Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 08:04 PM EDT

PDB ID	:	5D8Y
Title	:	2.05A resolution structure of iron bound BfrB (L68A E81A) from Pseudomonas aeruginosa
Authors	:	Lovell, S.; Battaile, K.P.; Wang, Y.; Yao, H.; Rivera, M.
Deposited on	:	2015-08-18
Resolution	:	2.05 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:

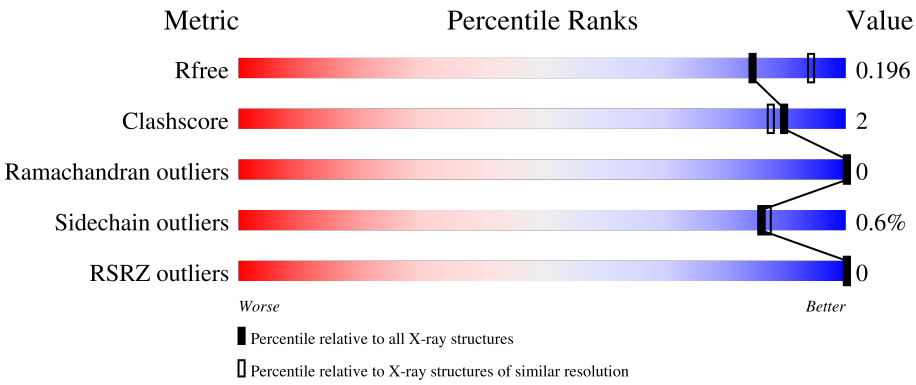
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	158	94%
1	B	158	96%
1	C	158	95%
1	D	158	94% 5%
1	E	158	93% 6%

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Mol	Chain	Length	Quality of chain
1	F	158	96%
1	G	158	96%
1	H	158	95%
1	I	158	96%
1	J	158	94% 5%
1	K	158	94%
1	L	158	94% 5%
1	M	158	96%
1	N	158	94% 5%
1	O	158	97%
1	P	158	93% 6%
1	Q	158	93% 6%
1	R	158	96%
1	S	158	97%
1	T	158	92% 6%
1	U	158	97%
1	V	158	97%
1	W	158	93% 6%
1	X	158	96%

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
3	ACT	C	207	-	-	X	-
3	ACT	H	207	-	-	X	-
3	ACT	J	207	-	-	X	-
3	ACT	K	208	-	-	X	-
3	ACT	M	209	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	O	205	-	-	X	-
3	ACT	Q	205	-	-	X	-
3	ACT	T	207	-	-	X	-
3	ACT	U	208	-	-	X	-
3	ACT	V	206	-	-	X	-
3	ACT	W	206	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 34099 atoms, of which 0 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1273	805	217	244	7	0	3	0
1	B	156	1272	804	218	243	7	0	2	0
1	C	156	1264	799	217	241	7	0	1	0
1	D	156	1269	803	217	242	7	0	2	0
1	E	156	1262	798	216	241	7	0	2	0
1	F	156	1253	792	214	240	7	0	1	0
1	G	156	1270	803	218	242	7	0	2	0
1	H	156	1271	803	218	243	7	0	2	0
1	I	156	1254	793	214	240	7	0	1	0
1	J	156	1255	794	214	240	7	0	1	0
1	K	156	1261	796	215	243	7	0	1	0
1	L	156	1259	797	215	240	7	0	1	0
1	M	156	1270	805	218	240	7	0	2	0
1	N	156	1271	803	218	243	7	0	2	0
1	O	156	1264	798	216	243	7	0	1	0
1	P	156	1254	793	214	240	7	0	1	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	156	1263	798	215	243	7	0	1	0
			Total	C	N	O	S			
1	R	156	1270	802	218	243	7	0	2	0
			Total	C	N	O	S			
1	S	156	1274	805	219	243	7	0	2	0
			Total	C	N	O	S			
1	T	156	1260	796	215	242	7	0	1	0
			Total	C	N	O	S			
1	U	156	1267	801	217	242	7	0	2	0
			Total	C	N	O	S			
1	V	156	1259	795	215	242	7	0	1	0
			Total	C	N	O	S			
1	W	156	1258	795	214	242	7	0	1	0
			Total	C	N	O	S			
1	X	156	1264	798	216	243	7	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	LEU	engineered mutation	UNP Q9HY79
A	81	ALA	GLU	engineered mutation	UNP Q9HY79
B	68	ALA	LEU	engineered mutation	UNP Q9HY79
B	81	ALA	GLU	engineered mutation	UNP Q9HY79
C	68	ALA	LEU	engineered mutation	UNP Q9HY79
C	81	ALA	GLU	engineered mutation	UNP Q9HY79
D	68	ALA	LEU	engineered mutation	UNP Q9HY79
D	81	ALA	GLU	engineered mutation	UNP Q9HY79
E	68	ALA	LEU	engineered mutation	UNP Q9HY79
E	81	ALA	GLU	engineered mutation	UNP Q9HY79
F	68	ALA	LEU	engineered mutation	UNP Q9HY79
F	81	ALA	GLU	engineered mutation	UNP Q9HY79
G	68	ALA	LEU	engineered mutation	UNP Q9HY79
G	81	ALA	GLU	engineered mutation	UNP Q9HY79
H	68	ALA	LEU	engineered mutation	UNP Q9HY79
H	81	ALA	GLU	engineered mutation	UNP Q9HY79
I	68	ALA	LEU	engineered mutation	UNP Q9HY79
I	81	ALA	GLU	engineered mutation	UNP Q9HY79
J	68	ALA	LEU	engineered mutation	UNP Q9HY79
J	81	ALA	GLU	engineered mutation	UNP Q9HY79
K	68	ALA	LEU	engineered mutation	UNP Q9HY79
K	81	ALA	GLU	engineered mutation	UNP Q9HY79
L	68	ALA	LEU	engineered mutation	UNP Q9HY79

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Chain	Residue	Modelled	Actual	Comment	Reference
L	81	ALA	GLU	engineered mutation	UNP Q9HY79
M	68	ALA	LEU	engineered mutation	UNP Q9HY79
M	81	ALA	GLU	engineered mutation	UNP Q9HY79
N	68	ALA	LEU	engineered mutation	UNP Q9HY79
N	81	ALA	GLU	engineered mutation	UNP Q9HY79
O	68	ALA	LEU	engineered mutation	UNP Q9HY79
O	81	ALA	GLU	engineered mutation	UNP Q9HY79
P	68	ALA	LEU	engineered mutation	UNP Q9HY79
P	81	ALA	GLU	engineered mutation	UNP Q9HY79
Q	68	ALA	LEU	engineered mutation	UNP Q9HY79
Q	81	ALA	GLU	engineered mutation	UNP Q9HY79
R	68	ALA	LEU	engineered mutation	UNP Q9HY79
R	81	ALA	GLU	engineered mutation	UNP Q9HY79
S	68	ALA	LEU	engineered mutation	UNP Q9HY79
S	81	ALA	GLU	engineered mutation	UNP Q9HY79
T	68	ALA	LEU	engineered mutation	UNP Q9HY79
T	81	ALA	GLU	engineered mutation	UNP Q9HY79
U	68	ALA	LEU	engineered mutation	UNP Q9HY79
U	81	ALA	GLU	engineered mutation	UNP Q9HY79
V	68	ALA	LEU	engineered mutation	UNP Q9HY79
V	81	ALA	GLU	engineered mutation	UNP Q9HY79
W	68	ALA	LEU	engineered mutation	UNP Q9HY79
W	81	ALA	GLU	engineered mutation	UNP Q9HY79
X	68	ALA	LEU	engineered mutation	UNP Q9HY79
X	81	ALA	GLU	engineered mutation	UNP Q9HY79

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	8	8	8	0	0
2	B	7	7	7	0	0
2	C	6	6	6	0	0
2	D	7	7	7	0	0
2	E	7	7	7	0	0
2	F	5	5	5	0	0
2	G	7	7	7	0	0

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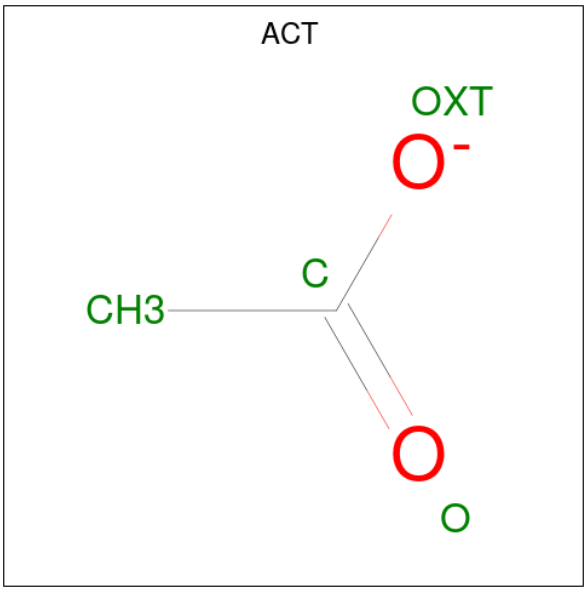
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	H	6	6	6	0	0
2	I	6	6	6	0	0
2	J	6	6	6	0	0
2	K	6	6	6	0	0
2	L	8	8	8	0	0
2	M	7	7	7	0	0
2	N	6	6	6	0	0
2	O	4	4	4	0	0
2	P	6	6	6	0	0
2	Q	4	4	4	0	0
2	R	7	7	7	0	0
2	S	5	5	5	0	0
2	T	6	6	6	0	0
2	U	6	6	6	0	0
2	V	5	5	5	0	0
2	W	4	4	4	0	0
2	X	5	5	5	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	F	1	4	2	2	0	0
3	G	1	4	2	2	0	0
3	H	1	4	2	2	0	0
3	I	1	4	2	2	0	0
3	J	1	4	2	2	0	0
3	K	1	4	2	2	0	0
3	L	1	4	2	2	0	0
3	M	1	4	2	2	0	0
3	N	1	4	2	2	0	0

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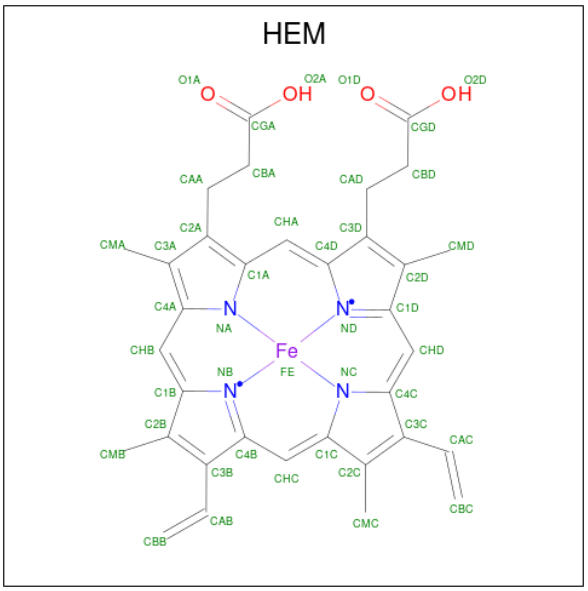
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	O	1	4	2	2	0	0
3	P	1	4	2	2	0	0
3	Q	1	4	2	2	0	0
3	R	1	4	2	2	0	0
3	S	1	4	2	2	0	0
3	T	1	4	2	2	0	0
3	U	1	4	2	2	0	0
3	V	1	4	2	2	0	0
3	W	1	4	2	2	0	0
3	X	1	4	2	2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	D	1	1	1	0	0
4	E	1	1	1	0	0
4	G	1	1	1	0	0
4	L	1	1	1	0	0

- Molecule 5 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	N	O		
5	B	1	43	34	1	4	4	0	0
5	D	1	43	34	1	4	4	0	0
5	E	1	43	34	1	4	4	0	0
5	G	1	43	34	1	4	4	0	0
5	I	1	43	34	1	4	4	0	0
5	K	1	43	34	1	4	4	0	0
5	M	1	43	34	1	4	4	0	0
5	P	1	43	34	1	4	4	0	0
5	R	1	43	34	1	4	4	0	0
5	S	1	43	34	1	4	4	0	0
5	U	1	43	34	1	4	4	0	0
5	W	1	43	34	1	4	4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	153	Total O 153 153	0	0
6	B	140	Total O 140 140	0	0
6	C	109	Total O 109 109	0	0
6	D	126	Total O 126 126	0	0
6	E	127	Total O 127 127	0	0
6	F	118	Total O 118 118	0	0
6	G	111	Total O 111 111	0	0
6	H	112	Total O 112 112	0	0
6	I	117	Total O 117 117	0	0
6	J	122	Total O 122 122	0	0
6	K	113	Total O 113 113	0	0
6	L	122	Total O 122 122	0	0
6	M	152	Total O 152 152	0	0
6	N	138	Total O 138 138	0	0
6	O	116	Total O 116 116	0	0
6	P	115	Total O 115 115	0	0
6	Q	132	Total O 132 132	0	0
6	R	118	Total O 118 118	0	0
6	S	143	Total O 143 143	0	0
6	T	136	Total O 136 136	0	0
6	U	127	Total O 127 127	0	0
6	V	103	Total O 103 103	0	0

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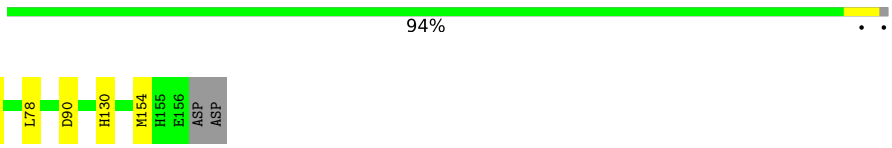
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	W	123	123	123	0	0
			Total	O		
6	X	127	127	127	0	0

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.

