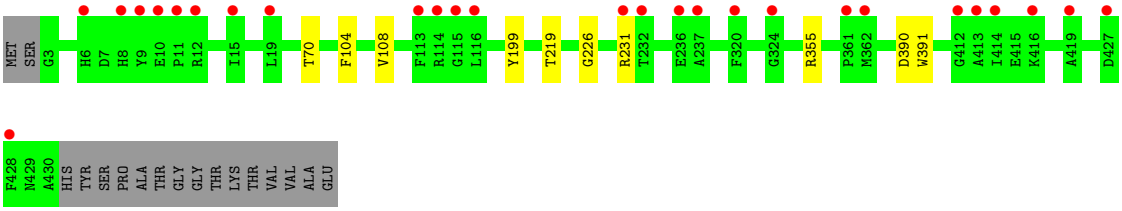
3 Residue-property plots (i)

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

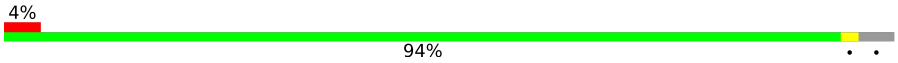
Chain A:

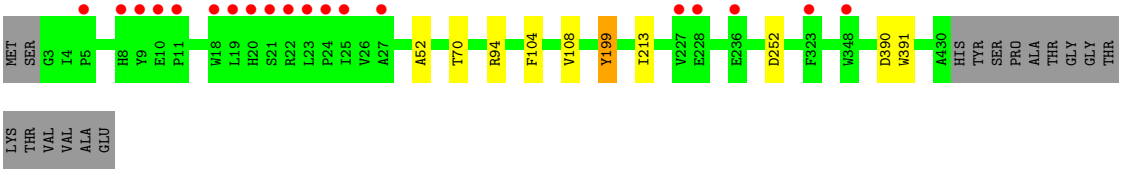




• Molecule 1: Cytochrome b

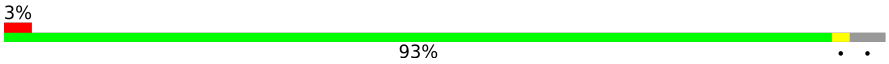
Chain E:

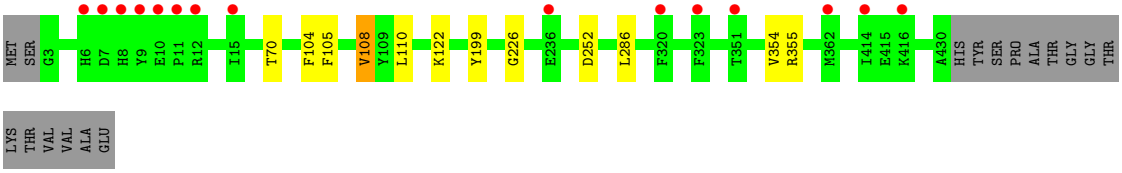




• Molecule 1: Cytochrome b

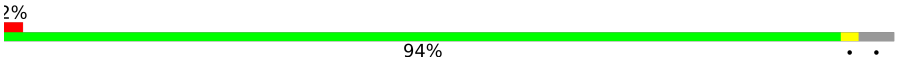
Chain K:

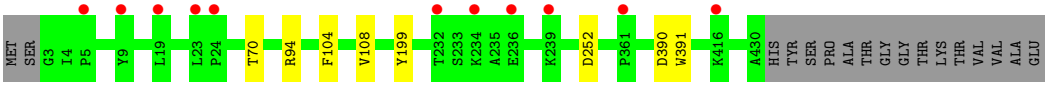




• Molecule 1: Cytochrome b

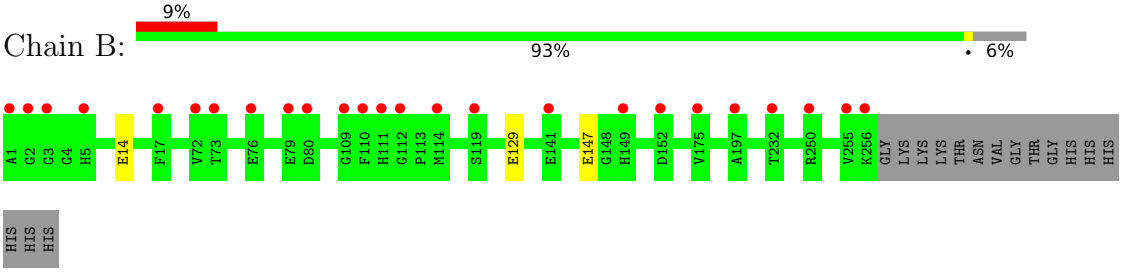
Chain O:





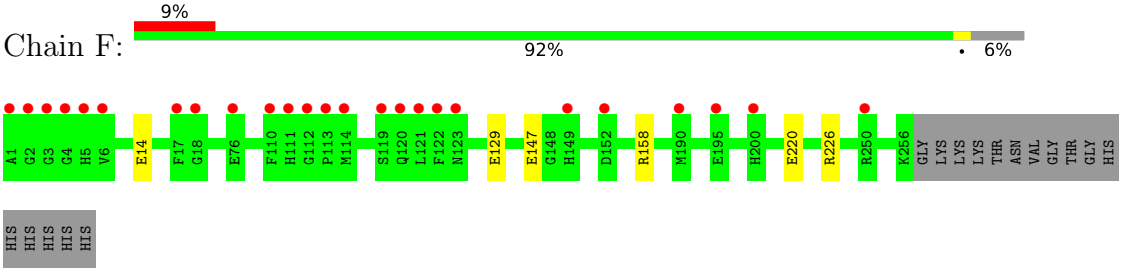
• Molecule 2: Cytochrome c1

Chain B:



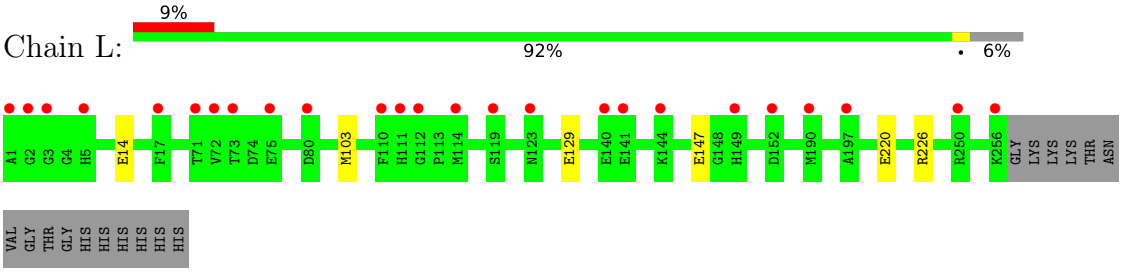
• Molecule 2: Cytochrome c1

Chain F:



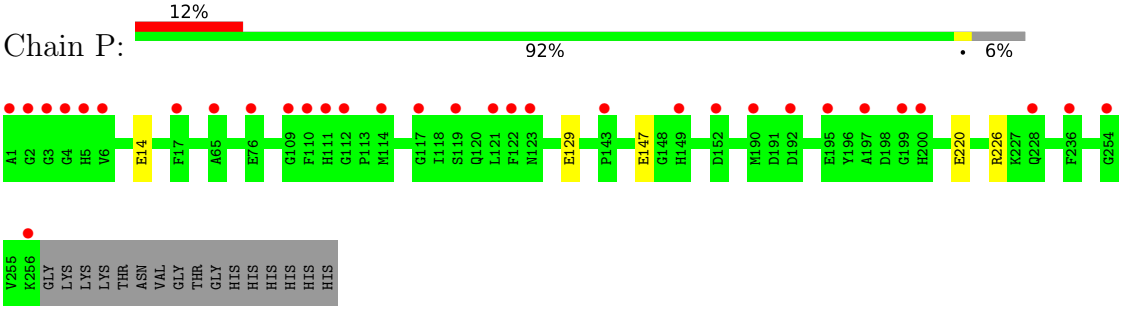
• Molecule 2: Cytochrome c1

Chain L:



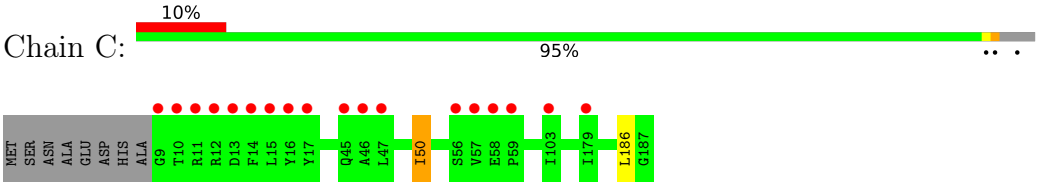
• Molecule 2: Cytochrome c1

Chain P:



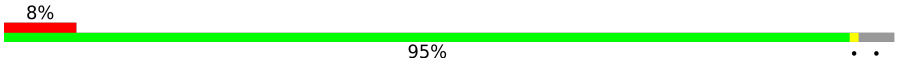
• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

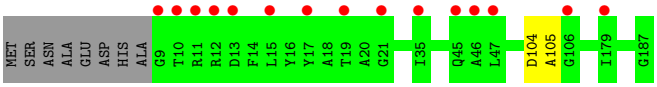
Chain C:



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

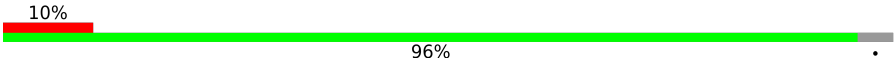
Chain G:

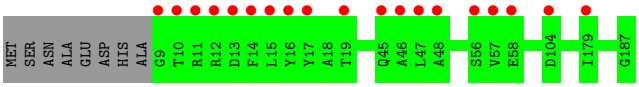




• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

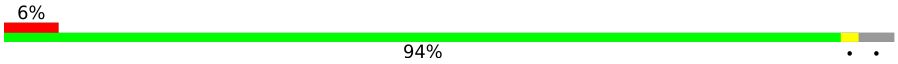
Chain M:

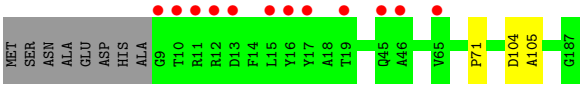




• Molecule 3: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain Q:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	118.86Å 126.93Å 127.89Å 64.64° 87.69° 61.80°	Depositor
Resolution (Å)	37.74 – 3.00 37.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (37.74-3.00) 79.5 (37.72-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11rc1_2513: ???)	Depositor
R, R_{free}	0.211 , 0.243 0.215 , 0.244	Depositor DCC
R_{free} test set	1866 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	55093	wwPDB-VP
Average B, all atoms (Å^2)	92.0	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 34.19 % 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 7.0909e-04. 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: SMA, ANJ, SR, FES, HEC, HEM, LOP

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	0.38	1/3565 (0.0%)	0.58	0/4891
1	E	0.38	1/3565 (0.0%)	0.58	0/4891
1	K	0.39	1/3565 (0.0%)	0.61	0/4891
1	O	0.37	1/3565 (0.0%)	0.58	0/4891
2	B	0.35	0/2010	0.57	0/2733
2	F	0.34	0/2010	0.58	1/2733 (0.0%)
2	L	0.35	0/2010	0.59	0/2733
2	P	0.33	0/2010	0.55	0/2733
3	C	0.35	0/1371	0.59	1/1868 (0.1%)
3	G	0.35	0/1371	0.57	0/1868
3	M	0.35	0/1371	0.58	0/1868
3	Q	0.36	0/1371	0.57	0/1868
All	All	0.37	4/27784 (0.0%)	0.58	2/37968 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	70	THR	C-N	7.44	1.48	1.34
1	K	70	THR	C-N	6.00	1.45	1.34
1	A	70	THR	C-N	5.91	1.45	1.34
1	O	70	THR	C-N	5.55	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	50	ILE	CG1-CB-CG2	5.21	122.87	111.40
2	F	158	ARG	NE-CZ-NH1	5.21	122.90	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	3435	3406	3420	3	0
1	E	3435	3406	3420	6	0
1	K	3435	3406	3420	6	0
1	O	3435	3406	3420	3	0
2	B	1953	1839	1848	1	0
2	F	1953	1839	1848	2	0
2	L	1953	1838	1848	3	0
2	P	1953	1839	1848	2	0
3	C	1341	1304	1307	1	0
3	G	1341	1304	1307	1	0
3	M	1341	1304	1307	0	0
3	Q	1341	1304	1307	2	0
4	A	86	60	60	2	0
4	E	86	60	60	2	0
4	K	86	60	60	2	0
4	O	86	60	60	2	0
5	A	37	42	42	0	0
5	E	37	42	42	0	0
5	K	37	42	42	0	0
5	O	37	42	42	0	0
6	A	39	39	39	0	0
6	E	39	39	39	3	0
6	K	39	39	40	1	0
6	O	39	39	39	1	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
8	O	45	67	67	0	0
9	B	43	32	30	2	0
9	F	43	32	30	2	0
9	L	43	32	30	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	P	43	32	30	2	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
All	All	27938	27155	27253	42	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.

All (42) 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)
2:B:14:GLU:OE2	2:B:129:GLU:OE2	2.10	0.70
2:F:14:GLU:OE2	2:F:129:GLU:OE2	2.18	0.60
9:B:1001:HEC:HBC3	9:B:1001:HEC:HMC1	1.83	0.60
2:F:220:GLU:OE1	2:F:226:ARG:NH1	2.35	0.59
9:F:1001:HEC:HMC1	9:F:1001:HEC:HBC3	1.86	0.58
9:L:1001:HEC:HBC3	9:L:1001:HEC:HMC1	1.86	0.58
9:L:1001:HEC:HBB3	9:L:1001:HEC:HMB1	1.87	0.57
9:P:1001:HEC:HMC1	9:P:1001:HEC:HBC3	1.86	0.57
9:F:1001:HEC:HMB1	9:F:1001:HEC:HBB3	1.87	0.56
2:P:220:GLU:OE1	2:P:226:ARG:NH1	2.38	0.56
1:E:52:ALA:HB2	6:E:1004:ANJ:H163	1.86	0.56
9:P:1001:HEC:HMB1	9:P:1001:HEC:HBB3	1.88	0.55
4:O:1001:HEM:HBB2	4:O:1001:HEM:HHC	1.89	0.55
1:A:219:THR:O	1:A:231:ARG:NH2	2.38	0.55
4:K:1001:HEM:HBC2	4:K:1001:HEM:HHD	1.90	0.53
2:L:14:GLU:OE2	2:L:129:GLU:OE2	2.27	0.53
4:K:1001:HEM:HBB2	4:K:1001:HEM:HHC	1.90	0.52
3:C:50:ILE:HD11	3:C:186:LEU:HD12	1.92	0.52
9:B:1001:HEC:HBB3	9:B:1001:HEC:HMB1	1.91	0.51
1:A:226:GLY:O	1:A:355:ARG:NH1	2.38	0.51
2:P:14:GLU:OE2	2:P:129:GLU:OE2	2.29	0.51
4:A:1001:HEM:HBB2	4:A:1001:HEM:HHC	1.94	0.49
1:K:110:LEU:HD11	8:K:1006:LOP:H14	1.95	0.49
1:O:94:ARG:NH2	4:O:1001:HEM:O1A	2.45	0.49
2:L:220:GLU:OE1	2:L:226:ARG:NH1	2.46	0.48
1:O:390:ASP:OD1	1:O:391:TRP:N	2.47	0.48
1:E:94:ARG:NH2	4:E:1001:HEM:O1A	2.47	0.48
3:G:104:ASP:OD1	3:G:105:ALA:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:ASP:OD2	6:E:1004:ANJ:O2	2.33	0.47
1:A:390:ASP:OD1	1:A:391:TRP:N	2.49	0.46
1:E:213:ILE:HD11	6:E:1004:ANJ:H162	1.97	0.46
1:E:199:TYR:CE2	4:E:1001:HEM:HBC1	2.50	0.46
2:L:103:MET:HG2	9:L:1001:HEC:HMA3	1.98	0.45
1:K:226:GLY:O	1:K:355:ARG:NH1	2.41	0.44
1:K:252:ASP:OD2	6:K:1004:ANJ:O2	2.34	0.43
1:O:252:ASP:OD2	6:O:1004:ANJ:O2	2.36	0.43
3:Q:104:ASP:OD1	3:Q:105:ALA:N	2.52	0.43
4:A:1002:HEM:HBA1	4:A:1002:HEM:HHA	2.00	0.43
1:K:122:LYS:NZ	1:K:354:VAL:O	2.47	0.42
1:E:390:ASP:OD1	1:E:391:TRP:N	2.53	0.42
1:K:105:PHE:HA	1:K:108:VAL:HG22	2.01	0.41
1:K:286:LEU:HA	3:Q:71:PRO:HG3	2.03	0.41

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%)	422 (99%)	4 (1%)	0	100	100
2	B	254/272 (93%)	246 (97%)	7 (3%)	1 (0%)	34	72
2	F	254/272 (93%)	246 (97%)	7 (3%)	1 (0%)	34	72
2	L	254/272 (93%)	246 (97%)	7 (3%)	1 (0%)	34	72
2	P	254/272 (93%)	246 (97%)	7 (3%)	1 (0%)	34	72
3	C	177/187 (95%)	171 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	177/187 (95%)	171 (97%)	6 (3%)	0	100	100
3	M	177/187 (95%)	170 (96%)	7 (4%)	0	100	100
3	Q	177/187 (95%)	170 (96%)	7 (4%)	0	100	100
All	All	3428/3616 (95%)	3351 (98%)	73 (2%)	4 (0%)	51	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	147	GLU
2	B	147	GLU
2	F	147	GLU
2	P	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	353/366 (96%)	350 (99%)	3 (1%)	81	93
1	E	353/366 (96%)	350 (99%)	3 (1%)	81	93
1	K	353/366 (96%)	350 (99%)	3 (1%)	81	93
1	O	353/366 (96%)	350 (99%)	3 (1%)	81	93
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	2776/2904 (96%)	2764 (100%)	12 (0%)	91	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	PHE
1	A	108	VAL
1	A	199	TYR
1	E	104	PHE
1	E	108	VAL
1	E	199	TYR
1	K	104	PHE
1	K	108	VAL
1	K	199	TYR
1	O	104	PHE
1	O	108	VAL
1	O	199	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
9	HEC	L	1001	2	32,50,50	2.07	3 (9%)	24,82,82	1.65	4 (16%)
10	FES	G	1001	3	0,4,4	-	-	-		
8	LOP	O	1005	-	44,44,44	0.92	1 (2%)	47,49,49	1.16	3 (6%)
5	SMA	A	1003	-	38,38,38	0.76	0	48,52,52	1.79	9 (18%)
4	HEM	A	1001	1	41,50,50	1.48	6 (14%)	45,82,82	1.45	8 (17%)
10	FES	C	1001	3	0,4,4	-	-	-		
5	SMA	K	1003	-	38,38,38	0.73	0	48,52,52	1.65	9 (18%)
8	LOP	K	1006	-	44,44,44	0.94	2 (4%)	47,49,49	1.07	4 (8%)
6	ANJ	O	1004	-	40,40,40	0.87	0	36,54,54	1.25	6 (16%)
9	HEC	B	1001	2	32,50,50	2.08	3 (9%)	24,82,82	1.80	6 (25%)
8	LOP	E	1005	-	44,44,44	0.93	1 (2%)	47,49,49	1.16	3 (6%)
4	HEM	K	1001	1	41,50,50	1.53	5 (12%)	45,82,82	1.55	6 (13%)
10	FES	Q	1001	3	0,4,4	-	-	-		
10	FES	M	1001	3	0,4,4	-	-	-		
4	HEM	E	1002	1	41,50,50	1.52	5 (12%)	45,82,82	1.68	9 (20%)
9	HEC	F	1001	2	32,50,50	2.03	3 (9%)	24,82,82	1.69	6 (25%)
4	HEM	O	1001	1	41,50,50	1.49	6 (14%)	45,82,82	1.50	7 (15%)
4	HEM	K	1002	1	41,50,50	1.55	6 (14%)	45,82,82	1.53	9 (20%)
6	ANJ	E	1004	-	40,40,40	0.90	1 (2%)	36,54,54	1.08	2 (5%)
6	ANJ	K	1004	-	40,40,40	0.89	1 (2%)	36,54,54	1.22	5 (13%)
4	HEM	A	1002	1	41,50,50	1.49	4 (9%)	45,82,82	1.49	9 (20%)
8	LOP	A	1006	-	44,44,44	0.91	1 (2%)	47,49,49	1.12	4 (8%)
5	SMA	O	1003	-	38,38,38	0.80	0	48,52,52	1.73	7 (14%)
6	ANJ	A	1004	-	40,40,40	0.84	0	36,54,54	1.42	7 (19%)
5	SMA	E	1003	-	38,38,38	0.76	1 (2%)	48,52,52	1.59	8 (16%)
4	HEM	E	1001	1	41,50,50	1.45	4 (9%)	45,82,82	1.34	7 (15%)
4	HEM	O	1002	1	41,50,50	1.50	6 (14%)	45,82,82	1.67	10 (22%)
9	HEC	P	1001	2	32,50,50	2.08	3 (9%)	24,82,82	1.64	5 (20%)

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
9	HEC	L	1001	2	-	4/10/54/54	-
10	FES	G	1001	3	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LOP	O	1005	-	-	20/48/48/48	-
5	SMA	A	1003	-	-	3/34/34/34	0/2/2/2
4	HEM	A	1001	1	-	4/12/54/54	-
10	FES	C	1001	3	-	-	0/1/1/1
5	SMA	K	1003	-	-	4/34/34/34	0/2/2/2
8	LOP	K	1006	-	-	24/48/48/48	-
6	ANJ	O	1004	-	-	11/40/55/55	0/1/2/2
9	HEC	B	1001	2	-	2/10/54/54	-
8	LOP	E	1005	-	-	25/48/48/48	-
4	HEM	K	1001	1	-	6/12/54/54	-
10	FES	Q	1001	3	-	-	0/1/1/1
10	FES	M	1001	3	-	-	0/1/1/1
4	HEM	E	1002	1	-	2/12/54/54	-
9	HEC	F	1001	2	-	2/10/54/54	-
4	HEM	O	1001	1	-	6/12/54/54	-
4	HEM	K	1002	1	-	2/12/54/54	-
6	ANJ	E	1004	-	-	7/40/55/55	0/1/2/2
6	ANJ	K	1004	-	-	13/40/55/55	0/1/2/2
4	HEM	A	1002	1	-	2/12/54/54	-
8	LOP	A	1006	-	-	26/48/48/48	-
5	SMA	O	1003	-	-	3/34/34/34	0/2/2/2
6	ANJ	A	1004	-	-	11/40/55/55	0/1/2/2
5	SMA	E	1003	-	-	2/34/34/34	0/2/2/2
4	HEM	E	1001	1	-	5/12/54/54	-
4	HEM	O	1002	1	-	2/12/54/54	-
9	HEC	P	1001	2	-	2/10/54/54	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1001	HEC	C2B-C3B	-6.74	1.33	1.40
9	P	1001	HEC	C2B-C3B	-6.53	1.33	1.40
9	L	1001	HEC	C2B-C3B	-5.96	1.34	1.40
9	F	1001	HEC	C2B-C3B	-5.95	1.34	1.40
9	L	1001	HEC	C3C-C2C	-5.79	1.34	1.40
9	F	1001	HEC	C3C-C2C	-5.03	1.35	1.40
9	B	1001	HEC	C3D-C2D	5.03	1.52	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1001	HEC	C3C-C2C	-5.02	1.35	1.40
9	F	1001	HEC	C3D-C2D	4.99	1.52	1.37
9	P	1001	HEC	C3D-C2D	4.99	1.52	1.37
9	L	1001	HEC	C3D-C2D	4.86	1.52	1.37
9	P	1001	HEC	C3C-C2C	-4.81	1.35	1.40
4	K	1001	HEM	C3C-C2C	-4.47	1.34	1.40
4	K	1002	HEM	C3C-CAC	4.31	1.56	1.47
4	O	1002	HEM	C3C-CAC	4.30	1.56	1.47
4	E	1002	HEM	C3C-CAC	4.27	1.56	1.47
4	A	1002	HEM	C3C-CAC	4.10	1.56	1.47
4	K	1001	HEM	C3C-CAC	4.10	1.56	1.47
4	A	1001	HEM	C3C-CAC	3.88	1.55	1.47
4	O	1001	HEM	C3C-C2C	-3.70	1.35	1.40
4	O	1001	HEM	C3C-CAC	3.66	1.55	1.47
4	E	1001	HEM	C3C-CAC	3.63	1.55	1.47
4	A	1002	HEM	C3C-C2C	-3.59	1.35	1.40
4	A	1002	HEM	CAB-C3B	3.44	1.56	1.47
4	O	1002	HEM	C3C-C2C	-3.42	1.35	1.40
4	K	1002	HEM	FE-NB	3.38	2.13	1.96
4	K	1002	HEM	C3C-C2C	-3.29	1.35	1.40
4	O	1002	HEM	CAB-C3B	3.26	1.56	1.47
4	K	1002	HEM	CAB-C3B	3.25	1.56	1.47
4	E	1001	HEM	C3C-C2C	-3.24	1.35	1.40
4	E	1002	HEM	FE-NB	3.24	2.12	1.96
4	E	1002	HEM	CAB-C3B	3.21	1.56	1.47
4	E	1002	HEM	C3C-C2C	-3.11	1.36	1.40
4	A	1001	HEM	C3C-C2C	-2.95	1.36	1.40
4	E	1001	HEM	CAB-C3B	2.86	1.55	1.47
4	O	1001	HEM	CAB-C3B	2.78	1.55	1.47
4	O	1001	HEM	FE-ND	2.77	2.10	1.96
4	A	1001	HEM	CAB-C3B	2.75	1.54	1.47
4	E	1002	HEM	CMB-C2B	2.73	1.56	1.50
4	K	1002	HEM	CMB-C2B	2.59	1.56	1.50
4	K	1001	HEM	CAB-C3B	2.58	1.54	1.47
4	O	1001	HEM	CMB-C2B	2.34	1.55	1.50
4	O	1002	HEM	FE-NB	2.28	2.08	1.96
4	A	1001	HEM	CMC-C2C	2.25	1.56	1.51
4	A	1002	HEM	CMB-C2B	2.25	1.55	1.50
8	K	1006	LOP	C7-C6	2.19	1.57	1.50
8	E	1005	LOP	C7-C6	2.17	1.57	1.50
4	K	1001	HEM	CMB-C2B	2.16	1.55	1.50
4	E	1001	HEM	CMB-C2B	2.14	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	HEM	CMB-C2B	2.14	1.55	1.50
8	A	1006	LOP	C7-C6	2.13	1.56	1.50
4	O	1001	HEM	CMD-C2D	2.12	1.55	1.50
4	O	1002	HEM	CMB-C2B	2.10	1.55	1.50
6	K	1004	ANJ	C1-N1	2.09	1.37	1.34
4	A	1001	HEM	C2C-C1C	2.08	1.47	1.42
8	K	1006	LOP	C25-C24	2.07	1.56	1.50
4	O	1002	HEM	CMD-C2D	2.07	1.55	1.50
5	E	1003	SMA	O1-C2	2.05	1.39	1.36
4	K	1001	HEM	CMC-C2C	2.04	1.56	1.51
4	K	1002	HEM	CAA-C2A	2.03	1.55	1.52
6	E	1004	ANJ	O8-C24	2.01	1.39	1.34
8	O	1005	LOP	C7-C6	2.01	1.56	1.50

