Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 03:28 PM EDT

PDB ID	:	6NHH
Title	:	Rhodobacter sphaeroides bc1 with azoxystrobin
Authors	:	Xia, D.; Zhou, F.; Yu, C.A.
Deposited on	:	2018-12-21
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:

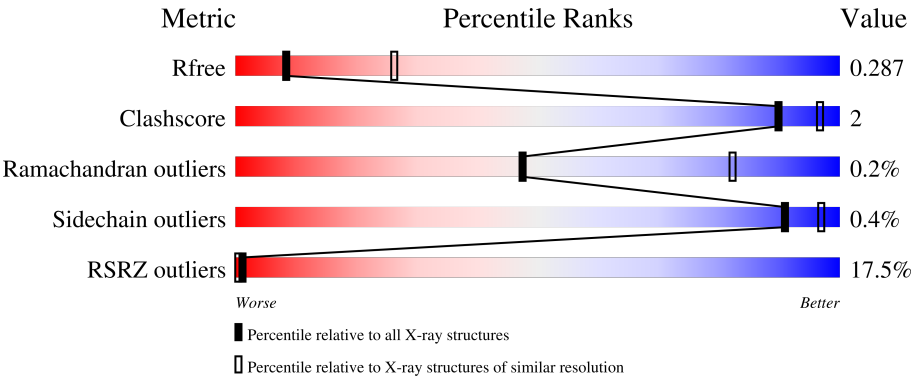
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	3% 92% 5% ·
1	E	445	3% 92% · ·
2	B	272	7% 89% 5% 6%
2	F	272	8% 90% · 6%
3	C	187	62% 91% · 6%

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Mol	Chain	Length	Quality of chain
3	G	187	64% 90% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	FES	G	1001	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 27403 atoms, of which 13476 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	430	Total	C	H	N	O	S	0	0	0
			6878	2334	3421	549	559	15			
1	E	430	Total	C	H	N	O	S	0	0	0
			6878	2334	3421	549	559	15			

- Molecule 2 is a protein called Cytochrome c1.

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

There are 18 discrepancies between the modelled and reference sequences:

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

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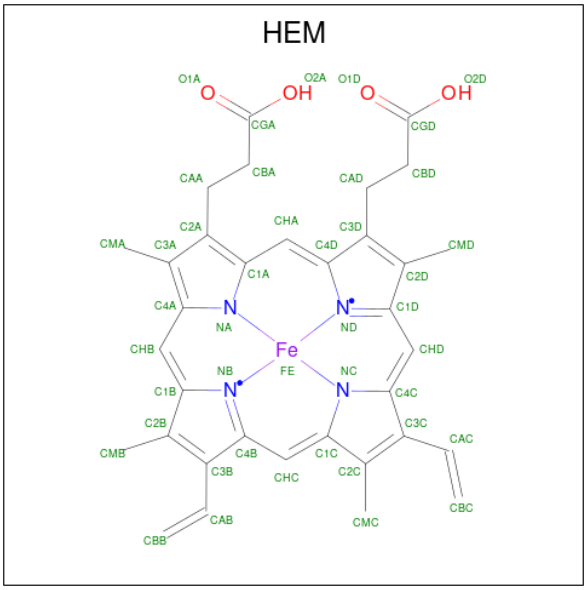
Chain	Residue	Modelled	Actual	Comment	Reference
F	271	HIS	-	expression tag	UNP A0A344Q9J2
F	272	HIS	-	expression tag	UNP A0A344Q9J2

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

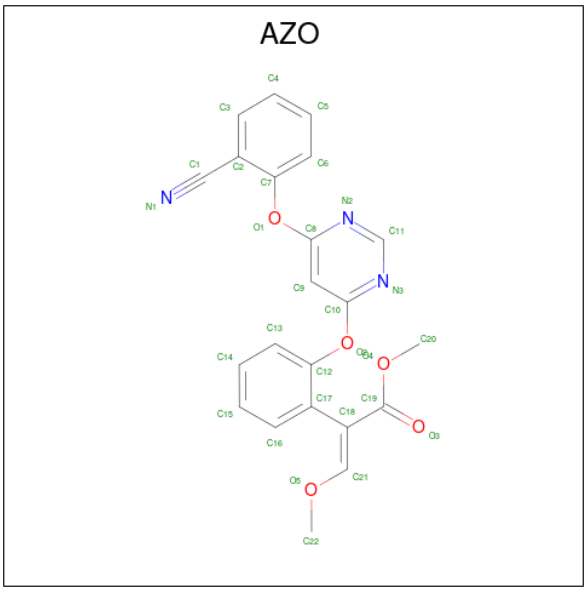
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	175	Total	C	H	N	O	S	0	0	0
			2576	827	1268	227	248	6			
3	G	175	Total	C	H	N	O	S	0	0	0
			2576	827	1268	227	248	6			

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



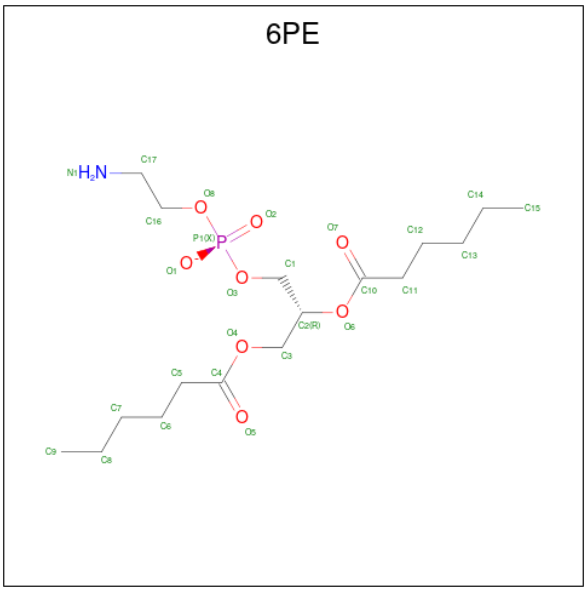
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
4	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 5 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (three-letter code: AZO) (formula: $C_{22}H_{17}N_3O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			47	22	17	3	5		
5	E	1	Total	C	H	N	O	0	0
			47	22	17	3	5		

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



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

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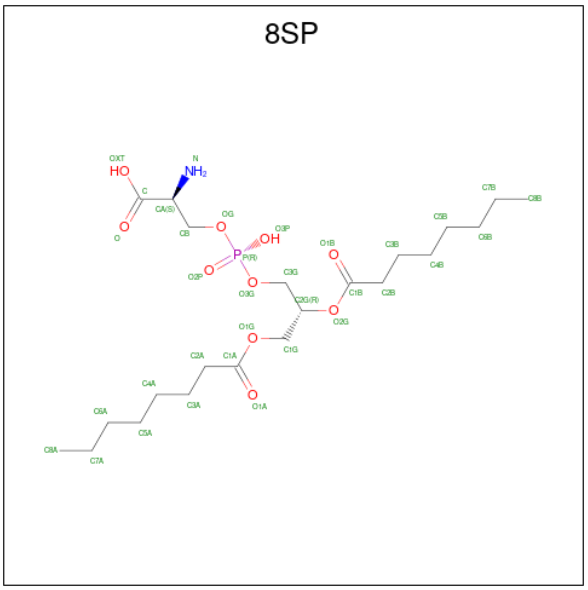
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		

- Molecule 7 is O-[(R)-{[(2R)-2,3-bis(octanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: 8SP) (formula: $C_{22}H_{42}NO_{10}P$).

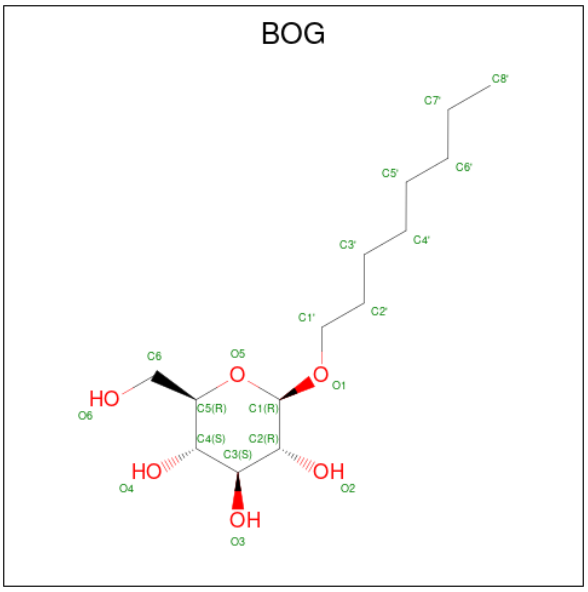


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	P	0	0
			74	22	40	1	10	1		
7	F	1	Total	C	H	N	O	P	0	0
			74	22	40	1	10	1		

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

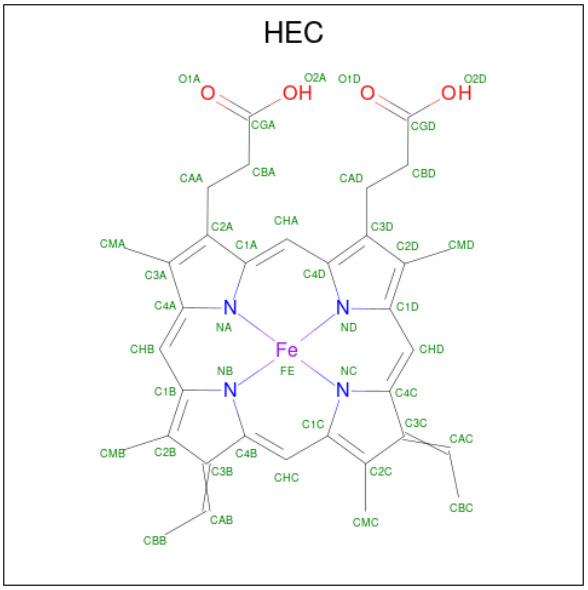
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Sr	0	0
			1	1		
8	B	1	Total	Sr	0	0
			1	1		
8	F	1	Total	Sr	0	0
			1	1		

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



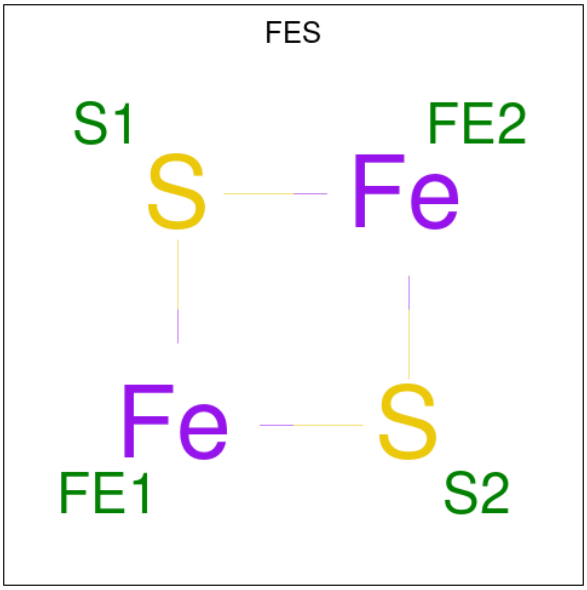
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			48	14	28	6		
9	F	1	Total	C	H	O	0	0
			48	14	28	6		

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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

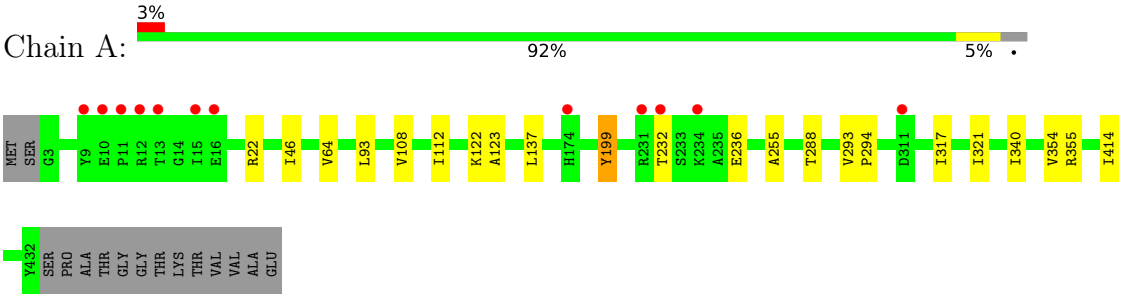


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total Fe S 4 2 2	0	0
11	G	1	Total Fe S 4 2 2	0	0

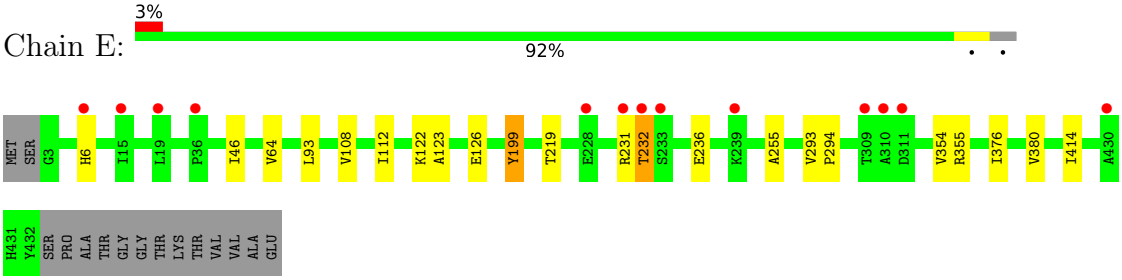
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

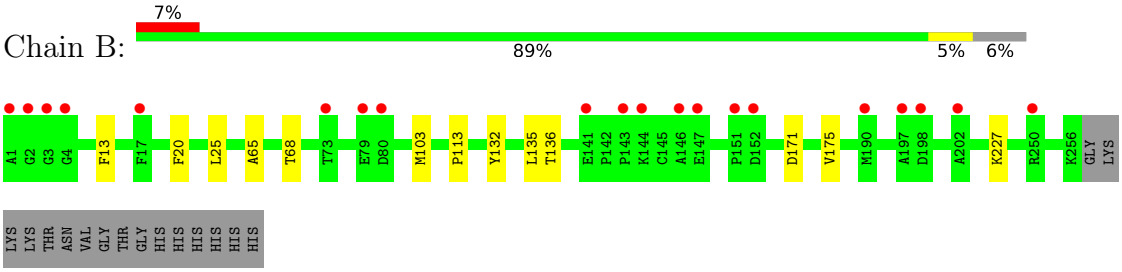
• Molecule 1: Cytochrome b



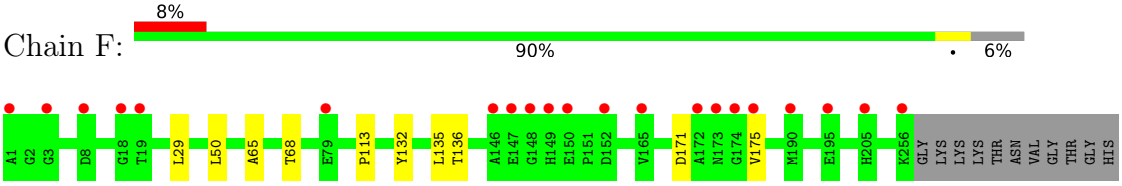
• Molecule 1: Cytochrome b



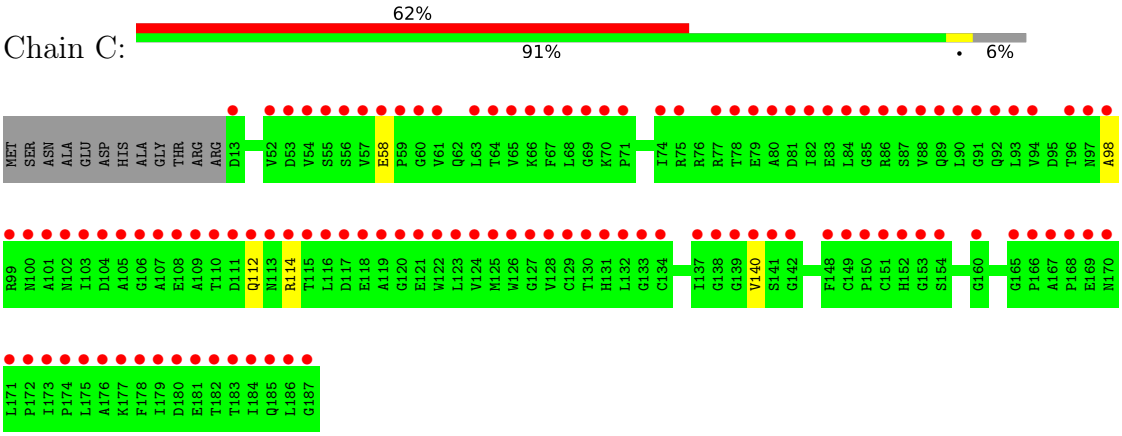
• Molecule 2: Cytochrome c1



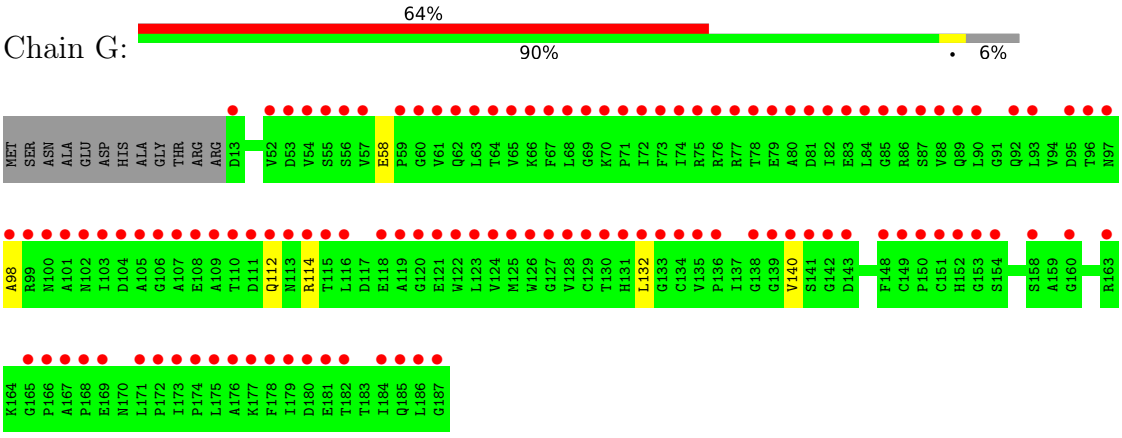
• Molecule 2: Cytochrome c1



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



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.31Å 154.66Å 100.94Å 90.00° 95.36° 90.00°	Depositor
Resolution (Å)	39.28 – 3.00 37.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.28-3.00) 92.8 (37.00-2.99)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_3339	Depositor
R, R_{free}	0.264 , 0.282 0.271 , 0.287	Depositor DCC
R_{free} test set	1991 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.935	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	27403	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8SP, BOG, SR, FES, AZO, HEC, 6PE, HEM