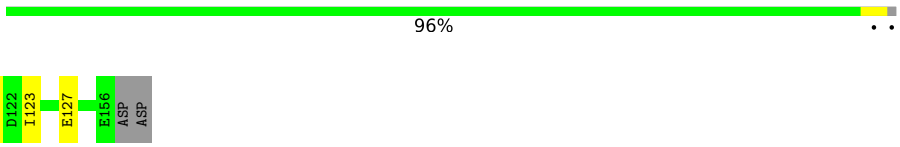
- Molecule 1: Ferroxidase

Chain A:



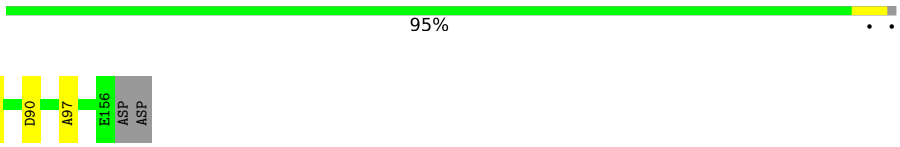
- Molecule 1: Ferroxidase

Chain B:



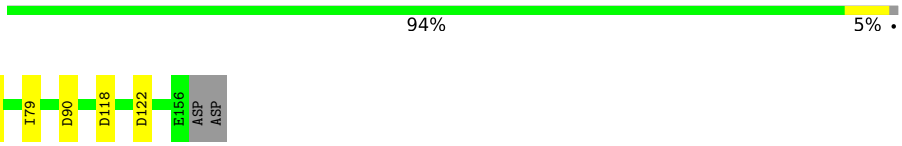
- Molecule 1: Ferroxidase

Chain C:



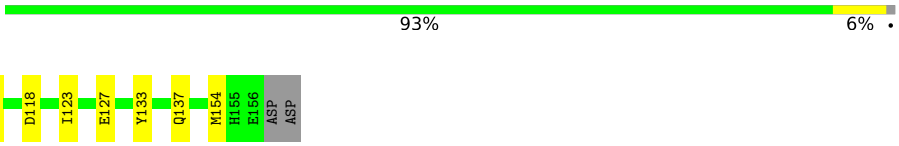
- Molecule 1: Ferroxidase

Chain D:



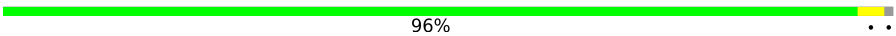
- Molecule 1: Ferroxidase

Chain E:



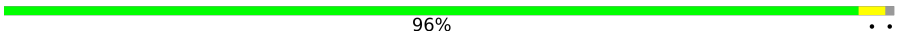
- Molecule 1: Ferroxidase

Chain F:



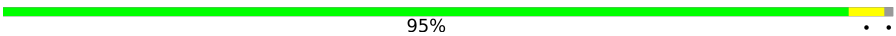
• Molecule 1: Ferroxidase

Chain G:



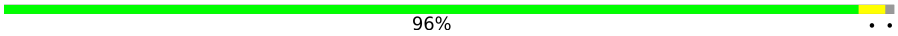
• Molecule 1: Ferroxidase

Chain H:



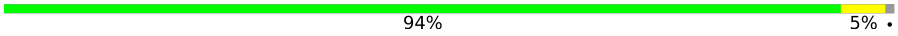
• Molecule 1: Ferroxidase

Chain I:



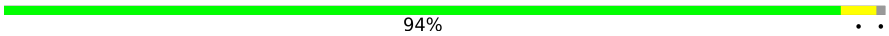
• Molecule 1: Ferroxidase

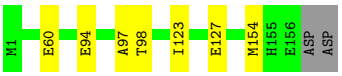
Chain J:



• Molecule 1: Ferroxidase

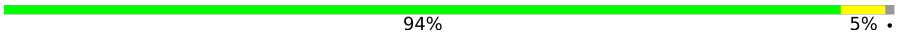
Chain K:

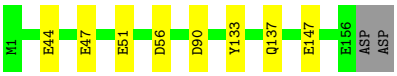




• Molecule 1: Ferroxidase

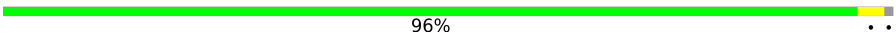
Chain L:

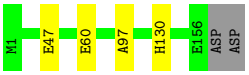




• Molecule 1: Ferroxidase

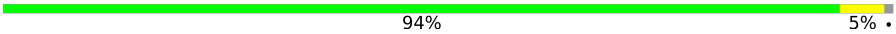
Chain M:

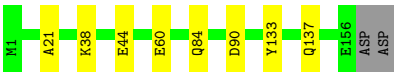




• Molecule 1: Ferroxidase

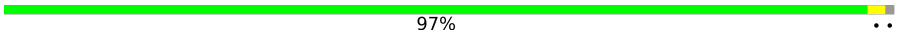
Chain N:

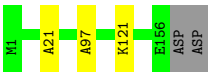




• Molecule 1: Ferroxidase

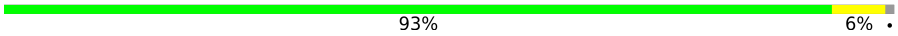
Chain O:

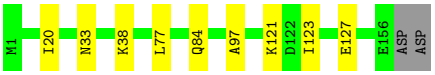




• Molecule 1: Ferroxidase

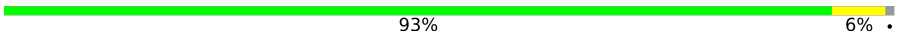
Chain P:





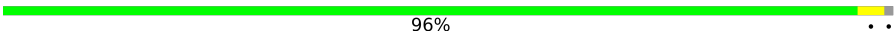
• Molecule 1: Ferroxidase

Chain Q:



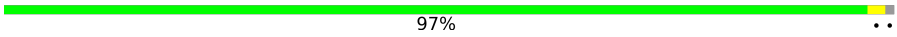
• Molecule 1: Ferroxidase

Chain R:



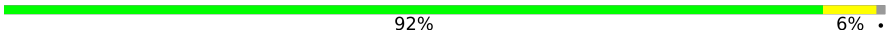
• Molecule 1: Ferroxidase

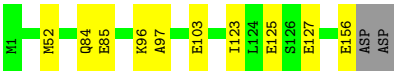
Chain S:



• Molecule 1: Ferroxidase

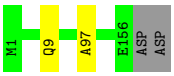
Chain T:





• Molecule 1: Ferroxidase

Chain U: 97%



• Molecule 1: Ferroxidase

Chain V: 97%

• Molecule 1: Ferroxidase

Chain W: 93% 6%

• Molecule 1: Ferroxidase

Chain X: 96%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	125.84Å 125.84Å 272.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.75 – 2.05 48.75 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.75-2.05) 100.0 (48.75-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.05Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.151 , 0.196 0.152 , 0.196	Depositor DCC
R_{free} test set	14740 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.027 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	34099	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, HEM, ACT, K

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	0.51	0/1304	0.59	0/1761
1	B	0.52	0/1300	0.59	0/1754
1	C	0.49	0/1288	0.58	1/1737 (0.1%)
1	D	0.51	0/1297	0.57	0/1750
1	E	0.49	0/1290	0.58	0/1743
1	F	0.48	0/1277	0.57	0/1725
1	G	0.49	0/1298	0.58	0/1751
1	H	0.47	0/1299	0.58	0/1753
1	I	0.48	0/1278	0.57	0/1726
1	J	0.49	0/1279	0.59	0/1727
1	K	0.47	0/1285	0.56	0/1735
1	L	0.53	1/1283 (0.1%)	0.59	1/1731 (0.1%)
1	M	0.52	0/1298	0.59	0/1750
1	N	0.50	0/1299	0.59	0/1753
1	O	0.47	0/1288	0.57	0/1738
1	P	0.50	0/1278	0.59	0/1726
1	Q	0.53	0/1287	0.57	0/1737
1	R	0.49	0/1298	0.56	0/1752
1	S	0.48	0/1302	0.57	0/1756
1	T	0.50	0/1284	0.60	0/1733
1	U	0.48	0/1295	0.55	0/1748
1	V	0.51	0/1283	0.58	0/1732
1	W	0.46	0/1282	0.56	0/1731
1	X	0.51	0/1288	0.57	0/1738
All	All	0.50	1/30960 (0.0%)	0.58	2/41787 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	147	GLU	CG-CD	5.11	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	90	ASP	CB-CG-OD1	5.12	122.91	118.30
1	L	56	ASP	CB-CG-OD1	5.02	122.81	118.30