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1003	SMA	O5-C5-C4A	7.37	126.12	115.85
5	O	1003	SMA	O5-C5-C4A	7.07	125.70	115.85
5	E	1003	SMA	O5-C5-C4A	6.11	124.36	115.85
5	K	1003	SMA	O5-C5-C4A	6.07	124.30	115.85
5	A	1003	SMA	O5-C5-C6	-5.36	114.90	124.12
5	O	1003	SMA	O5-C5-C6	-5.06	115.41	124.12
9	L	1001	HEC	CBD-CAD-C3D	-4.38	105.14	112.62
5	K	1003	SMA	O5-C5-C6	-4.25	116.80	124.12
5	E	1003	SMA	O5-C5-C6	-4.22	116.86	124.12
4	K	1001	HEM	C4C-CHD-C1D	4.18	128.07	122.56
4	K	1001	HEM	C4B-CHC-C1C	4.00	127.84	122.56
4	O	1001	HEM	C4B-CHC-C1C	3.96	127.79	122.56
4	A	1002	HEM	CMC-C2C-C3C	3.91	132.00	124.68
4	E	1002	HEM	C4D-ND-C1D	3.69	108.89	105.07
8	O	1005	LOP	O6-C24-C25	3.60	123.19	111.91
4	E	1002	HEM	C4B-CHC-C1C	3.59	127.30	122.56
4	K	1002	HEM	C4B-CHC-C1C	3.56	127.25	122.56
9	B	1001	HEC	C1D-C2D-C3D	-3.55	104.53	107.00
4	E	1002	HEM	CMC-C2C-C3C	3.53	131.28	124.68
4	E	1002	HEM	CBA-CAA-C2A	-3.51	106.63	112.62
4	A	1001	HEM	CHC-C4B-C3B	3.49	129.91	124.57
8	O	1005	LOP	O6-C5-C4	3.47	118.55	108.43
9	F	1001	HEC	C1D-C2D-C3D	-3.44	104.60	107.00
8	E	1005	LOP	O5-C6-C7	3.40	118.82	111.50
4	O	1002	HEM	C4D-ND-C1D	3.37	108.55	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1002	HEM	CMC-C2C-C3C	3.37	130.98	124.68
4	K	1002	HEM	CMC-C2C-C3C	3.35	130.94	124.68
4	K	1001	HEM	CHC-C4B-C3B	3.33	129.67	124.57
9	B	1001	HEC	CMC-C2C-C1C	-3.32	123.36	128.46
4	O	1002	HEM	CMB-C2B-C1B	-3.32	119.99	125.04
6	E	1004	ANJ	C14-O8-C24	3.27	123.40	117.78
4	O	1001	HEM	C1B-NB-C4B	3.26	108.44	105.07
4	O	1001	HEM	CBA-CAA-C2A	-3.25	107.08	112.62
8	E	1005	LOP	O6-C24-C25	3.24	122.08	111.91
6	A	1004	ANJ	O6-C17-C9	3.19	115.29	110.28
4	A	1001	HEM	C4C-CHD-C1D	3.18	126.75	122.56
8	A	1006	LOP	O5-C6-C7	3.18	118.35	111.50
4	K	1001	HEM	CBA-CAA-C2A	-3.17	107.20	112.62
4	E	1002	HEM	CMB-C2B-C1B	-3.16	120.23	125.04
9	B	1001	HEC	CAA-CBA-CGA	-3.15	104.92	113.76
8	E	1005	LOP	O6-C5-C4	3.13	117.56	108.43
4	O	1001	HEM	CHC-C4B-C3B	3.13	129.36	124.57
4	A	1001	HEM	C4B-CHC-C1C	3.13	126.68	122.56
9	P	1001	HEC	CMC-C2C-C1C	-3.13	123.66	128.46
4	O	1002	HEM	C4C-CHD-C1D	3.11	126.66	122.56
8	A	1006	LOP	O5-C4-C3	3.06	119.50	108.40
4	E	1001	HEM	CMC-C2C-C3C	3.06	130.41	124.68
4	A	1002	HEM	C4B-CHC-C1C	3.06	126.60	122.56
9	B	1001	HEC	CBD-CAD-C3D	-3.05	107.42	112.62
6	K	1004	ANJ	C14-O8-C24	3.01	122.95	117.78
4	K	1002	HEM	CMB-C2B-C1B	-3.01	120.46	125.04
4	E	1001	HEM	C4C-CHD-C1D	3.00	126.52	122.56
9	P	1001	HEC	C1D-C2D-C3D	-2.99	104.92	107.00
4	O	1002	HEM	C4B-CHC-C1C	2.99	126.50	122.56
4	O	1001	HEM	CMC-C2C-C3C	2.99	130.26	124.68
5	K	1003	SMA	C9-C10-C11	-2.98	109.08	114.52
4	O	1002	HEM	C4A-C3A-C2A	2.98	109.07	107.00
4	E	1001	HEM	CMB-C2B-C1B	-2.95	120.55	125.04
5	K	1003	SMA	C22-C11-C10	2.93	114.96	110.36
4	A	1001	HEM	C1B-NB-C4B	2.92	108.09	105.07
4	K	1001	HEM	C1B-NB-C4B	2.90	108.07	105.07
9	F	1001	HEC	CMC-C2C-C1C	-2.89	124.02	128.46
4	A	1002	HEM	CMB-C2B-C1B	-2.89	120.64	125.04
9	B	1001	HEC	CMC-C2C-C3C	2.86	129.18	125.82
9	P	1001	HEC	CAA-CBA-CGA	-2.84	105.79	113.76
6	A	1004	ANJ	C3-C2-N1	2.83	126.85	122.59
9	L	1001	HEC	CMC-C2C-C1C	-2.83	124.12	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1002	HEM	C4D-ND-C1D	2.81	107.97	105.07
9	F	1001	HEC	CBD-CAD-C3D	-2.79	107.86	112.62
4	A	1001	HEM	CMC-C2C-C3C	2.77	129.87	124.68
9	P	1001	HEC	CMC-C2C-C3C	2.76	129.07	125.82
5	E	1003	SMA	C9-C10-C11	-2.74	109.51	114.52
9	F	1001	HEC	CAA-CBA-CGA	-2.73	106.12	113.76
5	K	1003	SMA	C3M-C3-C4	-2.71	111.77	116.27
5	E	1003	SMA	C5M-O5-C5	2.67	121.57	117.53
6	O	1004	ANJ	O6-C17-C9	2.66	114.47	110.28
6	A	1004	ANJ	O8-C14-C15	-2.66	102.19	107.47
5	E	1003	SMA	C3M-C3-C4	-2.65	111.87	116.27
6	A	1004	ANJ	C9-N2-C8	2.62	126.27	121.52
5	O	1003	SMA	C3M-C3-C4	-2.62	111.93	116.27
4	E	1002	HEM	CAD-CBD-CGD	-2.61	107.98	113.60
4	O	1002	HEM	CBD-CAD-C3D	-2.61	105.39	112.63
8	K	1006	LOP	O6-C5-C4	2.59	115.97	108.43
4	A	1001	HEM	CBA-CAA-C2A	-2.58	108.21	112.62
6	K	1004	ANJ	O8-C14-C15	-2.57	102.36	107.47
9	L	1001	HEC	C1D-C2D-C3D	-2.57	105.21	107.00
6	A	1004	ANJ	C14-O8-C24	2.54	122.14	117.78
4	E	1002	HEM	C3D-C4D-ND	-2.51	107.38	110.17
4	O	1001	HEM	C4C-CHD-C1D	2.51	125.86	122.56
8	K	1006	LOP	O5-C6-C7	2.48	116.85	111.50
6	A	1004	ANJ	O6-C17-O7	-2.48	120.96	124.08
4	K	1002	HEM	C4C-CHD-C1D	2.48	125.83	122.56
6	O	1004	ANJ	C14-O8-C24	2.47	122.02	117.78
8	K	1006	LOP	C5-C4-C3	2.47	117.62	111.79
4	E	1001	HEM	C2C-C3C-C4C	2.46	108.62	106.90
4	A	1002	HEM	C1B-NB-C4B	2.46	107.62	105.07
5	K	1003	SMA	C7M-O7-C7	2.46	121.24	117.53
8	A	1006	LOP	O5-C6-O7	-2.44	117.80	123.70
5	K	1003	SMA	C3M-C3-C2	2.43	127.38	122.95
4	K	1002	HEM	CBD-CAD-C3D	-2.43	105.87	112.63
4	A	1002	HEM	C4D-ND-C1D	2.41	107.56	105.07
4	A	1002	HEM	C4A-C3A-C2A	2.40	108.67	107.00
5	E	1003	SMA	C7M-O7-C7	2.40	121.16	117.53
4	O	1002	HEM	CBA-CAA-C2A	-2.39	108.55	112.62
4	O	1002	HEM	C1B-NB-C4B	2.38	107.53	105.07
5	O	1003	SMA	C22-C11-C10	2.38	114.09	110.36
5	O	1003	SMA	C9-C2-C3	2.35	130.51	127.07
6	K	1004	ANJ	C6-C8-N2	2.34	121.13	116.80
4	O	1002	HEM	C3D-C4D-ND	-2.33	107.57	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	1003	SMA	C3M-C3-C2	2.33	127.18	122.95
6	K	1004	ANJ	O6-C17-O7	-2.32	121.16	124.08
8	O	1005	LOP	O5-C6-C7	2.31	116.47	111.50
4	E	1002	HEM	C4C-CHD-C1D	2.29	125.58	122.56
9	L	1001	HEC	CAA-CBA-CGA	-2.29	107.34	113.76
5	A	1003	SMA	C22-C11-C10	2.28	113.94	110.36
5	E	1003	SMA	C3M-C3-C2	2.28	127.09	122.95
5	A	1003	SMA	C3M-C3-C4	-2.28	112.50	116.27
5	O	1003	SMA	C5M-O5-C5	2.27	120.95	117.53
9	F	1001	HEC	CMC-C2C-C3C	2.27	128.48	125.82
4	E	1001	HEM	C1B-NB-C4B	2.26	107.41	105.07
5	A	1003	SMA	O12-C12-C13	2.24	111.28	107.97
5	A	1003	SMA	C7M-O7-C7	2.24	120.91	117.53
6	O	1004	ANJ	O8-C14-C15	-2.23	103.05	107.47
4	A	1002	HEM	C3B-C2B-C1B	2.22	108.13	106.49
6	E	1004	ANJ	C6-C8-N2	2.21	120.90	116.80
5	A	1003	SMA	O14-C14-C13	-2.21	103.36	107.98
6	O	1004	ANJ	C6-C8-N2	2.21	120.89	116.80
5	A	1003	SMA	C9-C10-C11	-2.19	110.51	114.52
5	K	1003	SMA	O14-C14-C13	-2.19	103.41	107.98
4	A	1001	HEM	C2C-C3C-C4C	2.19	108.43	106.90
6	K	1004	ANJ	O1-C1-N1	2.18	128.57	125.80
5	K	1003	SMA	C5M-O5-C5	2.18	120.82	117.53
8	K	1006	LOP	O6-C24-C25	2.18	118.74	111.91
4	K	1002	HEM	CHA-C4D-ND	2.16	127.05	124.38
8	A	1006	LOP	P1-O1-C2	-2.12	111.13	121.59
4	A	1001	HEM	CAB-C3B-C2B	-2.11	121.65	128.60
6	O	1004	ANJ	C9-N2-C8	2.08	125.28	121.52
5	E	1003	SMA	C22-C11-C10	2.07	113.61	110.36
4	O	1001	HEM	CBD-CAD-C3D	-2.06	106.91	112.63
9	P	1001	HEC	CAD-CBD-CGD	-2.04	108.03	113.76
4	E	1002	HEM	C2D-C1D-ND	-2.04	107.44	109.88
4	K	1002	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
4	E	1001	HEM	CBA-CAA-C2A	-2.03	109.16	112.62
6	O	1004	ANJ	O6-C17-O7	-2.02	121.53	124.08
9	F	1001	HEC	CMB-C2B-C1B	-2.02	125.36	128.46
6	A	1004	ANJ	C6-C8-N2	2.01	120.52	116.80
5	A	1003	SMA	C9-C2-C3	2.01	130.01	127.07
4	K	1001	HEM	CAB-C3B-C2B	-2.01	121.99	128.60
4	K	1002	HEM	C1B-NB-C4B	2.01	107.14	105.07
4	A	1002	HEM	CAD-CBD-CGD	-2.00	109.29	113.60
4	E	1001	HEM	CAD-CBD-CGD	-2.00	109.29	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	1001	HEC	C2B-C3B-C4B	2.00	108.51	106.35
4	A	1002	HEM	C4C-CHD-C1D	2.00	125.20	122.56

There are no chirality outliers.

All (188) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1004	ANJ	C9-C10-O4-C12
6	A	1004	ANJ	C16-C15-O6-C17
6	A	1004	ANJ	O7-C17-O6-C15
6	A	1004	ANJ	C9-C17-O6-C15
6	A	1004	ANJ	O8-C14-C15-O6
6	A	1004	ANJ	O8-C14-C15-C16
6	A	1004	ANJ	C13-C14-C15-O6
6	E	1004	ANJ	O7-C17-O6-C15
6	E	1004	ANJ	C9-C17-O6-C15
6	K	1004	ANJ	C9-C10-O4-C12
6	K	1004	ANJ	C16-C15-O6-C17
6	K	1004	ANJ	O7-C17-O6-C15
6	K	1004	ANJ	C9-C17-O6-C15
6	K	1004	ANJ	O8-C14-C15-O6
6	K	1004	ANJ	O8-C14-C15-C16
6	K	1004	ANJ	C13-C14-C15-O6
6	O	1004	ANJ	C9-C10-O4-C12
6	O	1004	ANJ	C16-C15-O6-C17
6	O	1004	ANJ	O7-C17-O6-C15
6	O	1004	ANJ	C9-C17-O6-C15
6	O	1004	ANJ	O8-C14-C15-O6
6	O	1004	ANJ	C13-C14-C15-O6
8	A	1006	LOP	C3-O2-P1-O4
8	E	1005	LOP	N1-C1-C2-O1
8	E	1005	LOP	C2-O1-P1-O2
8	E	1005	LOP	C2-O1-P1-O3
8	E	1005	LOP	C2-O1-P1-O4
8	E	1005	LOP	C3-O2-P1-O3
8	E	1005	LOP	C3-O2-P1-O4
8	K	1006	LOP	C2-O1-P1-O2
8	K	1006	LOP	C2-O1-P1-O3
8	K	1006	LOP	C2-O1-P1-O4
8	K	1006	LOP	C3-O2-P1-O3
8	K	1006	LOP	O5-C4-C5-O6
8	A	1006	LOP	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	1004	ANJ	C14-C13-C18-C19
6	K	1004	ANJ	C14-C13-C18-C19
6	E	1004	ANJ	C12-C13-C18-C19
6	K	1004	ANJ	C12-C13-C18-C19
6	O	1004	ANJ	C12-C13-C18-C19
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	E	1003	SMA	C6-C5-O5-C5M
8	K	1006	LOP	C13-C14-C15-C16
8	E	1005	LOP	C24-C25-C26-C27
5	A	1003	SMA	C4A-C5-O5-C5M
5	K	1003	SMA	C4A-C5-O5-C5M
5	O	1003	SMA	C4A-C5-O5-C5M
5	E	1003	SMA	C4A-C5-O5-C5M
6	A	1004	ANJ	O9-C24-C25-C26
8	A	1006	LOP	C3-O2-P1-O1
8	E	1005	LOP	C3-O2-P1-O1
8	K	1006	LOP	C3-O2-P1-O1
8	O	1005	LOP	C24-C25-C26-C27
8	A	1006	LOP	O7-C6-O5-C4
8	E	1005	LOP	C17-C18-C19-C20
8	O	1005	LOP	C17-C18-C19-C20
8	O	1005	LOP	O7-C6-O5-C4
8	A	1006	LOP	C16-C17-C18-C19
8	E	1005	LOP	C16-C17-C18-C19
8	E	1005	LOP	C9-C10-C11-C12
8	K	1006	LOP	C9-C10-C11-C12
8	O	1005	LOP	C9-C10-C11-C12
8	O	1005	LOP	C16-C17-C18-C19
6	E	1004	ANJ	C14-C13-C18-C19
8	K	1006	LOP	C15-C16-C17-C18
8	A	1006	LOP	C17-C18-C19-C20
8	O	1005	LOP	C30-C31-C32-C33
8	K	1006	LOP	C11-C12-C13-C14
8	K	1006	LOP	C27-C28-C29-C30
8	A	1006	LOP	C24-C25-C26-C27
6	E	1004	ANJ	C13-C18-C19-C20
8	K	1006	LOP	O8-C24-O6-C5
8	E	1005	LOP	C15-C16-C17-C18
8	O	1005	LOP	C11-C12-C13-C14
6	K	1004	ANJ	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	A	1006	LOP	C32-C33-C34-C35
8	K	1006	LOP	C3-C4-C5-O6
8	A	1006	LOP	C20-C21-C22-C23
8	A	1006	LOP	C28-C29-C30-C31
4	K	1001	HEM	C3D-CAD-CBD-CGD
8	E	1005	LOP	C6-C7-C8-C9
8	E	1005	LOP	C18-C19-C20-C21
8	E	1005	LOP	C30-C31-C32-C33
8	E	1005	LOP	C13-C14-C15-C16
8	O	1005	LOP	C13-C14-C15-C16
8	O	1005	LOP	C18-C19-C20-C21
5	K	1003	SMA	C9-C10-C11-C22
8	A	1006	LOP	O2-C3-C4-O5
6	A	1004	ANJ	O8-C24-C25-C26
8	K	1006	LOP	C28-C29-C30-C31
8	A	1006	LOP	O5-C4-C5-O6
8	A	1006	LOP	C9-C10-C11-C12
5	O	1003	SMA	C9-C10-C11-C22
8	K	1006	LOP	O2-C3-C4-O5
4	K	1001	HEM	C4B-C3B-CAB-CBB
4	O	1001	HEM	C4B-C3B-CAB-CBB
8	A	1006	LOP	C27-C28-C29-C30
6	K	1004	ANJ	O9-C24-C25-C26
6	O	1004	ANJ	O9-C24-C25-C26
8	A	1006	LOP	C2-O1-P1-O3
6	E	1004	ANJ	O8-C24-C25-C26
8	A	1006	LOP	C11-C12-C13-C14
4	K	1002	HEM	C1A-C2A-CAA-CBA
4	K	1002	HEM	C3A-C2A-CAA-CBA
6	O	1004	ANJ	O5-C12-O4-C10
8	A	1006	LOP	C18-C19-C20-C21
4	O	1001	HEM	C3D-CAD-CBD-CGD
8	E	1005	LOP	O2-C3-C4-C5
6	K	1004	ANJ	C26-C25-C27-C28
8	A	1006	LOP	C29-C30-C31-C32
8	O	1005	LOP	C2-O1-P1-O2
8	K	1006	LOP	C12-C13-C14-C15
8	O	1005	LOP	C28-C29-C30-C31
8	E	1005	LOP	C28-C29-C30-C31
4	A	1001	HEM	CAD-CBD-CGD-O1D
4	O	1001	HEM	CAA-CBA-CGA-O1A
8	E	1005	LOP	C3-C4-C5-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	K	1006	LOP	O7-C6-O5-C4
4	K	1001	HEM	CAA-CBA-CGA-O1A
8	K	1006	LOP	C30-C31-C32-C33
8	A	1006	LOP	C12-C13-C14-C15
4	O	1001	HEM	CAA-CBA-CGA-O2A
8	O	1005	LOP	C7-C8-C9-C10
5	A	1003	SMA	C26-C19-C20-C21
4	K	1001	HEM	CAA-CBA-CGA-O2A
4	A	1001	HEM	CAD-CBD-CGD-O2D
8	E	1005	LOP	O6-C24-C25-C26
8	O	1005	LOP	O6-C24-C25-C26
8	E	1005	LOP	C25-C26-C27-C28
8	O	1005	LOP	C25-C26-C27-C28
4	E	1001	HEM	C3D-CAD-CBD-CGD
8	O	1005	LOP	O2-C3-C4-O5
8	K	1006	LOP	C25-C24-O6-C5
4	A	1002	HEM	CAD-CBD-CGD-O2D
4	O	1002	HEM	CAA-CBA-CGA-O1A
8	O	1005	LOP	C29-C30-C31-C32
8	K	1006	LOP	O2-C3-C4-C5
4	K	1001	HEM	CAD-CBD-CGD-O2D
8	E	1005	LOP	C26-C27-C28-C29
4	A	1001	HEM	CAA-CBA-CGA-O2A
4	E	1001	HEM	CAD-CBD-CGD-O2D
9	B	1001	HEC	CAA-CBA-CGA-O2A
8	K	1006	LOP	O5-C6-C7-C8
8	A	1006	LOP	C26-C27-C28-C29
8	O	1005	LOP	C12-C13-C14-C15
8	A	1006	LOP	C7-C8-C9-C10
6	A	1004	ANJ	C19-C20-C21-C22
4	E	1001	HEM	CAA-CBA-CGA-O1A
4	E	1002	HEM	CAA-CBA-CGA-O1A
8	E	1005	LOP	C14-C15-C16-C17
6	O	1004	ANJ	O8-C24-C25-C26
4	O	1001	HEM	CAD-CBD-CGD-O2D
9	F	1001	HEC	CAA-CBA-CGA-O2A
4	A	1002	HEM	CAD-CBD-CGD-O1D
4	K	1001	HEM	CAD-CBD-CGD-O1D
8	O	1005	LOP	O5-C6-C7-C8
8	E	1005	LOP	C12-C13-C14-C15
8	A	1006	LOP	C25-C26-C27-C28
4	A	1001	HEM	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	1001	HEM	CAD-CBD-CGD-O1D
4	O	1001	HEM	CAD-CBD-CGD-O1D
4	E	1001	HEM	CAA-CBA-CGA-O2A
9	F	1001	HEC	CAA-CBA-CGA-O1A
9	L	1001	HEC	CAA-CBA-CGA-O1A
9	L	1001	HEC	CAA-CBA-CGA-O2A
6	K	1004	ANJ	O8-C24-C25-C27
9	B	1001	HEC	CAA-CBA-CGA-O1A
9	P	1001	HEC	CAA-CBA-CGA-O2A
6	E	1004	ANJ	C9-C10-O4-C12
4	E	1002	HEM	CAA-CBA-CGA-O2A
8	A	1006	LOP	O5-C6-C7-C8
8	A	1006	LOP	C7-C6-O5-C4
6	O	1004	ANJ	C18-C19-C20-C21
8	A	1006	LOP	C2-O1-P1-O2
4	O	1002	HEM	CAA-CBA-CGA-O2A
9	L	1001	HEC	CAD-CBD-CGD-O2D
8	K	1006	LOP	C3-O2-P1-O4
8	O	1005	LOP	C2-O1-P1-O4
9	P	1001	HEC	CAA-CBA-CGA-O1A
8	A	1006	LOP	O6-C24-C25-C26
8	E	1005	LOP	O2-C3-C4-O5
8	K	1006	LOP	C14-C15-C16-C17
8	K	1006	LOP	O8-C24-C25-C26
8	O	1005	LOP	C26-C27-C28-C29
5	K	1003	SMA	C15-C14-O14-C25
9	L	1001	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

13 monomers are involved in 23 short contacts:

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

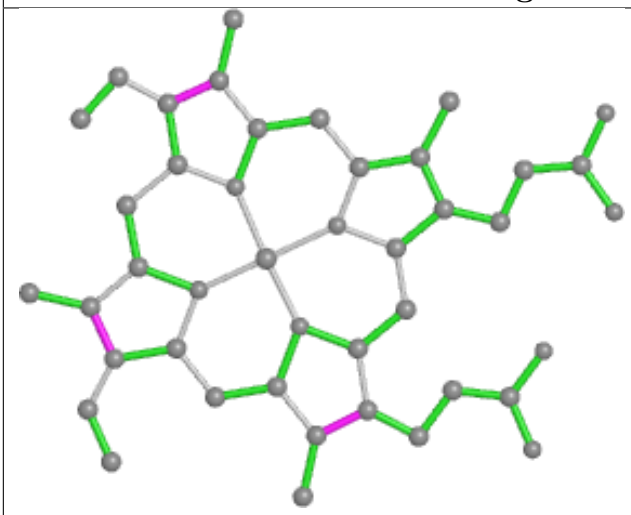
Continued on next page...