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	0.27	0/3589	0.46	0/4924
1	E	0.27	0/3589	0.46	0/4924
2	B	0.27	0/2010	0.46	0/2733
2	F	0.26	0/2010	0.45	0/2733
3	C	0.25	0/1338	0.47	0/1825
3	G	0.25	0/1338	0.47	0/1825
All	All	0.27	0/13874	0.46	0/18964

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3457	3421	3436	12	0
1	E	3457	3421	3436	11	0
2	B	1953	1839	1848	7	0
2	F	1953	1839	1848	5	0
3	C	1308	1268	1271	3	0
3	G	1308	1268	1271	4	0
4	A	86	60	60	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	86	60	60	2	0
5	A	30	17	17	0	0
5	E	30	17	17	0	0
6	A	27	33	33	0	0
6	E	27	33	33	0	0
7	A	34	40	40	0	0
7	F	34	40	40	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	F	1	0	0	0	0
9	B	20	28	28	0	0
9	F	20	28	28	0	0
10	B	43	32	30	4	0
10	F	43	32	30	3	0
11	C	4	0	0	0	0
11	G	4	0	0	0	0
All	All	13927	13476	13526	48	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:THR:OG1	1:E:236:GLU:OE1	2.09	0.68
10:F:302:HEC:HBC3	10:F:302:HEC:HMC1	1.76	0.68
10:B:302:HEC:HMC1	10:B:302:HEC:HBC3	1.76	0.67
1:E:123:ALA:O	1:E:355:ARG:NH1	2.28	0.65
1:A:123:ALA:O	1:A:355:ARG:NH1	2.31	0.63
1:A:122:LYS:NZ	1:A:354:VAL:O	2.25	0.61
1:E:64:VAL:HG11	1:E:93:LEU:HD13	1.85	0.57
1:E:219:THR:O	1:E:231:ARG:NH2	2.39	0.56
10:F:302:HEC:HBB3	10:F:302:HEC:HMB1	1.87	0.55
3:G:98:ALA:O	3:G:114:ARG:NH1	2.38	0.55
3:C:98:ALA:O	3:C:114:ARG:NH1	2.39	0.55
10:B:302:HEC:HMB1	10:B:302:HEC:HBB3	1.89	0.54
4:A:1001:HEM:HBB2	4:A:1001:HEM:HHC	1.91	0.52
1:A:64:VAL:HG11	1:A:93:LEU:HD13	1.92	0.52
2:B:103:MET:HG2	10:B:302:HEC:HMA3	1.92	0.51
3:G:58:GLU:N	3:G:58:GLU:OE1	2.44	0.50
3:C:58:GLU:N	3:C:58:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LYS:NZ	1:E:354:VAL:O	2.32	0.50
1:A:108:VAL:O	1:A:112:ILE:N	2.43	0.49
1:E:199:TYR:CZ	4:E:1001:HEM:HBC1	2.48	0.49
2:F:65:ALA:O	2:F:68:THR:OG1	2.28	0.49
4:E:1001:HEM:HBC2	4:E:1001:HEM:HMC1	1.94	0.49
2:F:171:ASP:OD1	2:F:175:VAL:N	2.46	0.49
1:A:232:THR:OG1	1:A:236:GLU:OE1	2.32	0.48
3:G:112:GLN:OE1	3:G:112:GLN:N	2.47	0.48
2:B:171:ASP:OD1	2:B:175:VAL:N	2.47	0.47
3:C:112:GLN:OE1	3:C:112:GLN:N	2.47	0.47
1:E:376:ILE:O	1:E:380:VAL:HG22	2.15	0.47
4:A:1002:HEM:HBB2	4:A:1002:HEM:HMB2	1.96	0.47
2:B:132:TYR:O	2:B:136:THR:HG22	2.15	0.47
1:A:288:THR:HB	3:G:132:LEU:HD22	1.96	0.47
2:B:65:ALA:O	2:B:68:THR:OG1	2.34	0.45
1:E:46:ILE:HD12	1:E:255:ALA:HB1	1.98	0.45
2:F:132:TYR:O	2:F:136:THR:HG22	2.17	0.45
1:A:199:TYR:CE2	4:A:1001:HEM:HBC1	2.52	0.45
2:B:20:PHE:HB3	2:B:25:LEU:HD11	2.00	0.44
1:E:108:VAL:O	1:E:112:ILE:N	2.46	0.43
4:A:1001:HEM:HHD	4:A:1001:HEM:HBC2	1.99	0.43
1:A:22:ARG:NE	1:E:126:GLU:OE1	2.47	0.43
1:A:46:ILE:HD12	1:A:255:ALA:HB1	2.01	0.42
1:A:137:LEU:HD21	1:A:340:ILE:HG21	2.01	0.42
2:F:135:LEU:HD21	10:F:302:HEC:HMB2	2.02	0.42
1:A:293:VAL:HG12	1:A:294:PRO:O	2.19	0.42
2:B:135:LEU:HD11	10:B:302:HEC:HMB2	2.01	0.42
2:B:13:PHE:O	2:B:227:LYS:NZ	2.53	0.41
1:A:317:ILE:HG22	1:A:321:ILE:HD12	2.03	0.41
2:F:29:LEU:HD22	2:F:50:LEU:HD22	2.02	0.41
1:E:293:VAL:HG12	1:E:294:PRO:O	2.21	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	428/445 (96%)	416 (97%)	12 (3%)	0	100	100
1	E	428/445 (96%)	416 (97%)	12 (3%)	0	100	100
2	B	254/272 (93%)	245 (96%)	8 (3%)	1 (0%)	34	72
2	F	254/272 (93%)	245 (96%)	8 (3%)	1 (0%)	34	72
3	C	173/187 (92%)	158 (91%)	14 (8%)	1 (1%)	25	64
3	G	173/187 (92%)	158 (91%)	14 (8%)	1 (1%)	25	64
All	All	1710/1808 (95%)	1638 (96%)	68 (4%)	4 (0%)	47	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	140	VAL
3	G	140	VAL
2	B	113	PRO
2	F	113	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/366 (97%)	353 (99%)	2 (1%)	86	95
1	E	355/366 (97%)	351 (99%)	4 (1%)	73	90
2	B	203/216 (94%)	203 (100%)	0	100	100
2	F	203/216 (94%)	203 (100%)	0	100	100
3	C	135/144 (94%)	135 (100%)	0	100	100
3	G	135/144 (94%)	135 (100%)	0	100	100
All	All	1386/1452 (96%)	1380 (100%)	6 (0%)	91	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	TYR
1	A	414	ILE
1	E	6	HIS
1	E	199	TYR
1	E	232	THR
1	E	414	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	113	ASN
3	G	113	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HEM	A	1002	1	41,50,50	1.53	6 (14%)	45,82,82	1.40	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	8SP	A	1005	-	32,33,33	0.88	1 (3%)	36,40,40	0.95	2 (5%)
11	FES	C	1001	3	0,4,4	-	-	-		
9	BOG	F	301	-	20,20,20	0.83	0	25,25,25	1.34	2 (8%)
6	6PE	A	1004	-	26,26,26	0.86	2 (7%)	29,31,31	0.68	0
5	AZO	A	1003	-	32,32,32	0.56	0	42,42,42	1.57	7 (16%)
7	8SP	F	303	-	32,33,33	0.87	1 (3%)	36,40,40	1.32	3 (8%)
4	HEM	E	1001	1	41,50,50	1.45	5 (12%)	45,82,82	1.38	6 (13%)
9	BOG	B	301	-	20,20,20	0.89	0	25,25,25	1.24	4 (16%)
6	6PE	E	1004	-	26,26,26	0.87	1 (3%)	29,31,31	0.68	1 (3%)
4	HEM	A	1001	1	41,50,50	1.54	5 (12%)	45,82,82	1.54	7 (15%)
5	AZO	E	1003	-	32,32,32	0.61	0	42,42,42	1.62	9 (21%)
10	HEC	B	302	2	32,50,50	2.09	3 (9%)	24,82,82	1.53	3 (12%)
4	HEM	E	1002	1	41,50,50	1.46	6 (14%)	45,82,82	1.41	7 (15%)
10	HEC	F	302	2	32,50,50	2.10	3 (9%)	24,82,82	1.42	3 (12%)
11	FES	G	1001	3	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	1002	1	-	5/12/54/54	-
7	8SP	A	1005	-	-	20/39/39/39	-
11	FES	C	1001	3	-	-	0/1/1/1
9	BOG	F	301	-	-	3/11/31/31	0/1/1/1
6	6PE	A	1004	-	-	10/30/30/30	-
5	AZO	A	1003	-	-	1/23/23/23	0/3/3/3
7	8SP	F	303	-	-	17/39/39/39	-
4	HEM	E	1001	1	-	4/12/54/54	-
9	BOG	B	301	-	-	6/11/31/31	0/1/1/1
6	6PE	E	1004	-	-	20/30/30/30	-
4	HEM	A	1001	1	-	4/12/54/54	-
5	AZO	E	1003	-	-	0/23/23/23	0/3/3/3
10	HEC	B	302	2	-	2/10/54/54	-
4	HEM	E	1002	1	-	0/12/54/54	-
10	HEC	F	302	2	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	FES	G	1001	3	-	-	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	302	HEC	C2B-C3B	-6.28	1.34	1.40
10	B	302	HEC	C2B-C3B	-6.25	1.34	1.40
10	B	302	HEC	C3D-C2D	5.32	1.53	1.37
10	F	302	HEC	C3D-C2D	5.31	1.53	1.37
10	B	302	HEC	C3C-C2C	-5.18	1.35	1.40
10	F	302	HEC	C3C-C2C	-5.17	1.35	1.40
4	A	1001	HEM	C3C-C2C	-4.60	1.34	1.40
4	E	1001	HEM	C3C-C2C	-4.01	1.34	1.40
4	E	1002	HEM	C3C-CAC	3.85	1.55	1.47
4	A	1002	HEM	C3C-CAC	3.77	1.55	1.47
4	A	1002	HEM	C3C-C2C	-3.69	1.35	1.40
4	A	1001	HEM	C3C-CAC	3.68	1.55	1.47
4	E	1002	HEM	C3C-C2C	-3.60	1.35	1.40
4	A	1002	HEM	FE-NB	3.30	2.13	1.96
4	E	1001	HEM	C3C-CAC	3.20	1.54	1.47
4	A	1002	HEM	CAB-C3B	3.12	1.55	1.47
4	A	1001	HEM	CAB-C3B	3.10	1.55	1.47
4	E	1002	HEM	CAB-C3B	2.91	1.55	1.47
4	E	1001	HEM	CAB-C3B	2.84	1.55	1.47
6	E	1004	6PE	P1-O3	2.64	1.70	1.59
4	E	1002	HEM	FE-NB	2.56	2.09	1.96
7	F	303	8SP	P-O3G	2.48	1.69	1.59
4	A	1002	HEM	CAA-C2A	2.43	1.55	1.52
6	A	1004	6PE	P1-O3	2.37	1.68	1.59
7	A	1005	8SP	P-O3G	2.34	1.68	1.59
4	A	1002	HEM	CMB-C2B	2.24	1.55	1.50
4	A	1001	HEM	FE-NB	2.15	2.07	1.96
4	E	1002	HEM	CMB-C2B	2.14	1.55	1.50
6	A	1004	6PE	P1-O8	2.13	1.67	1.59
4	E	1001	HEM	CMD-C2D	2.08	1.55	1.50
4	E	1001	HEM	CMB-C2B	2.06	1.55	1.50
4	E	1002	HEM	CAA-C2A	2.04	1.55	1.52
4	A	1001	HEM	CMB-C2B	2.02	1.55	1.50

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1003	AZO	C11-N3-C10	6.20	119.14	114.48
5	A	1003	AZO	C11-N3-C10	5.96	118.96	114.48
7	F	303	8SP	OG-CB-CA	-4.69	103.97	108.06
7	F	303	8SP	C2G-O2G-C1B	4.00	127.65	117.79
10	B	302	HEC	CMC-C2C-C1C	-3.83	122.58	128.46
4	A	1002	HEM	C4D-ND-C1D	3.44	108.62	105.07
4	A	1001	HEM	C1B-NB-C4B	3.37	108.55	105.07
4	E	1002	HEM	C4D-ND-C1D	3.34	108.52	105.07
9	F	301	BOG	C1-C2-C3	-3.32	103.08	110.00
10	F	302	HEC	CMC-C2C-C1C	-3.22	123.52	128.46
5	E	1003	AZO	C11-N2-C8	3.20	116.89	114.48
5	A	1003	AZO	C11-N2-C8	3.16	116.86	114.48
4	A	1001	HEM	C4B-CHC-C1C	3.11	126.67	122.56
4	A	1001	HEM	CBA-CAA-C2A	-3.09	107.34	112.62
5	A	1003	AZO	C12-O2-C10	3.02	124.88	118.47
5	E	1003	AZO	C9-C10-N3	-3.02	120.32	124.57
5	E	1003	AZO	N2-C11-N3	-2.91	124.06	128.60
4	A	1001	HEM	C3B-C2B-C1B	2.90	108.64	106.49
5	A	1003	AZO	N2-C11-N3	-2.88	124.09	128.60
10	B	302	HEC	CBD-CAD-C3D	-2.88	107.71	112.62
5	A	1003	AZO	C9-C10-N3	-2.87	120.53	124.57
5	E	1003	AZO	C12-O2-C10	2.85	124.50	118.47
4	A	1001	HEM	C4C-CHD-C1D	2.79	126.24	122.56
4	A	1001	HEM	C4D-ND-C1D	2.77	107.94	105.07
4	A	1002	HEM	C4B-CHC-C1C	2.75	126.19	122.56
4	E	1001	HEM	C1B-NB-C4B	2.75	107.91	105.07
4	E	1001	HEM	C4C-CHD-C1D	2.68	126.09	122.56
4	E	1001	HEM	CBA-CAA-C2A	-2.67	108.06	112.62
4	E	1002	HEM	C4B-CHC-C1C	2.67	126.08	122.56
4	A	1001	HEM	CHC-C4B-C3B	2.63	128.60	124.57
4	E	1001	HEM	C2C-C3C-C4C	2.61	108.72	106.90
5	A	1003	AZO	C20-O4-C19	2.58	120.74	115.86
9	F	301	BOG	O3-C3-C4	-2.57	104.40	110.35
4	E	1002	HEM	CMC-C2C-C3C	2.57	129.49	124.68
4	E	1001	HEM	C4D-ND-C1D	2.51	107.67	105.07
4	A	1002	HEM	C4C-CHD-C1D	2.50	125.86	122.56
4	A	1002	HEM	CMC-C2C-C3C	2.47	129.30	124.68
7	A	1005	8SP	OG-CB-CA	-2.42	105.94	108.06
5	E	1003	AZO	C20-O4-C19	2.39	120.38	115.86
7	F	303	8SP	OXT-C-O	2.39	129.51	124.09
4	A	1002	HEM	C3D-C4D-ND	-2.35	107.55	110.17
4	E	1002	HEM	C3D-C4D-ND	-2.32	107.58	110.17
4	E	1002	HEM	C1B-NB-C4B	2.29	107.43	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	302	HEC	CBD-CAD-C3D	-2.28	108.72	112.62
9	B	301	BOG	C1-C2-C3	-2.25	105.30	110.00
4	A	1002	HEM	C1B-NB-C4B	2.23	107.38	105.07
9	B	301	BOG	O3-C3-C4	-2.22	105.22	110.35
10	B	302	HEC	C1D-C2D-C3D	-2.20	105.47	107.00
4	A	1002	HEM	CMA-C3A-C4A	-2.19	125.10	128.46
10	F	302	HEC	C1D-C2D-C3D	-2.18	105.48	107.00
5	A	1003	AZO	C21-C18-C19	2.17	121.39	117.41
4	E	1001	HEM	C4B-CHC-C1C	2.14	125.39	122.56
5	E	1003	AZO	C21-C18-C19	2.12	121.29	117.41
5	E	1003	AZO	C17-C18-C21	-2.09	119.22	122.26
4	E	1002	HEM	C4C-CHD-C1D	2.09	125.31	122.56
7	A	1005	8SP	OXT-C-O	2.07	128.79	124.09
9	B	301	BOG	O2-C2-C3	-2.07	105.57	110.35
4	E	1002	HEM	CHA-C4D-ND	2.05	126.92	124.38
5	E	1003	AZO	C7-C2-C1	2.03	121.55	119.57
9	B	301	BOG	O5-C5-C4	-2.02	106.03	109.69
6	E	1004	6PE	O1-P1-O2	2.02	122.20	112.24