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	1273	0	1227	5	0
1	B	1272	0	1235	2	0
1	C	1264	0	1233	5	0
1	D	1269	0	1231	5	0
1	E	1262	0	1213	5	0
1	F	1253	0	1207	1	0
1	G	1270	0	1236	3	0
1	H	1271	0	1233	5	0
1	I	1254	0	1209	3	0
1	J	1255	0	1211	5	0
1	K	1261	0	1217	5	0
1	L	1259	0	1222	3	0
1	M	1270	0	1240	4	0
1	N	1271	0	1233	5	0
1	O	1264	0	1226	2	0
1	P	1254	0	1209	5	0
1	Q	1263	0	1221	7	0
1	R	1270	0	1231	3	0
1	S	1274	0	1242	2	0
1	T	1260	0	1220	7	0
1	U	1267	0	1227	2	0
1	V	1259	0	1218	3	0
1	W	1258	0	1213	6	0
1	X	1264	0	1226	3	0
2	A	8	0	0	0	0
2	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	0	0	0
2	D	7	0	0	0	0
2	E	7	0	0	0	0
2	F	5	0	0	0	0
2	G	7	0	0	0	0
2	H	6	0	0	0	0
2	I	6	0	0	0	0
2	J	6	0	0	0	0
2	K	6	0	0	0	0
2	L	8	0	0	0	0
2	M	7	0	0	0	0
2	N	6	0	0	0	0
2	O	4	0	0	0	0
2	P	6	0	0	0	0
2	Q	4	0	0	0	0
2	R	7	0	0	0	0
2	S	5	0	0	0	0
2	T	6	0	0	0	0
2	U	6	0	0	0	0
2	V	5	0	0	0	0
2	W	4	0	0	0	0
2	X	5	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	3	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	1	0
3	G	4	0	3	0	0
3	H	4	0	3	2	0
3	I	4	0	3	1	0
3	J	4	0	3	2	0
3	K	4	0	3	2	0
3	L	4	0	3	0	0
3	M	4	0	3	2	0
3	N	4	0	3	1	0
3	O	4	0	3	2	0
3	P	4	0	3	1	0
3	Q	4	0	3	2	0
3	R	4	0	3	0	0
3	S	4	0	3	1	0
3	T	4	0	3	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	4	0	3	2	0
3	V	4	0	3	2	0
3	W	4	0	3	2	0
3	X	4	0	3	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	L	1	0	0	0	0
5	B	43	0	30	2	0
5	D	43	0	30	1	0
5	E	43	0	30	2	0
5	G	43	0	30	1	0
5	I	43	0	30	1	0
5	K	43	0	30	2	0
5	M	43	0	30	1	0
5	P	43	0	30	1	0
5	R	43	0	30	3	0
5	S	43	0	30	3	0
5	U	43	0	30	0	0
5	W	43	0	30	4	0
6	A	153	0	0	1	0
6	B	140	0	0	1	0
6	C	109	0	0	1	0
6	D	126	0	0	2	0
6	E	127	0	0	2	0
6	F	118	0	0	0	0
6	G	111	0	0	1	0
6	H	112	0	0	1	0
6	I	117	0	0	0	0
6	J	122	0	0	0	0
6	K	113	0	0	1	0
6	L	122	0	0	0	0
6	M	152	0	0	1	0
6	N	138	0	0	2	0
6	O	116	0	0	0	0
6	P	115	0	0	1	0
6	Q	132	0	0	2	0
6	R	118	0	0	1	0
6	S	143	0	0	1	0
6	T	136	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	127	0	0	0	0
6	V	103	0	0	0	0
6	W	123	0	0	2	0
6	X	127	0	0	1	0
All	All	34099	0	29812	112	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 (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:ALA:HB2	3:K:208:ACT:H3	1.53	0.88
1:C:47:GLU:OE2	6:C:301:HOH:O	1.97	0.82
1:K:97:ALA:CB	3:K:208:ACT:H3	2.18	0.73
1:Q:97:ALA:HB2	3:Q:205:ACT:H3	1.73	0.71
1:D:118:ASP:OD2	6:D:301:HOH:O	2.08	0.70
1:M:97:ALA:HB2	3:M:209:ACT:H3	1.71	0.70
1:N:38:LYS:NZ	6:N:302:HOH:O	2.24	0.69
1:T:97:ALA:HB2	3:T:207:ACT:H3	1.77	0.66
1:V:97:ALA:HB2	3:V:206:ACT:H3	1.77	0.66
1:J:97:ALA:HB2	3:J:207:ACT:H3	1.77	0.65
1:K:60:GLU:OE1	6:K:301:HOH:O	2.15	0.64
1:H:97:ALA:HB2	3:H:207:ACT:H3	1.80	0.63
1:E:118:ASP:OD2	6:E:301:HOH:O	2.16	0.62
1:M:60:GLU:OE1	6:M:301:HOH:O	2.15	0.61
1:T:97:ALA:CB	3:T:207:ACT:H3	2.31	0.60
1:T:125:GLU:OE1	6:T:301:HOH:O	2.16	0.60
1:T:85:GLU:OE2	6:T:302:HOH:O	2.17	0.59
1:N:60:GLU:OE1	6:N:301:HOH:O	2.17	0.58
1:W:97:ALA:HB2	3:W:206:ACT:H3	1.85	0.58
1:U:97:ALA:HB2	3:U:208:ACT:H3	1.85	0.58
1:Q:96:LYS:NZ	1:Q:100:ASP:OD2	2.37	0.57
1:T:103:GLU:OE2	6:T:303:HOH:O	2.18	0.55
1:N:21:ALA:HB2	3:N:207:ACT:H2	1.88	0.55
5:B:208:HEM:HBB2	5:B:208:HEM:HMB2	1.89	0.55
1:P:84:GLN:NE2	6:P:301:HOH:O	2.35	0.55
1:A:154:MET:HE1	1:Q:153:HIS:HE1	1.73	0.53
1:E:84:GLN:OE1	6:E:302:HOH:O	2.19	0.52
1:O:97:ALA:HB2	3:O:205:ACT:H3	1.92	0.51
1:R:123:ILE:O	1:R:127:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:ASP:O	1:J:60:GLU:HG3	2.11	0.51
5:W:205:HEM:O1D	6:W:301:HOH:O	2.18	0.50
1:W:66:GLU:HG2	6:W:408:HOH:O	2.11	0.50
1:C:97:ALA:HB2	3:C:207:ACT:H3	1.94	0.49
1:W:123:ILE:O	1:W:127:GLU:HG2	2.13	0.49
5:G:208:HEM:HBC2	5:G:208:HEM:HMC1	1.96	0.48
1:V:97:ALA:CB	3:V:206:ACT:H3	2.42	0.48
1:W:21:ALA:HB2	3:W:206:ACT:H2	1.96	0.47
1:B:60:GLU:OE1	6:B:301:HOH:O	2.20	0.47
1:E:133:TYR:O	1:E:137:GLN:HG2	2.15	0.47
1:O:21:ALA:HB2	3:O:205:ACT:H2	1.96	0.47
1:P:123:ILE:O	1:P:127:GLU:HG2	2.14	0.46
1:H:97:ALA:CB	3:H:207:ACT:H3	2.45	0.46
1:T:123:ILE:O	1:T:127:GLU:HG2	2.16	0.46
5:K:207:HEM:HBC2	5:K:207:HEM:HMC1	1.98	0.46
1:M:47:GLU:OE1	1:M:130:HIS:CD2	2.70	0.45
1:A:52:MET:HB3	5:B:208:HEM:CHB	2.46	0.45
5:I:207:HEM:HBC2	5:I:207:HEM:HMC2	1.99	0.45
5:M:208:HEM:HMC2	5:M:208:HEM:HBC2	1.99	0.45
1:L:47:GLU:O	1:L:51:GLU:HG2	2.16	0.45
1:S:13:LYS:NZ	6:S:303:HOH:O	2.38	0.45
1:H:46[B]:HIS:CD2	6:H:368:HOH:O	2.71	0.44
1:R:38:LYS:NZ	6:R:306:HOH:O	2.51	0.44
1:A:44:GLU:OE2	1:A:90:ASP:OD2	2.35	0.44
1:I:20:ILE:HD11	1:I:75:GLY:HA3	2.00	0.44
1:P:33:ASN:O	1:P:38:LYS:HE3	2.18	0.44
1:E:123:ILE:O	1:E:127:GLU:HG2	2.18	0.44
1:V:123:ILE:O	1:V:127:GLU:HG2	2.17	0.44
5:D:208:HEM:HMC1	5:D:208:HEM:HBC2	1.99	0.43
5:R:208:HEM:HMC2	5:R:208:HEM:HBC2	1.99	0.43
1:U:97:ALA:CB	3:U:208:ACT:H3	2.47	0.43
1:B:123:ILE:O	1:B:127:GLU:HG2	2.18	0.43
1:M:97:ALA:CB	3:M:209:ACT:H3	2.43	0.43
5:W:205:HEM:HMB1	5:W:205:HEM:HBB2	2.01	0.43
1:H:123:ILE:O	1:H:127:GLU:HG2	2.18	0.43
1:A:47:GLU:OE1	1:A:130:HIS:CD2	2.72	0.43
1:D:44:GLU:OE2	1:D:90:ASP:OD2	2.36	0.43
1:F:21:ALA:HB2	3:F:206:ACT:H3	1.99	0.43
1:G:123:ILE:O	1:G:127:GLU:HG2	2.18	0.43
1:L:133:TYR:O	1:L:137:GLN:HG2	2.19	0.43
1:D:1:MET:O	1:D:65:LEU:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:123:ILE:O	1:Q:127:GLU:HG2	2.19	0.43
1:P:20:ILE:HG23	1:P:77:LEU:HD23	2.00	0.42
5:P:207:HEM:HBC2	5:P:207:HEM:HMC2	2.00	0.42
5:W:205:HEM:HMC2	5:W:205:HEM:HBC2	2.00	0.42
1:G:143:LYS:HE3	6:G:396:HOH:O	2.18	0.42
1:K:123:ILE:O	1:K:127:GLU:HG2	2.19	0.42
1:J:97:ALA:CB	3:J:207:ACT:H3	2.46	0.42
5:E:208:HEM:HBB2	5:E:208:HEM:HMB1	2.01	0.42
1:D:122:ASP:OD2	6:D:301:HOH:O	2.21	0.42
1:S:97:ALA:HB2	3:S:207:ACT:H2	2.02	0.42
5:R:208:HEM:HMB1	5:R:208:HEM:HBB2	2.00	0.41
1:C:21:ALA:HB2	3:C:207:ACT:H2	2.01	0.41
1:J:133:TYR:O	1:J:137:GLN:HG2	2.20	0.41
1:N:133:TYR:O	1:N:137:GLN:HG2	2.19	0.41
1:R:52:MET:HB3	5:R:208:HEM:CHD	2.49	0.41
1:A:78:LEU:HG	6:A:355:HOH:O	2.19	0.41
1:X:34:ASP:OD2	6:X:301:HOH:O	2.22	0.41
1:C:1:MET:O	1:C:65:LEU:HA	2.20	0.41
1:G:47:GLU:O	1:G:51:GLU:HG2	2.21	0.41
1:I:123:ILE:O	1:I:127:GLU:HG2	2.21	0.41
5:S:206:HEM:CHD	1:T:52:MET:HB3	2.49	0.41
1:W:19:LEU:CD2	5:W:205:HEM:HBB1	2.51	0.41
1:H:47:GLU:OE1	1:H:130:HIS:CD2	2.74	0.41
1:K:94:GLU:O	1:K:98:THR:HG23	2.20	0.41
1:D:27:LEU:HD23	1:D:79:ILE:HD12	2.03	0.41
5:E:208:HEM:HMC1	5:E:208:HEM:HBC2	2.03	0.41
5:K:207:HEM:CMB	5:K:207:HEM:HBB2	2.50	0.41
1:Q:97:ALA:CB	3:Q:205:ACT:H3	2.48	0.41
1:X:123:ILE:O	1:X:127:GLU:HG2	2.21	0.41
1:N:44:GLU:OE2	1:N:90:ASP:OD2	2.38	0.41
5:S:206:HEM:HMC1	5:S:206:HEM:HBC2	2.02	0.41
1:W:44:GLU:OE2	1:W:90:ASP:OD2	2.39	0.41
1:X:47:GLU:O	1:X:51:GLU:HG2	2.21	0.41
1:C:97:ALA:CB	3:C:207:ACT:H3	2.50	0.40
1:Q:147:GLU:HG3	6:Q:412:HOH:O	2.20	0.40
5:S:206:HEM:CMB	5:S:206:HEM:HBB2	2.52	0.40
1:Q:84:GLN:HG2	6:Q:309:HOH:O	2.21	0.40
1:E:44:GLU:OE2	1:E:90:ASP:OD2	2.39	0.40
1:P:97:ALA:HB2	3:P:208:ACT:H2	2.03	0.40
1:I:21:ALA:HB2	3:I:208:ACT:H3	2.02	0.40
1:J:123:ILE:O	1:J:127:GLU:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:44:GLU:OE2	1:L:90:ASP:OD2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/158 (99%)	155 (99%)	2 (1%)	0	100	100
1	B	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	C	155/158 (98%)	155 (100%)	0	0	100	100
1	D	156/158 (99%)	156 (100%)	0	0	100	100
1	E	156/158 (99%)	156 (100%)	0	0	100	100
1	F	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	G	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
1	H	156/158 (99%)	154 (99%)	2 (1%)	0	100	100
1	I	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	J	155/158 (98%)	155 (100%)	0	0	100	100
1	K	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	L	155/158 (98%)	155 (100%)	0	0	100	100
1	M	156/158 (99%)	155 (99%)	1 (1%)	0	100	100
1	N	156/158 (99%)	156 (100%)	0	0	100	100
1	O	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	P	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	Q	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	R	156/158 (99%)	156 (100%)	0	0	100	100
1	S	156/158 (99%)	155 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	155/158 (98%)	155 (100%)	0	0	100	100
1	U	156/158 (99%)	156 (100%)	0	0	100	100
1	V	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	W	155/158 (98%)	155 (100%)	0	0	100	100
1	X	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
All	All	3732/3792 (98%)	3711 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/142 (95%)	135 (100%)	0	100	100
1	B	136/142 (96%)	134 (98%)	2 (2%)	65	62
1	C	135/142 (95%)	135 (100%)	0	100	100
1	D	135/142 (95%)	135 (100%)	0	100	100
1	E	133/142 (94%)	132 (99%)	1 (1%)	81	82
1	F	132/142 (93%)	129 (98%)	3 (2%)	50	44
1	G	136/142 (96%)	136 (100%)	0	100	100
1	H	136/142 (96%)	136 (100%)	0	100	100
1	I	132/142 (93%)	132 (100%)	0	100	100
1	J	132/142 (93%)	131 (99%)	1 (1%)	81	82
1	K	134/142 (94%)	133 (99%)	1 (1%)	84	84
1	L	133/142 (94%)	133 (100%)	0	100	100
1	M	135/142 (95%)	135 (100%)	0	100	100
1	N	136/142 (96%)	135 (99%)	1 (1%)	84	84
1	O	135/142 (95%)	134 (99%)	1 (1%)	84	84
1	P	132/142 (93%)	131 (99%)	1 (1%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	134/142 (94%)	133 (99%)	1 (1%)	84	84
1	R	136/142 (96%)	135 (99%)	1 (1%)	84	84
1	S	137/142 (96%)	136 (99%)	1 (1%)	84	84
1	T	134/142 (94%)	131 (98%)	3 (2%)	52	46
1	U	135/142 (95%)	134 (99%)	1 (1%)	84	84
1	V	134/142 (94%)	134 (100%)	0	100	100
1	W	133/142 (94%)	132 (99%)	1 (1%)	81	82
1	X	135/142 (95%)	135 (100%)	0	100	100
All	All	3225/3408 (95%)	3206 (99%)	19 (1%)	86	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	LYS
1	B	121	LYS
1	E	154	MET
1	F	84	GLN
1	F	112	HIS
1	F	121	LYS
1	J	121	LYS
1	K	154	MET
1	N	84	GLN
1	O	121	LYS
1	P	121	LYS
1	Q	154	MET
1	R	121	LYS
1	S	121	LYS
1	T	84	GLN
1	T	96	LYS
1	T	156	GLU
1	U	9	GLN
1	W	121	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	112	HIS

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 186 ligands modelled in this entry, 150 are monoatomic - leaving 36 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	$\#\|Z\| > 2$
3	ACT	Q	205	2	3,3,3	0.89	0	3,3,3	1.46	0
3	ACT	H	207	2	3,3,3	0.94	0	3,3,3	1.70	1 (33%)
3	ACT	G	209	2	3,3,3	0.87	0	3,3,3	1.59	1 (33%)
3	ACT	L	209	2	3,3,3	0.85	0	3,3,3	1.76	2 (66%)
5	HEM	M	208	1	41,50,50	1.48	5 (12%)	45,82,82	1.93	12 (26%)
5	HEM	U	207	1	41,50,50	1.52	7 (17%)	45,82,82	2.19	14 (31%)
3	ACT	D	209	2	3,3,3	0.80	0	3,3,3	1.80	2 (66%)
3	ACT	P	208	2	3,3,3	0.73	0	3,3,3	1.64	1 (33%)
3	ACT	V	206	2	3,3,3	0.78	0	3,3,3	1.35	0
5	HEM	R	208	1	41,50,50	1.45	5 (12%)	45,82,82	2.03	13 (28%)
3	ACT	C	207	2	3,3,3	0.84	0	3,3,3	1.16	0
5	HEM	W	205	1	41,50,50	1.36	4 (9%)	45,82,82	1.85	10 (22%)
3	ACT	E	209	2	3,3,3	0.79	0	3,3,3	1.80	2 (66%)
3	ACT	X	206	2	3,3,3	0.84	0	3,3,3	1.28	0
5	HEM	P	207	1	41,50,50	1.41	3 (7%)	45,82,82	1.99	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ACT	W	206	2	3,3,3	0.91	0	3,3,3	1.42	0
3	ACT	T	207	2	3,3,3	0.89	0	3,3,3	1.84	1 (33%)
3	ACT	R	209	2	3,3,3	0.78	0	3,3,3	1.70	1 (33%)
3	ACT	O	205	2	3,3,3	0.82	0	3,3,3	1.42	0
5	HEM	I	207	1	41,50,50	1.46	6 (14%)	45,82,82	1.94	10 (22%)
3	ACT	S	207	2	3,3,3	0.80	0	3,3,3	1.66	1 (33%)
3	ACT	J	207	2	3,3,3	0.86	0	3,3,3	1.50	0
3	ACT	M	209	2	3,3,3	0.91	0	3,3,3	1.56	1 (33%)
5	HEM	G	208	1	41,50,50	1.48	6 (14%)	45,82,82	2.07	14 (31%)
3	ACT	I	208	2	3,3,3	0.73	0	3,3,3	1.70	1 (33%)
5	HEM	B	208	1	41,50,50	1.47	4 (9%)	45,82,82	1.91	13 (28%)
3	ACT	N	207	2	3,3,3	0.93	0	3,3,3	1.58	1 (33%)
5	HEM	D	208	1	41,50,50	1.43	6 (14%)	45,82,82	2.15	15 (33%)
5	HEM	K	207	1	41,50,50	1.47	4 (9%)	45,82,82	1.91	13 (28%)
3	ACT	B	209	2	3,3,3	0.87	0	3,3,3	1.97	2 (66%)
5	HEM	E	208	1	41,50,50	1.44	4 (9%)	45,82,82	2.10	16 (35%)
3	ACT	U	208	2	3,3,3	0.86	0	3,3,3	1.54	1 (33%)
5	HEM	S	206	1	41,50,50	1.45	4 (9%)	45,82,82	1.87	11 (24%)
3	ACT	A	209	2	3,3,3	0.66	0	3,3,3	1.64	1 (33%)
3	ACT	F	206	2	3,3,3	0.74	0	3,3,3	1.69	1 (33%)
3	ACT	K	208	2	3,3,3	0.89	0	3,3,3	1.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	D	208	1	-	4/12/54/54	-
5	HEM	I	207	1	-	4/12/54/54	-
5	HEM	K	207	1	-	4/12/54/54	-
5	HEM	E	208	1	-	4/12/54/54	-
5	HEM	S	206	1	-	4/12/54/54	-
5	HEM	R	208	1	-	4/12/54/54	-
5	HEM	G	208	1	-	4/12/54/54	-
5	HEM	W	205	1	-	4/12/54/54	-
5	HEM	M	208	1	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	P	207	1	-	4/12/54/54	-
5	HEM	B	208	1	-	4/12/54/54	-
5	HEM	U	207	1	-	4/12/54/54	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	207	HEM	C3C-C2C	-4.18	1.34	1.40
5	M	208	HEM	C3C-C2C	-4.10	1.34	1.40
5	I	207	HEM	C3C-C2C	-4.05	1.34	1.40
5	D	208	HEM	C3C-C2C	-4.05	1.34	1.40
5	U	207	HEM	FE-ND	3.80	2.15	1.96
5	R	208	HEM	C3C-C2C	-3.74	1.35	1.40
5	S	206	HEM	FE-NB	3.73	2.15	1.96
5	K	207	HEM	C3C-C2C	-3.68	1.35	1.40
5	W	205	HEM	C3C-C2C	-3.63	1.35	1.40
5	B	208	HEM	C3C-C2C	-3.60	1.35	1.40
5	U	207	HEM	C3C-C2C	-3.59	1.35	1.40
5	E	208	HEM	C3C-C2C	-3.52	1.35	1.40
5	M	208	HEM	C3C-CAC	3.50	1.55	1.47
5	E	208	HEM	FE-NB	3.48	2.14	1.96
5	G	208	HEM	C3C-C2C	-3.42	1.35	1.40
5	S	206	HEM	C3C-C2C	-3.38	1.35	1.40
5	W	205	HEM	C3C-CAC	3.34	1.54	1.47
5	B	208	HEM	C3C-CAC	3.33	1.54	1.47
5	K	207	HEM	C3C-CAC	3.31	1.54	1.47
5	U	207	HEM	C3C-CAC	3.28	1.54	1.47
5	D	208	HEM	FE-ND	3.26	2.13	1.96
5	P	207	HEM	C3C-CAC	3.26	1.54	1.47
5	G	208	HEM	FE-ND	3.19	2.12	1.96
5	E	208	HEM	C3C-CAC	3.16	1.54	1.47
5	G	208	HEM	C3C-CAC	3.12	1.54	1.47
5	S	206	HEM	C3C-CAC	3.12	1.54	1.47
5	I	207	HEM	C3C-CAC	3.09	1.54	1.47
5	B	208	HEM	FE-NB	3.02	2.11	1.96
5	K	207	HEM	FE-NB	2.98	2.11	1.96
5	R	208	HEM	C3C-CAC	2.98	1.53	1.47
5	I	207	HEM	FE-NB	2.96	2.11	1.96
5	W	205	HEM	FE-NB	2.95	2.11	1.96
5	R	208	HEM	FE-NB	2.93	2.11	1.96
5	P	207	HEM	CAB-C3B	2.74	1.54	1.47
5	R	208	HEM	FE-ND	2.61	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	207	HEM	CAB-C3B	2.60	1.54	1.47
5	B	208	HEM	CAB-C3B	2.56	1.54	1.47
5	M	208	HEM	FE-NB	2.55	2.09	1.96
5	D	208	HEM	C3C-CAC	2.55	1.53	1.47
5	G	208	HEM	CAB-C3B	2.50	1.54	1.47
5	I	207	HEM	CAB-C3B	2.48	1.54	1.47
5	G	208	HEM	FE-NB	2.46	2.09	1.96
5	U	207	HEM	CAB-C3B	2.40	1.54	1.47
5	R	208	HEM	CAB-C3B	2.40	1.54	1.47
5	G	208	HEM	CMB-C2B	2.39	1.55	1.50
5	W	205	HEM	CAB-C3B	2.36	1.53	1.47
5	D	208	HEM	CAB-C3B	2.34	1.53	1.47
5	I	207	HEM	CMB-C2B	2.26	1.55	1.50
5	S	206	HEM	CAB-C3B	2.23	1.53	1.47
5	U	207	HEM	FE-NB	2.18	2.07	1.96
5	M	208	HEM	CAB-C3B	2.16	1.53	1.47
5	I	207	HEM	CHA-C4D	2.15	1.40	1.35
5	D	208	HEM	FE-NB	2.13	2.07	1.96
5	E	208	HEM	CMC-C2C	2.10	1.56	1.51
5	D	208	HEM	CHA-C4D	2.10	1.40	1.35
5	U	207	HEM	CHA-C4D	2.05	1.40	1.35
5	U	207	HEM	C1B-NB	-2.01	1.36	1.40
5	M	208	HEM	CMB-C2B	2.01	1.55	1.50