Continued from previous page...

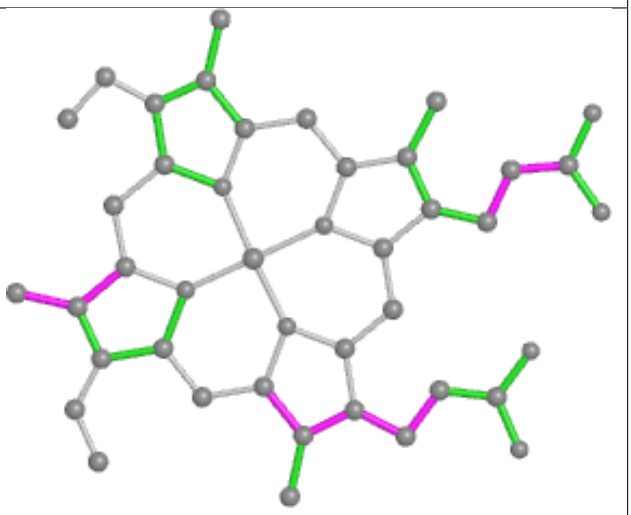
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	HEM	1	0
4	E	1001	HEM	2	0
9	P	1001	HEC	2	0

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.

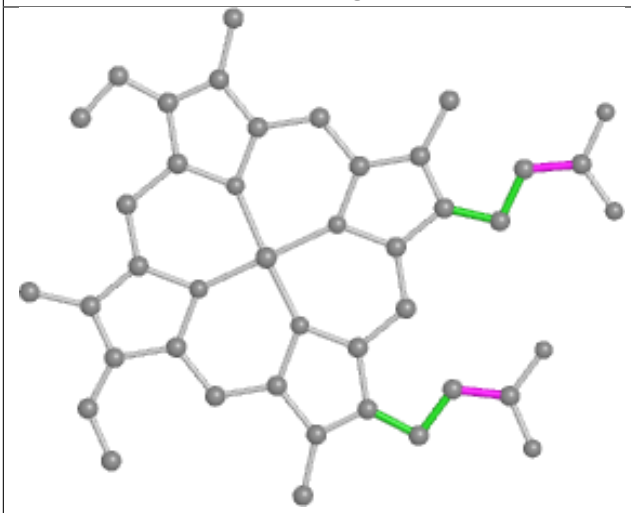
Ligand HEC L 1001



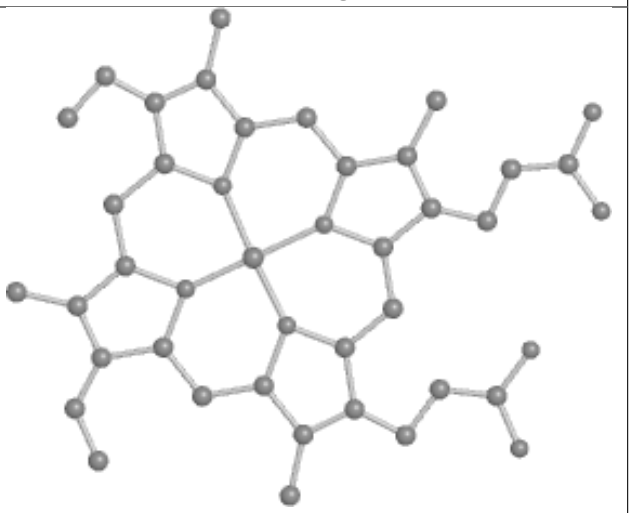
Bond lengths



Bond angles

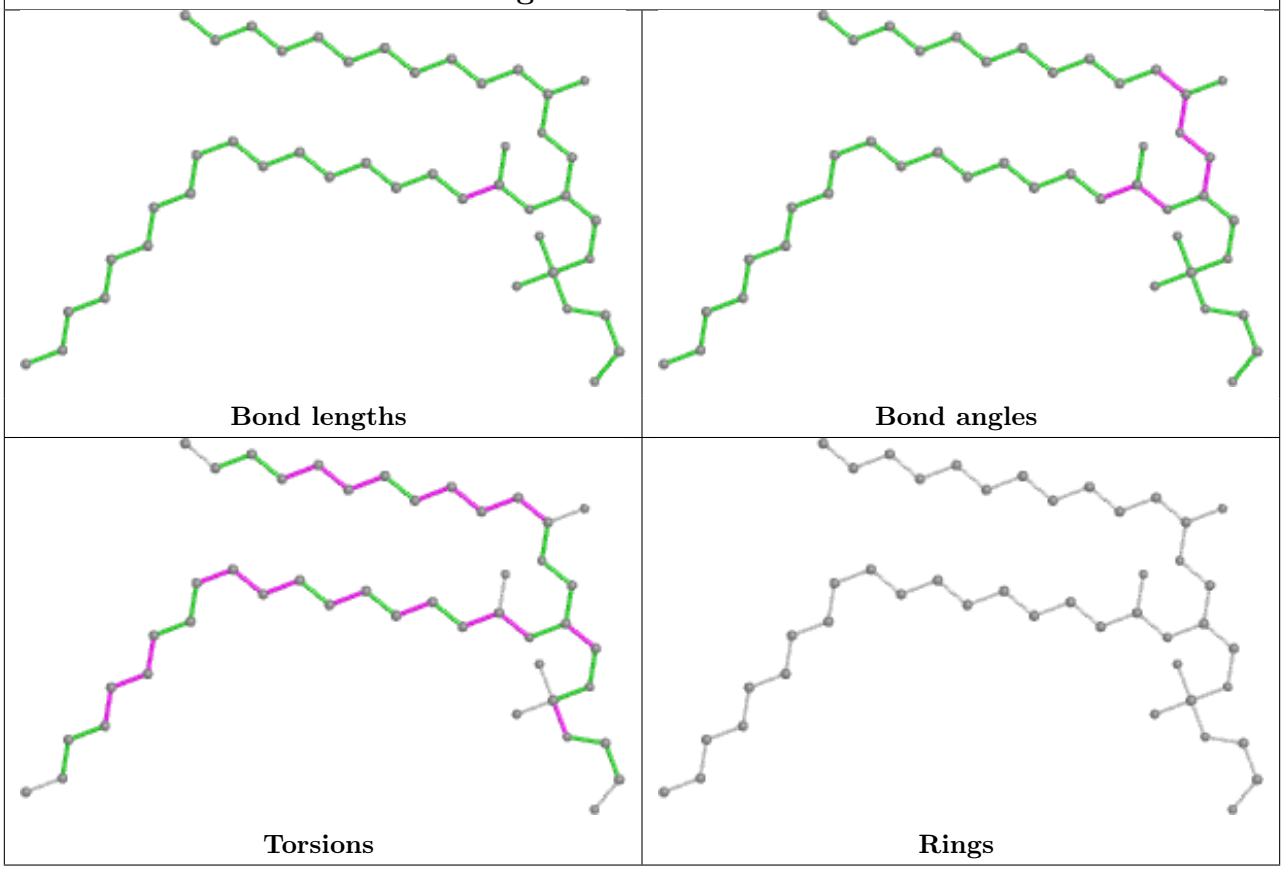


Torsions

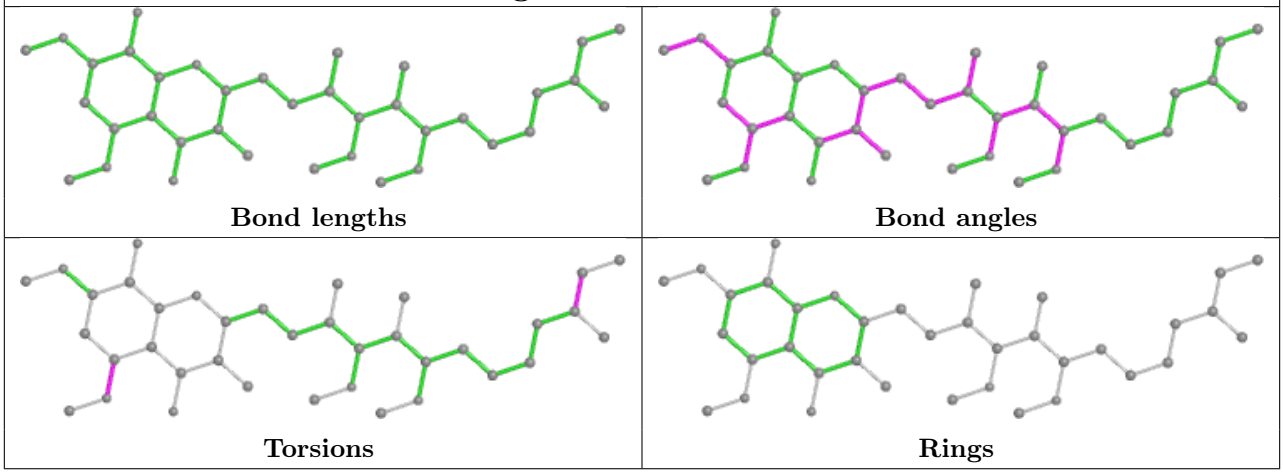


Rings

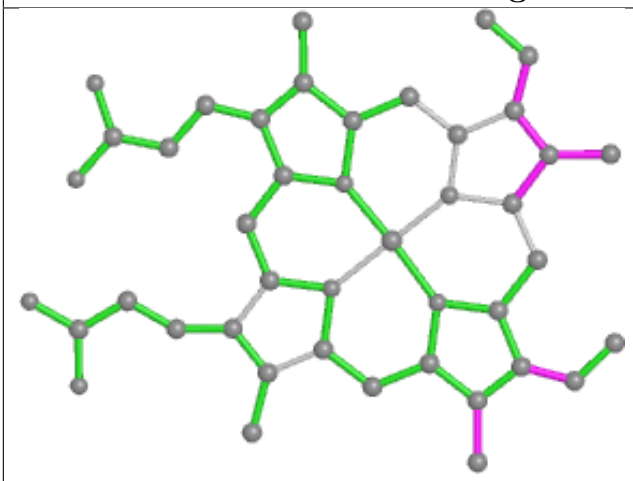
Ligand LOP O 1005



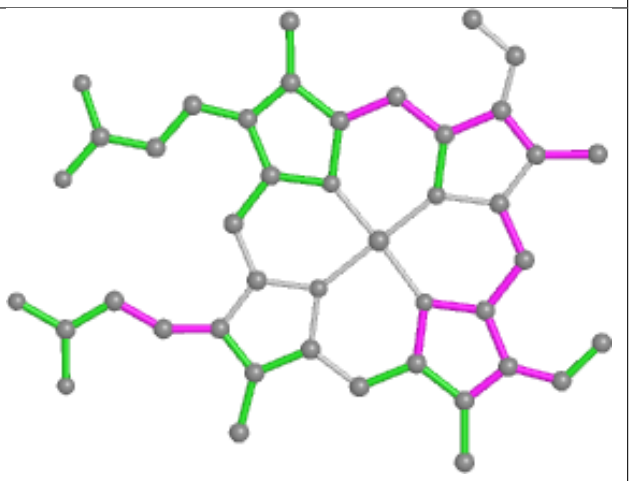
Ligand SMA A 1003



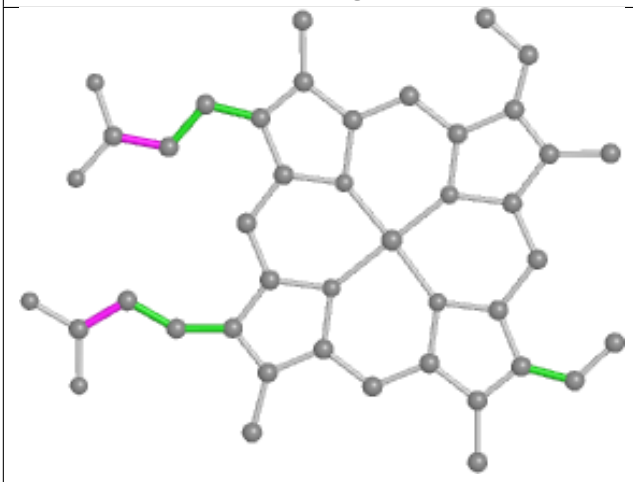
Ligand HEM A 1001



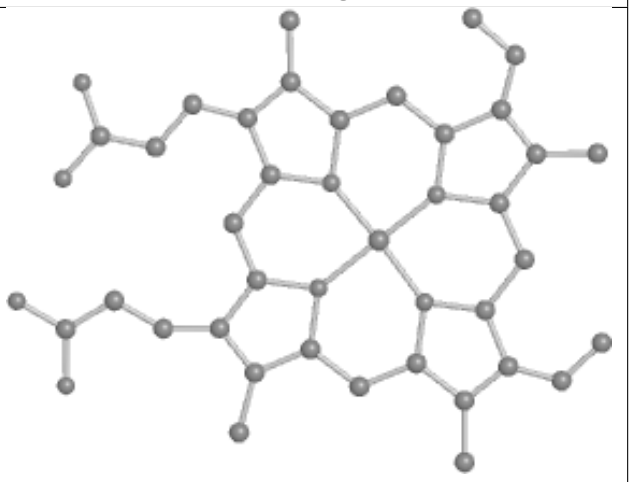
Bond lengths



Bond angles

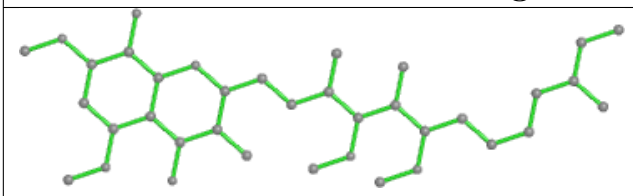


Torsions

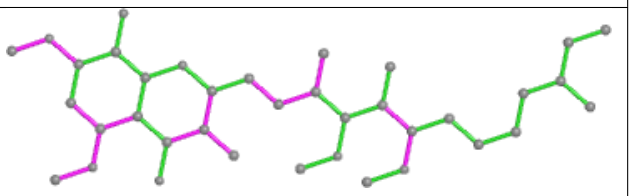


Rings

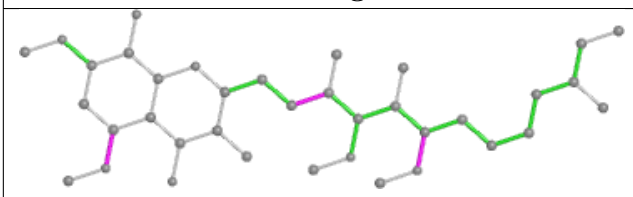
Ligand SMA K 1003



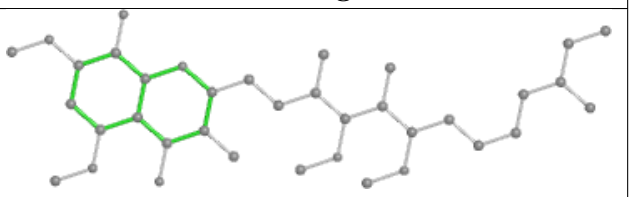
Bond lengths



Bond angles

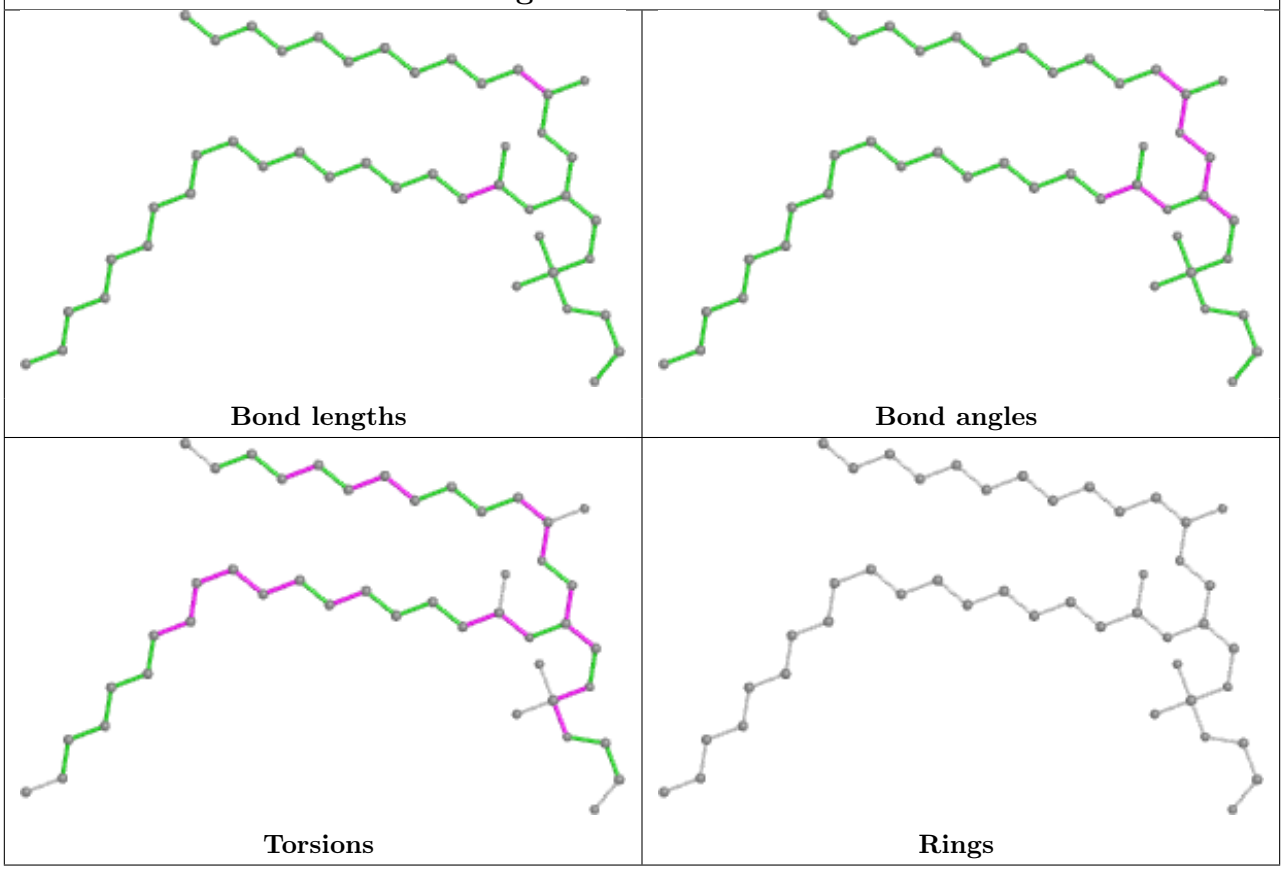


Torsions

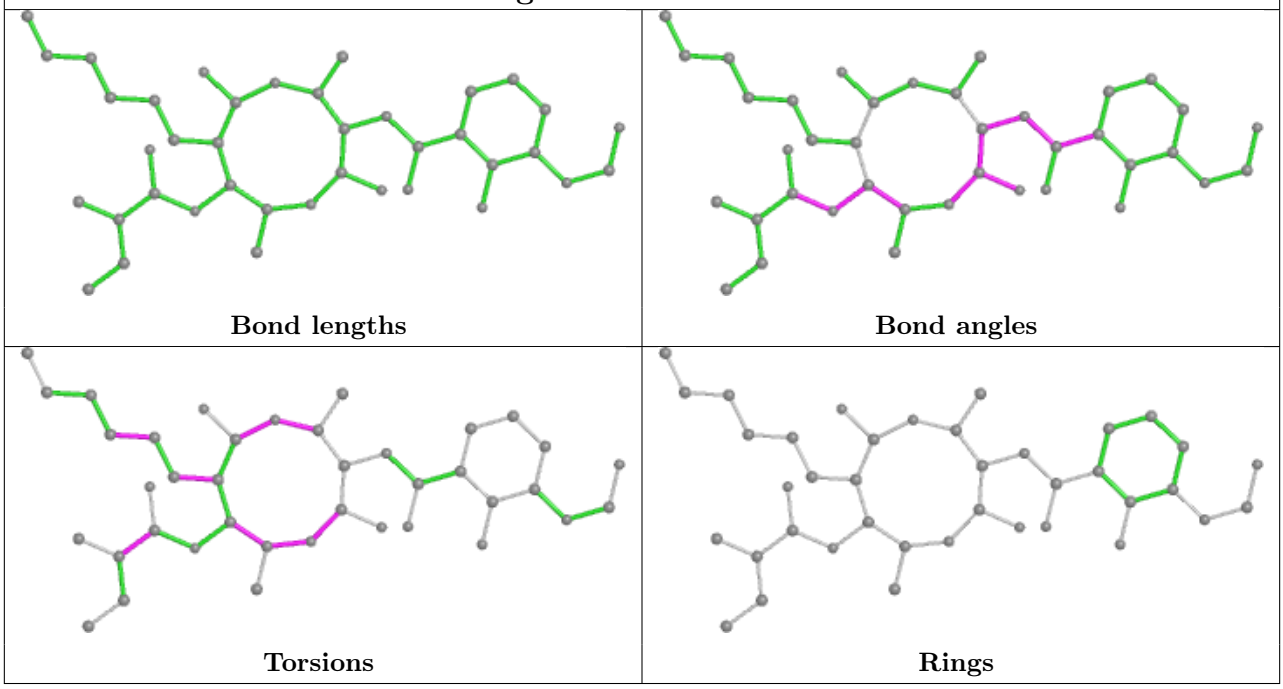


Rings

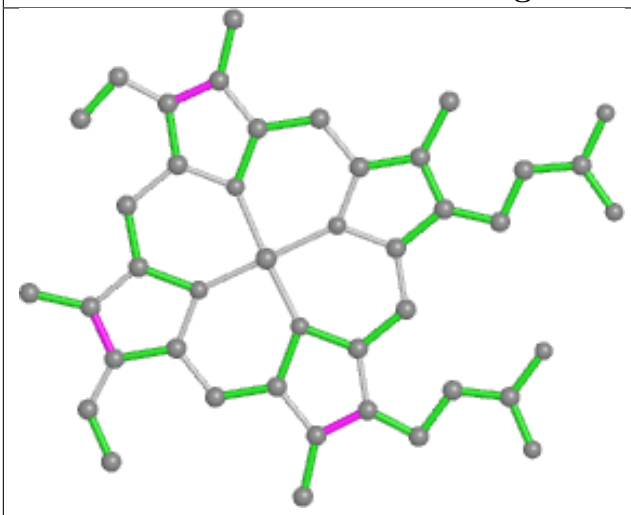
Ligand LOP K 1006



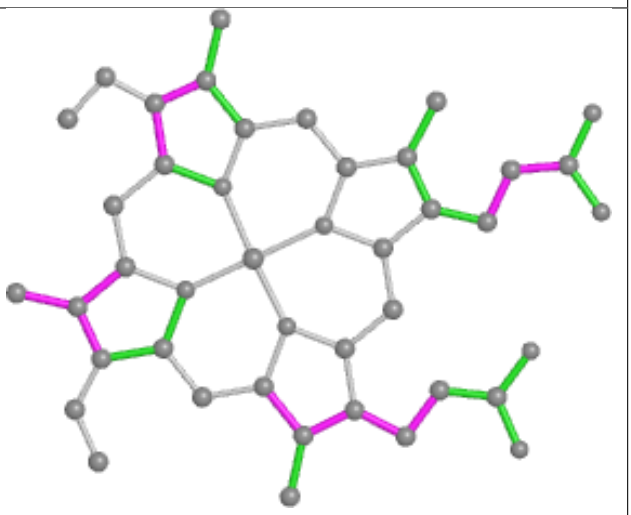
Ligand ANJ O 1004



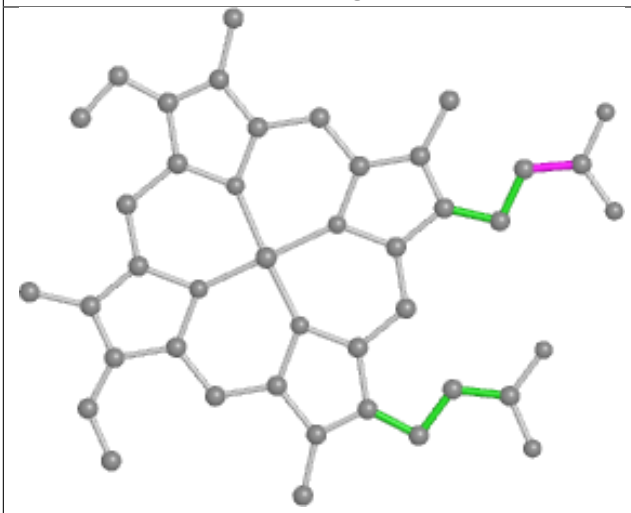
Ligand HEC B 1001



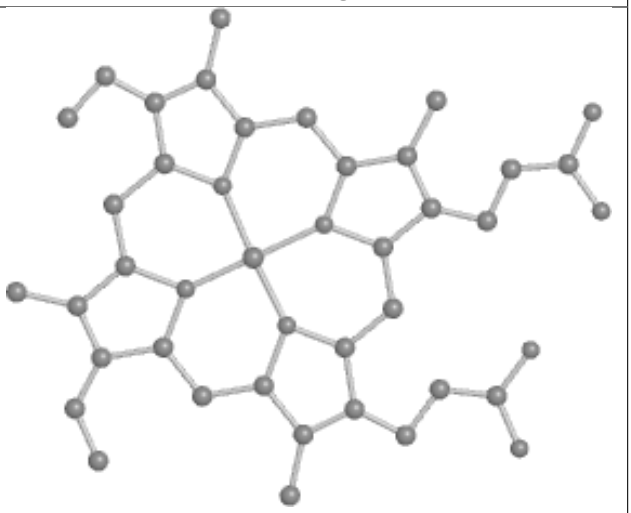
Bond lengths



Bond angles

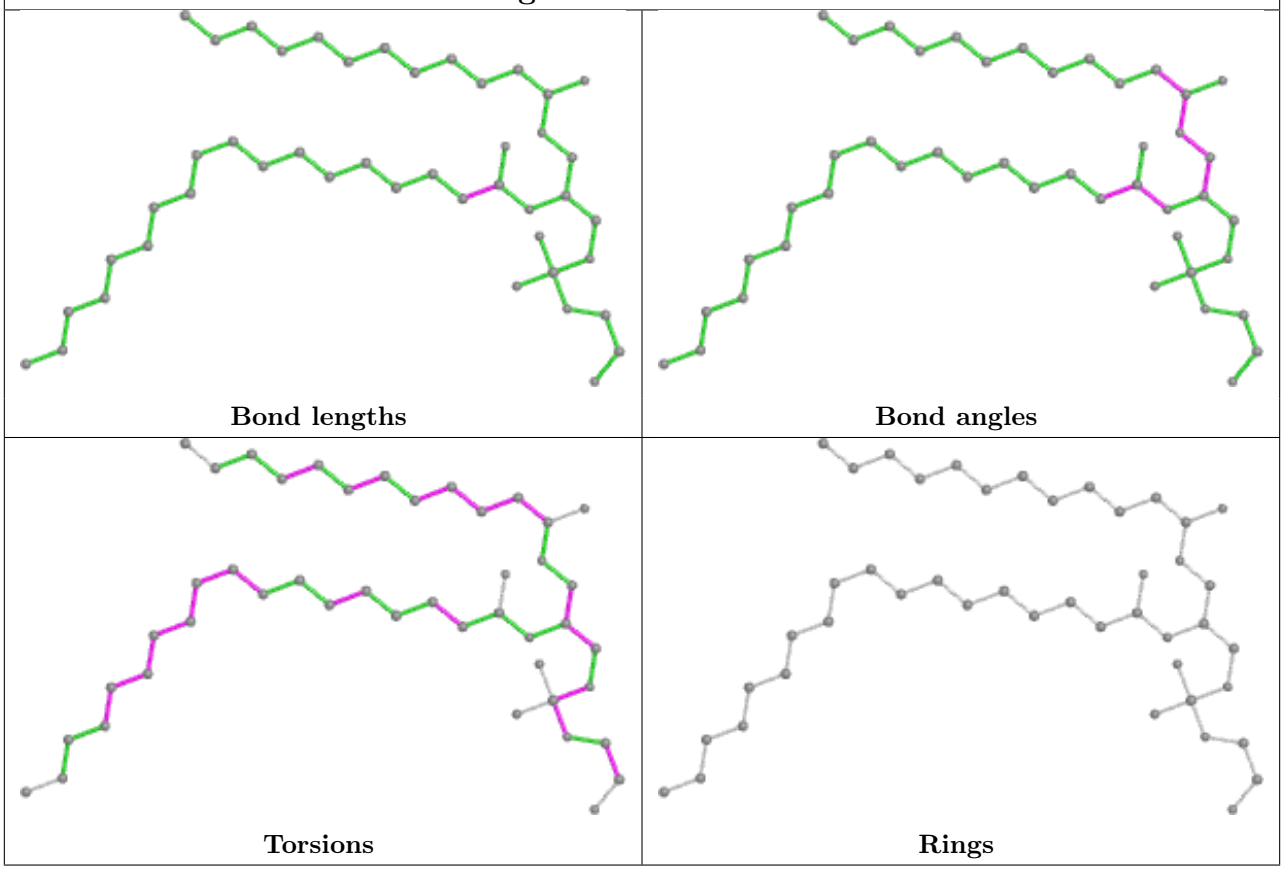


Torsions

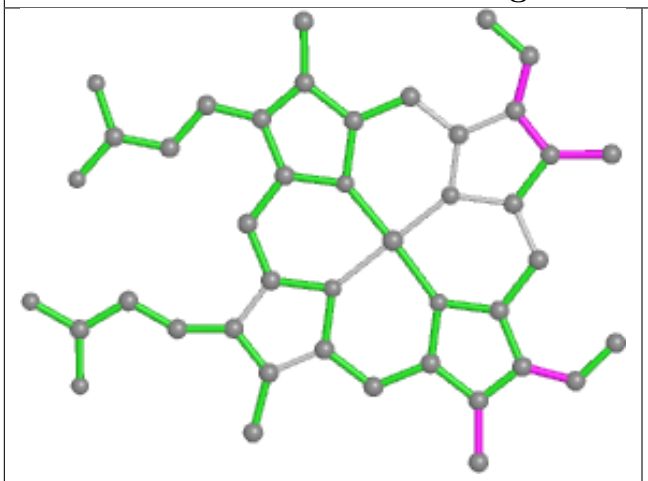


Rings

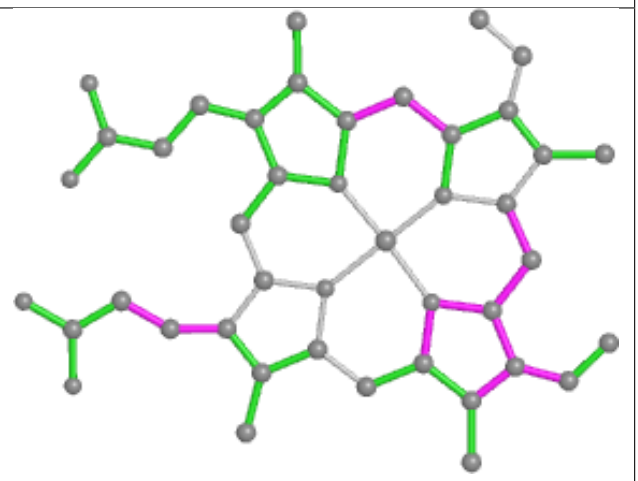
Ligand LOP E 1005



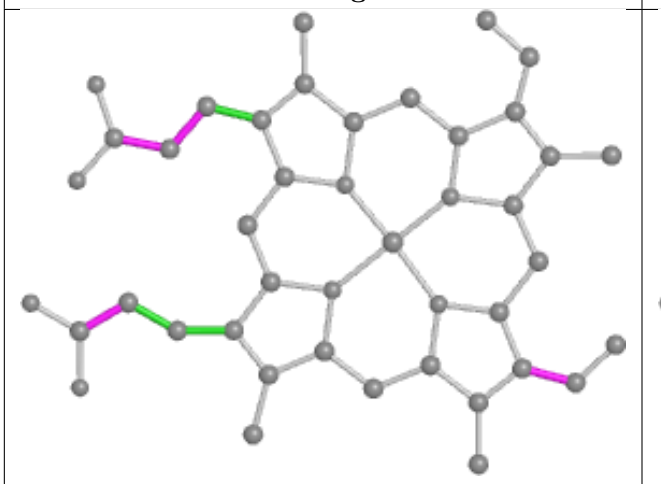
Ligand HEM K 1001



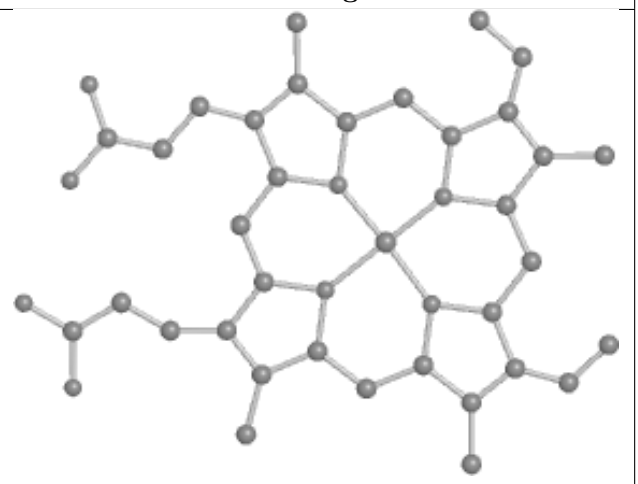
Bond lengths



Bond angles

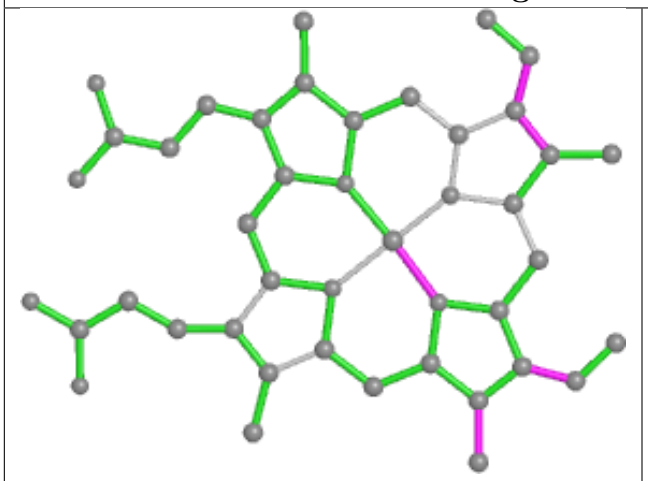


Torsions

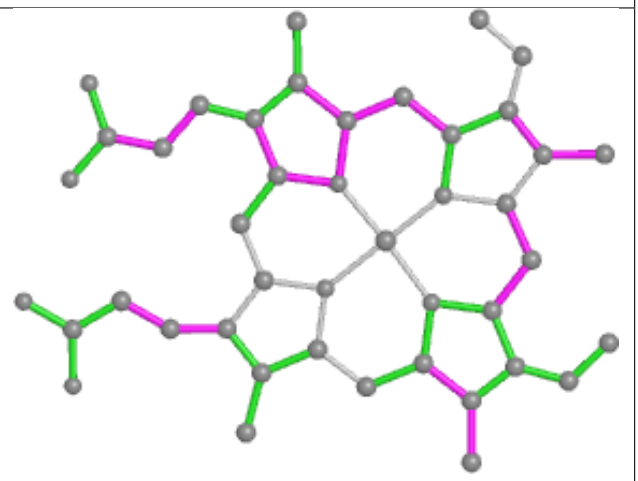


Rings

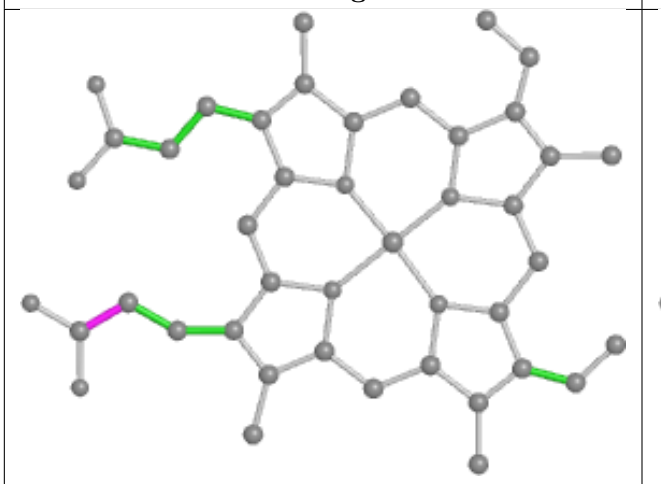
Ligand HEM E 1002



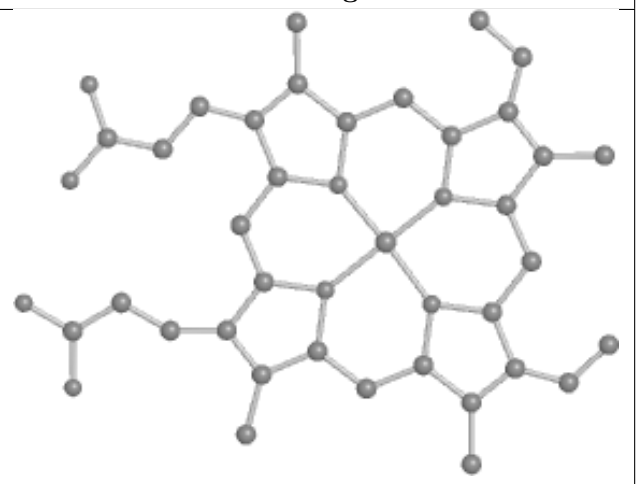
Bond lengths



Bond angles

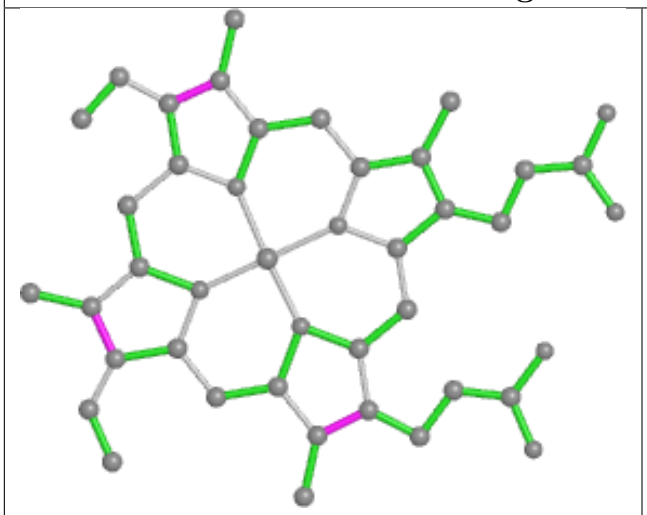


Torsions

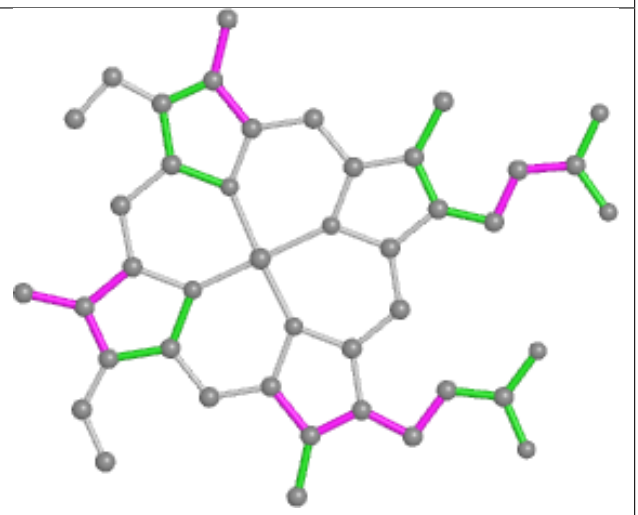


Rings

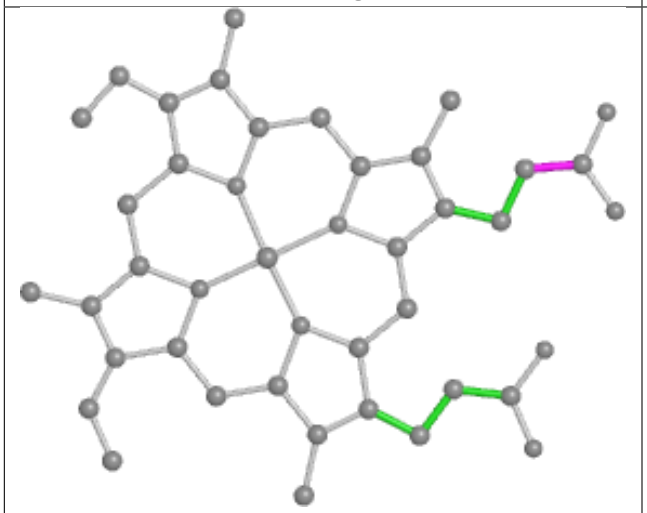
Ligand HEC F 1001



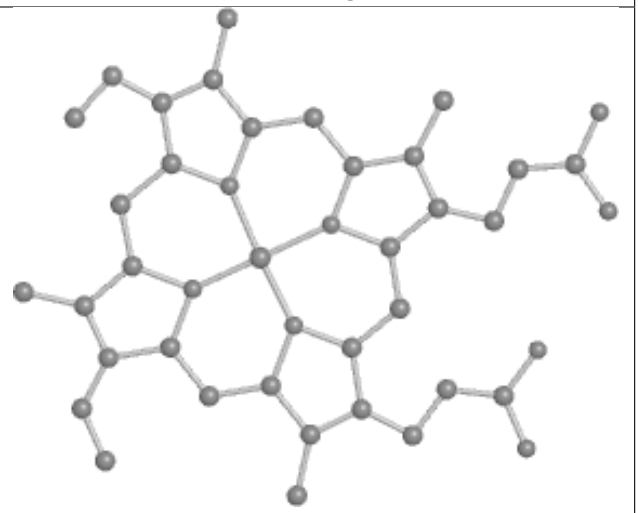
Bond lengths



Bond angles

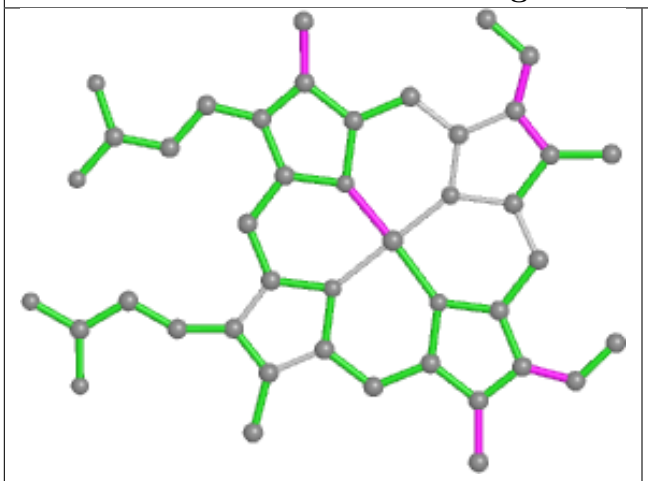


Torsions

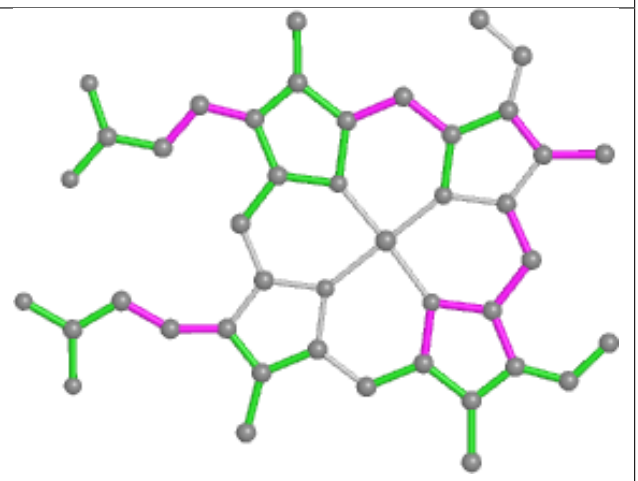


Rings

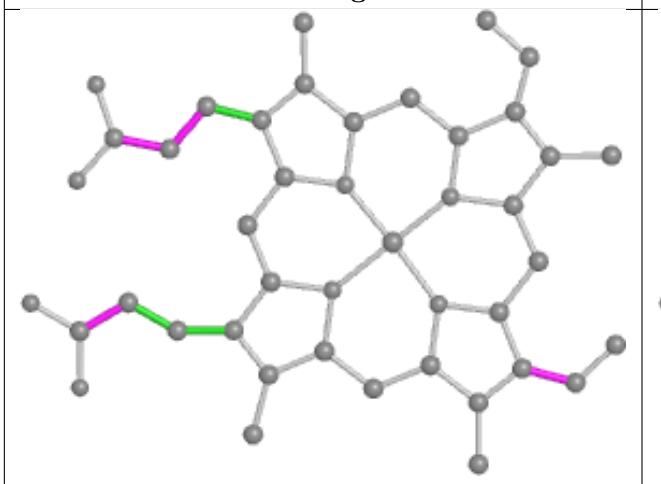
Ligand HEM O 1001



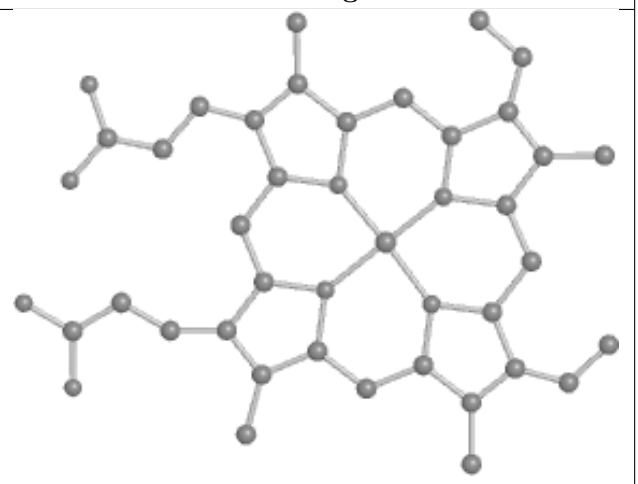
Bond lengths



Bond angles

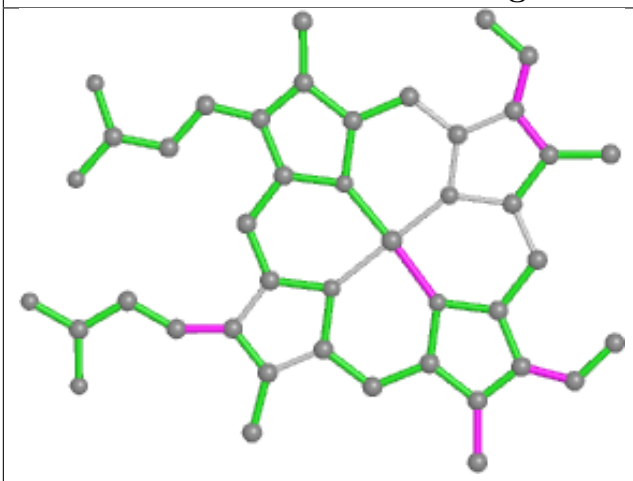


Torsions

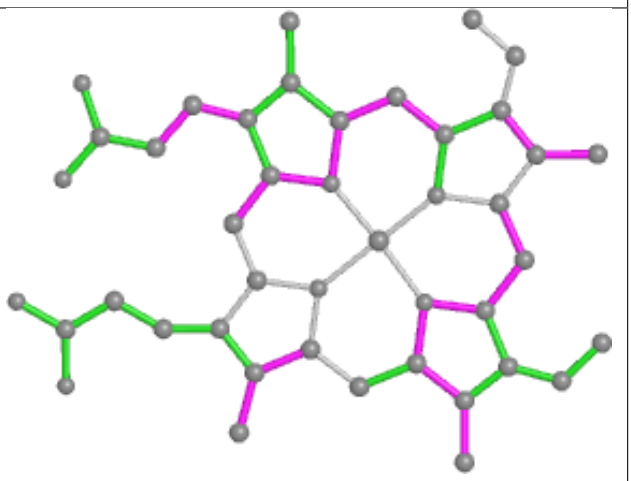


Rings

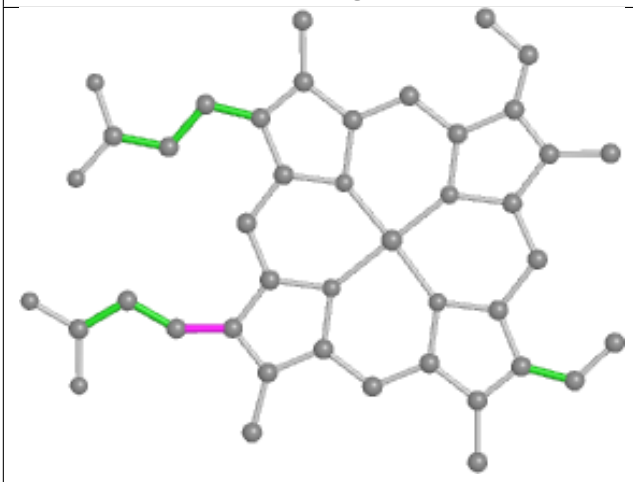
Ligand HEM K 1002



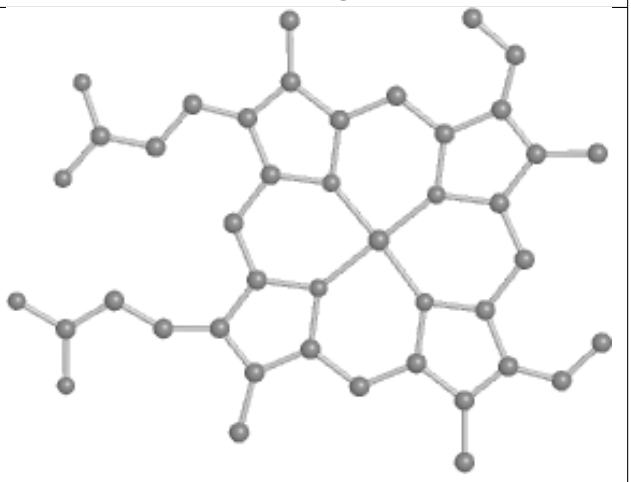
Bond lengths



Bond angles

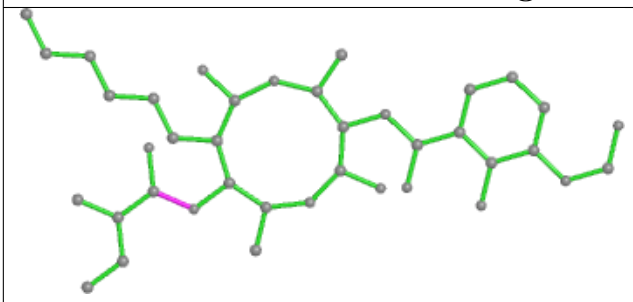


Torsions

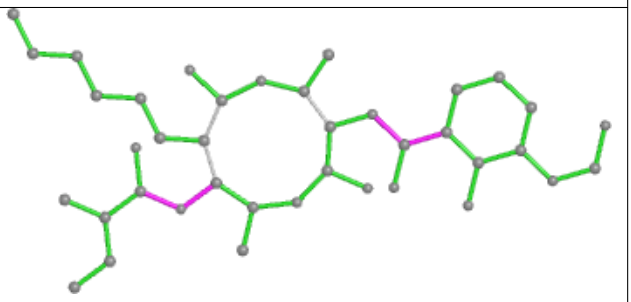


Rings

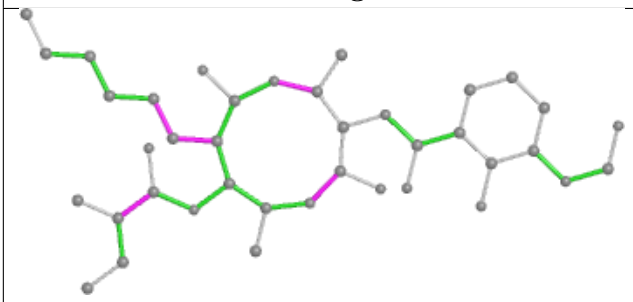
Ligand ANJ E 1004