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1004	6PE	C1-O3-P1-O1
6	E	1004	6PE	C16-O8-P1-O2
6	E	1004	6PE	O8-C16-C17-N1
7	A	1005	8SP	CB-OG-P-O3G
7	A	1005	8SP	CB-OG-P-O3P
7	A	1005	8SP	C3G-O3G-P-OG
7	A	1005	8SP	C3G-O3G-P-O2P
7	A	1005	8SP	C2B-C1B-O2G-C2G
7	F	303	8SP	CB-OG-P-O2P
7	F	303	8SP	N-CA-CB-OG
7	F	303	8SP	C-CA-CB-OG
9	F	301	BOG	C2'-C1'-O1-C1
7	A	1005	8SP	O1A-C1A-O1G-C1G
7	A	1005	8SP	O1B-C1B-O2G-C2G
7	A	1005	8SP	C2A-C1A-O1G-C1G
9	B	301	BOG	C4-C5-C6-O6
7	F	303	8SP	C2A-C1A-O1G-C1G
7	F	303	8SP	O1A-C1A-O1G-C1G
9	B	301	BOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	E	1004	6PE	C10-C11-C12-C13
4	A	1002	HEM	C2A-CAA-CBA-CGA
7	F	303	8SP	CB-OG-P-O3G
6	A	1004	6PE	C10-C11-C12-C13
6	A	1004	6PE	C5-C4-O4-C3
6	E	1004	6PE	C5-C4-O4-C3
9	F	301	BOG	O1-C1'-C2'-C3'
7	A	1005	8SP	C2A-C3A-C4A-C5A
6	E	1004	6PE	C1-C2-C3-O4
7	A	1005	8SP	C1A-C2A-C3A-C4A
6	A	1004	6PE	O5-C4-O4-C3
6	E	1004	6PE	O5-C4-O4-C3
7	F	303	8SP	C2B-C1B-O2G-C2G
7	A	1005	8SP	C3B-C4B-C5B-C6B
4	A	1001	HEM	C4B-C3B-CAB-CBB
9	F	301	BOG	O5-C5-C6-O6
6	E	1004	6PE	C1-O3-P1-O8
6	A	1004	6PE	O3-C1-C2-C3
7	F	303	8SP	O1B-C1B-O2G-C2G
7	F	303	8SP	O1G-C1G-C2G-C3G
6	E	1004	6PE	C5-C6-C7-C8
9	B	301	BOG	C4'-C5'-C6'-C7'
6	E	1004	6PE	C11-C10-O6-C2
6	E	1004	6PE	O6-C2-C3-O4
9	B	301	BOG	C2'-C3'-C4'-C5'
6	E	1004	6PE	O3-C1-C2-C3
6	A	1004	6PE	C1-C2-C3-O4
7	A	1005	8SP	O2G-C2G-C3G-O3G
6	E	1004	6PE	O7-C10-O6-C2
6	E	1004	6PE	C12-C13-C14-C15
7	A	1005	8SP	C1G-C2G-C3G-O3G
7	F	303	8SP	C1G-C2G-C3G-O3G
7	A	1005	8SP	C1G-C2G-O2G-C1B
7	F	303	8SP	C3G-C2G-O2G-C1B
6	A	1004	6PE	O3-C1-C2-O6
7	F	303	8SP	O1G-C1G-C2G-O2G
7	F	303	8SP	C3B-C4B-C5B-C6B
7	A	1005	8SP	O-C-CA-CB
7	A	1005	8SP	OXT-C-CA-CB
6	E	1004	6PE	C1-O3-P1-O2
7	A	1005	8SP	CB-OG-P-O2P
7	F	303	8SP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
6	E	1004	6PE	O3-C1-C2-O6
7	F	303	8SP	O2G-C2G-C3G-O3G
4	A	1002	HEM	C1A-C2A-CAA-CBA
4	A	1002	HEM	C3A-C2A-CAA-CBA
7	F	303	8SP	C1A-C2A-C3A-C4A
7	F	303	8SP	C3G-O3G-P-OG
4	A	1001	HEM	CAA-CBA-CGA-O1A
7	A	1005	8SP	C4A-C5A-C6A-C7A
6	A	1004	6PE	O6-C2-C3-O4
4	A	1001	HEM	CAA-CBA-CGA-O2A
10	F	302	HEC	CAA-CBA-CGA-O2A
4	A	1001	HEM	C3D-CAD-CBD-CGD
9	B	301	BOG	O1-C1'-C2'-C3'
4	A	1002	HEM	CAA-CBA-CGA-O2A
4	E	1001	HEM	CAD-CBD-CGD-O1D
6	A	1004	6PE	O7-C10-O6-C2
6	A	1004	6PE	O4-C4-C5-C6
10	F	302	HEC	CAA-CBA-CGA-O1A
4	A	1002	HEM	CAA-CBA-CGA-O1A
6	E	1004	6PE	O4-C4-C5-C6
6	E	1004	6PE	O6-C10-C11-C12
5	A	1003	AZO	N1-C1-C2-C7
6	E	1004	6PE	O5-C4-C5-C6
7	A	1005	8SP	C4B-C5B-C6B-C7B
4	E	1001	HEM	CAD-CBD-CGD-O2D
9	B	301	BOG	C3'-C4'-C5'-C6'
6	A	1004	6PE	O5-C4-C5-C6
4	E	1001	HEM	CAA-CBA-CGA-O2A
10	B	302	HEC	CAA-CBA-CGA-O2A
6	E	1004	6PE	O7-C10-C11-C12
7	A	1005	8SP	O1G-C1A-C2A-C3A
4	E	1001	HEM	CAA-CBA-CGA-O1A
10	B	302	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	HEM	1	0
4	E	1001	HEM	2	0
4	A	1001	HEM	3	0
10	B	302	HEC	4	0

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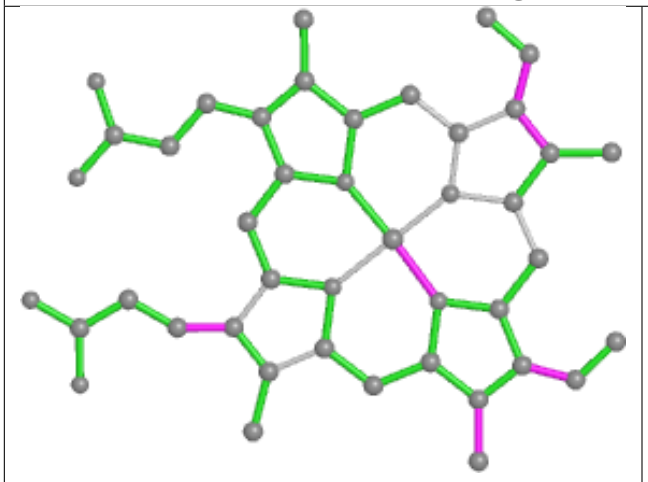
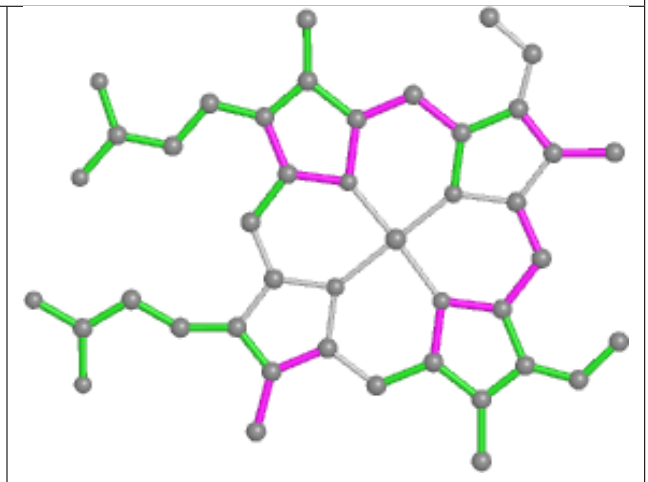
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	302	HEC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