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	207	HEM	C4D-ND-C1D	5.82	111.08	105.07
5	E	208	HEM	C4D-ND-C1D	5.16	110.41	105.07
5	S	206	HEM	C4D-ND-C1D	5.08	110.32	105.07
5	I	207	HEM	C4D-ND-C1D	4.98	110.22	105.07
5	R	208	HEM	C4D-ND-C1D	4.96	110.19	105.07
5	D	208	HEM	C4D-ND-C1D	4.92	110.15	105.07
5	K	207	HEM	C4D-ND-C1D	4.72	109.95	105.07
5	G	208	HEM	C1B-NB-C4B	4.59	109.81	105.07
5	P	207	HEM	C4D-ND-C1D	4.57	109.80	105.07
5	G	208	HEM	C4D-ND-C1D	4.55	109.77	105.07
5	D	208	HEM	C4C-CHD-C1D	4.53	128.54	122.56
5	G	208	HEM	C4B-CHC-C1C	4.50	128.50	122.56
5	U	207	HEM	CBA-CAA-C2A	-4.48	104.97	112.62
5	I	207	HEM	CMC-C2C-C3C	4.48	133.06	124.68
5	U	207	HEM	C1B-NB-C4B	4.47	109.69	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	208	HEM	CMC-C2C-C3C	4.37	132.86	124.68
5	M	208	HEM	C4D-ND-C1D	4.33	109.55	105.07
5	D	208	HEM	C1B-NB-C4B	4.29	109.51	105.07
5	I	207	HEM	C4B-CHC-C1C	4.29	128.22	122.56
5	R	208	HEM	C4B-CHC-C1C	4.29	128.21	122.56
5	B	208	HEM	C4D-ND-C1D	4.28	109.50	105.07
5	D	208	HEM	CMC-C2C-C3C	4.25	132.64	124.68
5	E	208	HEM	C4C-CHD-C1D	4.21	128.12	122.56
5	M	208	HEM	CBA-CAA-C2A	-4.17	105.50	112.62
5	U	207	HEM	C3D-C4D-ND	-4.17	105.53	110.17
5	S	206	HEM	CMC-C2C-C3C	4.09	132.32	124.68
5	I	207	HEM	CBA-CAA-C2A	-4.04	105.73	112.62
5	W	205	HEM	CMC-C2C-C3C	4.02	132.20	124.68
5	W	205	HEM	C4D-ND-C1D	4.01	109.22	105.07
5	P	207	HEM	CBA-CAA-C2A	-4.01	105.78	112.62
5	B	208	HEM	CMC-C2C-C3C	3.98	132.13	124.68
5	S	206	HEM	CBA-CAA-C2A	-3.93	105.92	112.62
5	K	207	HEM	C4B-CHC-C1C	3.92	127.74	122.56
5	K	207	HEM	CMC-C2C-C3C	3.91	131.99	124.68
5	G	208	HEM	CBA-CAA-C2A	-3.90	105.97	112.62
5	M	208	HEM	C4B-CHC-C1C	3.88	127.68	122.56
5	R	208	HEM	CMC-C2C-C3C	3.88	131.93	124.68
5	B	208	HEM	CBA-CAA-C2A	-3.86	106.03	112.62
5	P	207	HEM	C4B-CHC-C1C	3.86	127.65	122.56
5	R	208	HEM	C1B-NB-C4B	3.81	109.01	105.07
5	W	205	HEM	CBA-CAA-C2A	-3.76	106.20	112.62
5	W	205	HEM	C4B-CHC-C1C	3.75	127.50	122.56
5	U	207	HEM	C4B-CHC-C1C	3.74	127.49	122.56
5	R	208	HEM	CBA-CAA-C2A	-3.71	106.29	112.62
5	D	208	HEM	C3D-C4D-ND	-3.70	106.05	110.17
5	P	207	HEM	C3D-C4D-ND	-3.69	106.06	110.17
5	B	208	HEM	C4C-CHD-C1D	3.64	127.36	122.56
5	I	207	HEM	C3D-C4D-ND	-3.61	106.14	110.17
5	P	207	HEM	C1B-NB-C4B	3.60	108.79	105.07
5	K	207	HEM	CBA-CAA-C2A	-3.59	106.50	112.62
5	M	208	HEM	CMC-C2C-C3C	3.56	131.34	124.68
5	D	208	HEM	C4B-CHC-C1C	3.54	127.22	122.56
5	G	208	HEM	CMC-C2C-C3C	3.50	131.23	124.68
5	E	208	HEM	C3D-C4D-ND	-3.50	106.27	110.17
5	U	207	HEM	CMC-C2C-C3C	3.47	131.16	124.68
5	E	208	HEM	C1B-NB-C4B	3.40	108.59	105.07
5	K	207	HEM	C4C-CHD-C1D	3.39	127.03	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	207	HEM	CMC-C2C-C3C	3.38	131.00	124.68
5	R	208	HEM	C4C-CHD-C1D	3.38	127.02	122.56
5	B	208	HEM	C4B-CHC-C1C	3.31	126.92	122.56
5	G	208	HEM	CMB-C2B-C1B	-3.26	120.08	125.04
5	D	208	HEM	C2C-C3C-C4C	3.25	109.17	106.90
5	E	208	HEM	C4B-CHC-C1C	3.25	126.84	122.56
5	M	208	HEM	C4C-CHD-C1D	3.21	126.79	122.56
5	K	207	HEM	C1B-NB-C4B	3.21	108.39	105.07
5	S	206	HEM	C2D-C1D-ND	-3.19	106.06	109.88
5	W	205	HEM	CMB-C2B-C1B	-3.17	120.22	125.04
5	W	205	HEM	C1B-NB-C4B	3.16	108.34	105.07
5	U	207	HEM	C4C-CHD-C1D	3.16	126.72	122.56
5	B	208	HEM	C2C-C3C-C4C	3.15	109.10	106.90
5	D	208	HEM	CBD-CAD-C3D	-3.15	103.88	112.63
5	E	208	HEM	C2D-C1D-ND	-3.14	106.12	109.88
5	B	208	HEM	CBD-CAD-C3D	-3.12	103.96	112.63
5	E	208	HEM	CBA-CAA-C2A	-3.11	107.31	112.62
5	M	208	HEM	C1B-NB-C4B	3.10	108.28	105.07
5	R	208	HEM	C3D-C4D-ND	-3.04	106.78	110.17
5	E	208	HEM	C2C-C3C-C4C	3.04	109.02	106.90
5	M	208	HEM	CMA-C3A-C4A	-3.03	123.80	128.46
5	B	208	HEM	C1B-NB-C4B	3.03	108.20	105.07
5	S	206	HEM	C3D-C4D-ND	-3.03	106.80	110.17
5	U	207	HEM	C2D-C1D-ND	-3.01	106.28	109.88
5	G	208	HEM	C3D-C4D-ND	-3.00	106.83	110.17
5	S	206	HEM	C4B-CHC-C1C	2.99	126.51	122.56
5	M	208	HEM	C3D-C4D-ND	-2.98	106.85	110.17
5	K	207	HEM	C3D-C4D-ND	-2.97	106.86	110.17
5	R	208	HEM	C2D-C1D-ND	-2.96	106.34	109.88
5	P	207	HEM	CHA-C4D-ND	2.92	127.99	124.38
5	S	206	HEM	C1B-NB-C4B	2.92	108.09	105.07
5	U	207	HEM	CAD-CBD-CGD	-2.90	107.37	113.60
5	P	207	HEM	CHC-C4B-NB	2.89	127.57	124.43
5	D	208	HEM	CBA-CAA-C2A	-2.88	107.70	112.62
5	M	208	HEM	C2C-C3C-C4C	2.86	108.89	106.90
5	B	208	HEM	C2D-C1D-ND	-2.86	106.46	109.88
5	G	208	HEM	C2D-C1D-ND	-2.83	106.49	109.88
5	R	208	HEM	C4A-C3A-C2A	2.80	108.94	107.00
5	D	208	HEM	CMA-C3A-C4A	-2.78	124.19	128.46
5	I	207	HEM	C2D-C1D-ND	-2.77	106.56	109.88
5	K	207	HEM	C2D-C1D-ND	-2.76	106.58	109.88
5	P	207	HEM	C4C-CHD-C1D	2.75	126.19	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	207	HEM	CMA-C3A-C4A	-2.73	124.27	128.46
5	D	208	HEM	CHC-C4B-NB	2.68	127.35	124.43
5	M	208	HEM	C2D-C1D-ND	-2.67	106.68	109.88
5	D	208	HEM	C2D-C1D-ND	-2.66	106.70	109.88
5	U	207	HEM	CBD-CAD-C3D	-2.65	105.27	112.63
5	E	208	HEM	CMB-C2B-C1B	-2.60	121.08	125.04
5	W	205	HEM	C3D-C4D-ND	-2.60	107.28	110.17
5	E	208	HEM	C4B-C3B-C2B	2.57	109.16	107.11
5	K	207	HEM	CBD-CAD-C3D	-2.56	105.53	112.63
5	G	208	HEM	C4B-C3B-C2B	2.54	109.13	107.11
5	M	208	HEM	CBD-CAD-C3D	-2.54	105.58	112.63
5	P	207	HEM	C2D-C1D-ND	-2.53	106.85	109.88
3	B	209	ACT	OXT-C-O	-2.52	112.76	122.05
5	I	207	HEM	C4C-CHD-C1D	2.51	125.87	122.56
5	W	205	HEM	C2D-C1D-ND	-2.50	106.89	109.88
3	T	207	ACT	OXT-C-O	-2.49	112.86	122.05
5	R	208	HEM	C2C-C3C-C4C	2.45	108.61	106.90
5	E	208	HEM	C3C-C4C-NC	-2.44	106.34	110.94
5	S	206	HEM	C4C-CHD-C1D	2.42	125.75	122.56
5	B	208	HEM	C3D-C4D-ND	-2.42	107.47	110.17
5	S	206	HEM	C2C-C3C-C4C	2.41	108.58	106.90
5	G	208	HEM	C4C-CHD-C1D	2.41	125.74	122.56
5	R	208	HEM	CMA-C3A-C4A	-2.39	124.80	128.46
5	D	208	HEM	C2B-C1B-NB	-2.37	107.03	109.84
5	B	208	HEM	CMB-C2B-C1B	-2.34	121.47	125.04
5	P	207	HEM	CMB-C2B-C1B	-2.34	121.48	125.04
5	U	207	HEM	CMA-C3A-C4A	-2.32	124.90	128.46
5	I	207	HEM	C1B-NB-C4B	2.31	107.46	105.07
5	D	208	HEM	C3C-C4C-NC	-2.31	106.58	110.94
3	B	209	ACT	OXT-C-CH3	2.30	124.69	115.18
5	G	208	HEM	C2C-C3C-C4C	2.27	108.48	106.90
5	B	208	HEM	CHD-C1D-C2D	2.27	128.52	124.98
5	P	207	HEM	CBD-CAD-C3D	-2.26	106.35	112.63
3	H	207	ACT	OXT-C-O	-2.25	113.74	122.05
3	E	209	ACT	OXT-C-CH3	2.23	124.41	115.18
5	K	207	HEM	C3B-C2B-C1B	2.23	108.14	106.49
5	G	208	HEM	CHC-C4B-NB	2.22	126.84	124.43
5	G	208	HEM	C3C-C4C-NC	-2.21	106.77	110.94
3	A	209	ACT	OXT-C-CH3	2.21	124.31	115.18
5	B	208	HEM	C3C-C4C-NC	-2.21	106.77	110.94
3	L	209	ACT	OXT-C-O	-2.21	113.92	122.05
5	M	208	HEM	CMB-C2B-C1B	-2.21	121.68	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	209	ACT	OXT-C-O	-2.20	113.93	122.05
5	K	207	HEM	CHA-C4D-ND	2.20	127.10	124.38
3	F	206	ACT	OXT-C-CH3	2.20	124.25	115.18
3	D	209	ACT	OXT-C-CH3	2.19	124.25	115.18
3	R	209	ACT	OXT-C-CH3	2.19	124.23	115.18
5	G	208	HEM	CHD-C1D-C2D	2.19	128.40	124.98
3	I	208	ACT	OXT-C-CH3	2.18	124.19	115.18
3	M	209	ACT	OXT-C-O	-2.18	114.03	122.05
5	W	205	HEM	CBD-CAD-C3D	-2.18	106.58	112.63
5	P	207	HEM	C3B-C2B-C1B	2.17	108.10	106.49
3	P	208	ACT	OXT-C-CH3	2.15	124.08	115.18
3	E	209	ACT	OXT-C-O	-2.15	114.12	122.05
5	W	205	HEM	C4C-CHD-C1D	2.15	125.39	122.56
5	S	206	HEM	CBD-CAD-C3D	-2.14	106.68	112.63
5	E	208	HEM	CBD-CAD-C3D	-2.12	106.73	112.63
3	N	207	ACT	OXT-C-O	-2.12	114.23	122.05
5	E	208	HEM	C4A-C3A-C2A	2.12	108.47	107.00
3	L	209	ACT	OXT-C-CH3	2.10	123.86	115.18
5	R	208	HEM	CHC-C4B-NB	2.10	126.71	124.43
5	U	207	HEM	C2B-C1B-NB	-2.09	107.36	109.84
3	S	207	ACT	OXT-C-O	-2.09	114.36	122.05
5	R	208	HEM	C3C-C4C-NC	-2.08	107.02	110.94
5	U	207	HEM	CMB-C2B-C1B	-2.08	121.88	125.04
5	P	207	HEM	C2C-C3C-C4C	2.07	108.34	106.90
5	I	207	HEM	C1D-C2D-C3D	2.07	109.13	106.96
3	U	208	ACT	OXT-C-O	-2.06	114.48	122.05
5	S	206	HEM	CHA-C4D-ND	2.04	126.90	124.38
5	E	208	HEM	CMA-C3A-C4A	-2.04	125.33	128.46
5	K	207	HEM	C3C-C4C-NC	-2.03	107.10	110.94
3	G	209	ACT	OXT-C-O	-2.03	114.58	122.05
5	K	207	HEM	C2C-C3C-C4C	2.02	108.31	106.90
5	U	207	HEM	CHC-C4B-NB	2.02	126.62	124.43
5	E	208	HEM	CAA-CBA-CGA	-2.00	108.14	113.76
5	D	208	HEM	C4B-C3B-C2B	2.00	108.70	107.11