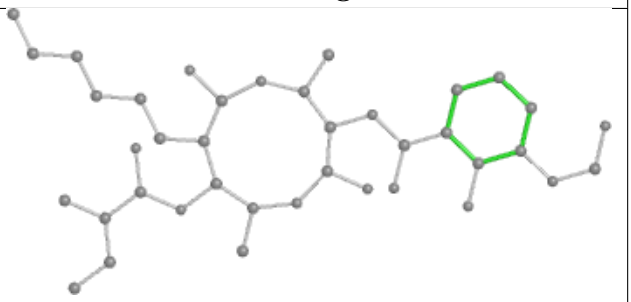
Bond lengths



Bond angles

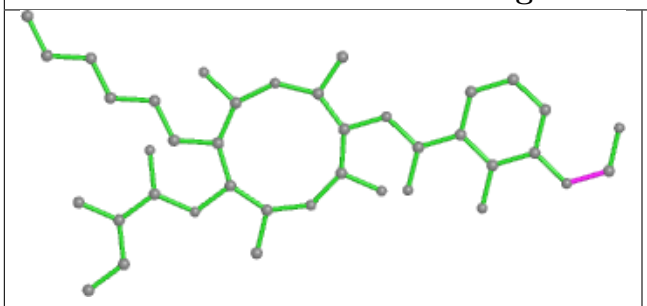


Torsions

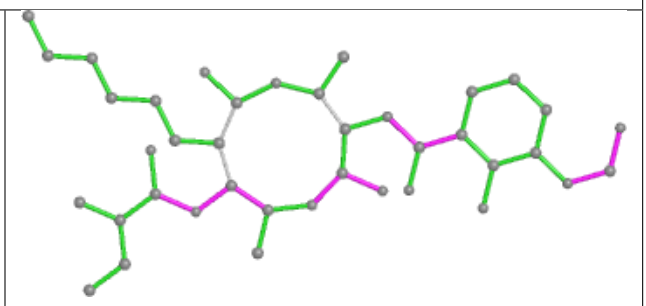


Rings

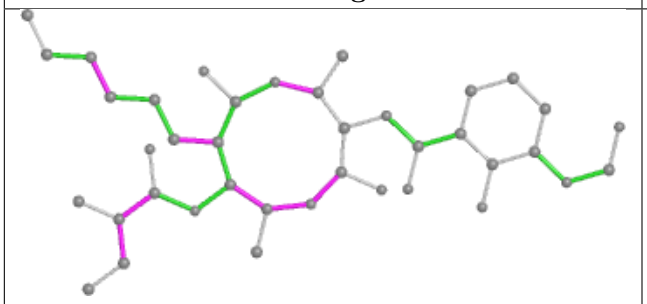
Ligand ANJ K 1004



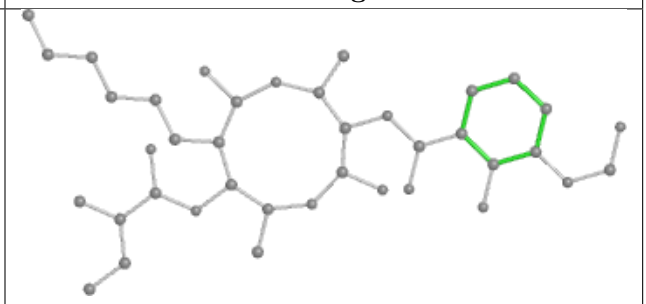
Bond lengths



Bond angles

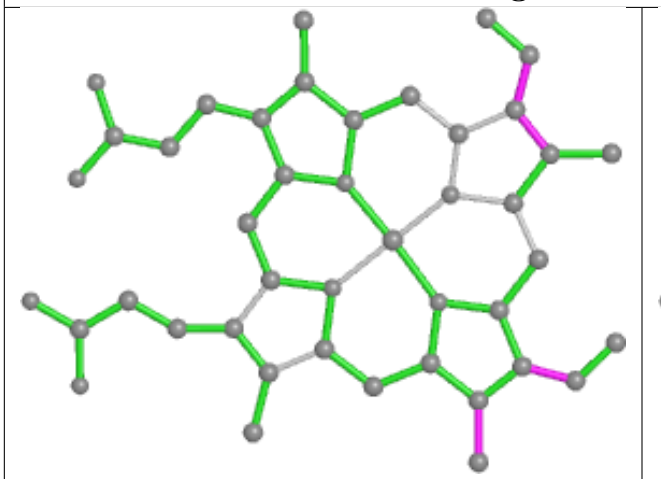


Torsions

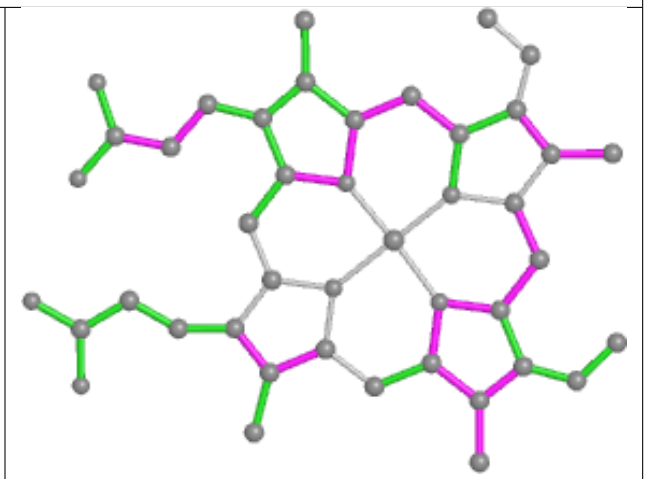


Rings

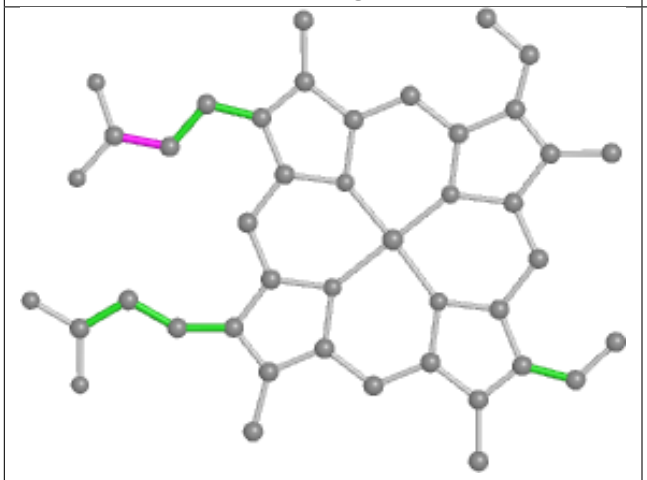
Ligand HEM A 1002



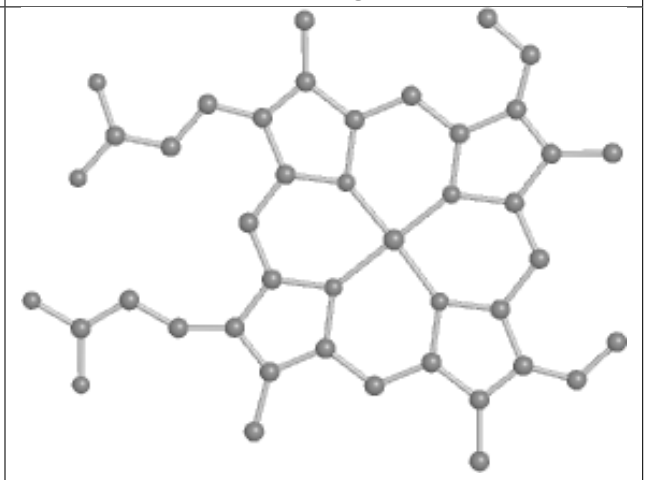
Bond lengths



Bond angles

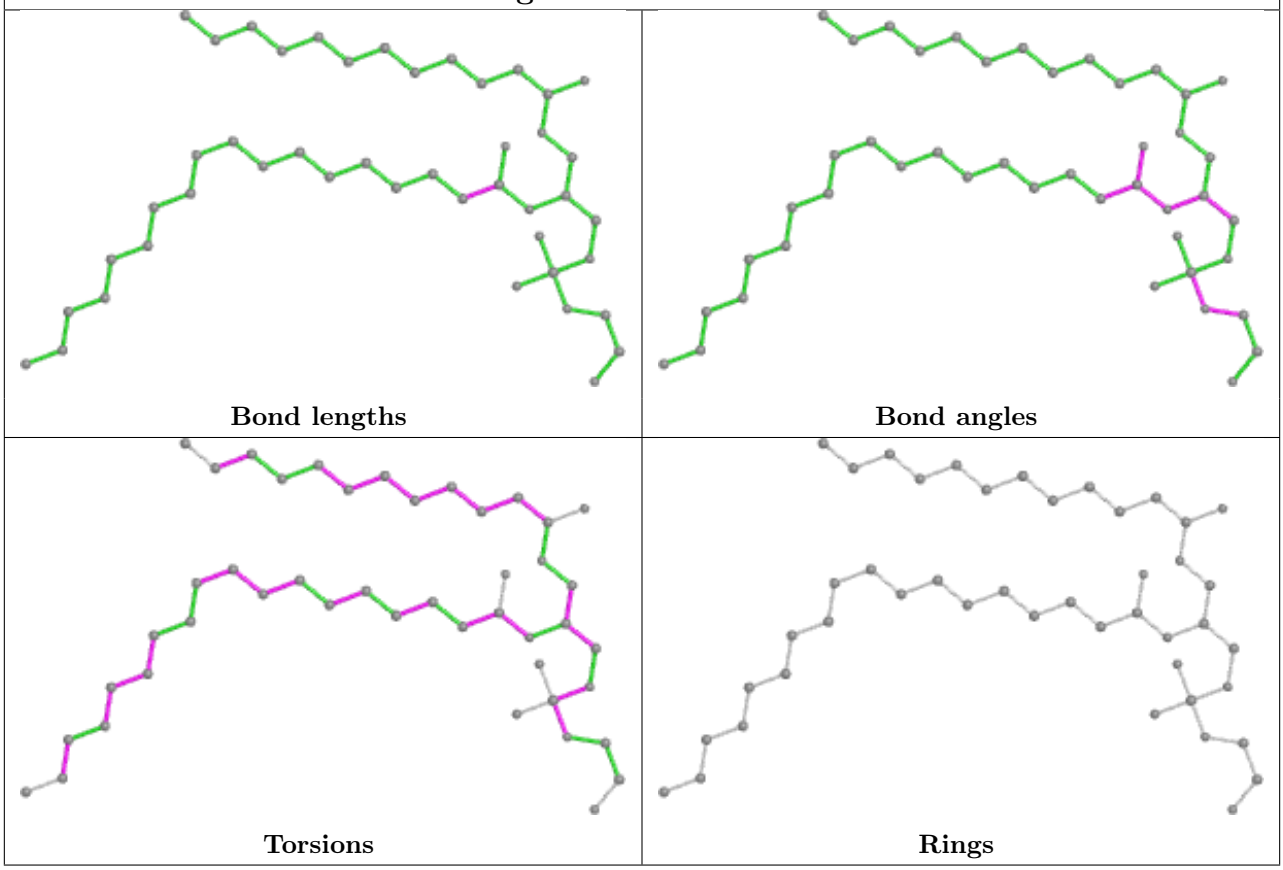


Torsions

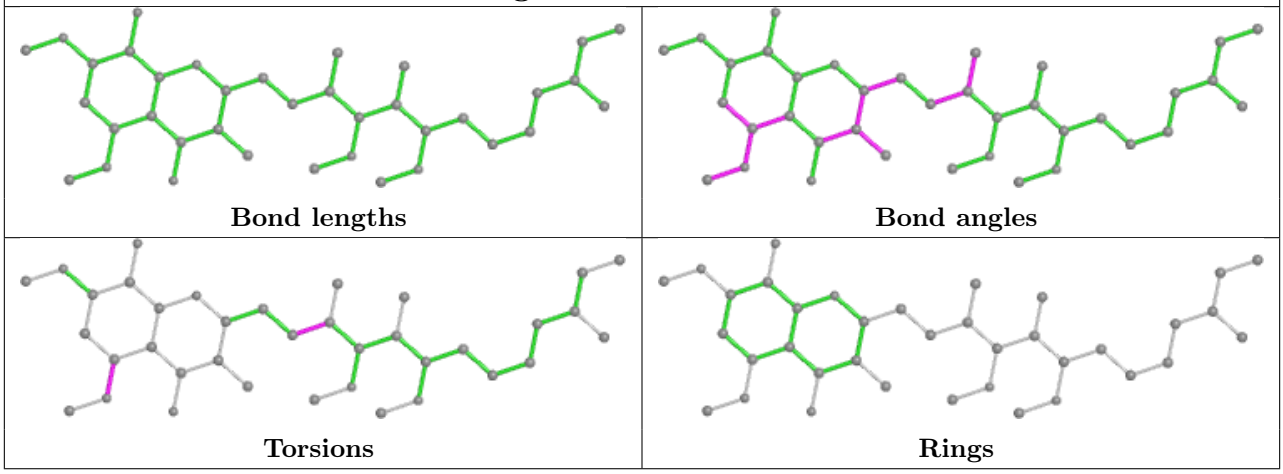


Rings

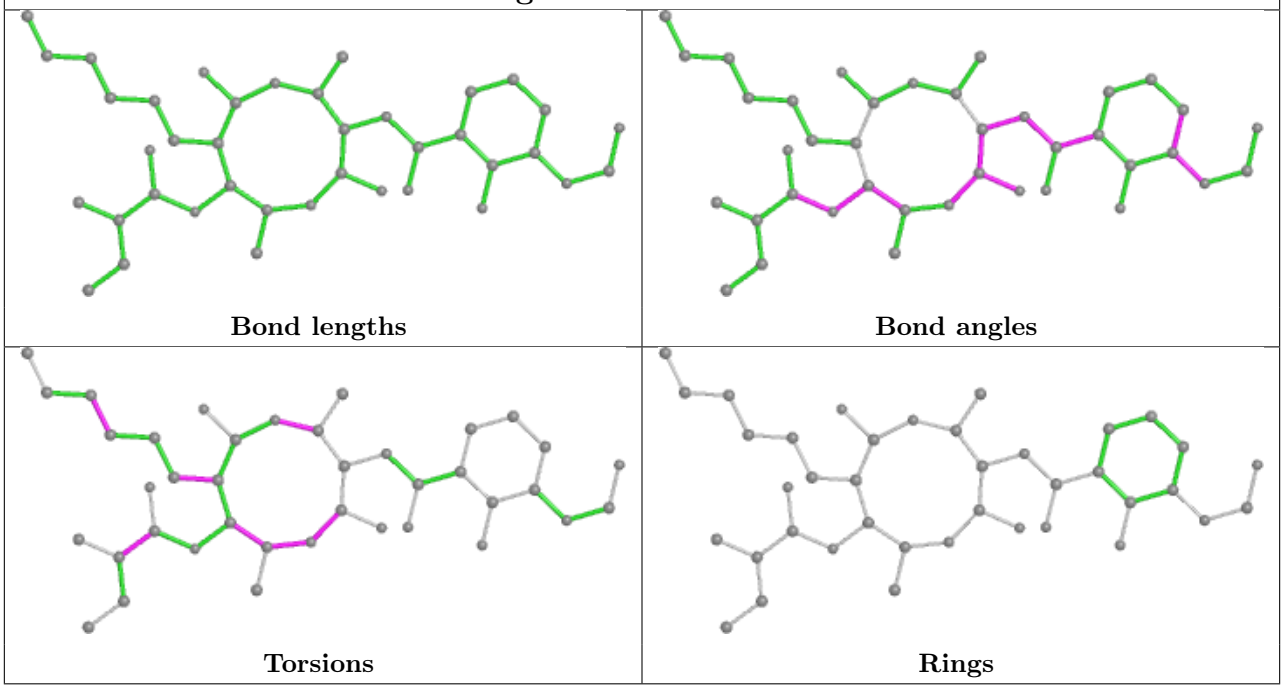
Ligand LOP A 1006



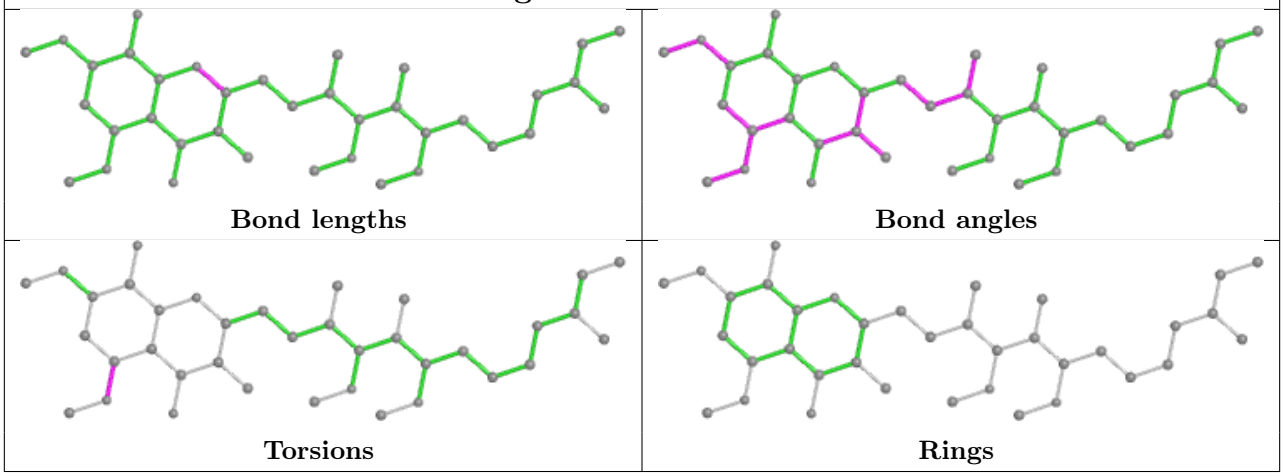
Ligand SMA O 1003



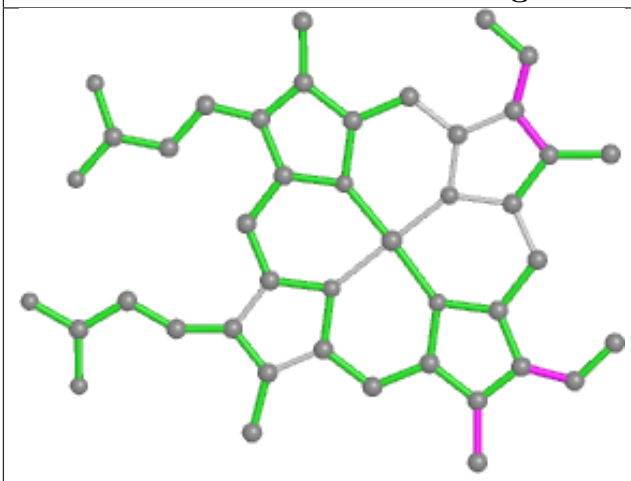
Ligand ANJ A 1004



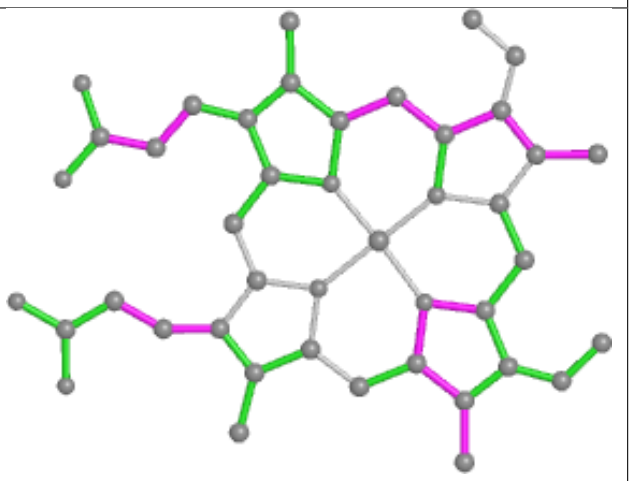
Ligand SMA E 1003



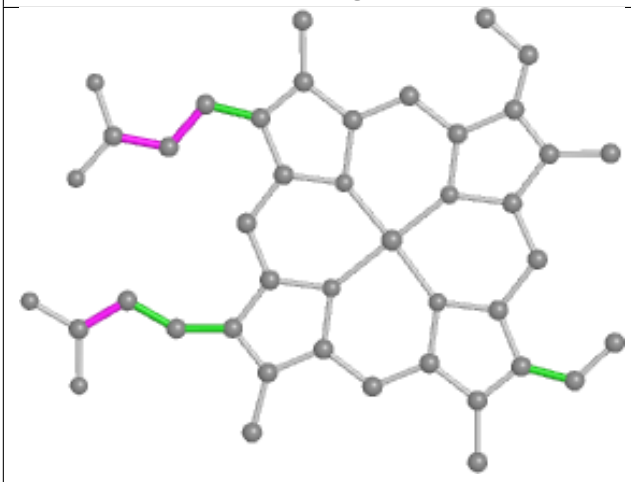
Ligand HEM E 1001



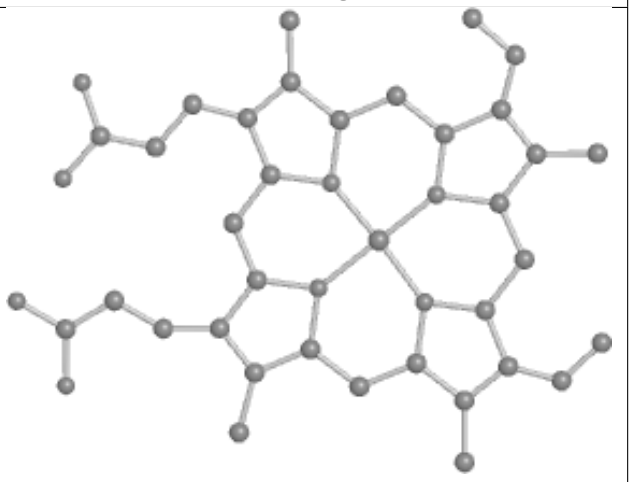
Bond lengths



Bond angles

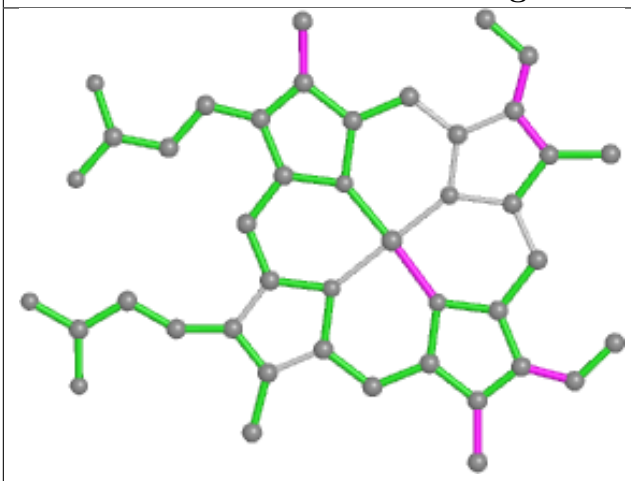


Torsions

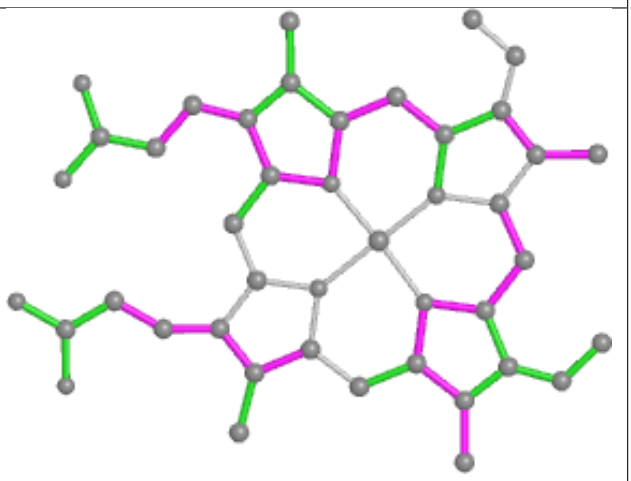


Rings

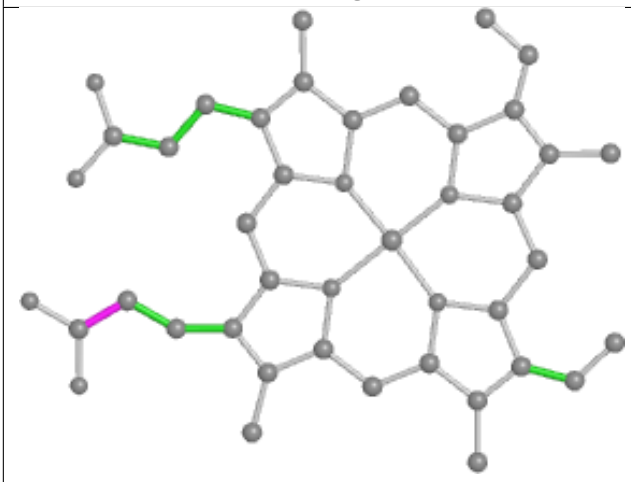
Ligand HEM O 1002



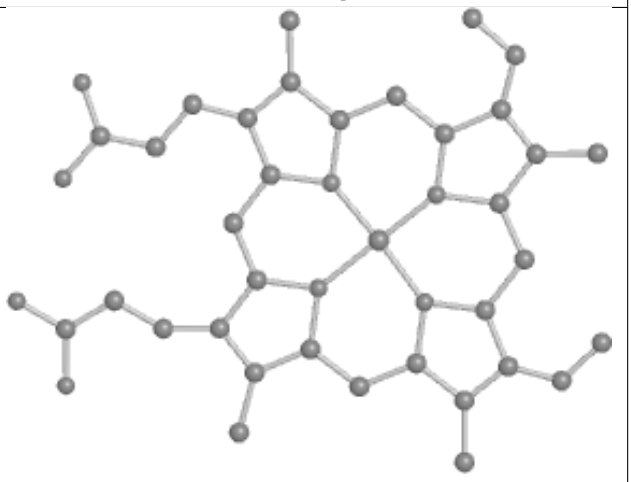
Bond lengths



Bond angles

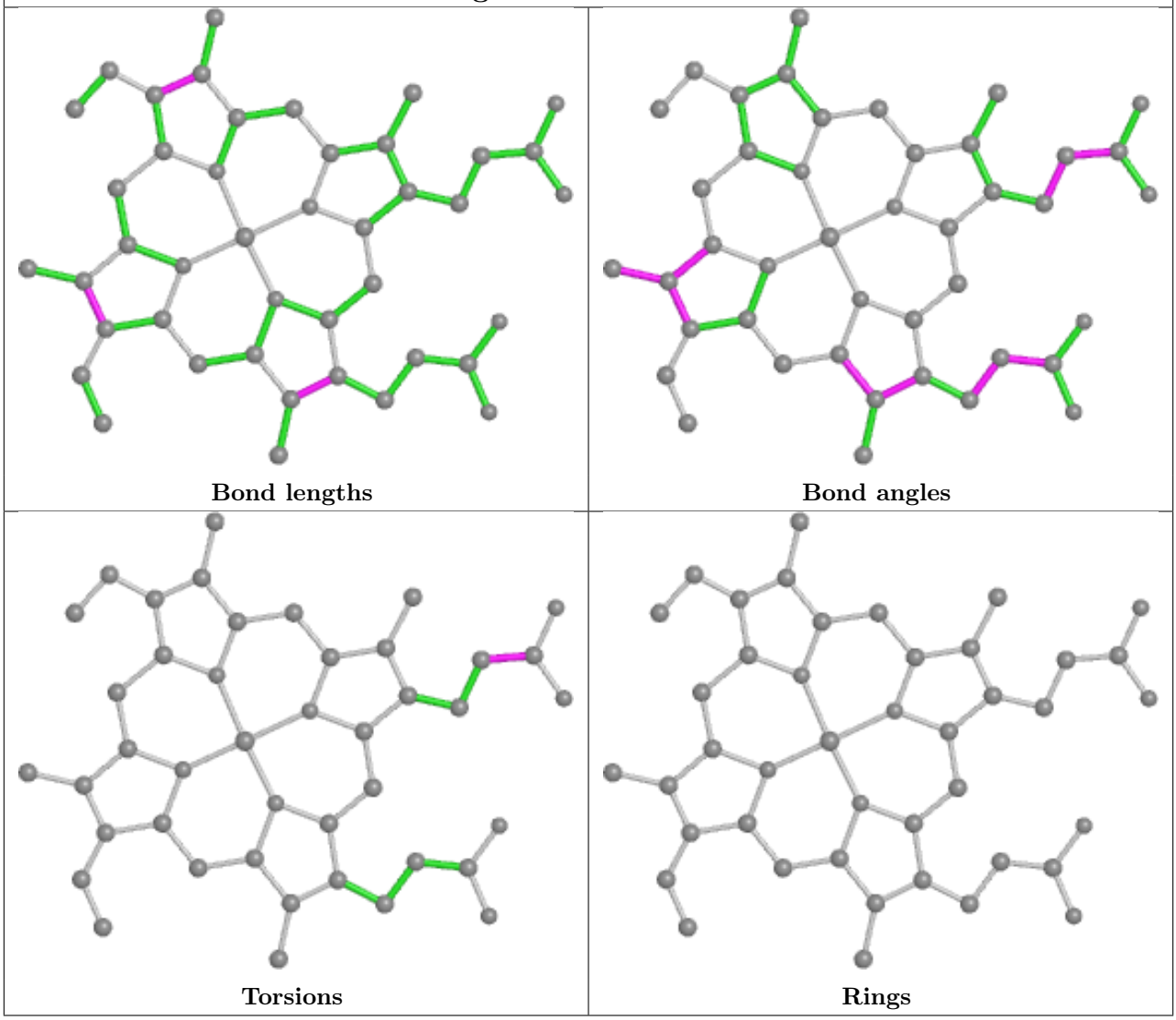


Torsions



Rings

Ligand HEC P 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	428/445 (96%)	0.38	27 (6%)	20	6	53, 88, 132, 178	0
1	E	428/445 (96%)	0.18	19 (4%)	34	13	49, 73, 119, 169	0
1	K	428/445 (96%)	0.10	15 (3%)	44	18	40, 63, 99, 154	0
1	O	428/445 (96%)	0.14	11 (2%)	56	27	49, 76, 119, 149	0
2	B	256/272 (94%)	0.40	25 (9%)	7	2	56, 85, 134, 199	0
2	F	256/272 (94%)	0.41	25 (9%)	7	2	57, 89, 130, 164	0
2	L	256/272 (94%)	0.41	25 (9%)	7	2	45, 75, 123, 167	0
2	P	256/272 (94%)	0.50	32 (12%)	3	1	64, 95, 130, 168	0
3	C	179/187 (95%)	0.56	18 (10%)	7	2	53, 87, 141, 184	0
3	G	179/187 (95%)	0.48	15 (8%)	11	3	67, 90, 133, 182	0
3	M	179/187 (95%)	0.60	19 (10%)	6	2	61, 85, 132, 172	0
3	Q	179/187 (95%)	0.39	12 (6%)	17	5	49, 86, 138, 190	0
All	All	3452/3616 (95%)	0.33	243 (7%)	16	5	40, 81, 128, 199	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	GLY	13.3
2	P	2	GLY	11.9
2	L	2	GLY	11.2
3	Q	46	ALA	10.9
3	C	10	THR	10.4
3	C	9	GLY	9.5
2	F	1	ALA	9.3
3	M	46	ALA	9.3
2	L	1	ALA	9.2
3	M	9	GLY	8.9
3	C	46	ALA	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	10	THR	8.7
2	B	1	ALA	8.7
3	Q	9	GLY	8.6
2	F	2	GLY	7.5
3	Q	10	THR	7.0
3	M	12	ARG	6.7
2	P	5	HIS	6.4
2	L	3	GLY	6.4
2	P	1	ALA	6.0
3	G	46	ALA	5.7
2	F	3	GLY	5.5
3	G	17	TYR	5.4
2	B	256	LYS	5.4
3	G	12	ARG	5.4
1	A	362	MET	5.3
3	C	12	ARG	5.2
3	C	11	ARG	5.0
2	L	114	MET	4.9
2	L	152	ASP	4.8
3	G	10	THR	4.7
3	C	17	TYR	4.6
3	M	47	LEU	4.6
3	M	17	TYR	4.6