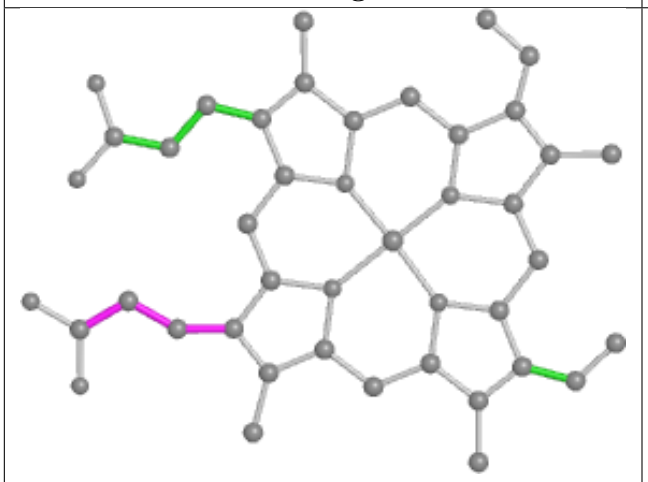
Ligand HEM A 1002



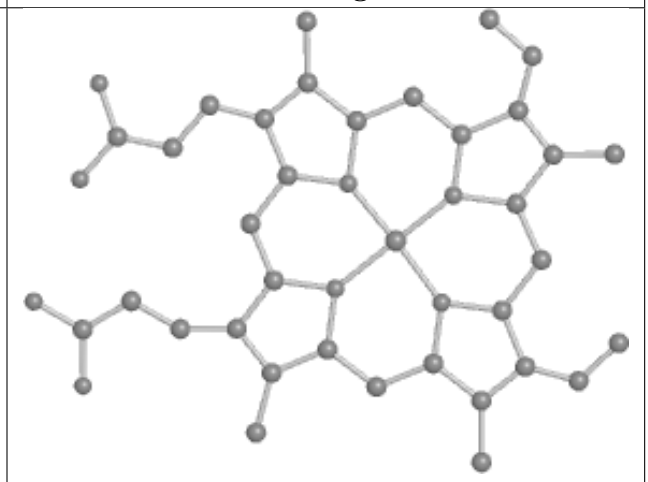
Bond lengths



Bond angles

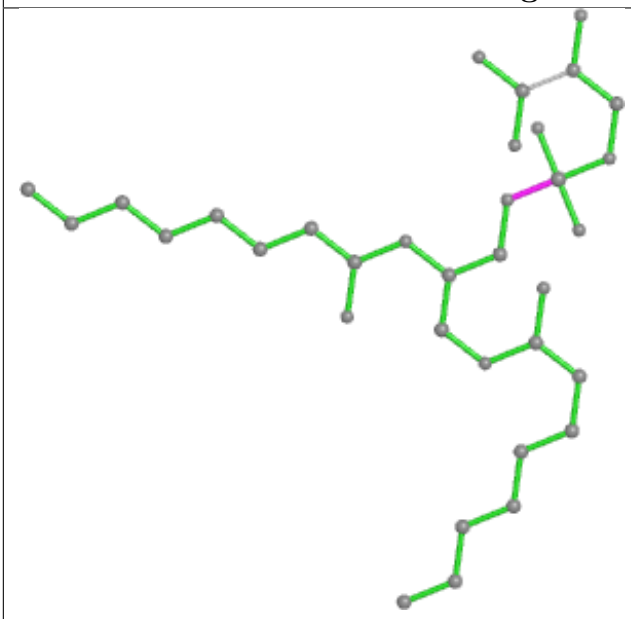


Torsions

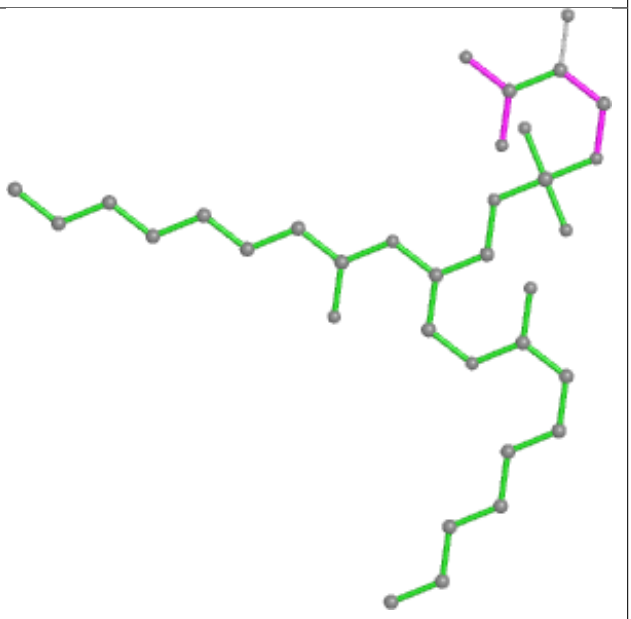


Rings

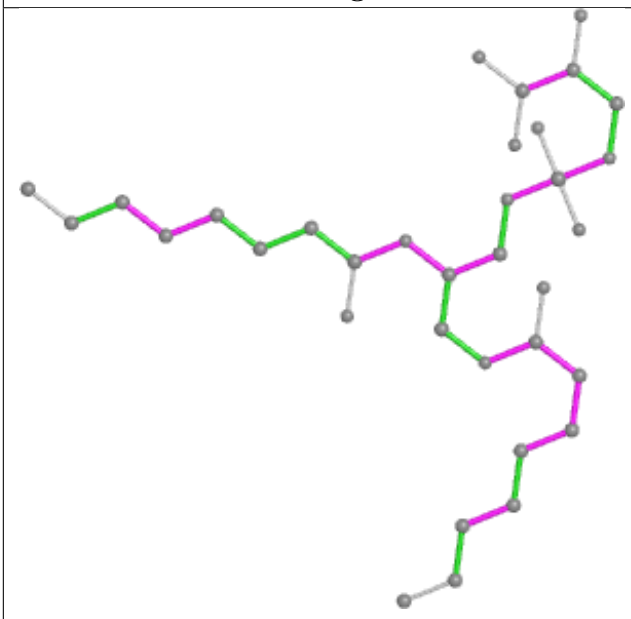
Ligand 8SP A 1005



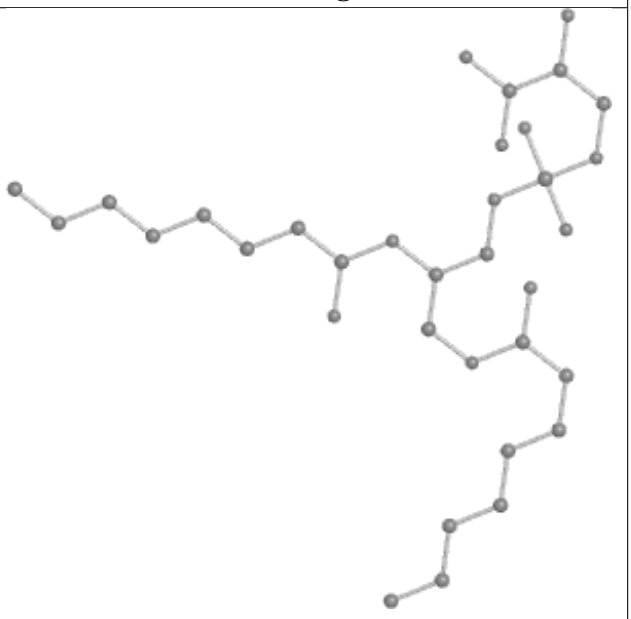
Bond lengths



Bond angles

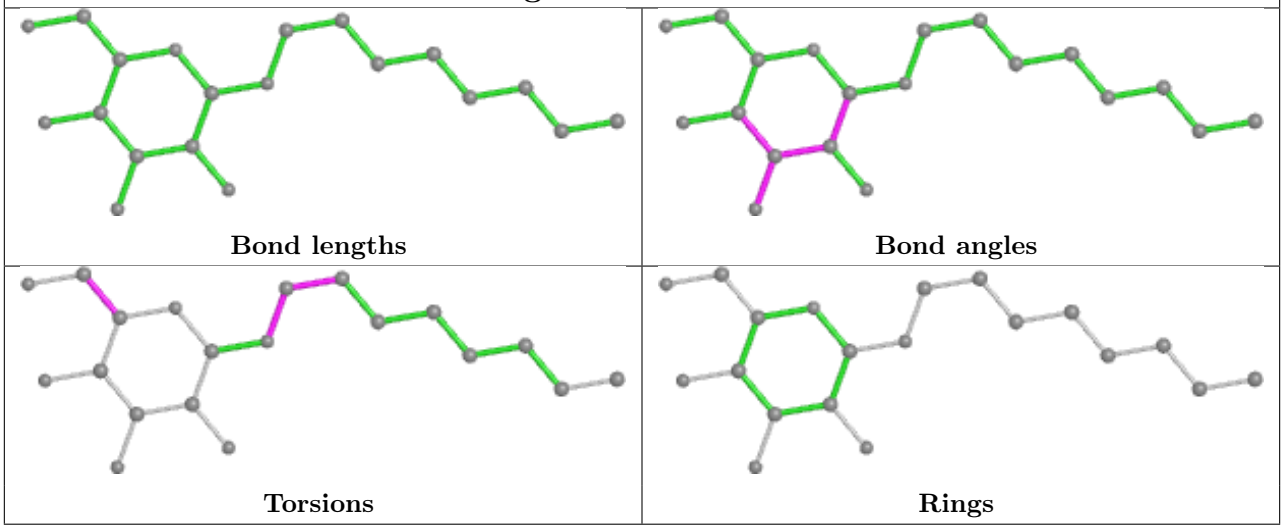


Torsions

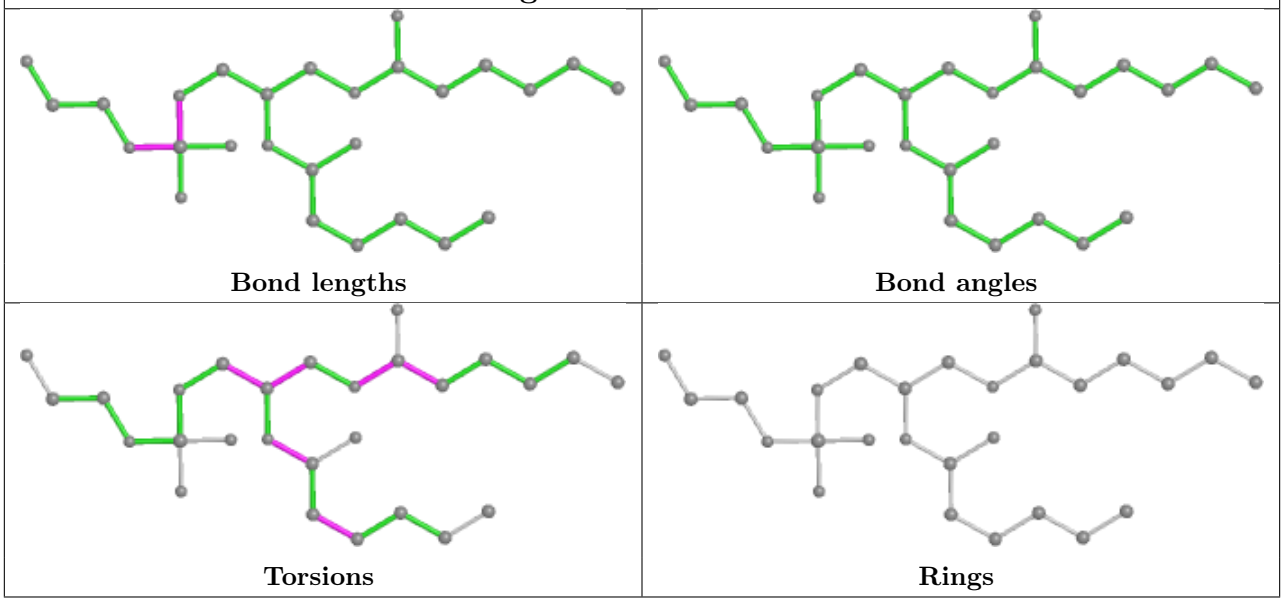


Rings

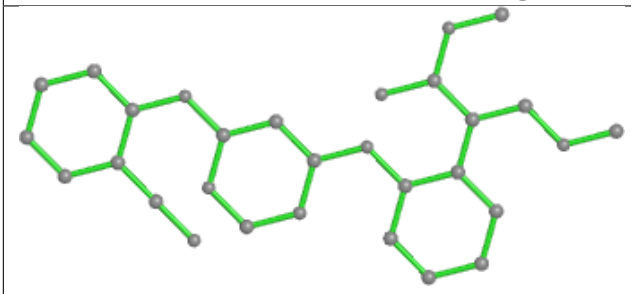
Ligand BOG F 301



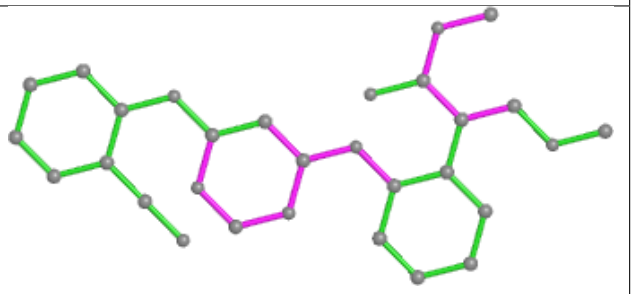
Ligand 6PE A 1004



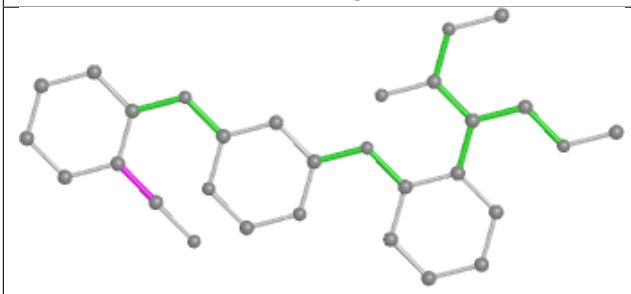
Ligand AZO A 1003



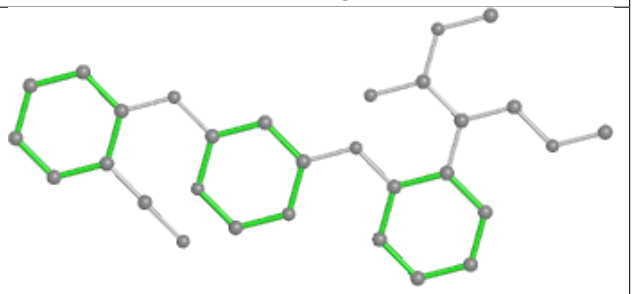
Bond lengths



Bond angles

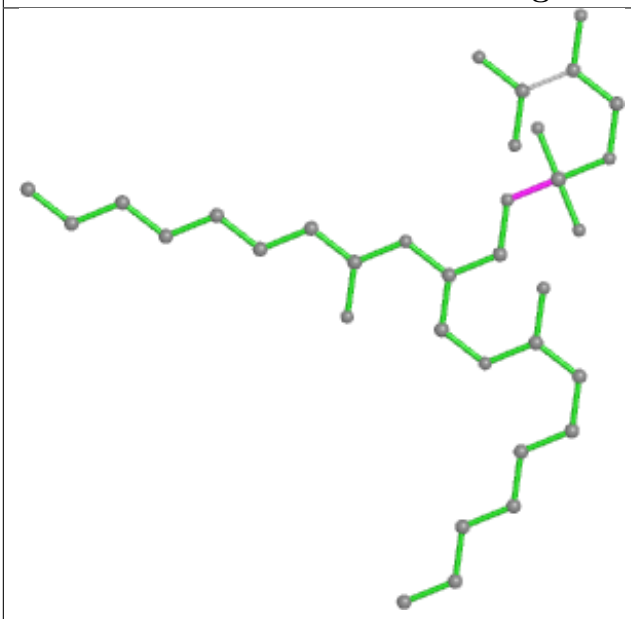


Torsions

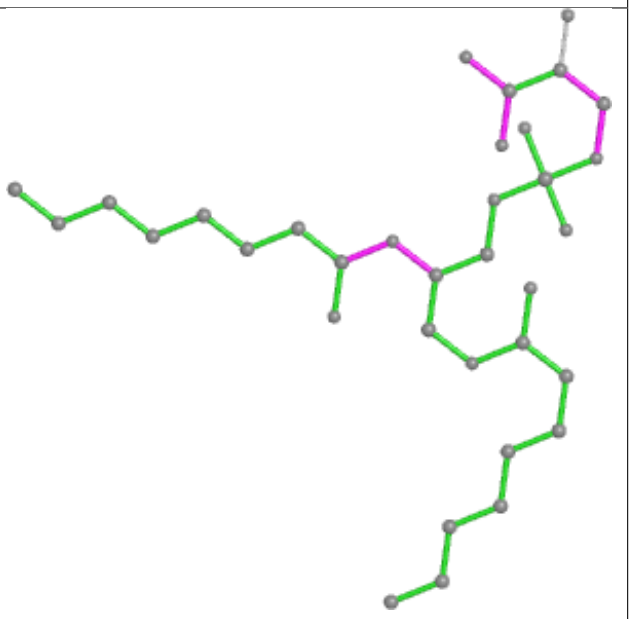


Rings

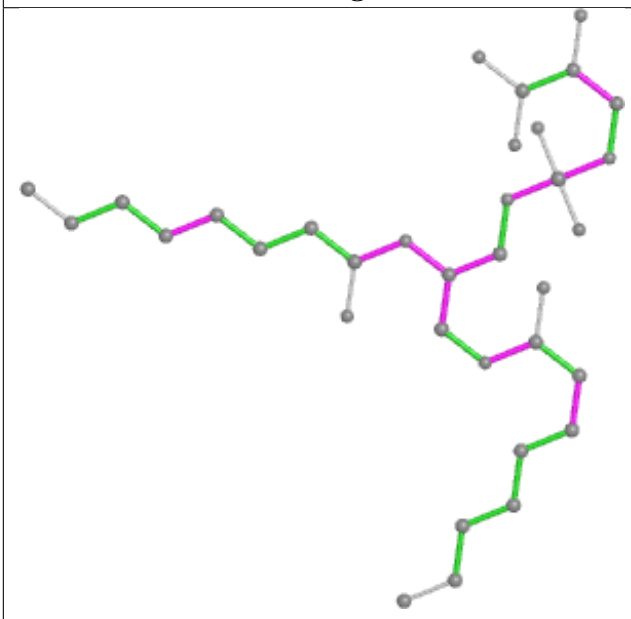
Ligand 8SP F 303



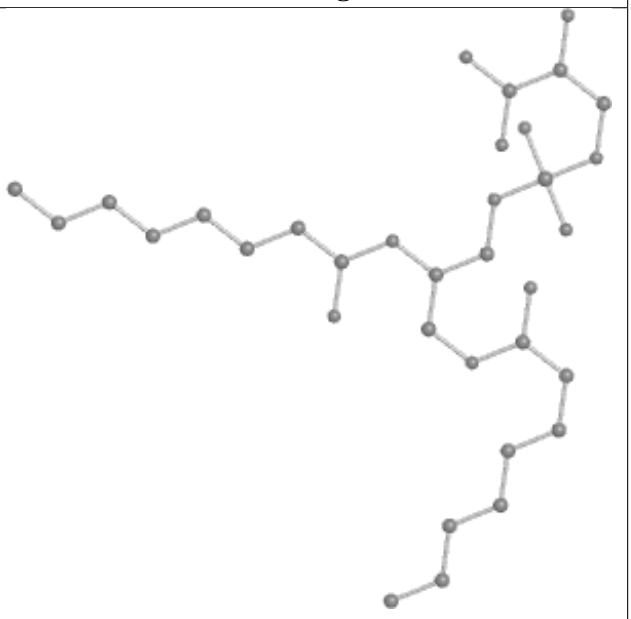
Bond lengths



Bond angles

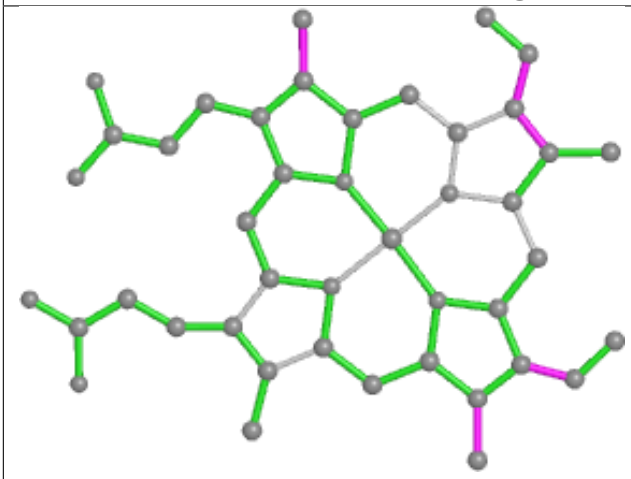


Torsions

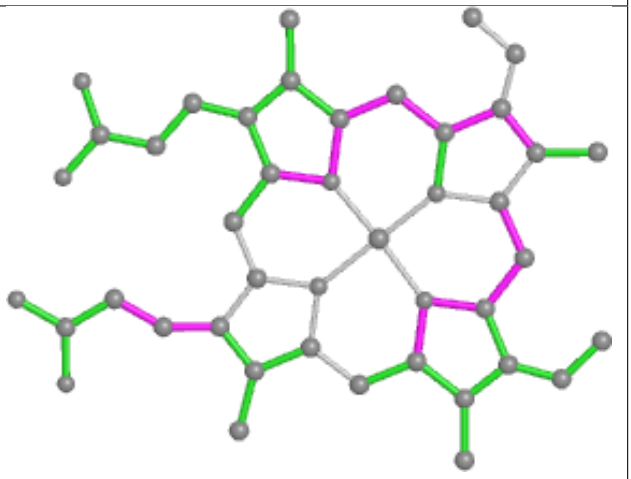


Rings

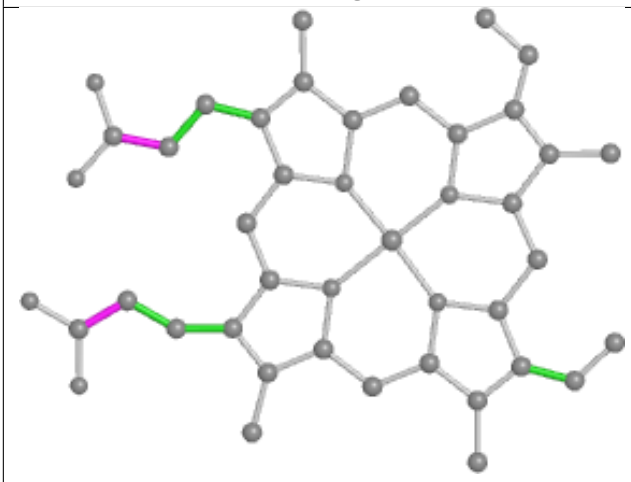
Ligand HEM E 1001



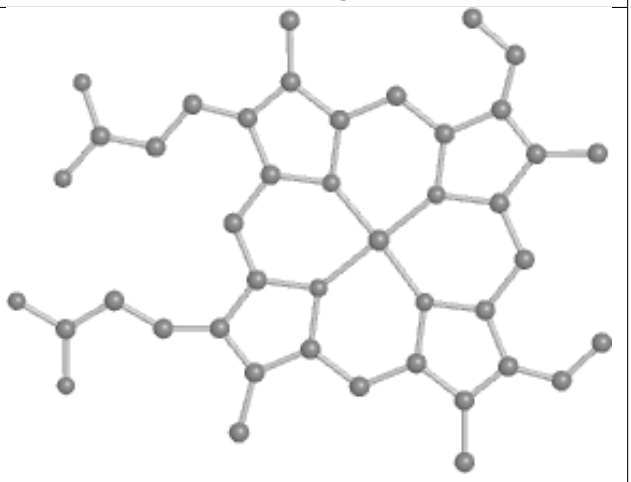
Bond lengths



Bond angles

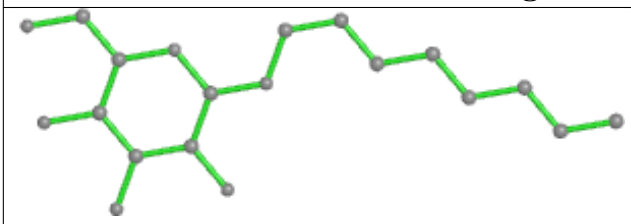


Torsions

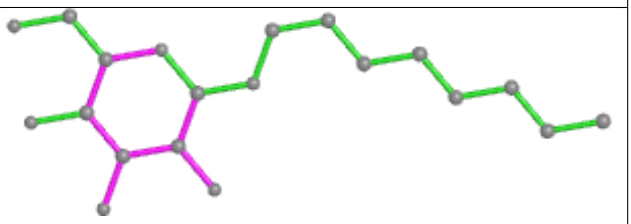


Rings

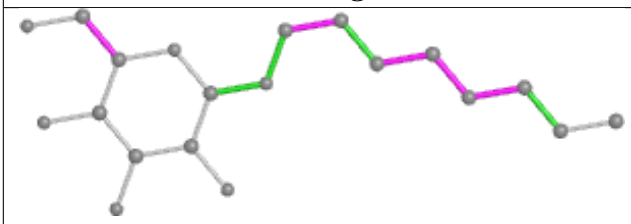
Ligand BOG B 301



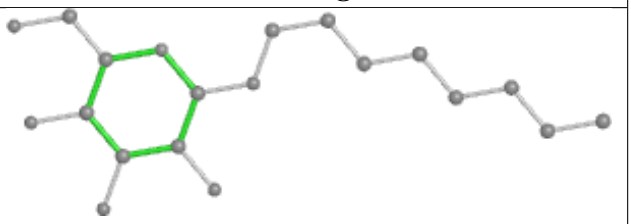
Bond lengths



Bond angles

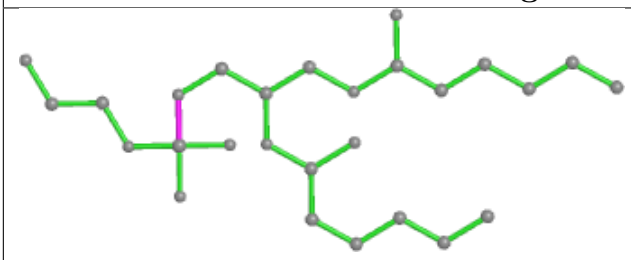


Torsions

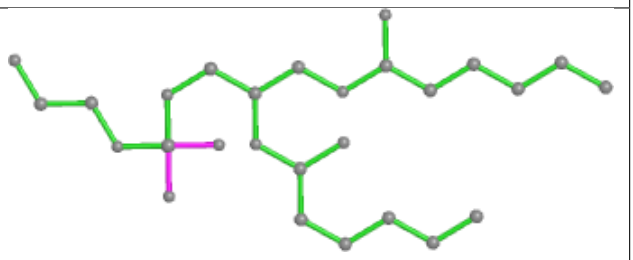


Rings

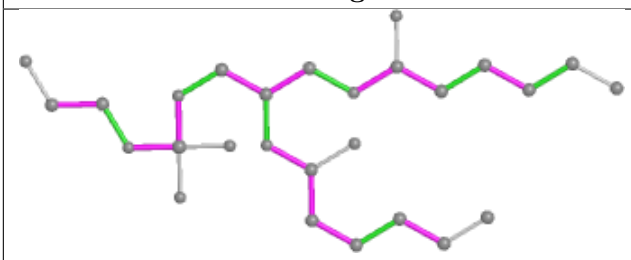
Ligand 6PE E 1004



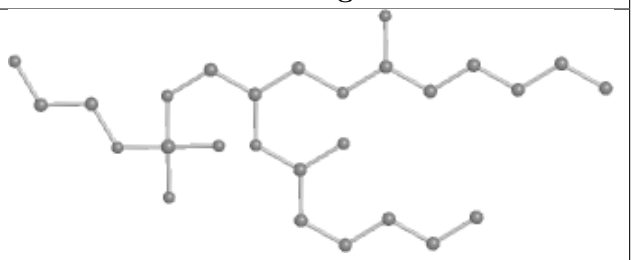
Bond lengths



Bond angles

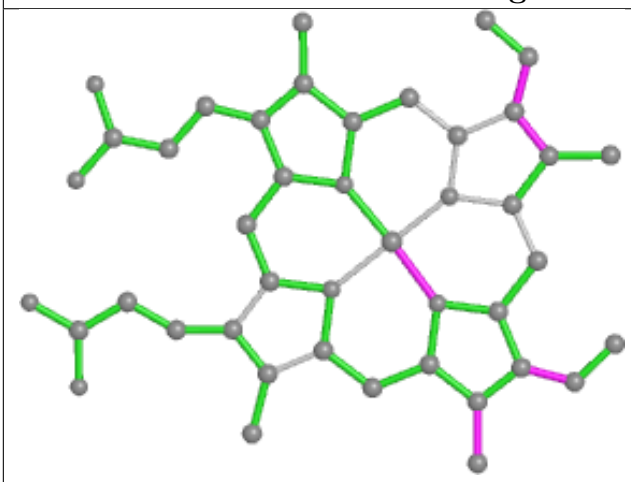


Torsions

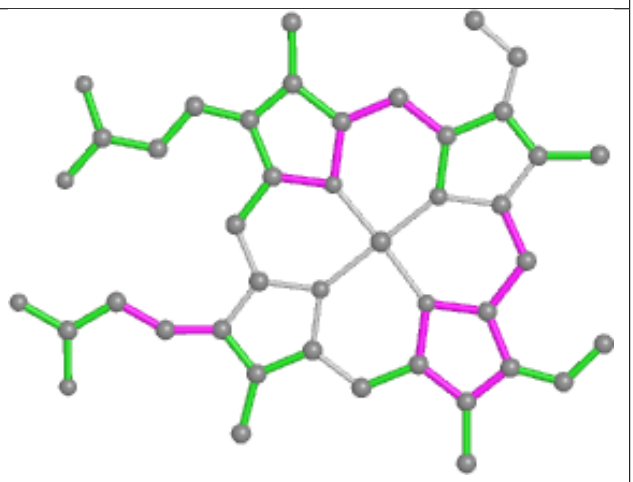


Rings

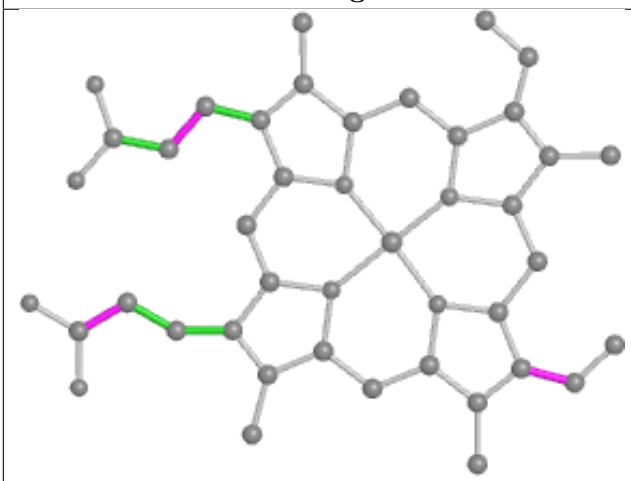
Ligand HEM A 1001



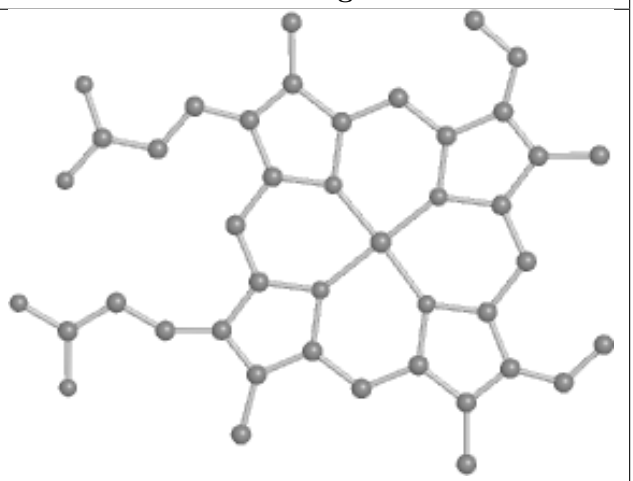
Bond lengths



Bond angles

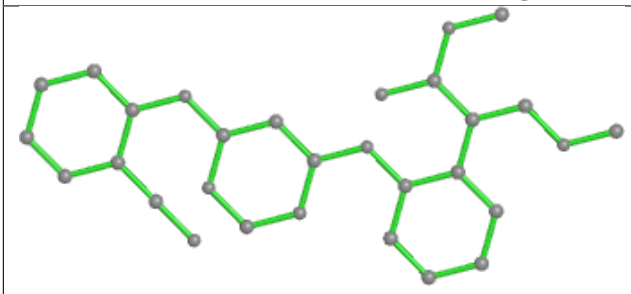


Torsions

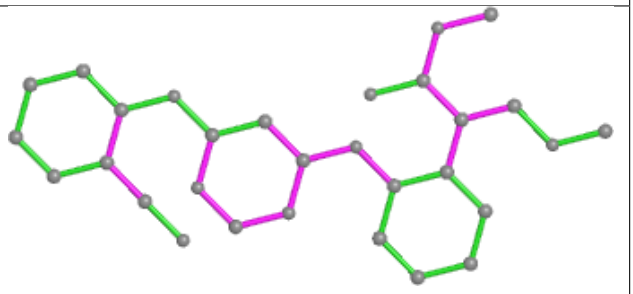


Rings

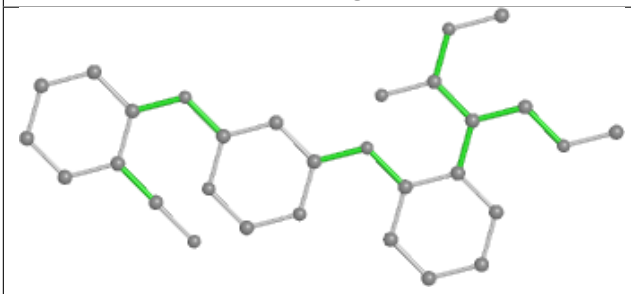
Ligand AZO E 1003



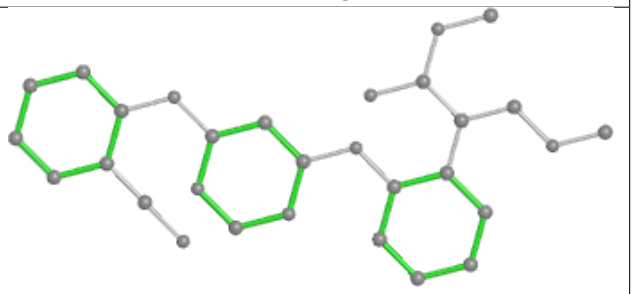
Bond lengths



Bond angles

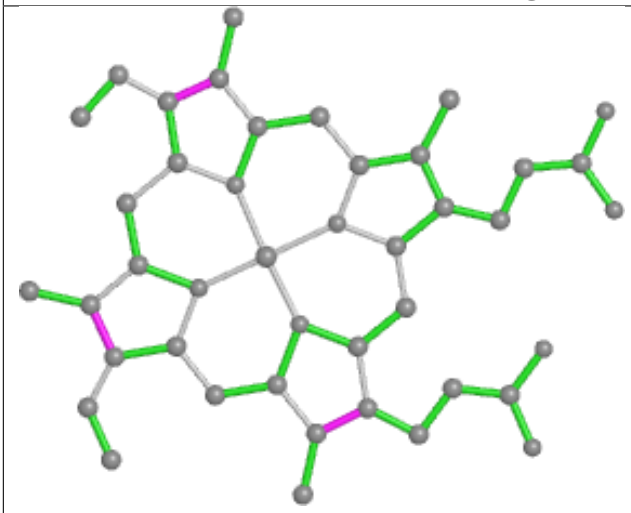


Torsions

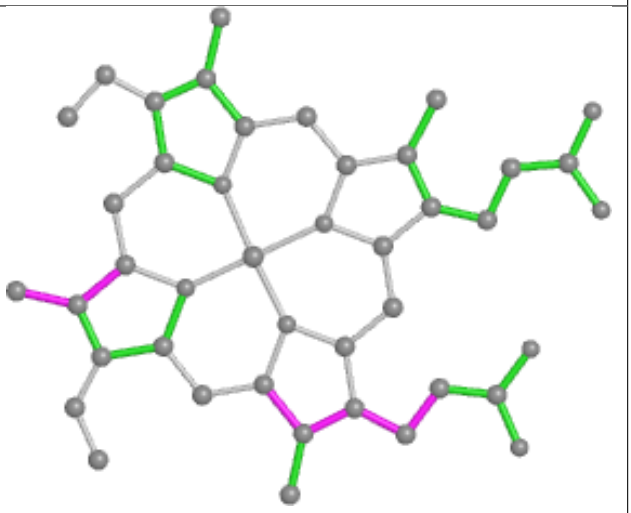


Rings

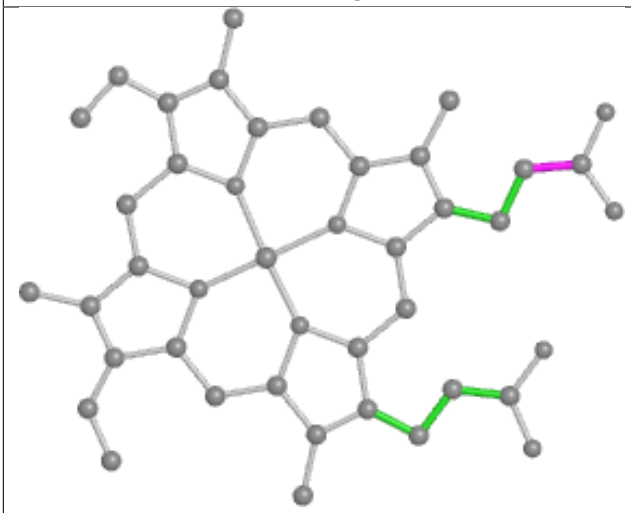
Ligand HEC B 302



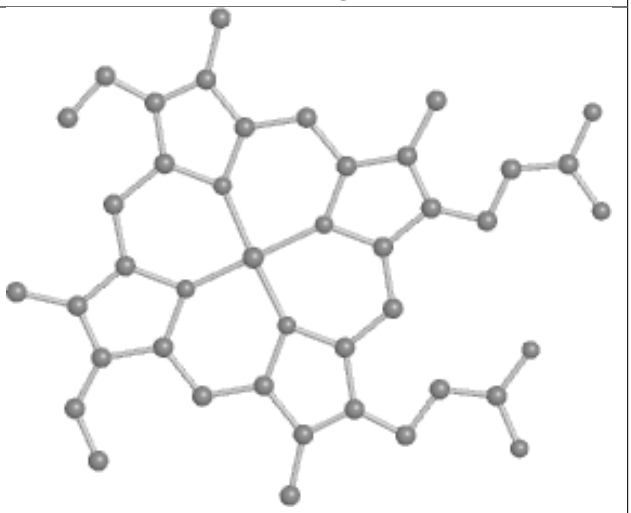
Bond lengths



Bond angles

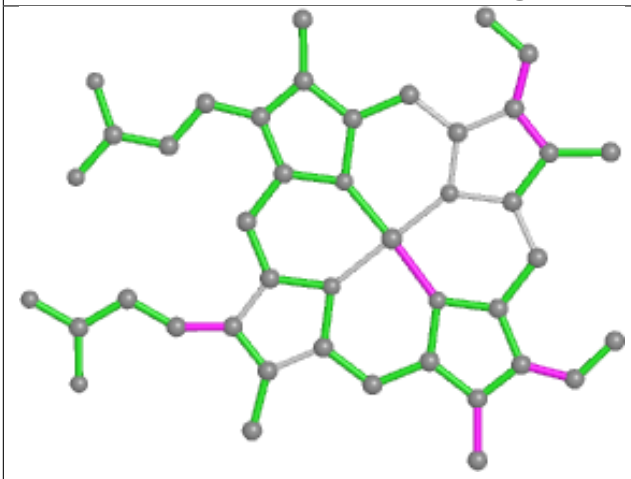


Torsions

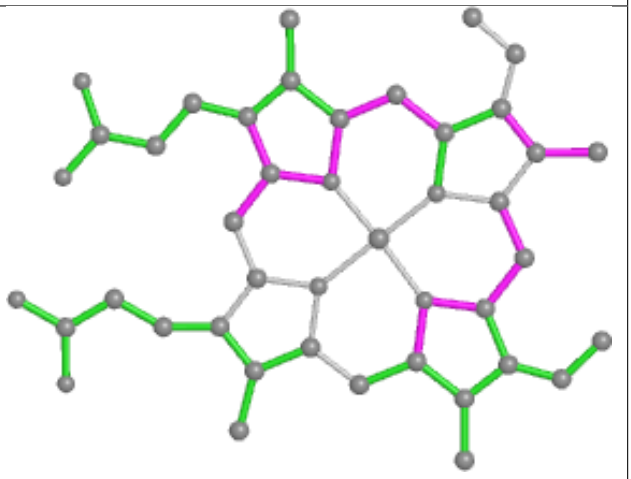


Rings

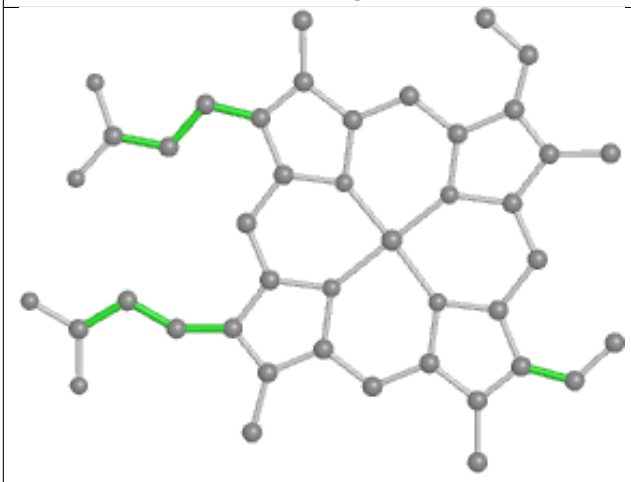
Ligand HEM E 1002



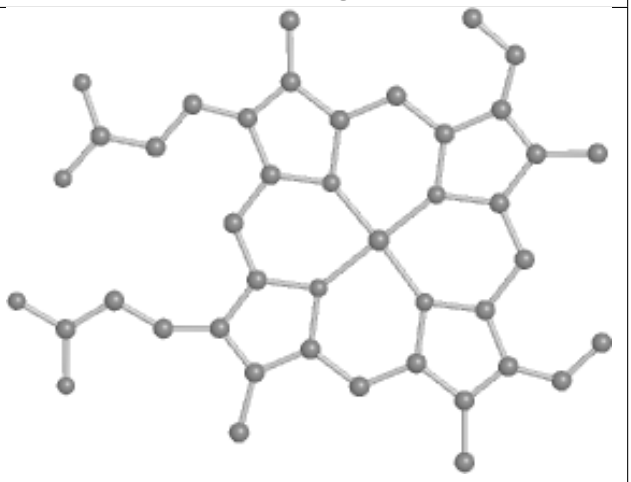
Bond lengths



Bond angles

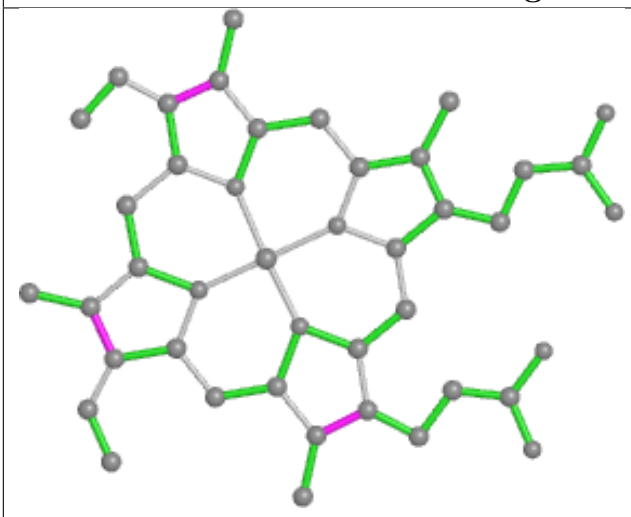


Torsions

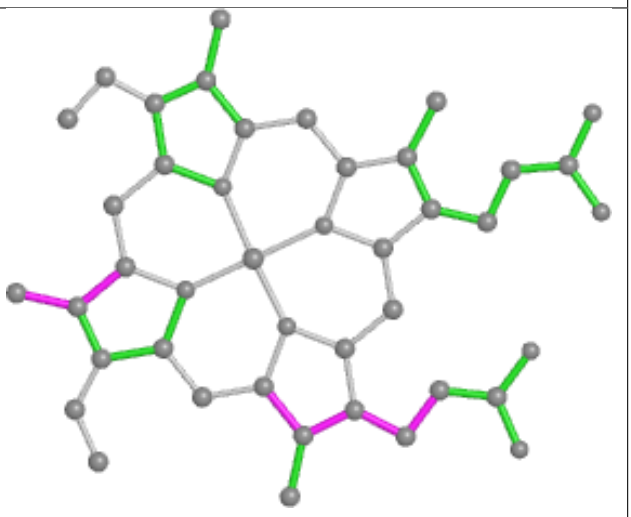


Rings

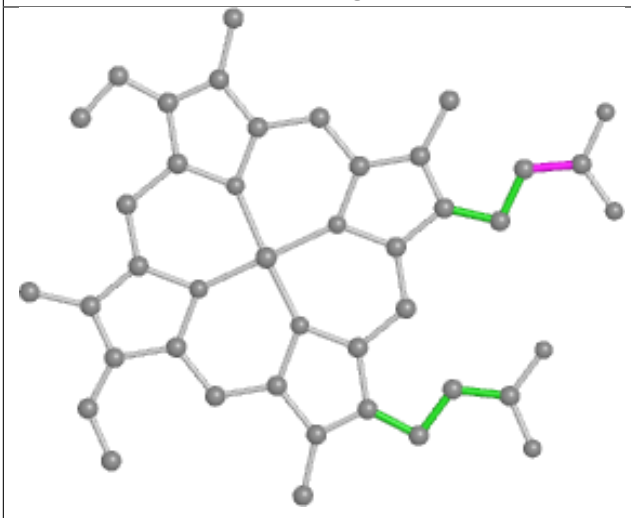
Ligand HEC F 302



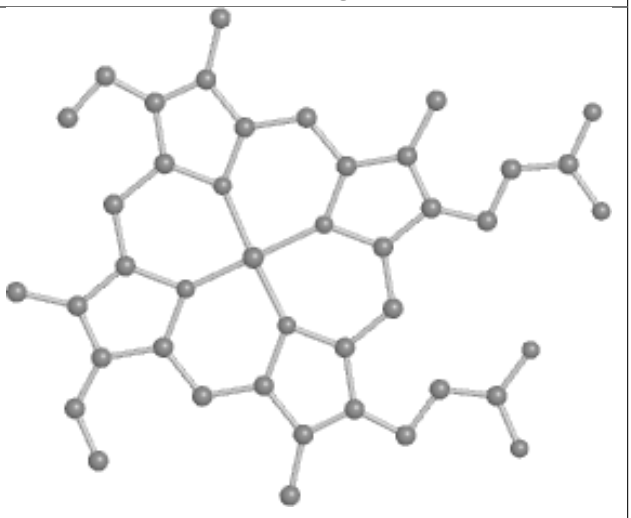