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	208	HEM	CAD-CBD-CGD-O2D
5	D	208	HEM	CAD-CBD-CGD-O2D
5	P	207	HEM	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
5	D	208	HEM	CAD-CBD-CGD-O1D
5	E	208	HEM	CAD-CBD-CGD-O1D
5	M	208	HEM	CAA-CBA-CGA-O1A
5	B	208	HEM	CAA-CBA-CGA-O1A
5	G	208	HEM	CAA-CBA-CGA-O2A
5	M	208	HEM	CAD-CBD-CGD-O2D
5	B	208	HEM	CAA-CBA-CGA-O2A
5	E	208	HEM	CAD-CBD-CGD-O2D
5	M	208	HEM	CAD-CBD-CGD-O1D
5	G	208	HEM	CAA-CBA-CGA-O1A
5	M	208	HEM	CAA-CBA-CGA-O2A
5	U	207	HEM	CAA-CBA-CGA-O1A
5	E	208	HEM	CAA-CBA-CGA-O2A
5	K	207	HEM	CAD-CBD-CGD-O2D
5	E	208	HEM	CAA-CBA-CGA-O1A
5	D	208	HEM	CAA-CBA-CGA-O1A
5	G	208	HEM	CAD-CBD-CGD-O1D
5	U	207	HEM	CAA-CBA-CGA-O2A
5	I	207	HEM	CAD-CBD-CGD-O2D
5	P	207	HEM	CAD-CBD-CGD-O1D
5	D	208	HEM	CAA-CBA-CGA-O2A
5	P	207	HEM	CAA-CBA-CGA-O2A
5	U	207	HEM	CAD-CBD-CGD-O2D
5	K	207	HEM	CAA-CBA-CGA-O2A
5	K	207	HEM	CAD-CBD-CGD-O1D
5	W	205	HEM	CAA-CBA-CGA-O2A
5	I	207	HEM	CAD-CBD-CGD-O1D
5	S	206	HEM	CAA-CBA-CGA-O1A
5	U	207	HEM	CAD-CBD-CGD-O1D
5	W	205	HEM	CAD-CBD-CGD-O1D
5	W	205	HEM	CAD-CBD-CGD-O2D
5	I	207	HEM	CAA-CBA-CGA-O1A
5	S	206	HEM	CAD-CBD-CGD-O2D
5	S	206	HEM	CAA-CBA-CGA-O2A
5	I	207	HEM	CAA-CBA-CGA-O2A
5	K	207	HEM	CAA-CBA-CGA-O1A
5	W	205	HEM	CAA-CBA-CGA-O1A
5	R	208	HEM	CAD-CBD-CGD-O2D
5	S	206	HEM	CAD-CBD-CGD-O1D
5	P	207	HEM	CAA-CBA-CGA-O1A
5	R	208	HEM	CAA-CBA-CGA-O1A
5	R	208	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
5	B	208	HEM	CAD-CBD-CGD-O1D
5	R	208	HEM	CAA-CBA-CGA-O2A
5	B	208	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

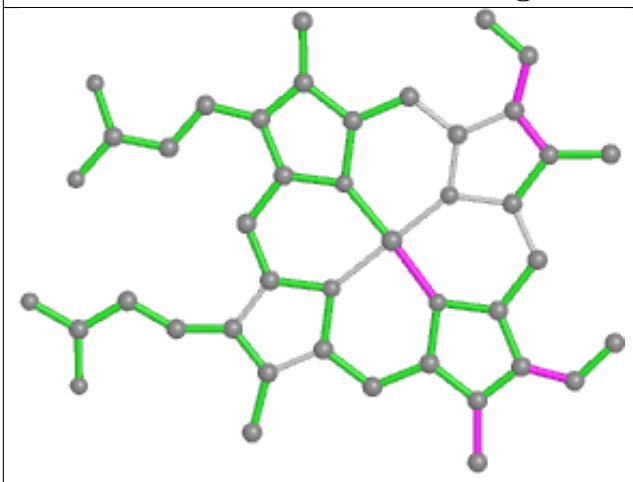
27 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	205	ACT	2	0
3	H	207	ACT	2	0
5	M	208	HEM	1	0
3	P	208	ACT	1	0
3	V	206	ACT	2	0
5	R	208	HEM	3	0
3	C	207	ACT	3	0
5	W	205	HEM	4	0
5	P	207	HEM	1	0
3	W	206	ACT	2	0
3	T	207	ACT	2	0
3	O	205	ACT	2	0
5	I	207	HEM	1	0
3	S	207	ACT	1	0
3	J	207	ACT	2	0
3	M	209	ACT	2	0
5	G	208	HEM	1	0
3	I	208	ACT	1	0
5	B	208	HEM	2	0
3	N	207	ACT	1	0
5	D	208	HEM	1	0
5	K	207	HEM	2	0
5	E	208	HEM	2	0
3	U	208	ACT	2	0
5	S	206	HEM	3	0
3	F	206	ACT	1	0
3	K	208	ACT	2	0

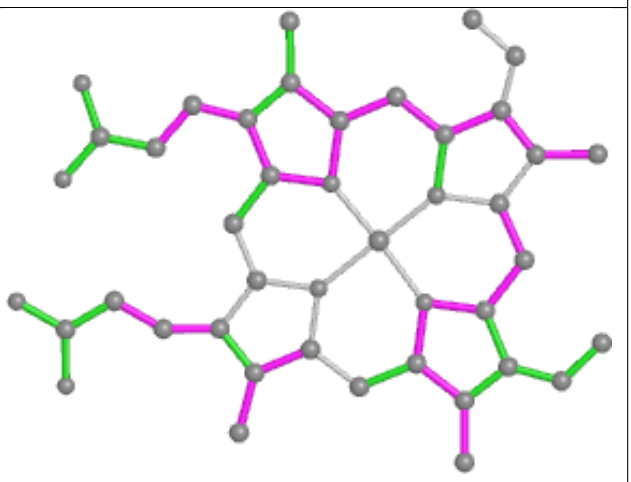
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