3	C	58	GLU	4.5
2	L	111	HIS	4.5
1	E	20	HIS	4.5
2	B	114	MET	4.4
3	G	13	ASP	4.4
3	C	47	LEU	4.4
1	K	9	TYR	4.4
1	A	12	ARG	4.4
2	B	3	GLY	4.4
1	E	19	LEU	4.4
3	M	13	ASP	4.3
1	A	9	TYR	4.3
3	M	15	LEU	4.1
1	O	19	LEU	4.1
3	G	15	LEU	4.1
1	E	5	PRO	4.0
2	L	256	LYS	4.0
3	M	16	TYR	4.0
3	G	47	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	3	GLY	3.9
2	F	122	PHE	3.9
1	K	8	HIS	3.9
1	A	236	GLU	3.9
2	F	111	HIS	3.9
2	P	190	MET	3.8
2	P	152	ASP	3.8
2	B	152	ASP	3.8
2	L	17	PHE	3.8
1	A	10	GLU	3.8
1	A	414	ILE	3.8
3	C	15	LEU	3.8
2	F	119	SER	3.8
3	M	56	SER	3.8
1	K	416	LYS	3.7
1	E	23	LEU	3.7
2	P	17	PHE	3.6
1	E	236	GLU	3.6
1	K	320	PHE	3.6
3	Q	17	TYR	3.6
1	A	412	GLY	3.6
3	M	48	ALA	3.5
2	F	17	PHE	3.5
1	K	323	PHE	3.4
2	F	112	GLY	3.4
2	L	112	GLY	3.4
3	G	9	GLY	3.4
2	L	141	GLU	3.4
2	F	114	MET	3.4
1	E	9	TYR	3.4
2	B	255	VAL	3.4
3	C	13	ASP	3.4
2	F	190	MET	3.4
1	A	428	PHE	3.3
2	P	192	ASP	3.3
1	E	21	SER	3.3
2	F	5	HIS	3.3
2	L	250	ARG	3.3
1	A	416	LYS	3.3
3	G	179	ILE	3.3
3	C	14	PHE	3.2
1	E	8	HIS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	123	ASN	3.2
1	E	22	ARG	3.2
2	L	72	VAL	3.2
1	A	361	PRO	3.2
2	L	149	HIS	3.2
1	A	232	THR	3.1
3	C	59	PRO	3.1
1	O	232	THR	3.1
1	K	362	MET	3.1
3	M	179	ILE	3.1
2	F	195	GLU	3.1
3	Q	45	GLN	3.1
2	B	111	HIS	3.1
2	F	152	ASP	3.1
3	Q	15	LEU	3.0
2	B	110	PHE	3.0
1	A	413	ALA	3.0
2	P	121	LEU	3.0
2	F	149	HIS	3.0
1	E	18	TRP	3.0
2	B	17	PHE	3.0
1	E	227	VAL	3.0
1	O	23	LEU	3.0
3	M	45	GLN	3.0
1	O	24	PRO	3.0
2	F	123	ASN	3.0
1	A	324	GLY	3.0
2	F	110	PHE	3.0
2	L	110	PHE	2.9
2	L	123	ASN	2.9
2	B	76	GLU	2.9
1	O	9	TYR	2.9
3	C	16	TYR	2.9
1	E	11	PRO	2.9
2	P	111	HIS	2.9
3	G	45	GLN	2.9
1	O	234	LYS	2.8
2	B	175	VAL	2.8
3	M	11	ARG	2.8
3	Q	16	TYR	2.8
3	M	58	GLU	2.8
2	P	119	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	190	MET	2.8
2	L	140	GLU	2.8
3	Q	13	ASP	2.8
2	B	119	SER	2.7
3	Q	12	ARG	2.7
1	O	236	GLU	2.7
2	P	112	GLY	2.7
2	L	119	SER	2.6
2	B	72	VAL	2.6
3	Q	11	ARG	2.6
2	P	6	VAL	2.6
1	A	19	LEU	2.6
3	C	56	SER	2.6
1	K	6	HIS	2.6
1	A	237	ALA	2.6
1	A	113	PHE	2.6
2	F	250	ARG	2.6
2	F	121	LEU	2.6
3	G	106	GLY	2.6
2	P	199	GLY	2.6
2	P	76	GLU	2.5
1	K	12	ARG	2.5
2	B	197	ALA	2.5
2	P	122	PHE	2.5
1	O	239	LYS	2.5
2	L	144	LYS	2.5
3	M	57	VAL	2.5
1	E	228	GLU	2.5
2	P	117	GLY	2.5
1	A	15	ILE	2.5
1	A	320	PHE	2.5
1	K	414	ILE	2.5
1	E	10	GLU	2.5
2	P	228	GLN	2.5
2	B	141	GLU	2.4
1	O	5	PRO	2.4
1	K	7	ASP	2.4
1	E	323	PHE	2.4
3	C	57	VAL	2.4
1	K	236	GLU	2.4
2	B	250	ARG	2.4
3	Q	65	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	6	HIS	2.4
3	G	21	GLY	2.4
1	K	10	GLU	2.4
2	P	236	PHE	2.4
2	B	149	HIS	2.3
2	B	80	ASP	2.3
1	A	11	PRO	2.3
2	P	110	PHE	2.3
1	E	25	ILE	2.3
3	C	103	ILE	2.3
3	M	19	THR	2.3
2	B	109	GLY	2.3
1	A	116	LEU	2.3
2	F	4	GLY	2.3
2	L	75	GLU	2.3
3	Q	19	THR	2.3
2	P	195	GLU	2.3
2	P	149	HIS	2.3
3	M	14	PHE	2.3
1	A	231	ARG	2.3