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	430/445 (96%)	-0.19	12 (2%)	53	25	34, 50, 98, 124	0
1	E	430/445 (96%)	-0.06	13 (3%)	50	22	17, 59, 105, 158	0
2	B	256/272 (94%)	0.29	20 (7%)	13	4	46, 67, 126, 172	0
2	F	256/272 (94%)	0.34	21 (8%)	11	3	47, 79, 148, 192	0
3	C	175/187 (93%)	4.12	116 (66%)	0	0	64, 110, 138, 143	136 (77%)
3	G	175/187 (93%)	3.25	119 (68%)	0	0	45, 100, 119, 141	136 (77%)
All	All	1722/1808 (95%)	0.78	301 (17%)	1	0	17, 70, 128, 192	272 (15%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	78	THR	19.0
3	C	80	ALA	18.3
3	G	78	THR	16.7
3	G	134	CYS	14.6
3	C	87	SER	14.5
3	C	119	ALA	14.0
3	C	120	GLY	13.9
3	C	113	ASN	13.3
3	G	77	ARG	12.8
3	C	140	VAL	11.8
3	G	141	SER	11.6
3	C	109	ALA	11.6
3	C	104	ASP	11.4
3	C	108	GLU	10.8
3	G	181	GLU	10.5
3	C	79	GLU	10.0
3	C	85	GLY	9.8
3	C	181	GLU	9.8
3	C	115	THR	9.7

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Mol	Chain	Res	Type	RSRZ
3	C	55	SER	9.7
3	C	112	GLN	9.3
3	G	133	GLY	9.3
3	C	91	GLY	9.1
3	G	142	GLY	8.7
3	C	56	SER	8.7
3	C	86	ARG	8.7
3	G	60	GLY	7.9
3	C	90	LEU	7.9
3	C	96	THR	7.8
3	G	87	SER	7.6
3	C	133	GLY	7.6
3	G	171	LEU	7.6
3	C	134	CYS	7.5
3	C	114	ARG	7.5
3	G	122	TRP	7.4
3	G	96	THR	7.4
3	C	118	GLU	7.3
3	G	88	VAL	7.3
3	C	149	CYS	7.2
3	G	83	GLU	7.1
3	C	65	VAL	7.0
3	C	180	ASP	6.9
3	C	122	TRP	6.8
3	C	178	PHE	6.7
3	C	83	GLU	6.7
3	C	182	THR	6.7
3	C	151	CYS	6.6
3	C	84	LEU	6.5
3	G	74	ILE	6.5
3	C	97	ASN	6.5
3	G	113	ASN	6.5
3	C	117	ASP	6.4
3	G	130	THR	6.4
3	C	110	THR	6.4
3	G	108	GLU	6.4
3	G	151	CYS	6.3
3	G	119	ALA	6.2
3	G	61	VAL	6.2
3	C	57	VAL	6.2
3	G	121	GLU	6.2
3	C	106	GLY	6.1

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Mol	Chain	Res	Type	RSRZ
3	G	90	LEU	6.1
2	B	2	GLY	6.0
3	G	80	ALA	6.0
3	C	69	GLY	5.9
3	G	118	GLU	5.9
3	C	68	LEU	5.8
3	C	166	PRO	5.8
3	G	125	MET	5.7
3	C	124	VAL	5.7
2	F	256	LYS	5.7
3	G	128	VAL	5.6
3	C	116	LEU	5.6
3	C	171	LEU	5.5
3	C	165	GLY	5.5
3	C	103	ILE	5.5
3	C	111	ASP	5.5
3	C	66	LYS	5.5
3	G	67	PHE	5.5
3	C	130	THR	5.4
3	C	88	VAL	5.4
3	G	114	ARG	5.4
3	C	13	ASP	5.4
3	C	67	PHE	5.3
3	G	126	TRP	5.3
3	G	140	VAL	5.2
3	G	178	PHE	5.2
3	G	139	GLY	5.2
3	C	126	TRP	5.1
3	G	89	GLN	5.1
3	C	125	MET	5.0
3	C	177	LYS	5.0
2	B	1	ALA	4.9
3	C	138	GLY	4.9
3	G	110	THR	4.9
3	G	71	PRO	4.9
3	G	127	GLY	4.9
3	C	81	ASP	4.9
3	C	60	GLY	4.9
3	G	105	ALA	4.9
3	C	185	GLN	4.8
2	B	3	GLY	4.8
3	C	107	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	123	LEU	4.8
3	C	131	HIS	4.8
2	F	8	ASP	4.7
3	C	92	GLN	4.7
3	G	56	SER	4.7
3	G	129	CYS	4.7
3	C	77	ARG	4.7
3	C	105	ALA	4.7
2	F	172	ALA	4.7
3	C	176	ALA	4.6
3	G	106	GLY	4.6
3	C	179	ILE	4.6
3	C	175	LEU	4.5
3	G	112	GLN	4.5
3	G	172	PRO	4.5
3	G	92	GLN	4.5
3	C	128	VAL	4.4
3	G	135	VAL	4.4
3	C	98	ALA	4.4
3	C	168	PRO	4.4
3	C	137	ILE	4.4
3	G	182	THR	4.4
3	G	116	LEU	4.4
3	C	183	THR	4.4
3	C	174	PRO	4.4
3	C	141	SER	4.4
2	F	149	HIS	4.3
3	C	70	LYS	4.3
3	G	187	GLY	4.3
3	C	173	ILE	4.3
2	B	4	GLY	4.3