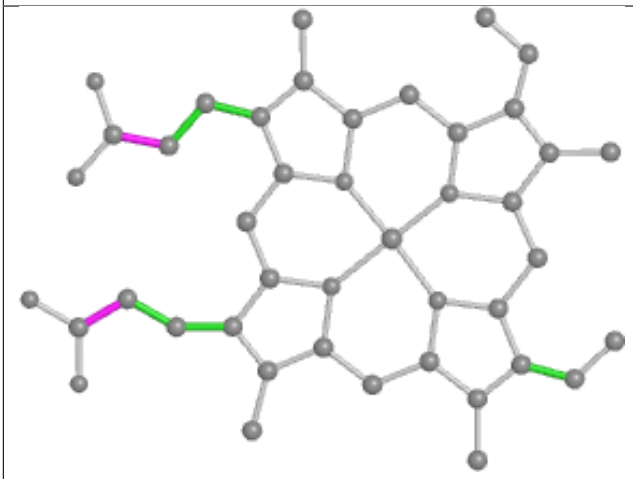
Ligand HEM M 208



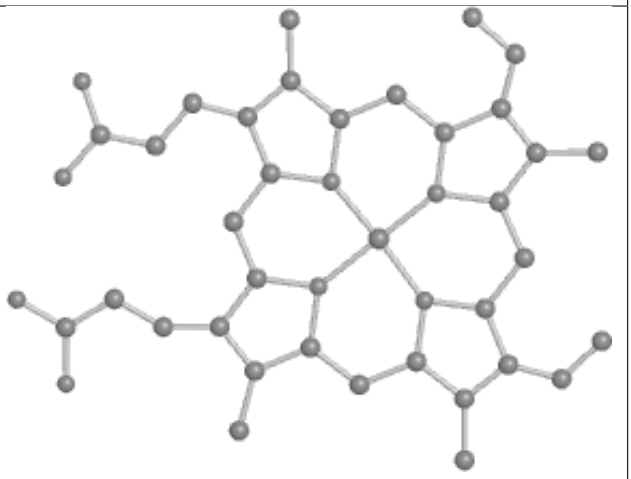
Bond lengths



Bond angles

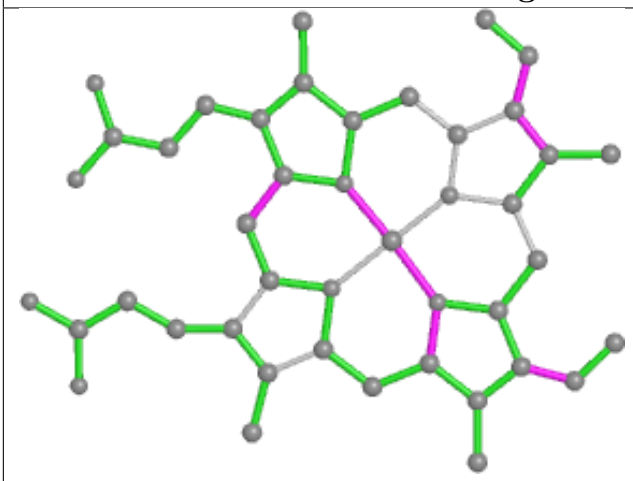


Torsions

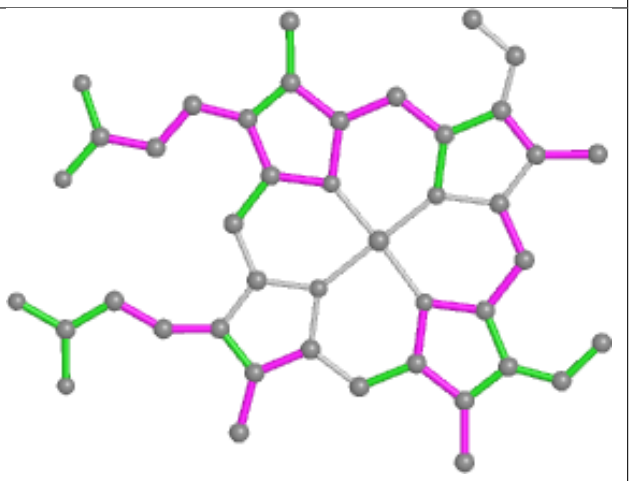


Rings

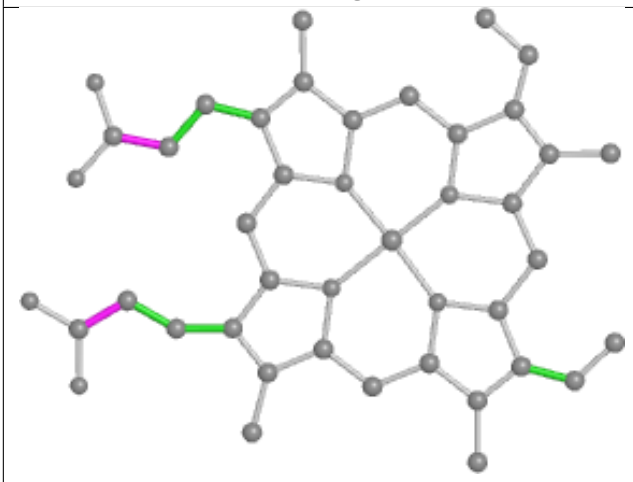
Ligand HEM U 207



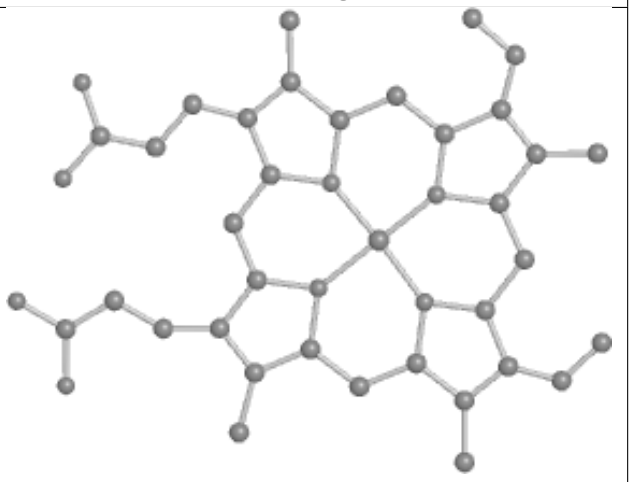
Bond lengths



Bond angles

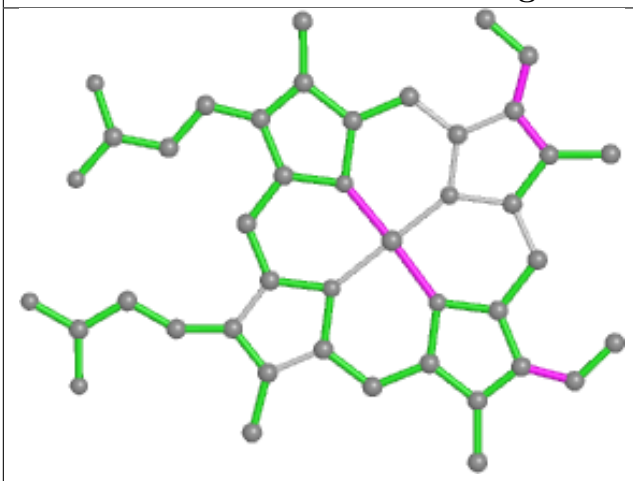


Torsions

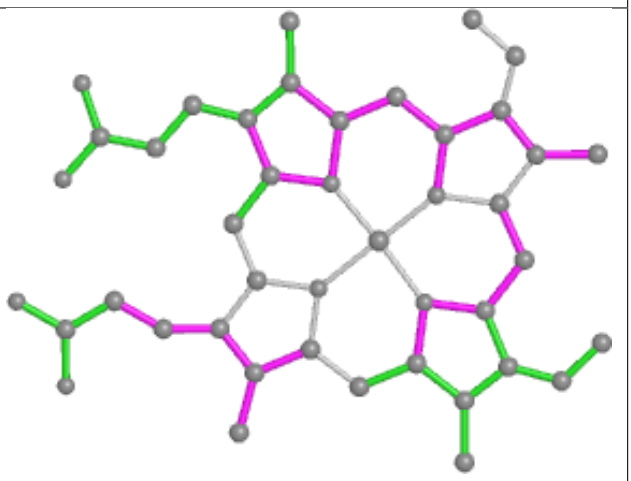


Rings

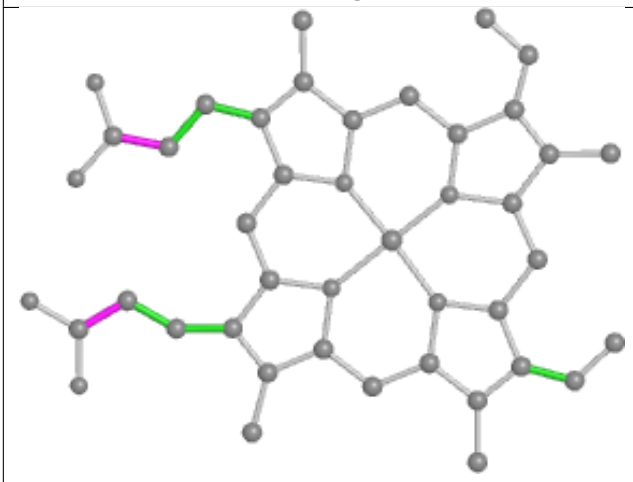
Ligand HEM R 208



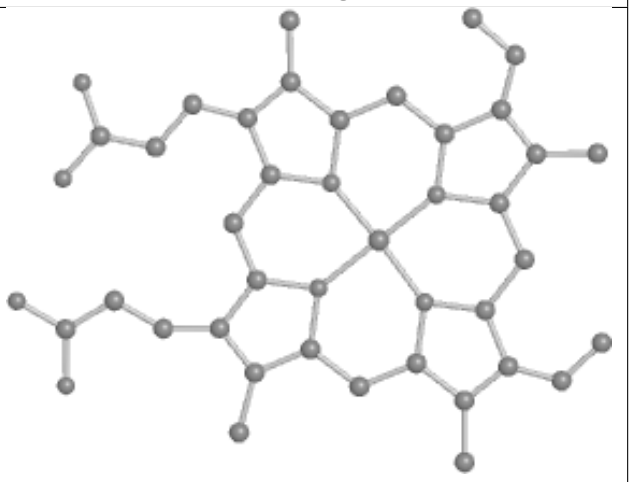
Bond lengths



Bond angles

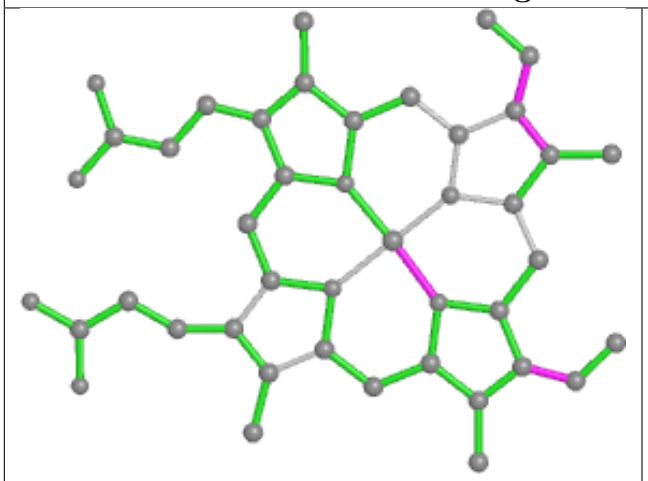


Torsions



Rings

Ligand HEM W 205



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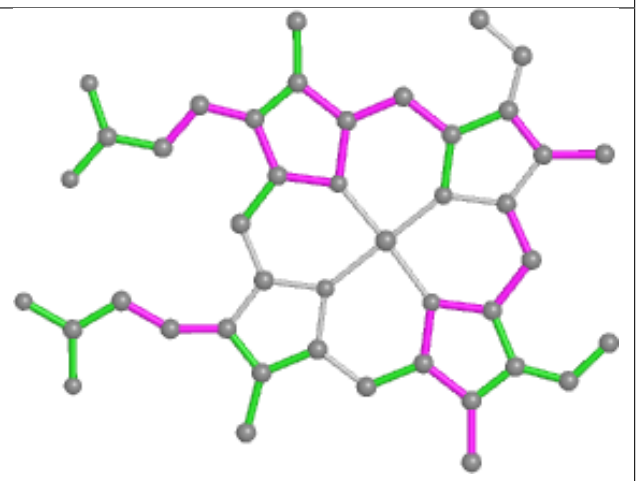
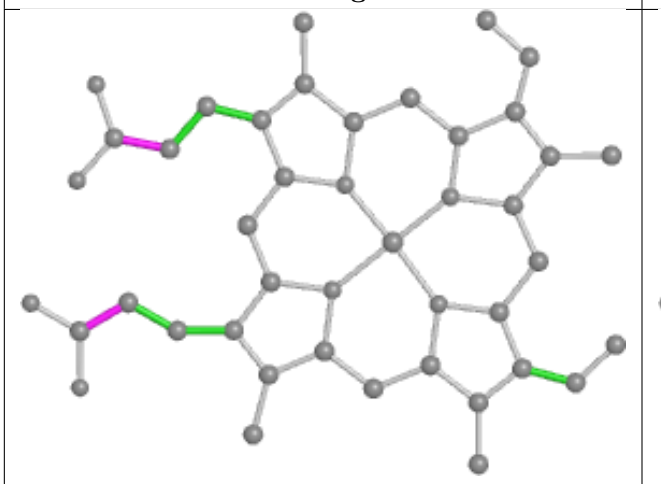
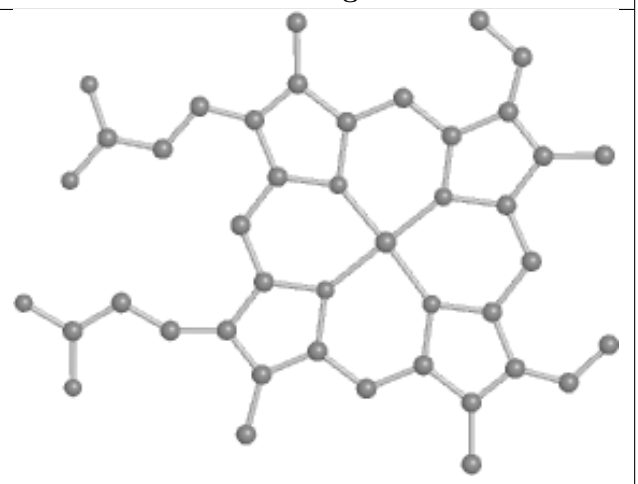