1	E	24	PRO	2.3
1	O	361	PRO	2.3
2	P	256	LYS	2.3
1	A	114	ARG	2.2
3	C	45	GLN	2.2
1	O	416	LYS	2.2
1	E	348	TRP	2.2
3	G	35	ILE	2.2
2	B	232	THR	2.2
2	F	6	VAL	2.2
2	B	73	THR	2.2
2	P	197	ALA	2.2
2	B	5	HIS	2.2
2	L	80	ASP	2.2
2	L	5	HIS	2.2
1	A	115	GLY	2.2
2	F	200	HIS	2.2
2	P	143	PRO	2.2
1	A	419	ALA	2.1
1	K	11	PRO	2.1
2	P	200	HIS	2.1
2	F	120	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	65	ALA	2.1
2	P	114	MET	2.1
1	A	8	HIS	2.1
2	P	109	GLY	2.1
3	M	104	ASP	2.1
2	B	112	GLY	2.1
2	F	18	GLY	2.1
3	G	11	ARG	2.1
2	B	79	GLU	2.1
3	G	19	THR	2.1
2	F	113	PRO	2.1
2	L	71	THR	2.1
1	A	427	ASP	2.1
1	K	15	ILE	2.1
2	L	197	ALA	2.1
2	F	76	GLU	2.1
2	P	254	GLY	2.0
1	K	351	THR	2.0
3	C	179	ILE	2.0
1	E	27	ALA	2.0
2	P	4	GLY	2.0
2	L	73	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	LOP	A	1006	45/45	0.77	0.36	80,104,114,116	0

Continued on next page...

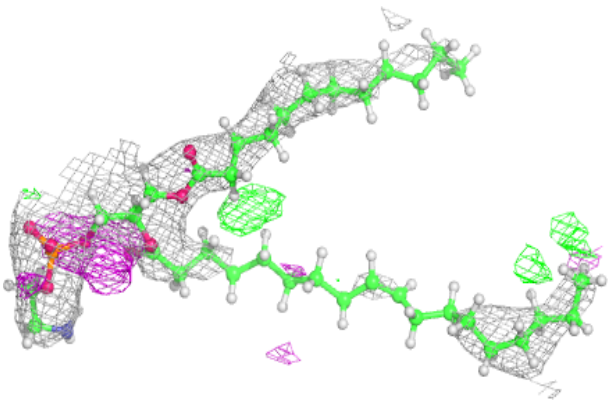
Continued from previous page...

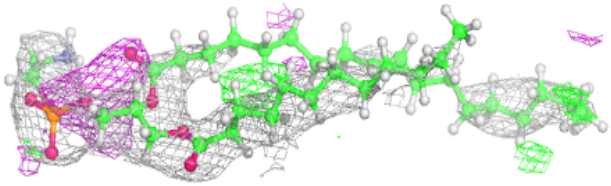
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	LOP	K	1006	45/45	0.83	0.31	64,85,101,106	0
8	LOP	O	1005	45/45	0.84	0.33	78,100,116,117	0
7	SR	A	1005	1/1	0.86	0.16	133,133,133,133	0
6	ANJ	A	1004	39/39	0.86	0.22	77,89,107,108	0
8	LOP	E	1005	45/45	0.87	0.35	75,95,109,113	0
6	ANJ	E	1004	39/39	0.87	0.19	58,74,101,101	0
6	ANJ	O	1004	39/39	0.87	0.24	67,84,107,108	0
7	SR	K	1005	1/1	0.88	0.16	121,121,121,121	0
6	ANJ	K	1004	39/39	0.91	0.20	49,71,100,101	0
7	SR	F	1002	1/1	0.92	0.07	132,132,132,132	0
5	SMA	O	1003	37/37	0.92	0.22	53,68,90,93	0
5	SMA	E	1003	37/37	0.92	0.21	47,67,88,88	0
5	SMA	K	1003	37/37	0.93	0.24	47,64,83,86	0
7	SR	P	1002	1/1	0.93	0.04	144,144,144,144	0
5	SMA	A	1003	37/37	0.93	0.22	56,69,83,89	0
4	HEM	A	1002	43/43	0.94	0.30	80,96,114,126	0
7	SR	B	1002	1/1	0.95	0.04	117,117,117,117	0
4	HEM	O	1002	43/43	0.95	0.25	75,80,97,98	0
9	HEC	F	1001	43/43	0.95	0.23	47,61,82,85	0
4	HEM	K	1002	43/43	0.96	0.25	64,72,89,96	0
4	HEM	A	1001	43/43	0.96	0.26	61,72,87,95	0
9	HEC	P	1001	43/43	0.96	0.21	47,62,75,83	0
4	HEM	O	1001	43/43	0.97	0.23	48,64,79,81	0
4	HEM	E	1002	43/43	0.97	0.22	65,78,94,98	0
7	SR	L	1002	1/1	0.97	0.04	113,113,113,113	0
9	HEC	B	1001	43/43	0.97	0.19	41,56,69,76	0
4	HEM	K	1001	43/43	0.97	0.23	51,62,79,83	0
9	HEC	L	1001	43/43	0.97	0.18	40,55,69,69	0
4	HEM	E	1001	43/43	0.97	0.23	56,69,85,89	0
10	FES	C	1001	4/4	0.99	0.23	59,62,64,64	0
10	FES	G	1001	4/4	0.99	0.27	71,74,74,76	0
10	FES	M	1001	4/4	0.99	0.25	72,72,75,77	0
10	FES	Q	1001	4/4	0.99	0.26	58,63,64,66	0

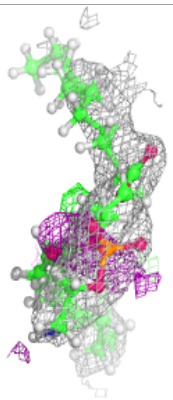
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

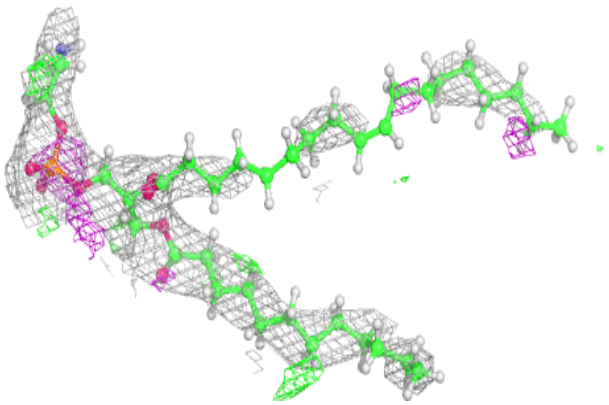


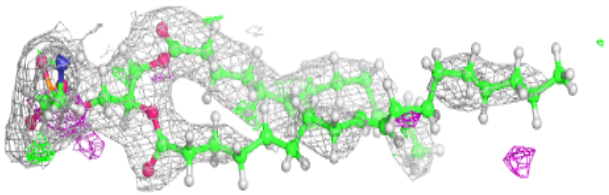


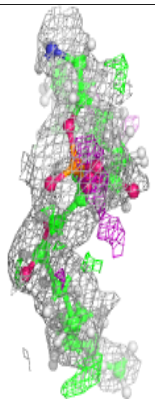


Electron density around LOP K 1006:

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

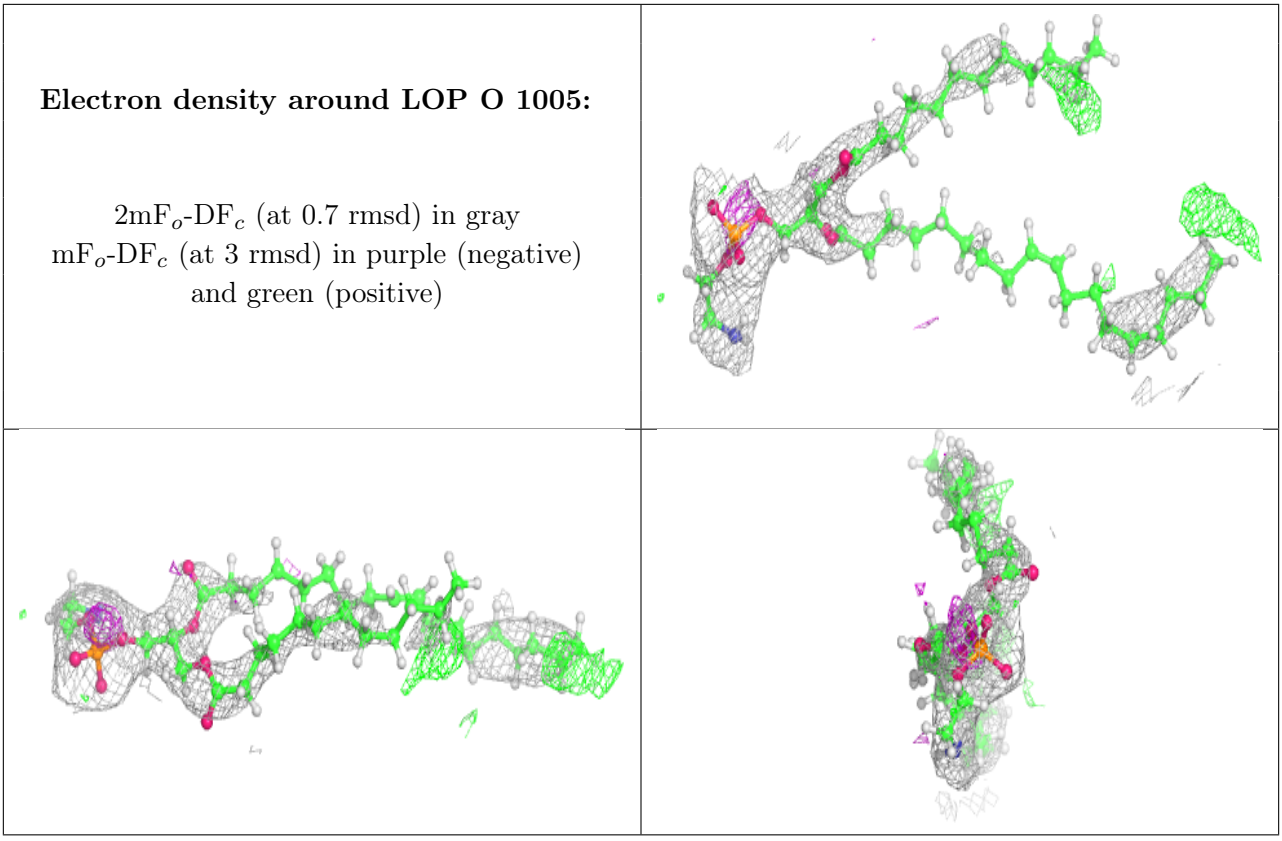






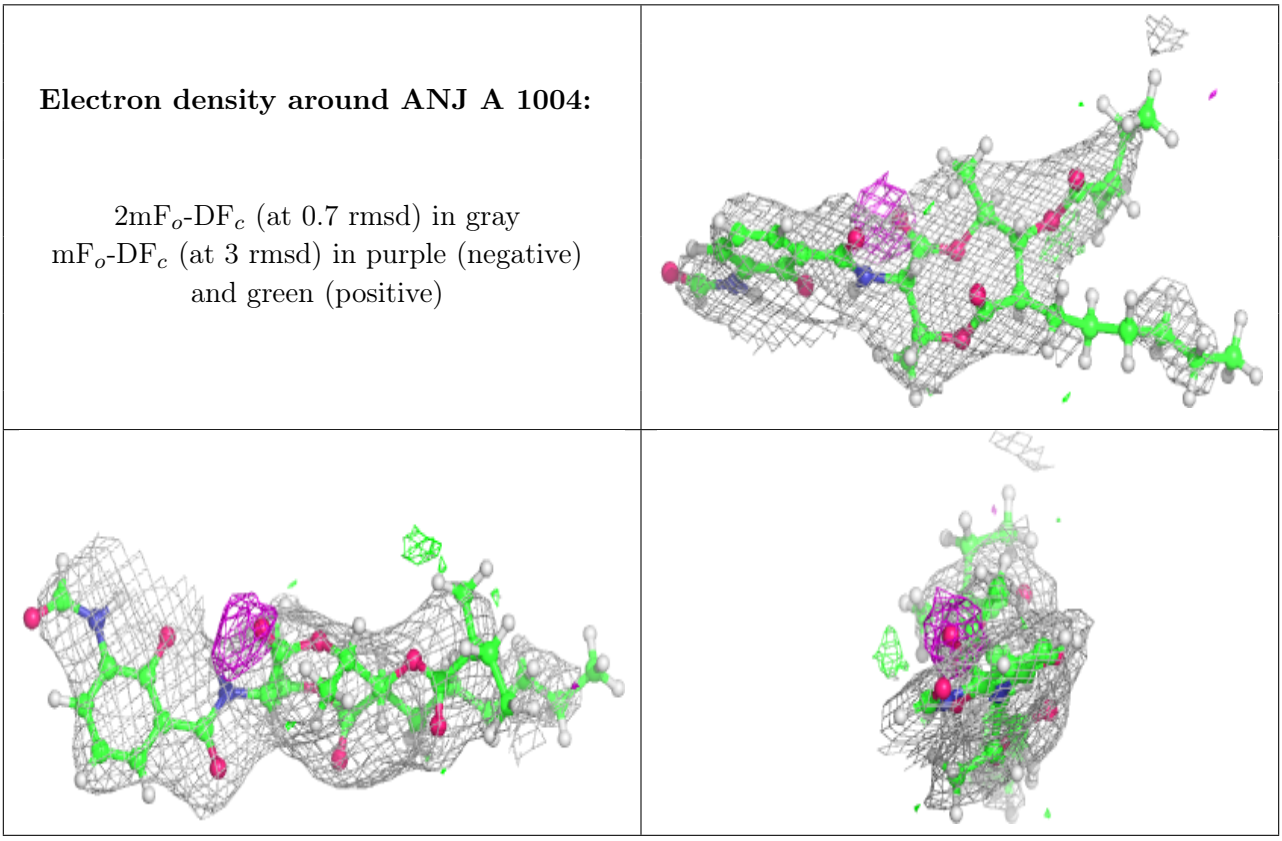
Electron density around LOP O 1005:

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



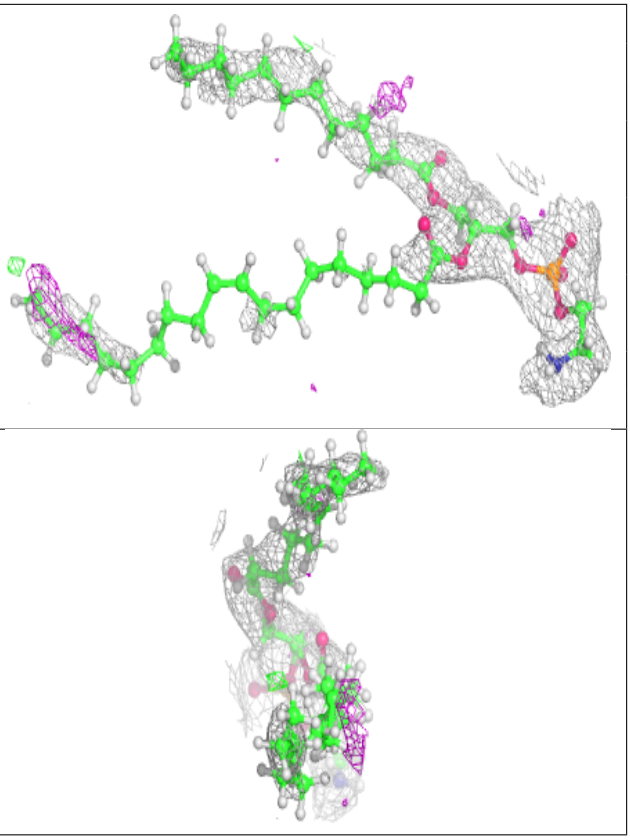
Electron density around ANJ A 1004:

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



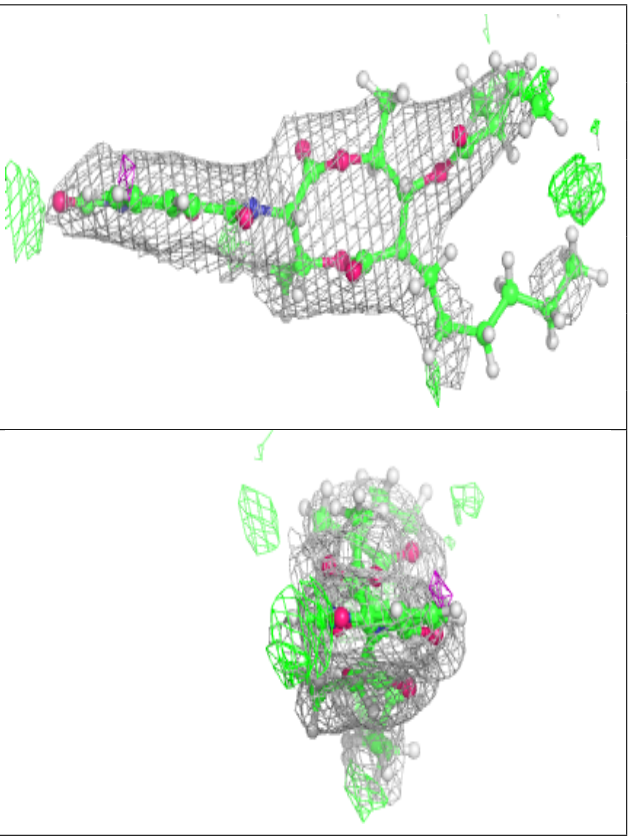
Electron density around LOP E 1005:

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



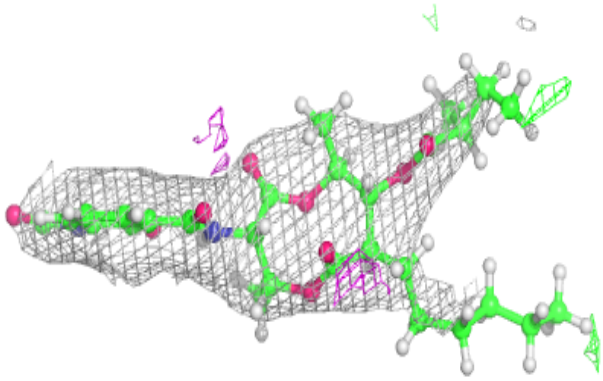
Electron density around ANJ E 1004:

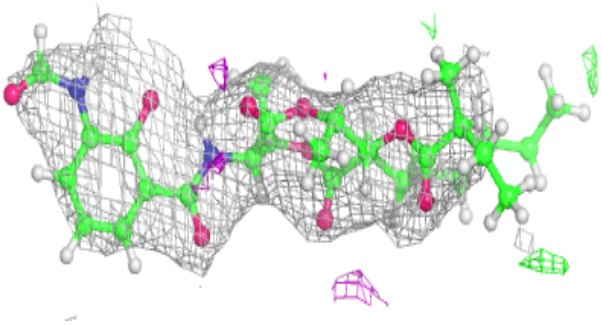
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

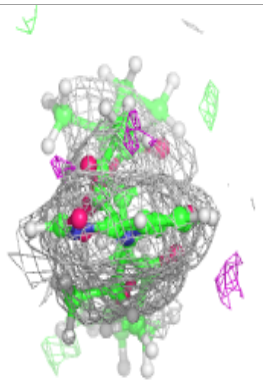


Electron density around ANJ O 1004:

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

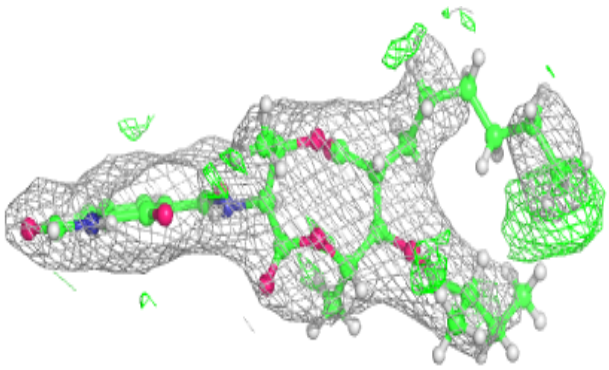


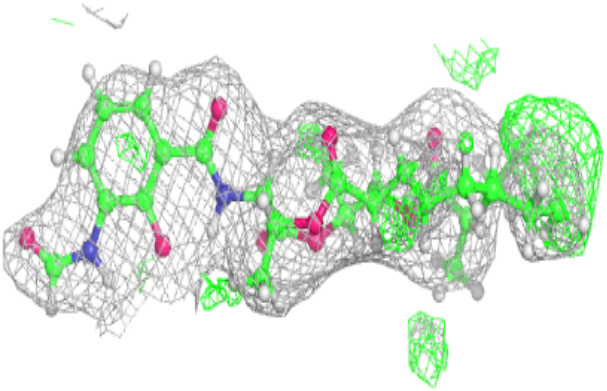


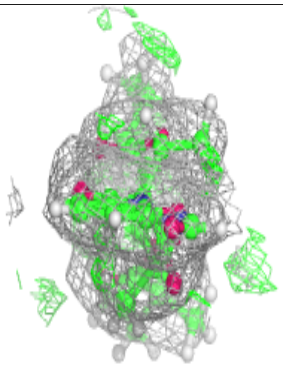


Electron density around ANJ K 1004:

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

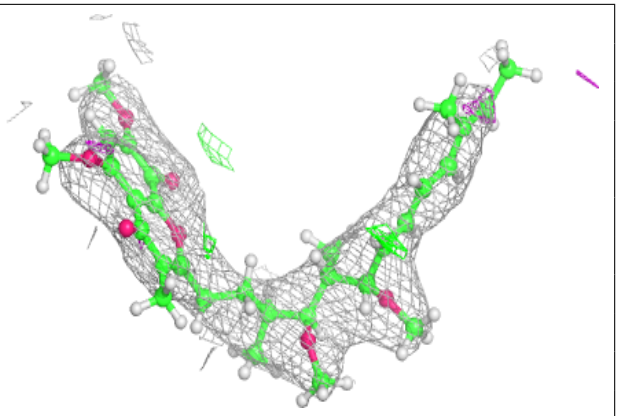


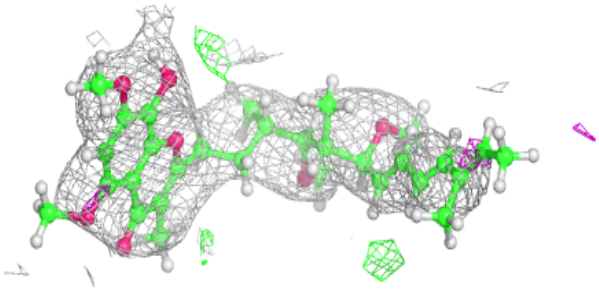


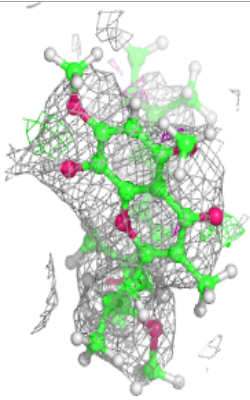


Electron density around SMA O 1003:

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

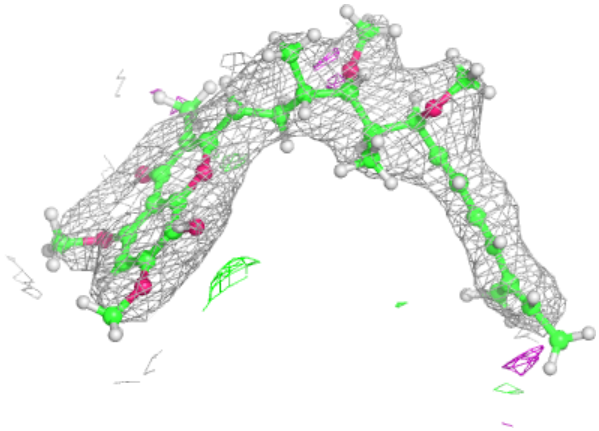


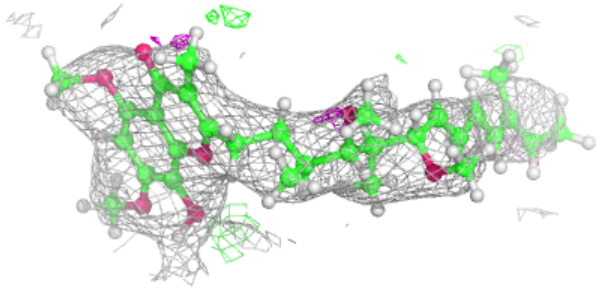


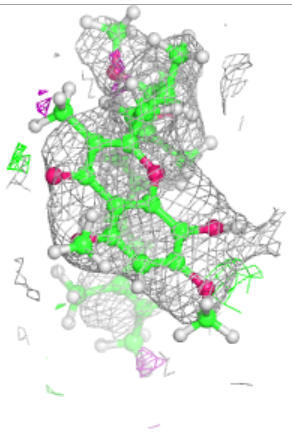


Electron density around SMA E 1003:

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

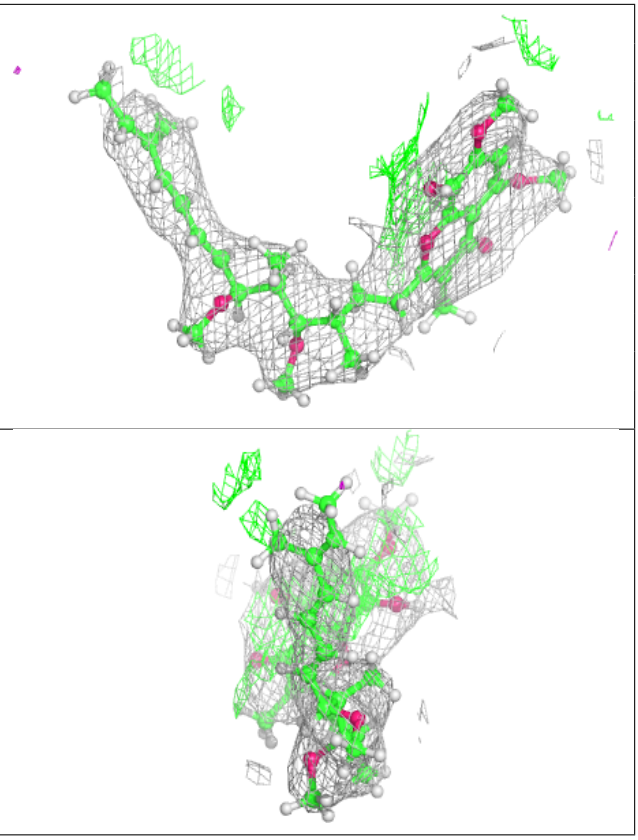






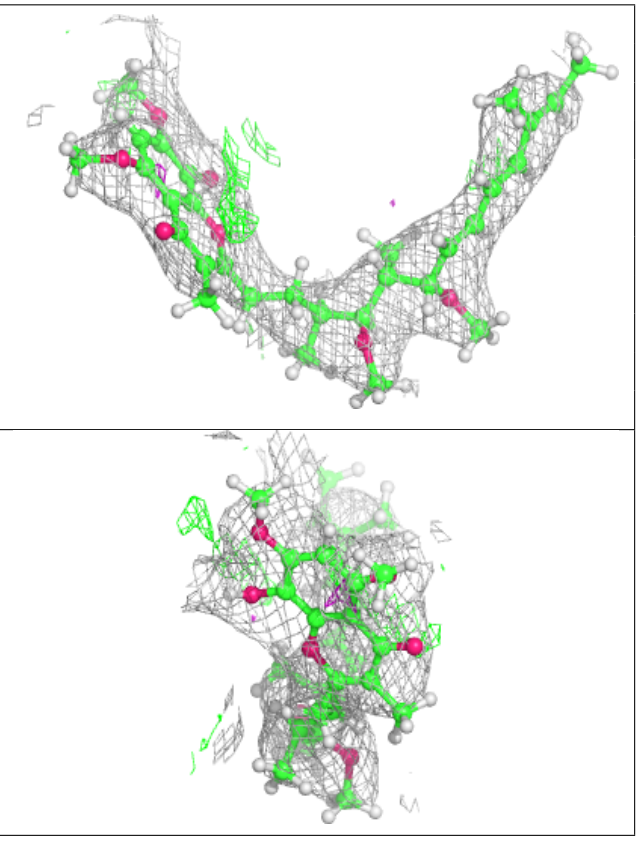
Electron density around SMA K 1003:

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



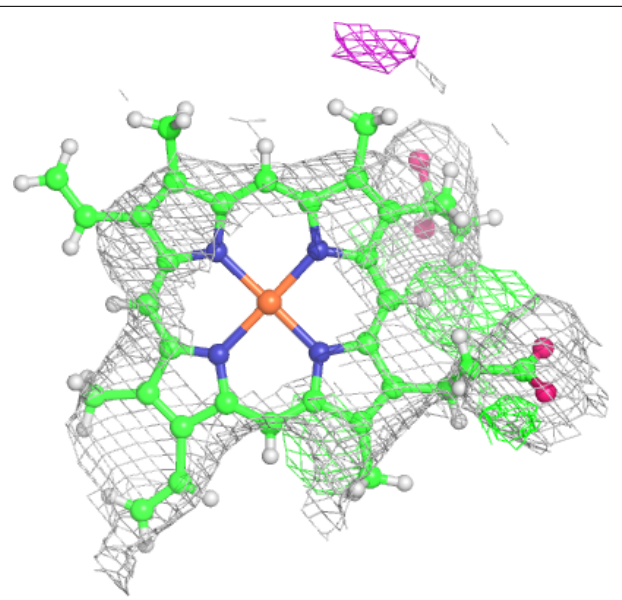
Electron density around SMA A 1003:

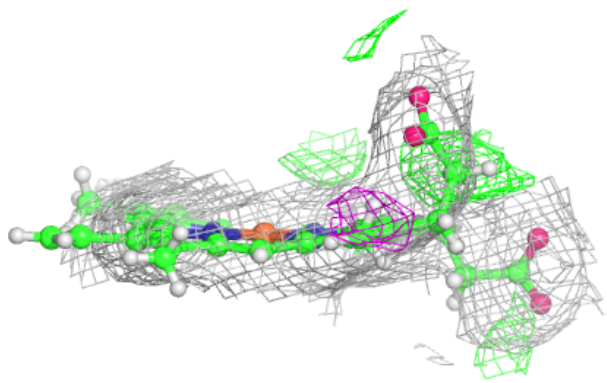
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

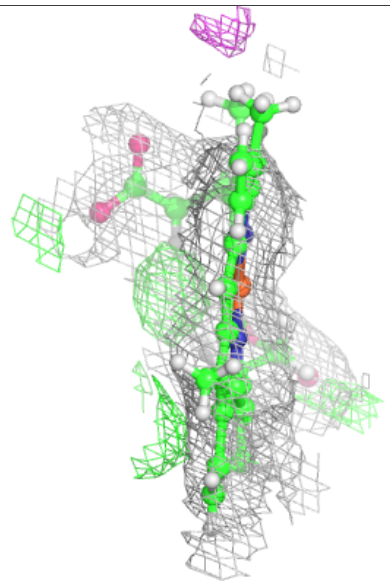


Electron density around HEM A 1002:

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

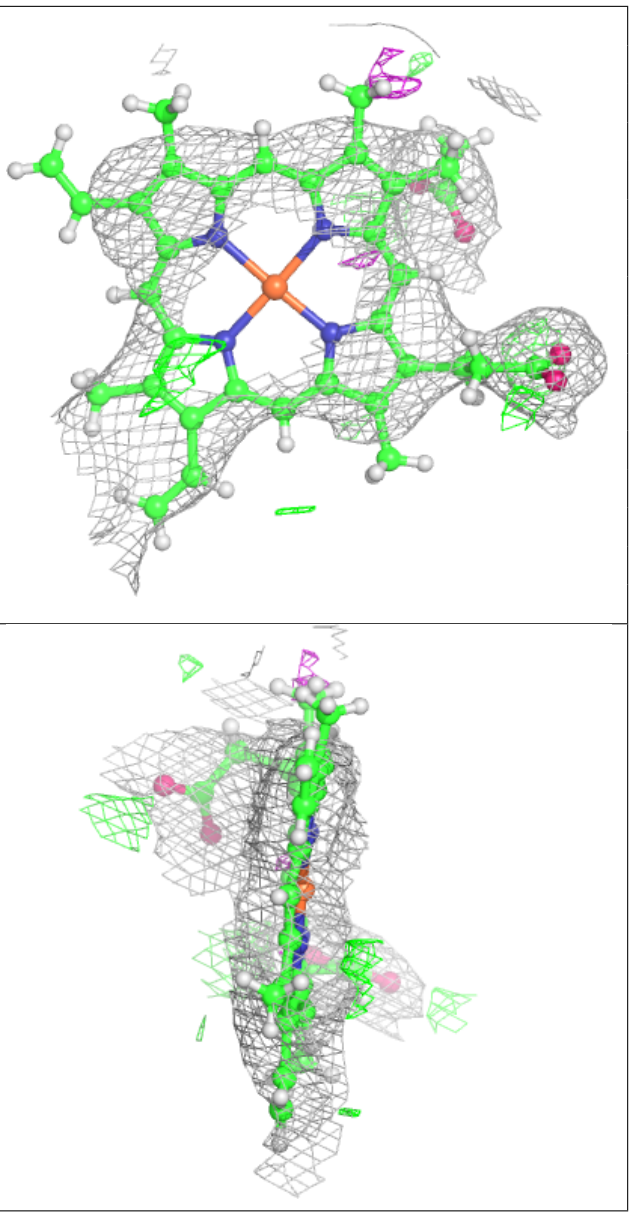






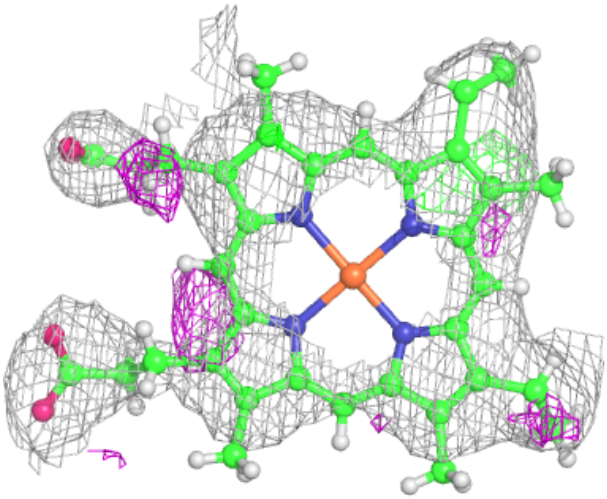
Electron density around HEM O 1002:

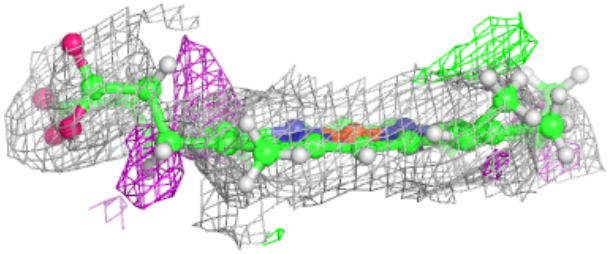
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC F 1001:

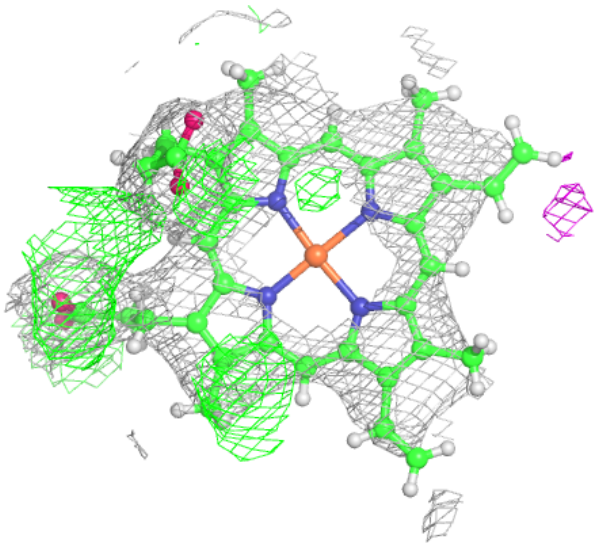
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

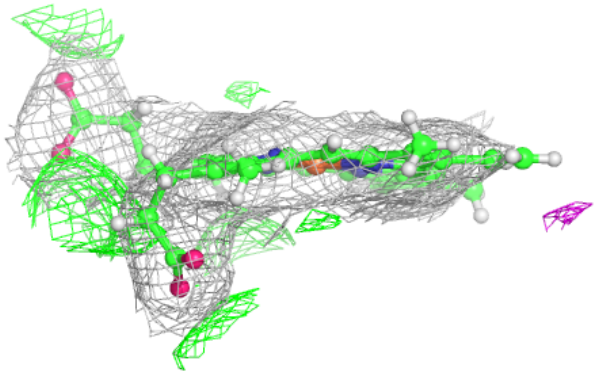


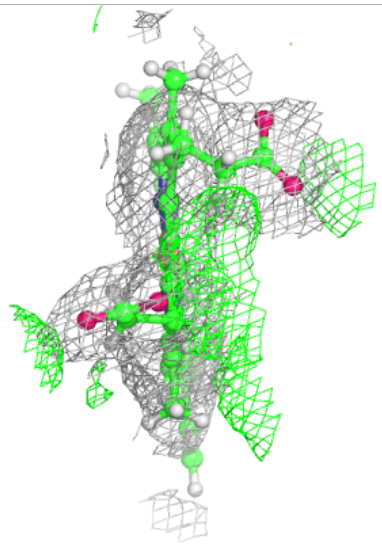


Electron density around HEM K 1002:

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

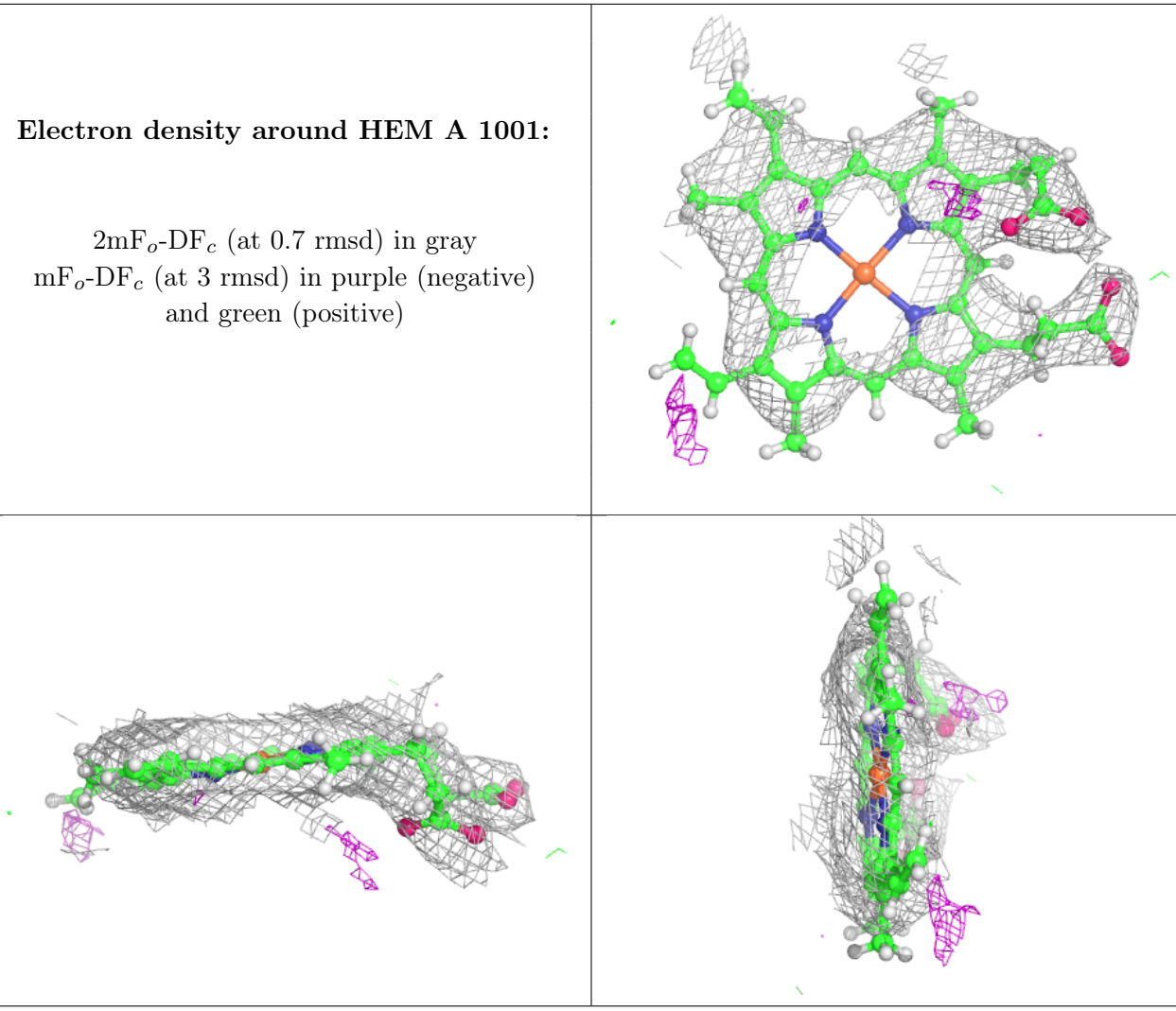






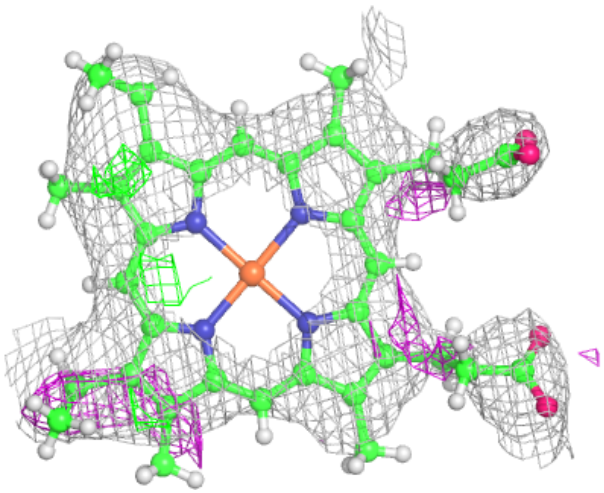
Electron density around HEM A 1001:

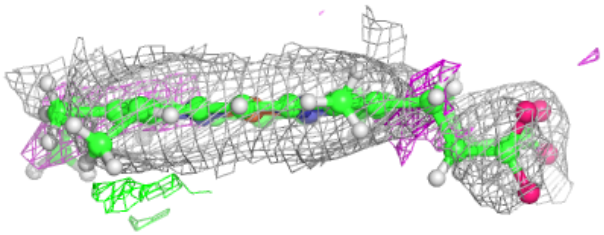
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

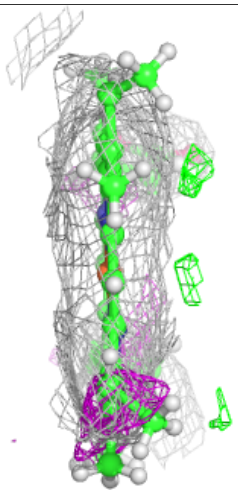


Electron density around HEC P 1001:

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

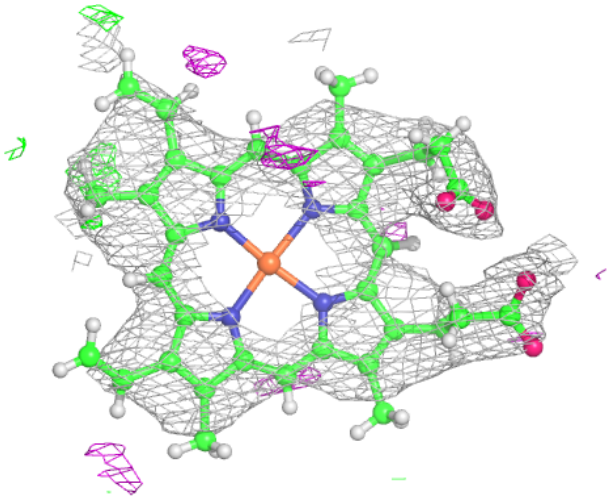


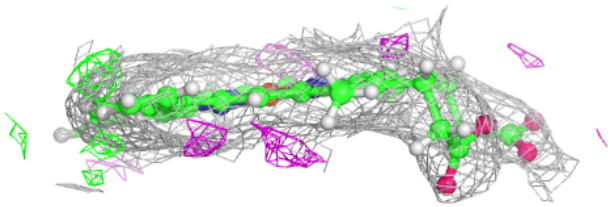


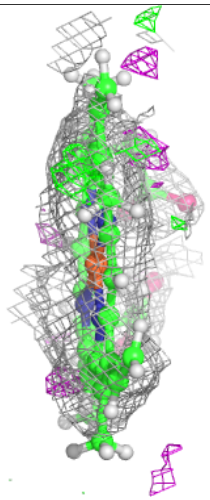


Electron density around HEM O 1001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

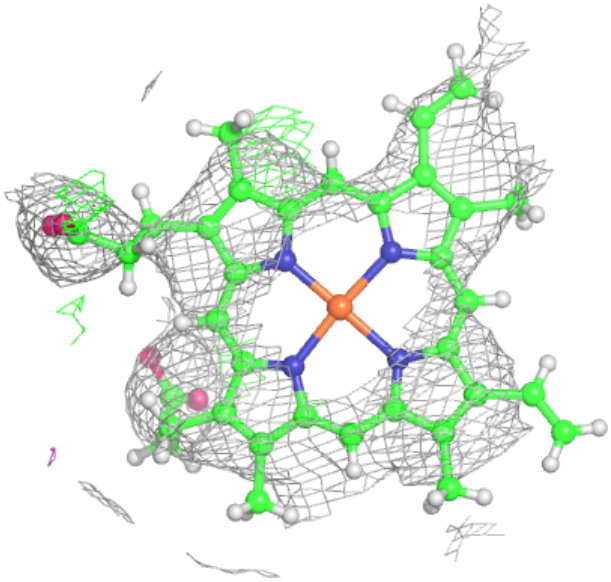


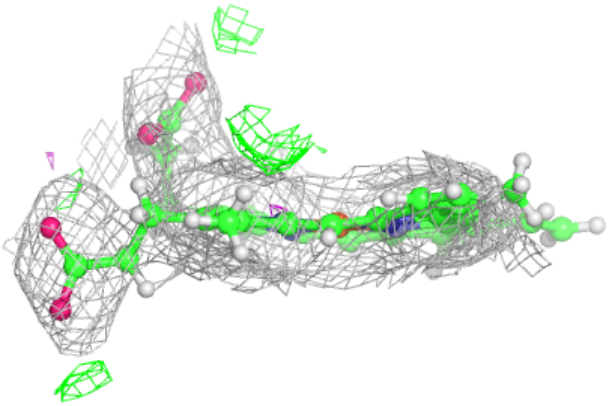


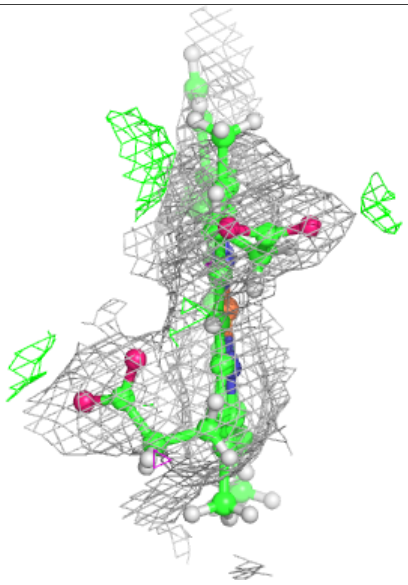


Electron density around HEM E 1002:

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

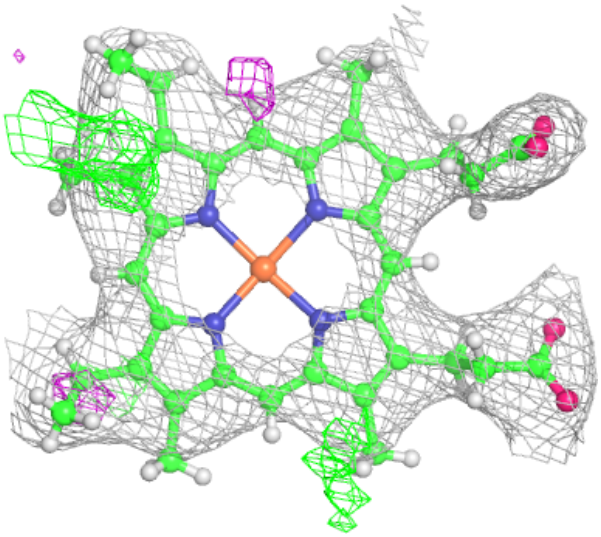


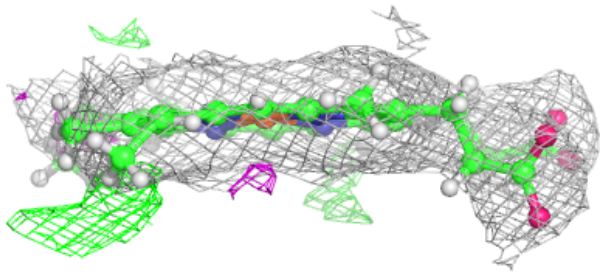


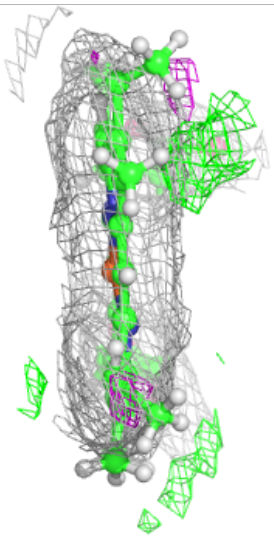


Electron density around HEC B 1001:

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

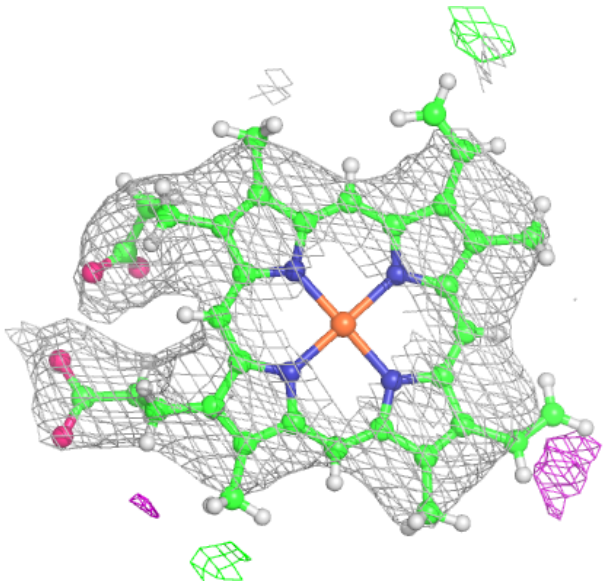


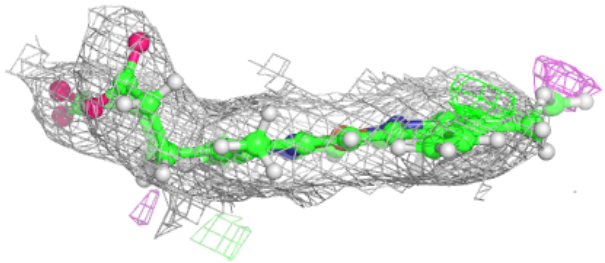


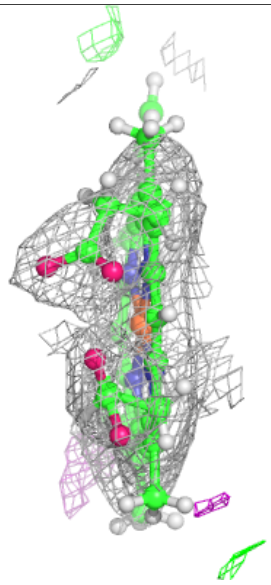


Electron density around HEM K 1001:

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

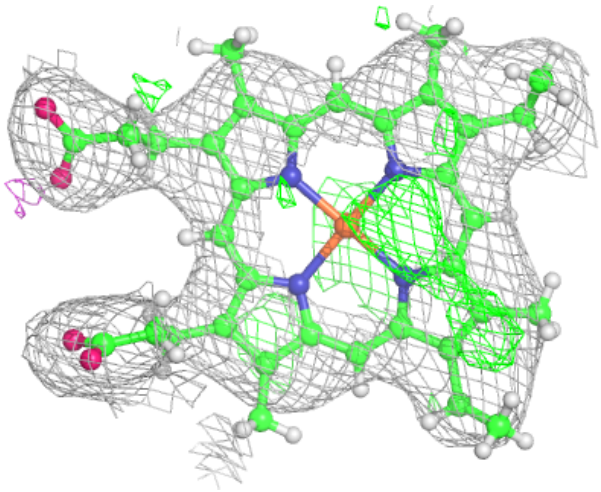


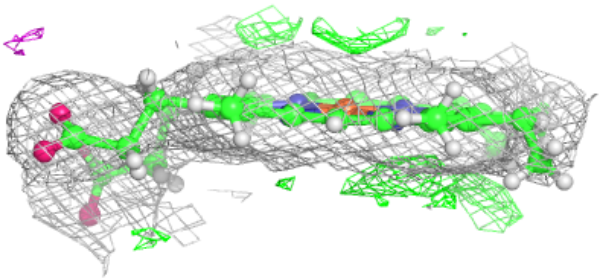


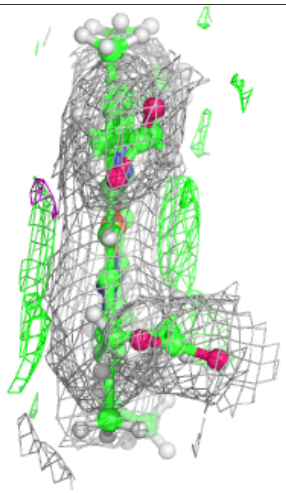


Electron density around HEC L 1001:

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

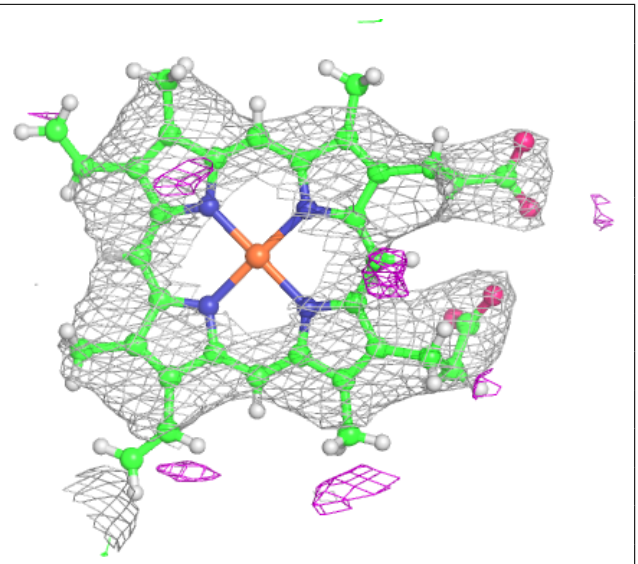


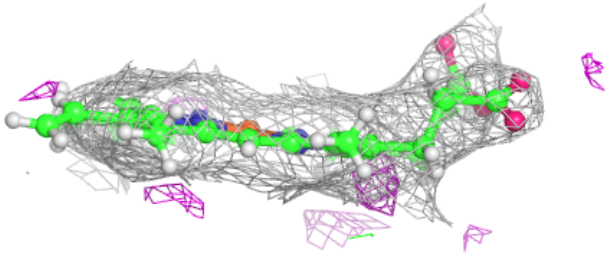


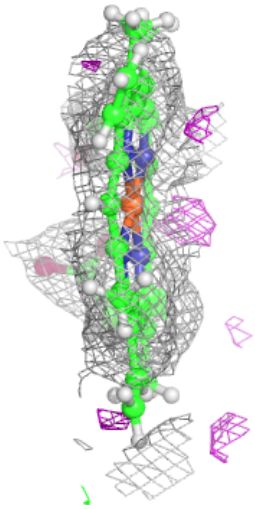


Electron density around HEM E 1001:

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







6.5 Other polymers (i)

There are no such residues in this entry.