3	G	177	LYS	4.2
3	C	187	GLY	4.2
3	G	68	LEU	4.2
3	C	100	ASN	4.2
3	G	150	PRO	4.2
3	C	52	VAL	4.2
3	G	185	GLN	4.1
3	G	174	PRO	4.1
3	G	79	GLU	4.1
3	G	131	HIS	4.1
3	C	93	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	F	175	VAL	4.1
3	G	107	ALA	4.1
3	G	124	VAL	4.0
3	G	82	ILE	4.0
3	C	139	GLY	4.0
3	C	160	GLY	4.0
3	C	82	ILE	4.0
3	G	111	ASP	3.9
3	C	148	PHE	3.9
3	G	101	ALA	3.9
3	C	150	PRO	3.9
2	F	195	GLU	3.9
3	C	53	ASP	3.9
3	G	143	ASP	3.9
1	E	309	THR	3.8
3	G	64	THR	3.8
3	G	175	LEU	3.8
3	C	74	ILE	3.8
3	G	152	HIS	3.8
3	G	115	THR	3.8
3	G	81	ASP	3.8
3	G	55	SER	3.8
3	C	54	VAL	3.7
3	G	176	ALA	3.7
3	G	184	ILE	3.7
3	C	186	LEU	3.7
3	G	173	ILE	3.7
3	C	169	GLU	3.7
3	G	62	GLN	3.6
3	C	172	PRO	3.6
2	F	146	ALA	3.5
3	G	166	PRO	3.5
3	G	186	LEU	3.5
3	C	184	ILE	3.5
3	G	120	GLY	3.5
3	G	72	ILE	3.5
1	A	13	THR	3.5
2	F	147	GLU	3.4
3	G	86	ARG	3.4
3	C	59	PRO	3.4
3	G	73	PHE	3.4
1	E	233	SER	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	89	GLN	3.4
2	F	152	ASP	3.3
3	C	102	ASN	3.3
2	F	150	GLU	3.3
3	C	61	VAL	3.3
3	C	153	GLY	3.3
3	G	57	VAL	3.3
3	G	123	LEU	3.3
3	G	54	VAL	3.3
3	G	160	GLY	3.3
3	G	76	ARG	3.2
2	F	3	GLY	3.2
2	B	143	PRO	3.2
3	C	152	HIS	3.2
3	G	149	CYS	3.2
3	G	53	ASP	3.2
3	G	59	PRO	3.2
3	G	98	ALA	3.2
3	G	103	ILE	3.2
3	G	93	LEU	3.1
3	C	99	ARG	3.1
3	C	101	ALA	3.1
1	E	232	THR	3.1
3	C	75	ARG	3.1
3	C	121	GLU	3.1
3	G	75	ARG	3.1
3	G	65	VAL	3.0
2	B	146	ALA	3.0
3	G	104	ASP	3.0
3	G	179	ILE	3.0
3	G	132	LEU	3.0
3	C	64	THR	3.0
1	E	311	ASP	2.9
2	B	144	LYS	2.9
2	F	148	GLY	2.9
3	G	66	LYS	2.8
3	G	109	ALA	2.8
2	F	174	GLY	2.8
2	B	152	ASP	2.8
2	B	197	ALA	2.8
3	C	71	PRO	2.8
3	G	84	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	142	GLY	2.8
2	F	19	THR	2.7
3	G	85	GLY	2.7
3	G	102	ASN	2.7
3	G	13	ASP	2.7
3	G	138	GLY	2.7
3	C	127	GLY	2.7
3	C	167	ALA	2.7
1	A	11	PRO	2.7
3	G	148	PHE	2.6
2	F	173	ASN	2.6
2	F	1	ALA	2.6
3	C	154	SER	2.6
2	B	80	ASP	2.6
3	G	180	ASP	2.6
1	E	19	LEU	2.6
2	F	205	HIS	2.6
2	B	151	PRO	2.6
3	G	97	ASN	2.6
3	C	132	LEU	2.6
3	G	95	ASP	2.5
1	E	239	LYS	2.5
1	E	6	HIS	2.5
3	C	170	ASN	2.5
3	G	154	SER	2.5
3	G	158	SER	2.5
3	G	167	ALA	2.5
2	F	18	GLY	2.4
3	G	63	LEU	2.4
2	B	190	MET	2.4
1	A	174	HIS	2.4
3	C	94	VAL	2.4
2	B	147	GLU	2.4
3	G	52	VAL	2.4
3	G	168	PRO	2.4
1	A	15	ILE	2.4
3	G	69	GLY	2.3
1	E	228	GLU	2.3
3	G	99	ARG	2.3
1	E	231	ARG	2.3
1	A	311	ASP	2.3
3	C	63	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	73	THR	2.3
3	G	153	GLY	2.3
2	B	250	ARG	2.3
3	G	100	ASN	2.3
1	A	234	LYS	2.2
1	E	430	ALA	2.2
2	B	198	ASP	2.2
3	G	136	PRO	2.2
2	F	190	MET	2.2
3	C	129	CYS	2.2
3	G	165	GLY	2.2
1	E	310	ALA	2.2
3	C	58	GLU	2.2
2	F	79	GLU	2.2
1	A	12	ARG	2.2
1	E	15	ILE	2.1
1	A	9	TYR	2.1
1	A	16	GLU	2.1
3	G	163	ARG	2.1
3	G	169	GLU	2.1
1	E	36	PRO	2.1
2	B	141	GLU	2.1
1	A	231	ARG	2.1
1	A	232	THR	2.1
2	B	202	ALA	2.1
3	G	70	LYS	2.0
1	A	10	GLU	2.0
2	F	165	VAL	2.0
2	B	79	GLU	2.0
2	B	17	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