Bond angles

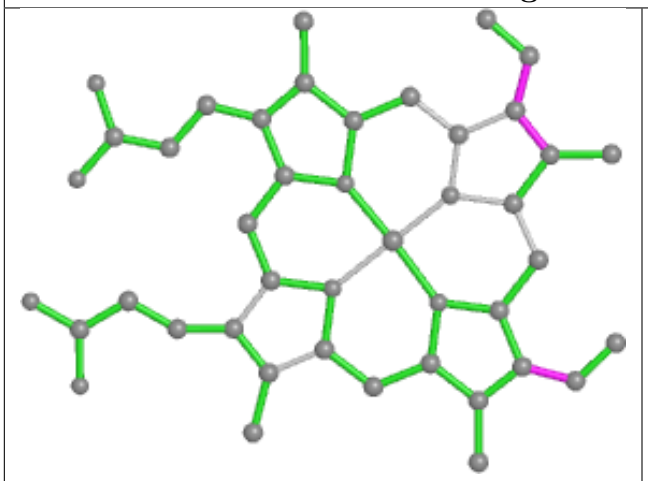


Torsions

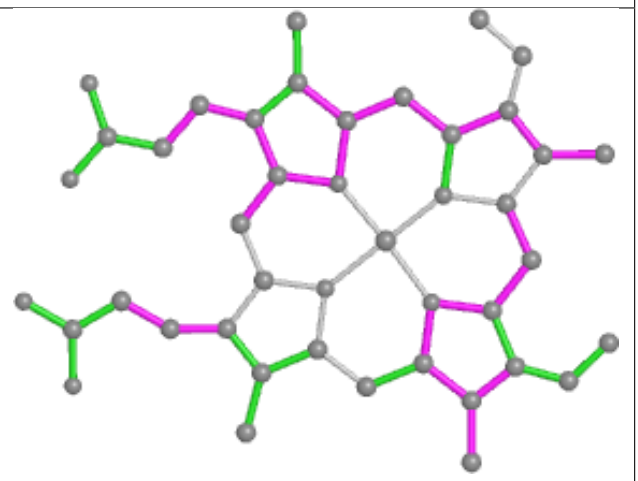


Rings

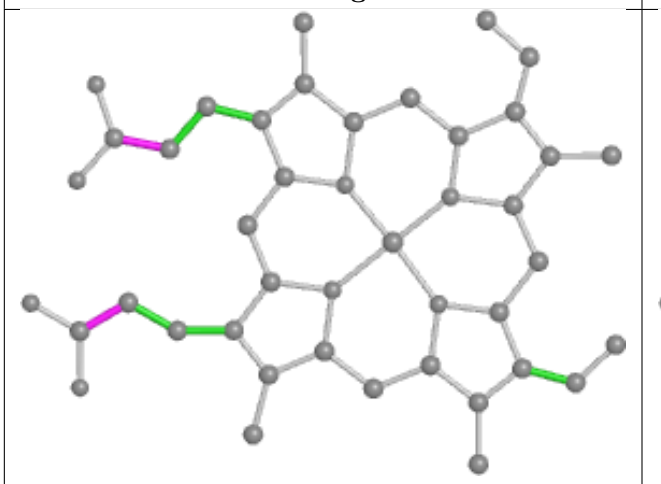
Ligand HEM P 207



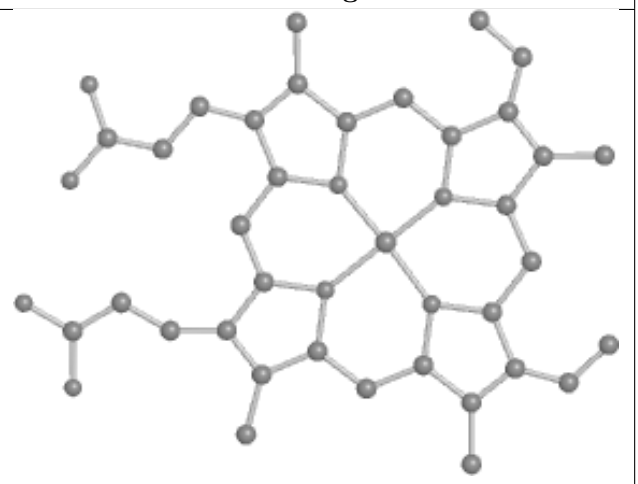
Bond lengths



Bond angles

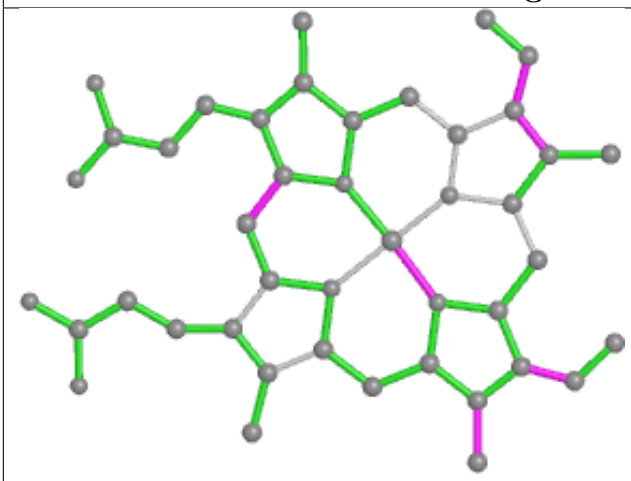


Torsions



Rings

Ligand HEM I 207



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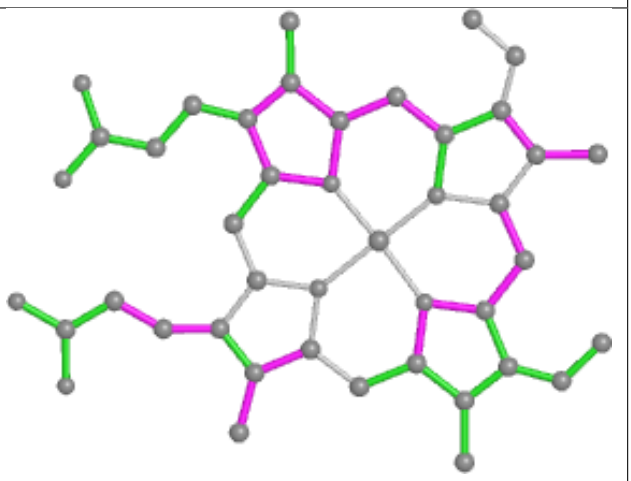
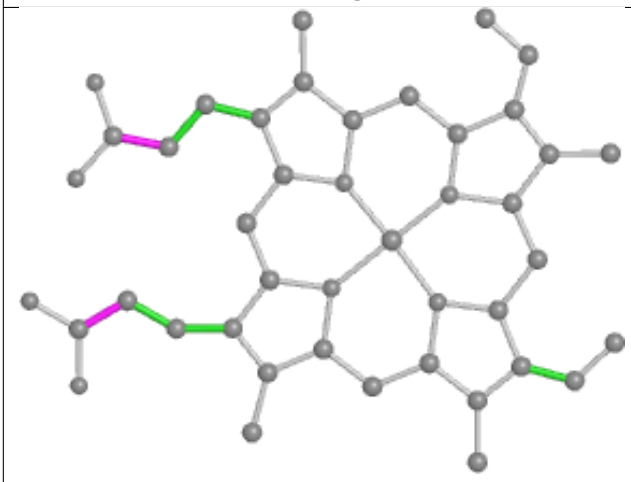
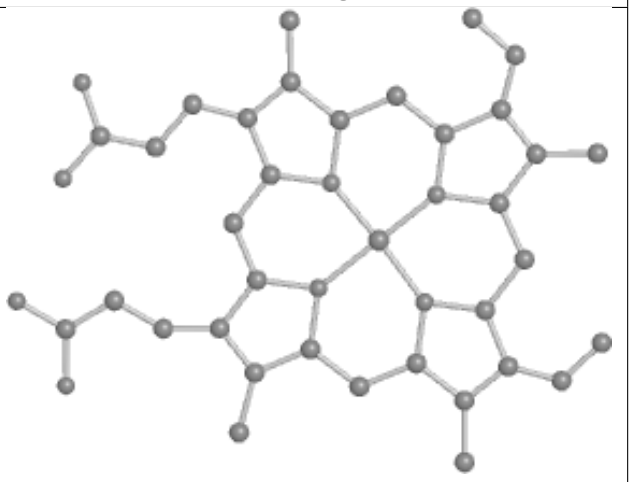


Bond angles

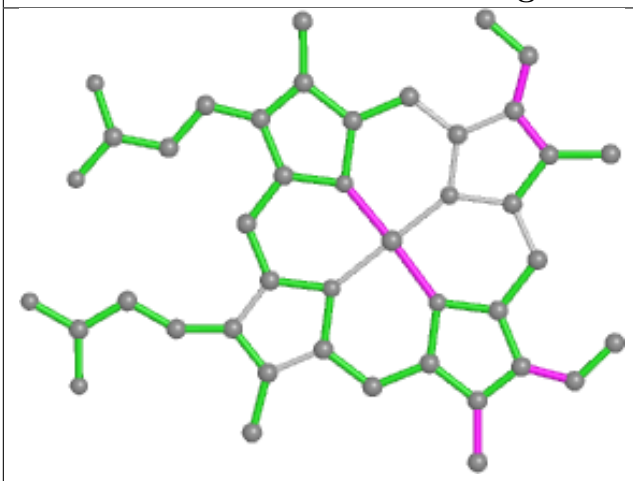


Torsions

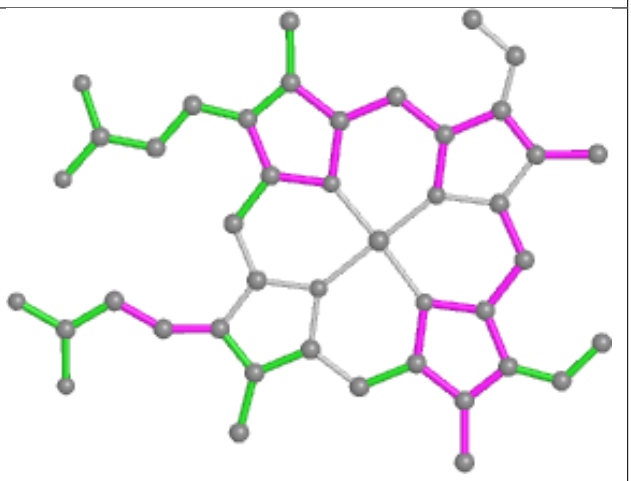


Rings

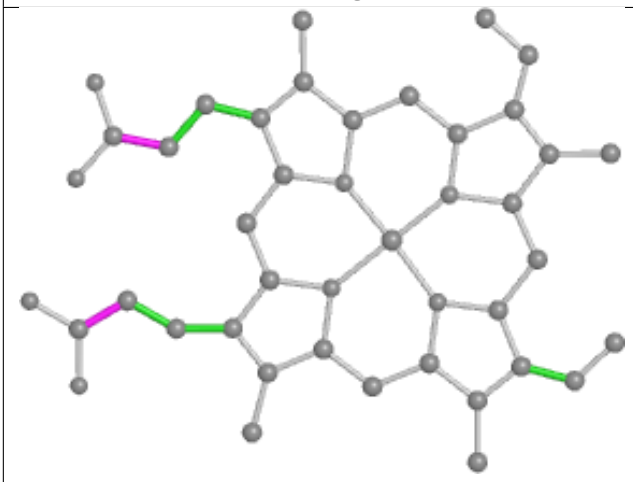
Ligand HEM G 208



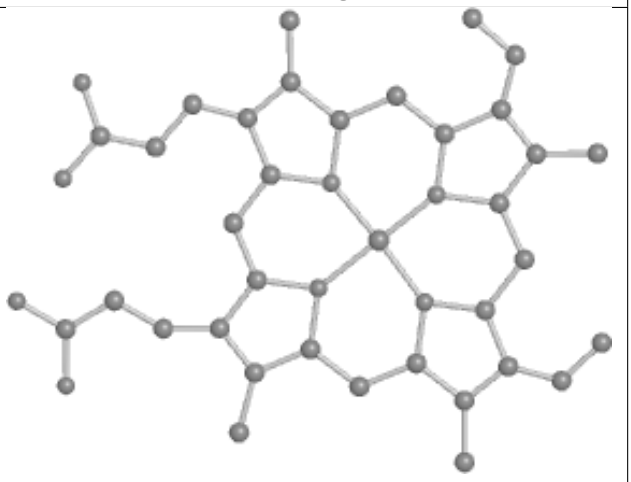
Bond lengths



Bond angles

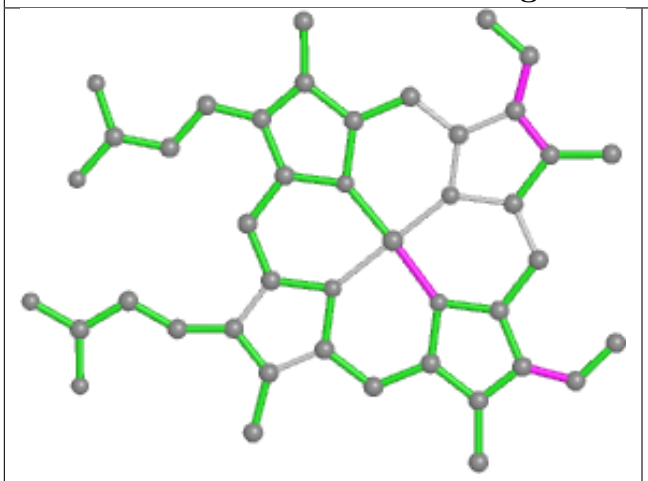


Torsions



Rings

Ligand HEM B 208



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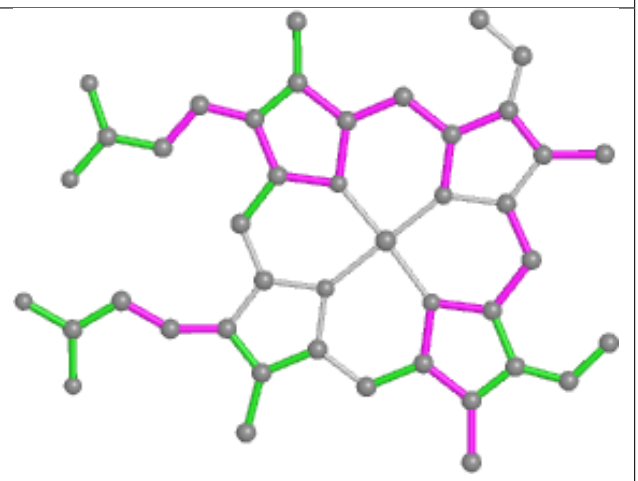
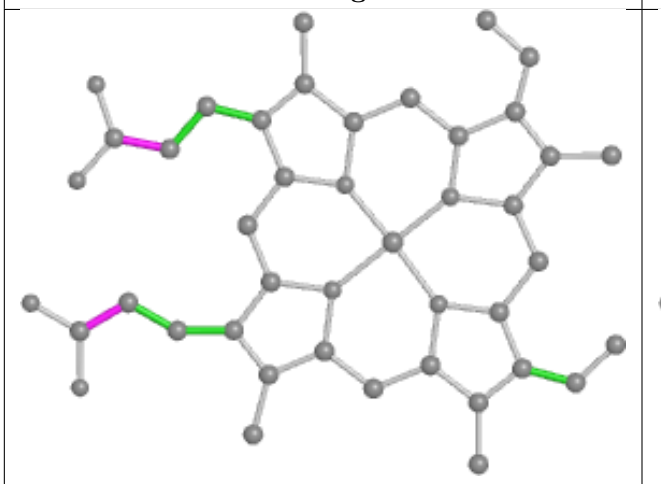


Bond angles



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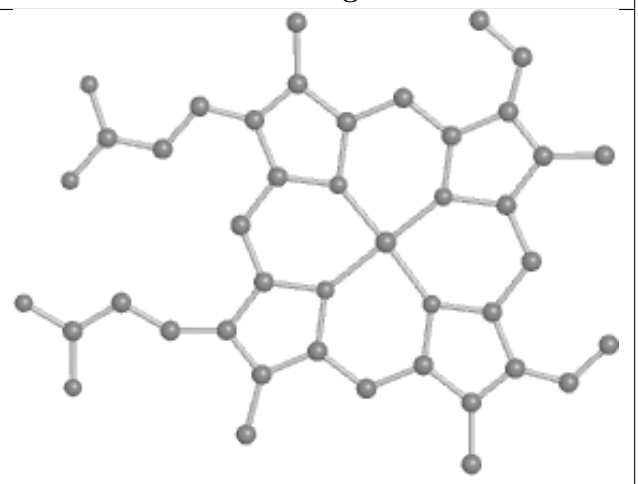

Rings

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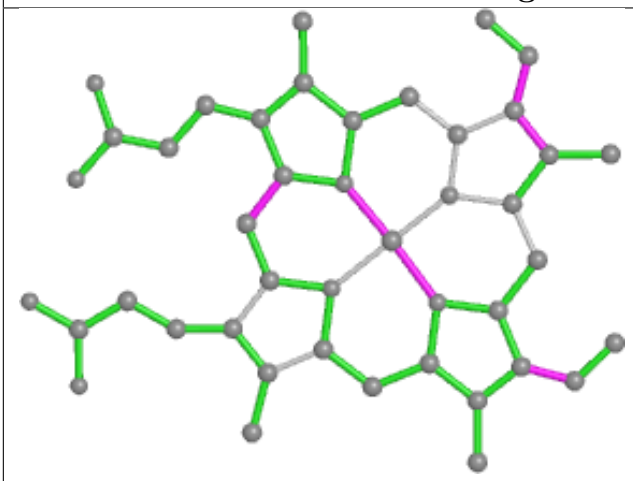