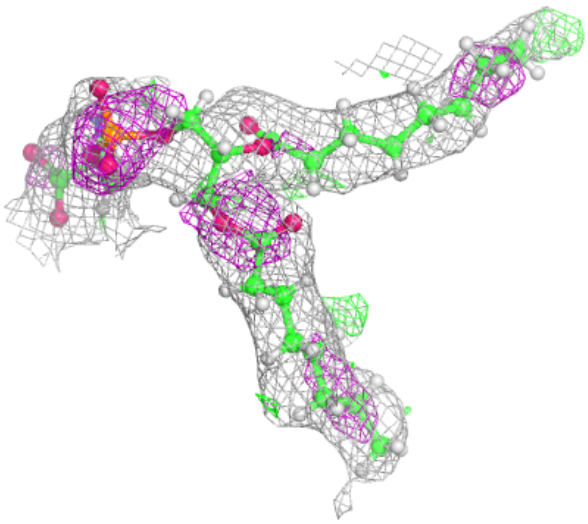
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

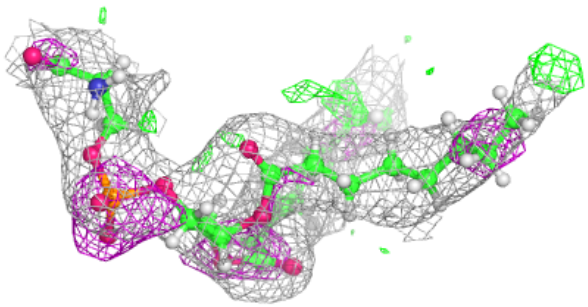
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	FES	C	1001	4/4	0.73	0.30	128,129,132,132	4
11	FES	G	1001	4/4	0.77	0.43	106,107,109,109	4
7	8SP	F	303	34/34	0.87	0.31	11,17,48,49	0
8	SR	A	1006	1/1	0.87	0.07	103,103,103,103	0
7	8SP	A	1005	34/34	0.88	0.24	6,12,35,35	0
9	BOG	F	301	20/20	0.88	0.30	12,16,21,25	0
6	6PE	A	1004	27/27	0.91	0.26	9,15,19,21	0
10	HEC	F	302	43/43	0.91	0.22	43,48,58,58	0
5	AZO	A	1003	30/30	0.91	0.23	32,35,43,44	0
9	BOG	B	301	20/20	0.91	0.27	9,12,15,19	0
6	6PE	E	1004	27/27	0.92	0.28	7,14,19,20	0
4	HEM	A	1001	43/43	0.93	0.28	47,53,64,64	0
5	AZO	E	1003	30/30	0.93	0.22	39,39,47,49	0
4	HEM	A	1002	43/43	0.93	0.28	49,54,66,66	0
4	HEM	E	1002	43/43	0.93	0.25	48,54,65,66	0
10	HEC	B	302	43/43	0.94	0.20	43,48,58,58	0
4	HEM	E	1001	43/43	0.94	0.24	46,52,63,63	0
8	SR	F	304	1/1	0.96	0.04	108,108,108,108	0
8	SR	B	303	1/1	0.97	0.10	102,102,102,102	0

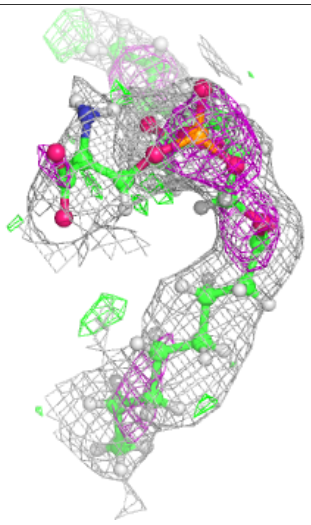
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8SP F 303:

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

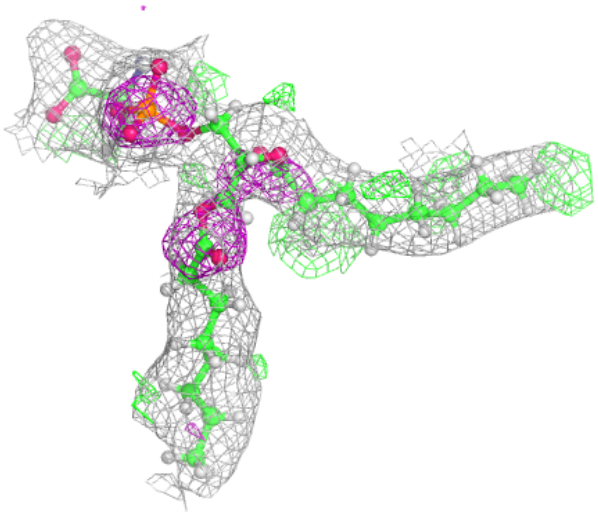


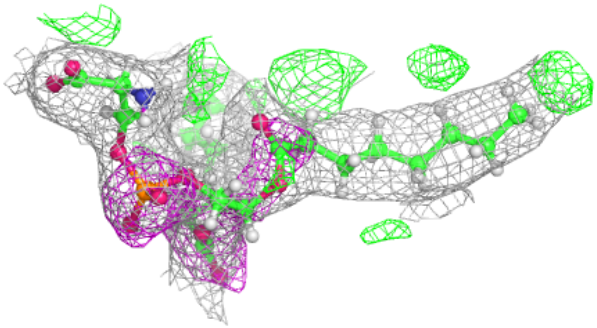


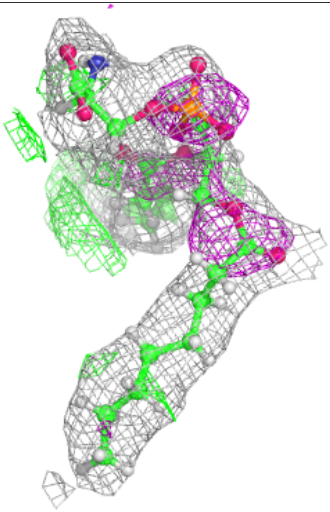


Electron density around 8SP A 1005:

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

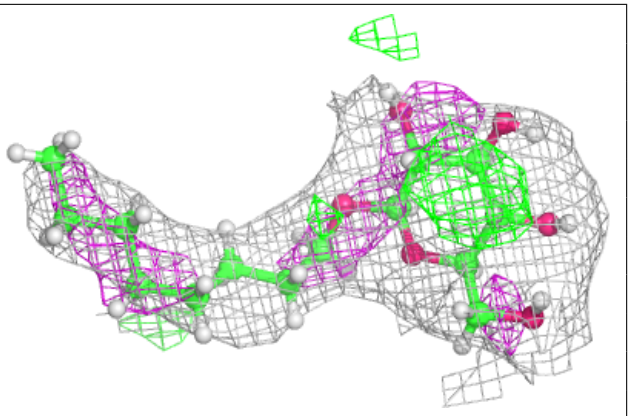


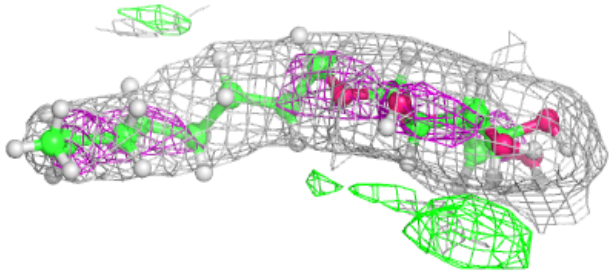


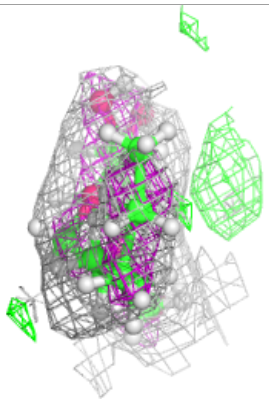


Electron density around BOG F 301:

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

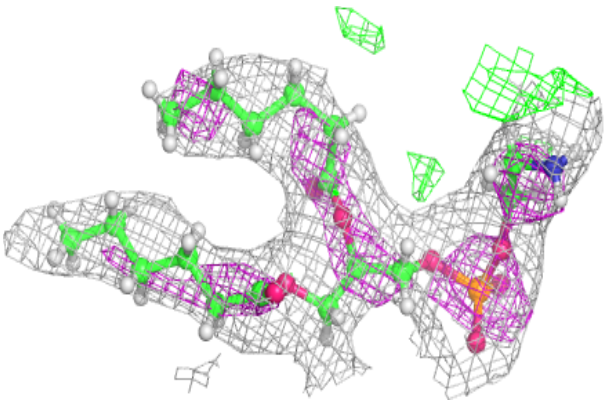


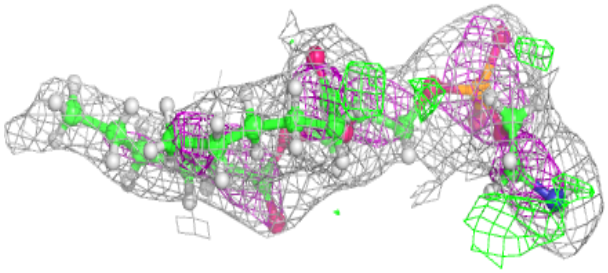


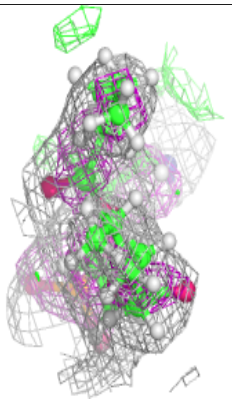


Electron density around 6PE A 1004:

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

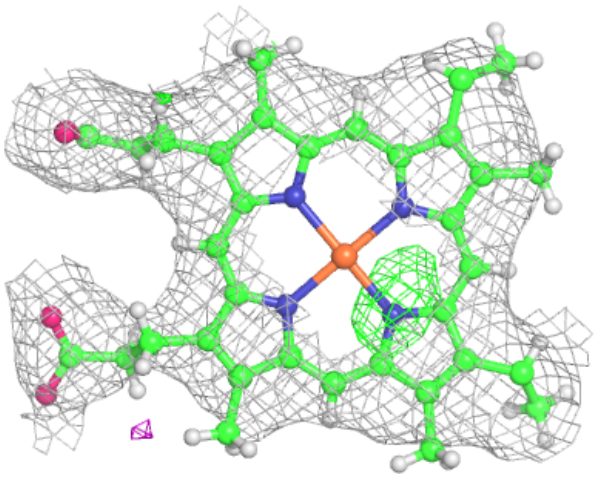


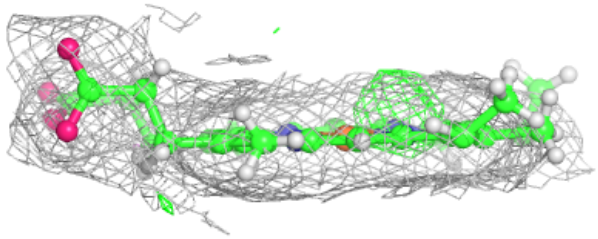


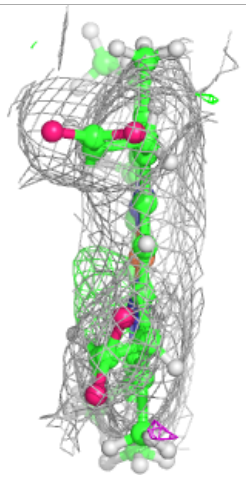


Electron density around HEC F 302:

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

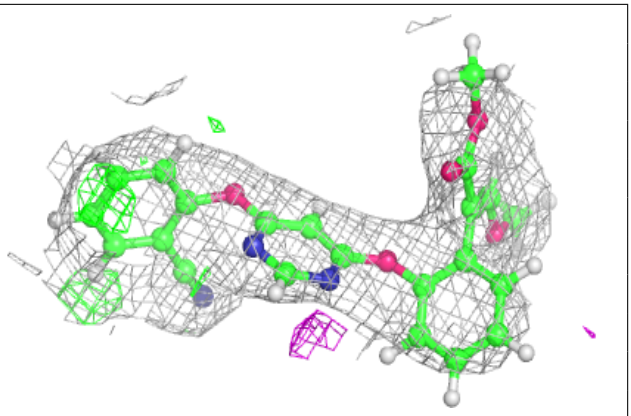


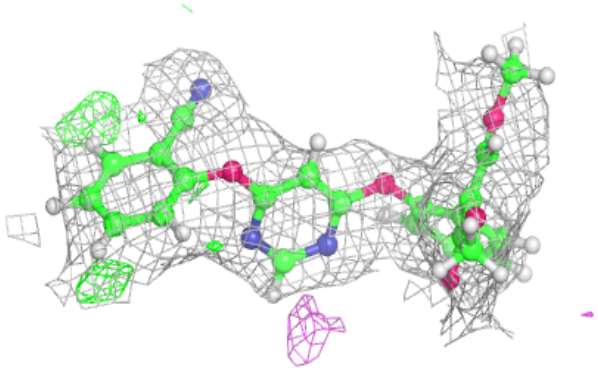


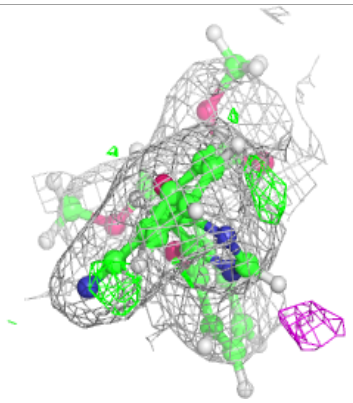


Electron density around AZO A 1003:

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

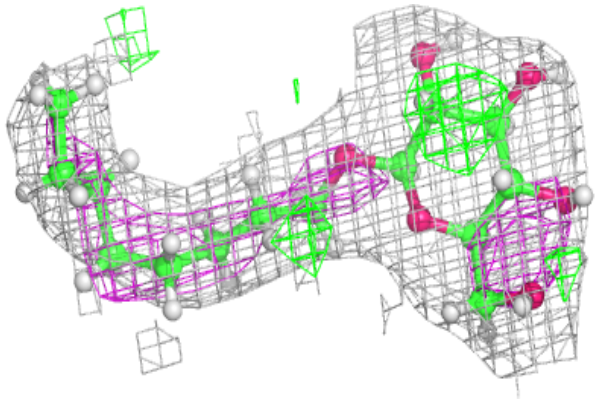


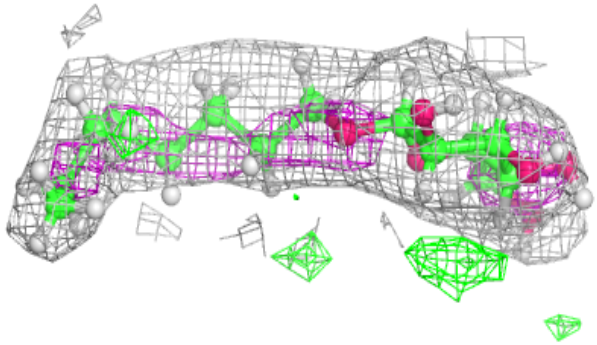


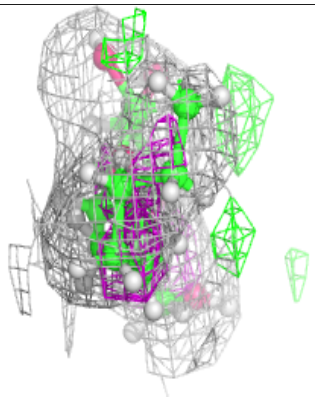


Electron density around BOG B 301:

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

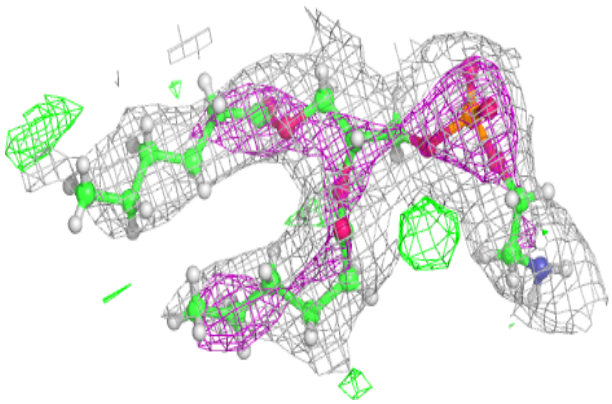


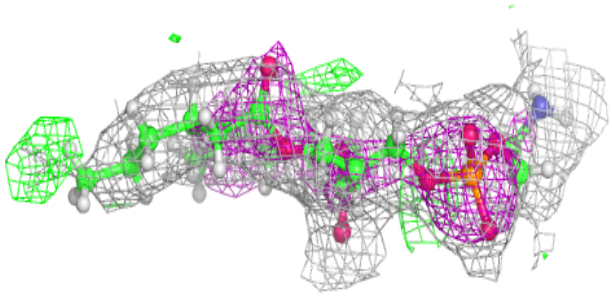


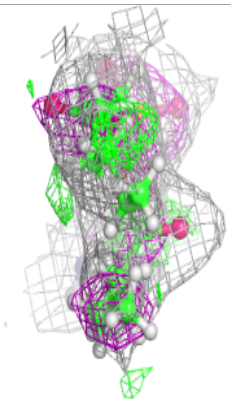


Electron density around 6PE E 1004:

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

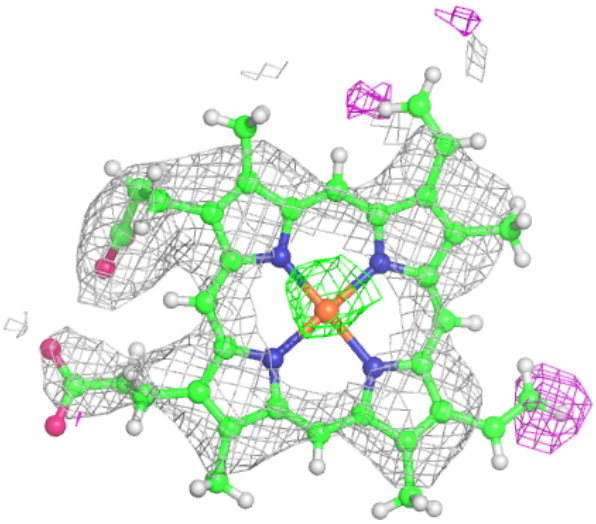


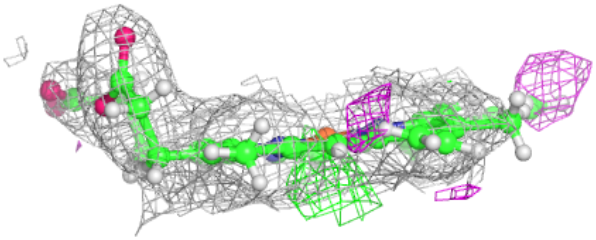


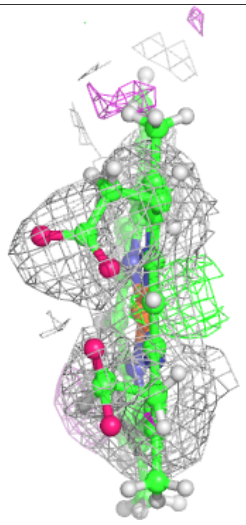


Electron density around HEM A 1001:

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

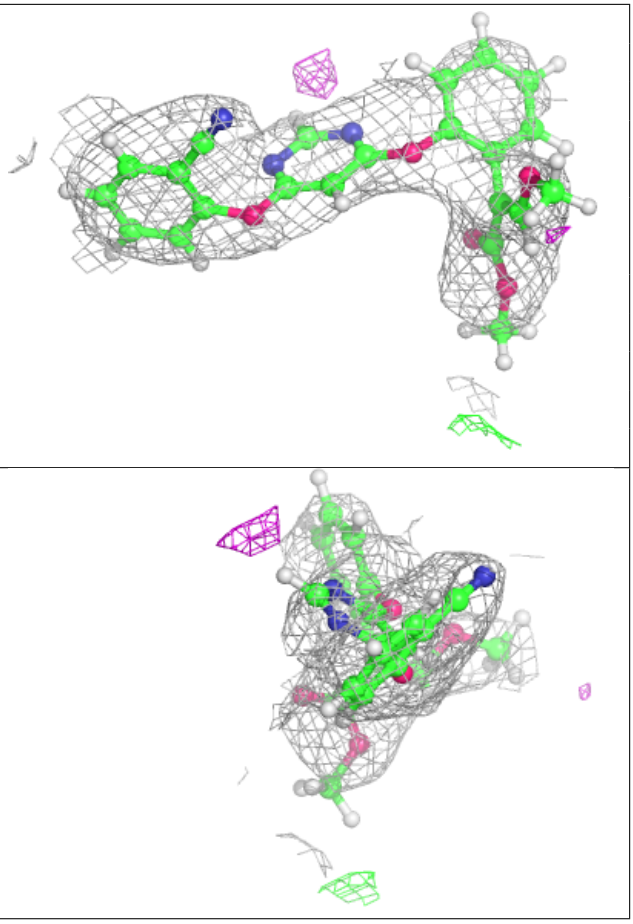


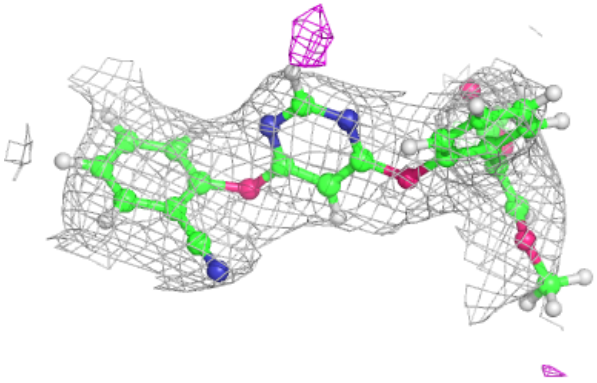




Electron density around AZO E 1003:

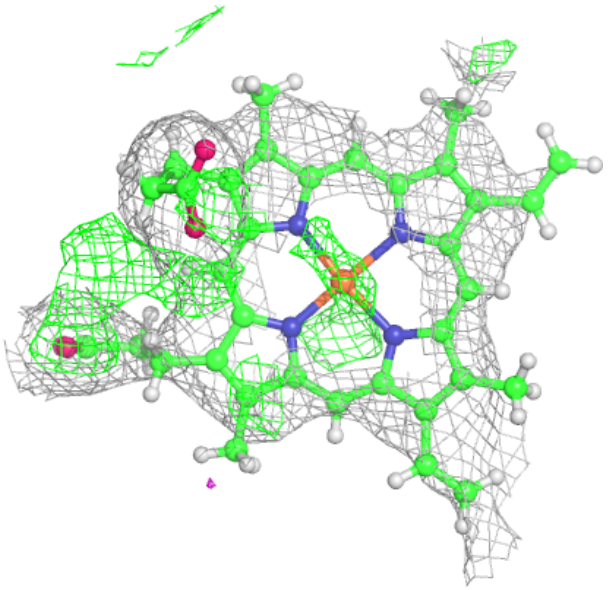
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

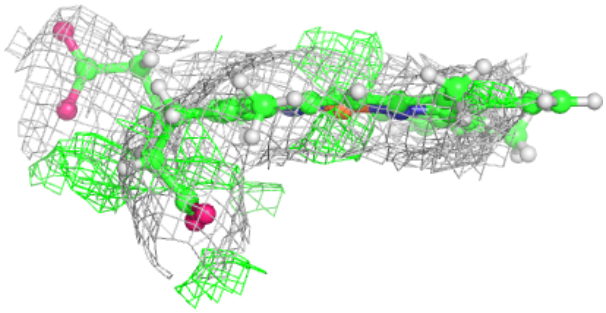


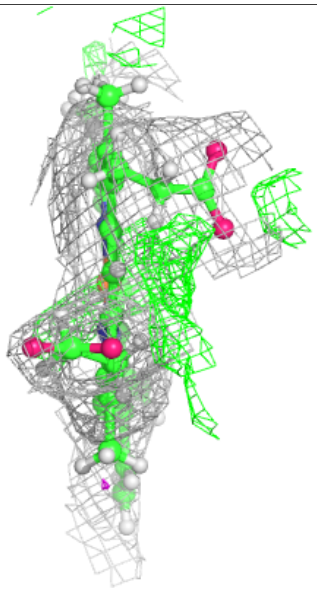


Electron density around HEM A 1002:

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

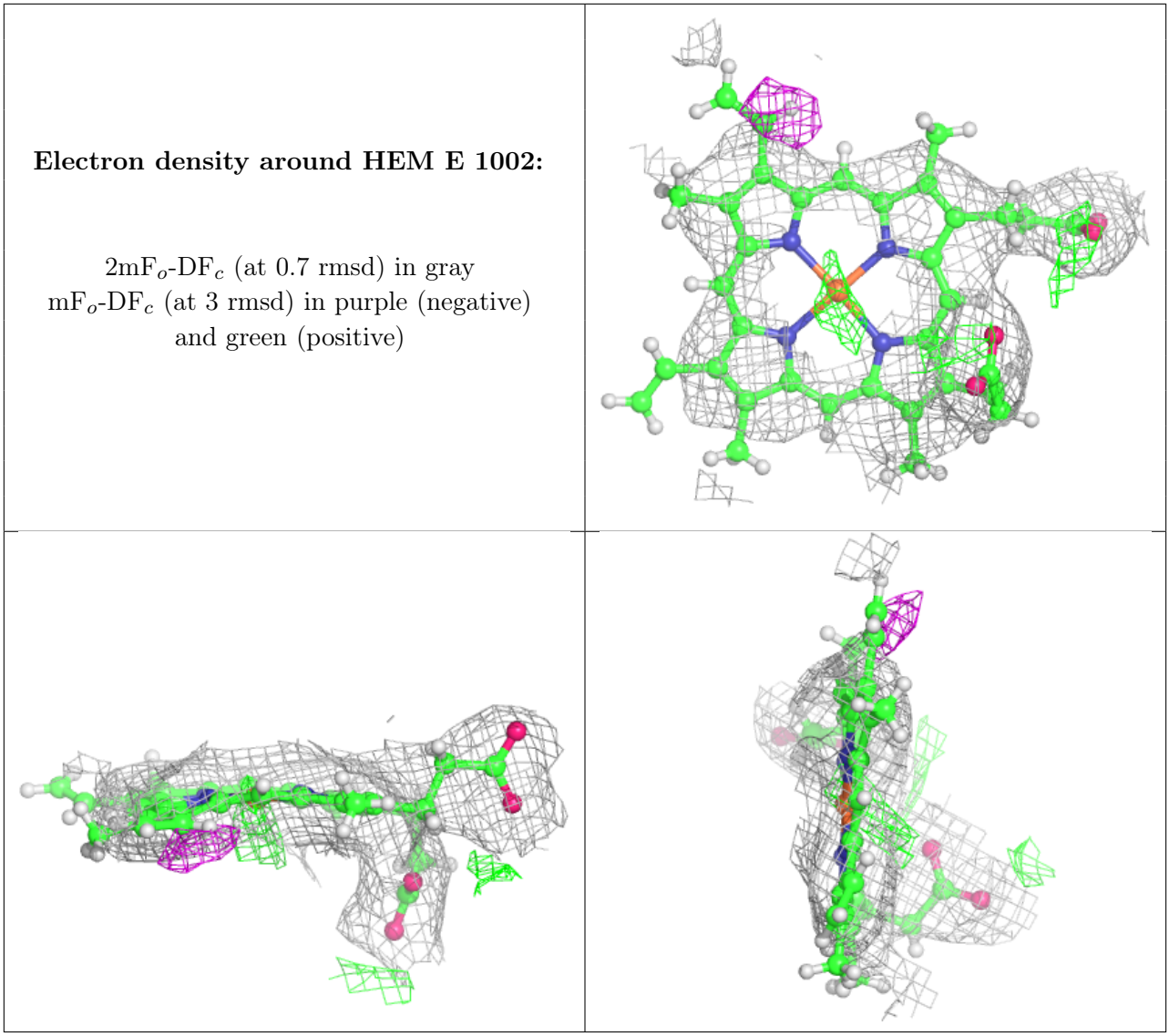






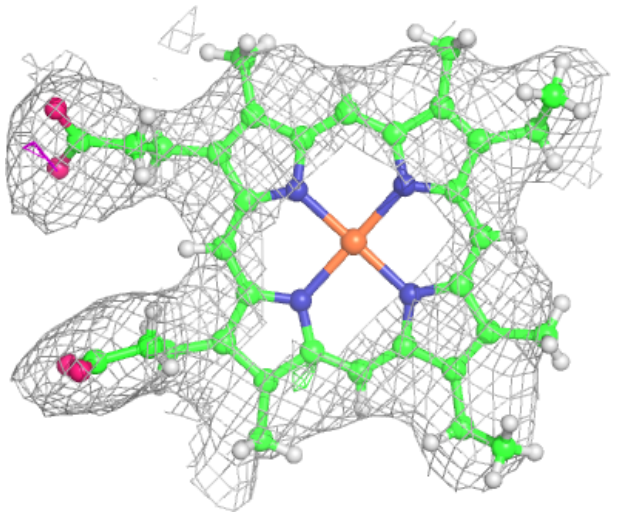
Electron density around HEM E 1002:

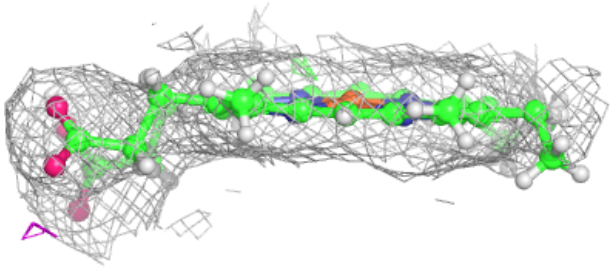
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

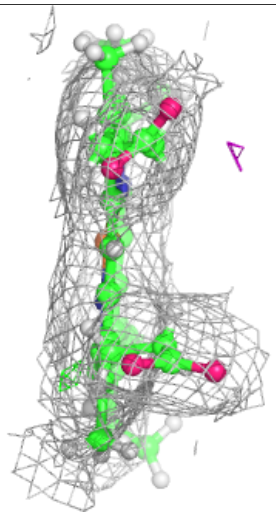


Electron density around HEC B 302:

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

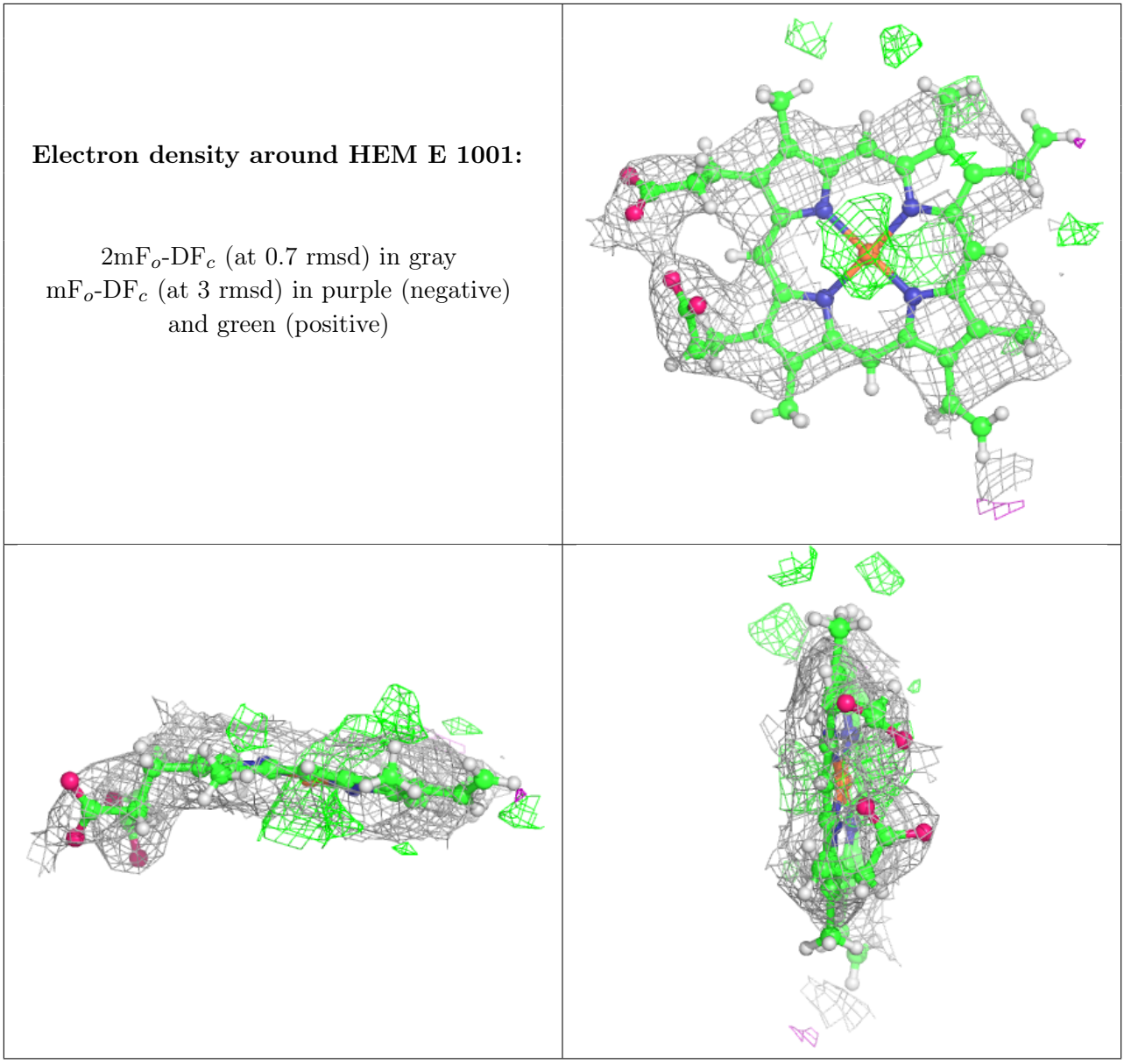






Electron density around HEM E 1001:

$2mF_o$-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

There are no such residues in this entry.