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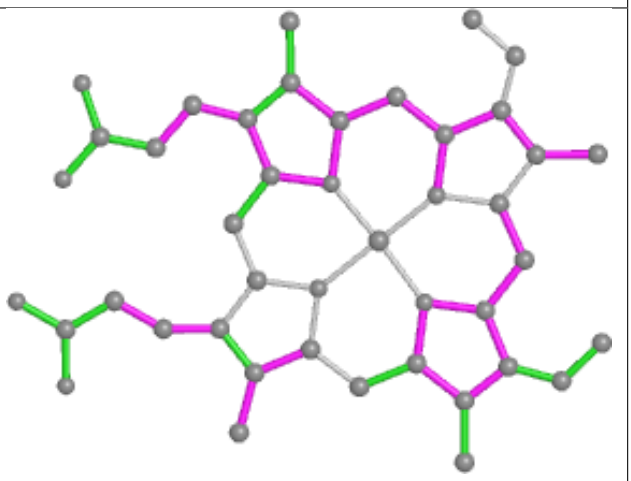
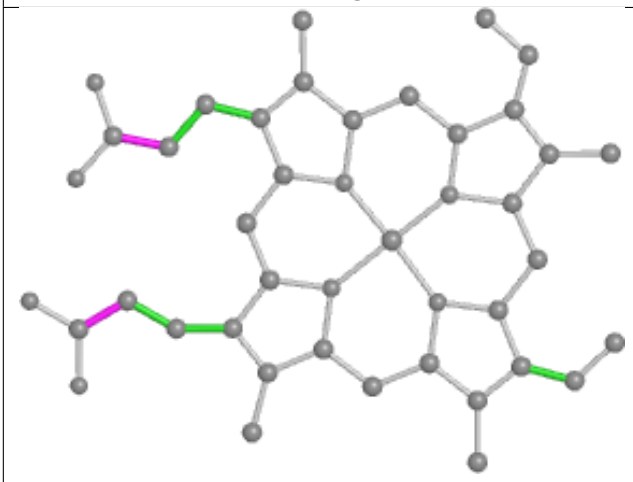
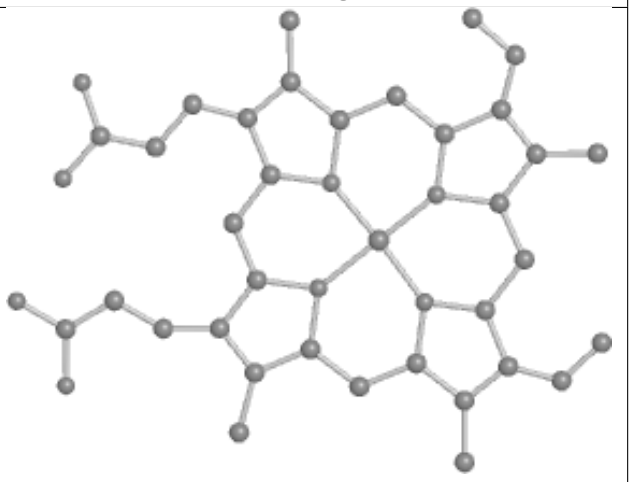


Bond angles



Torsions



Rings

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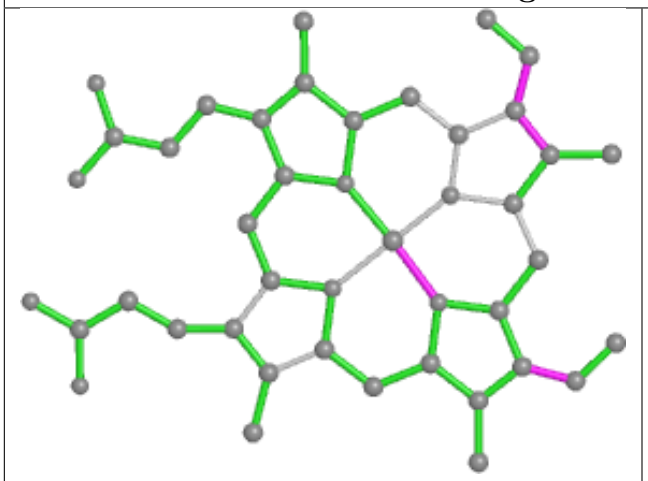

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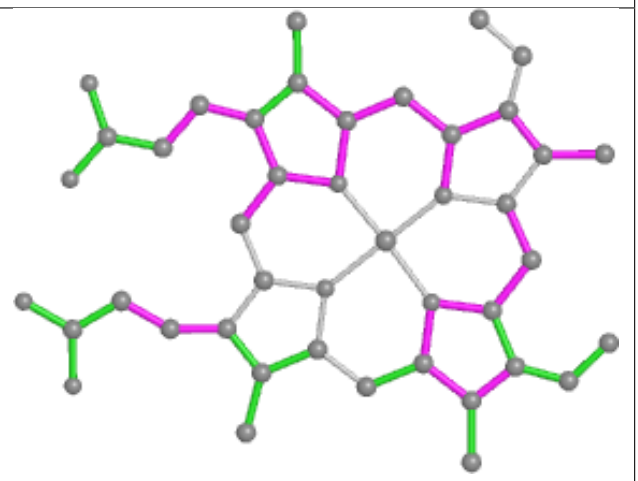
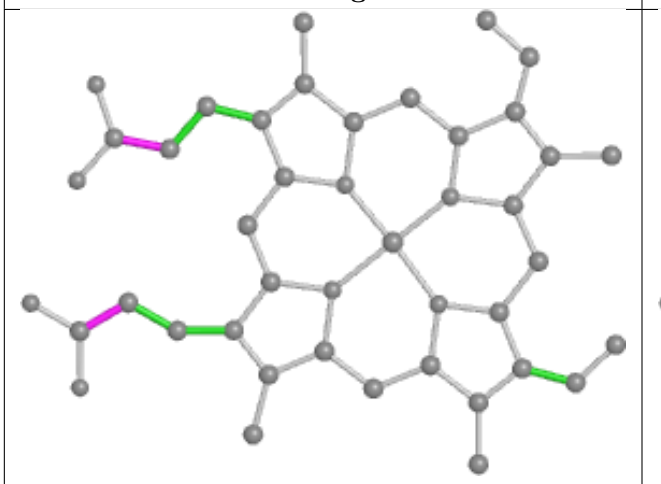
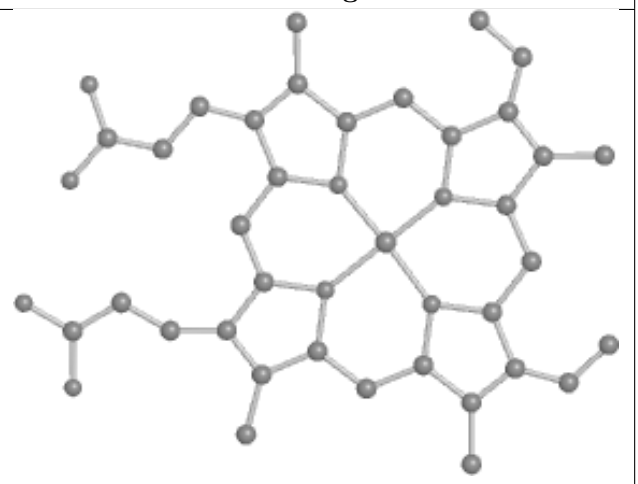


Bond angles

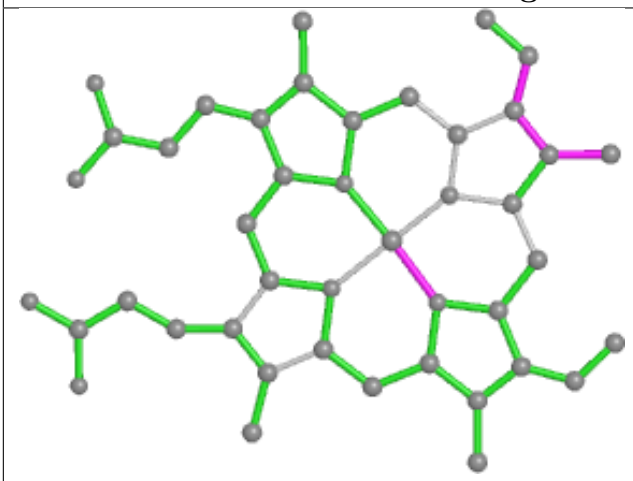


Torsions

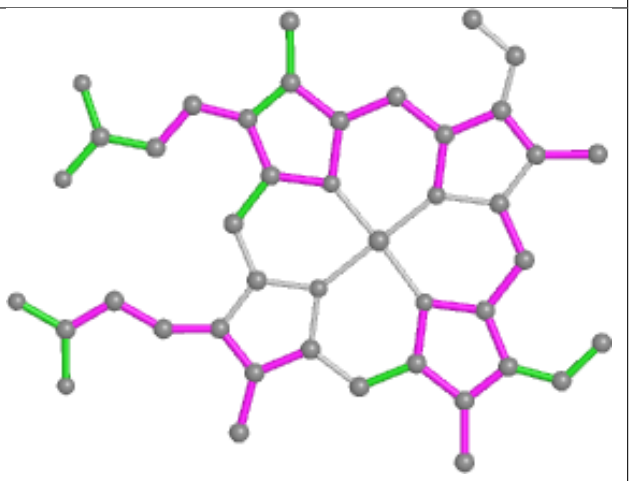


Rings

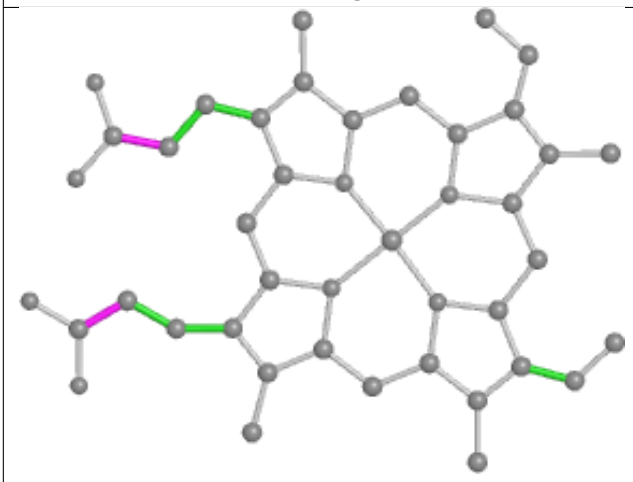
Ligand HEM E 208



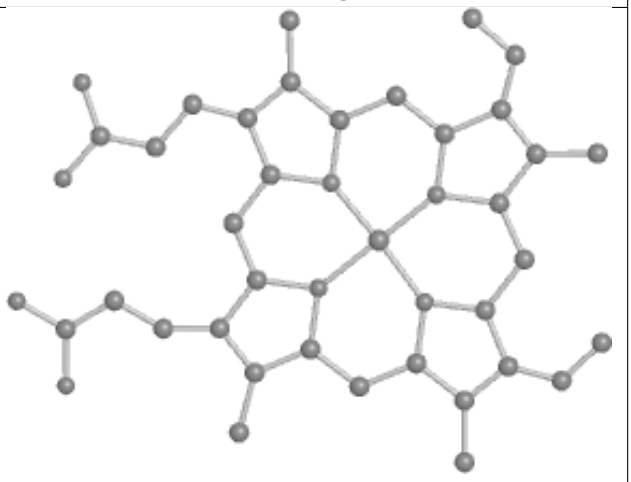
Bond lengths



Bond angles

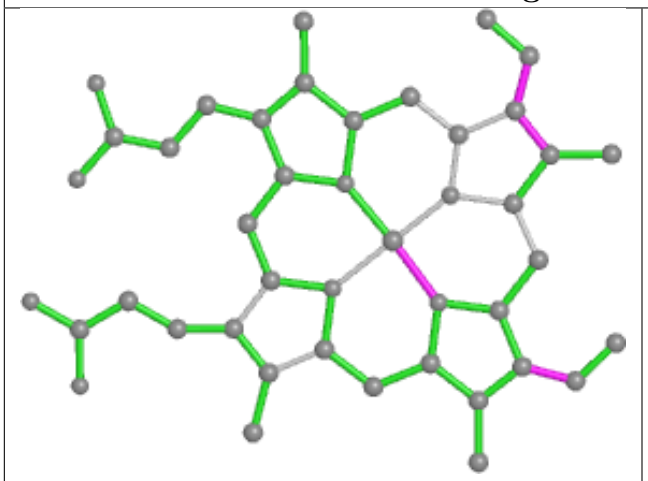


Torsions

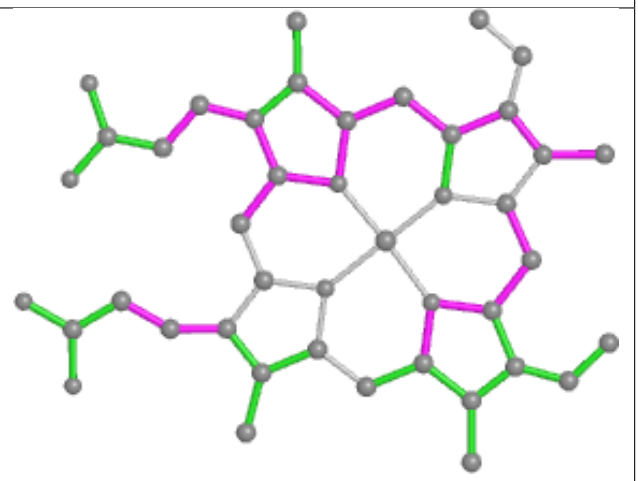


Rings

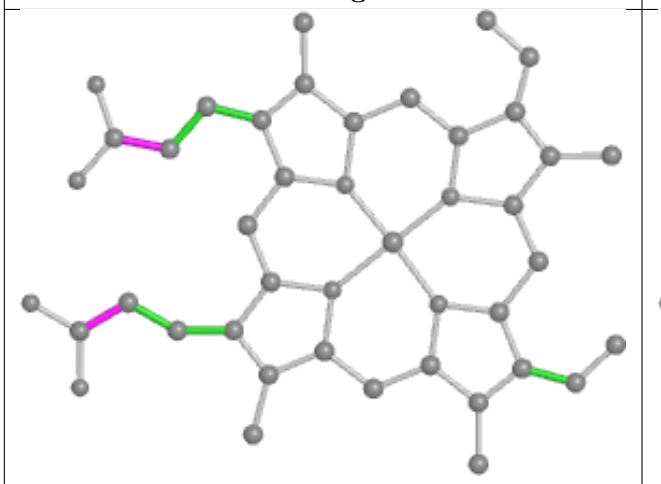
Ligand HEM S 206



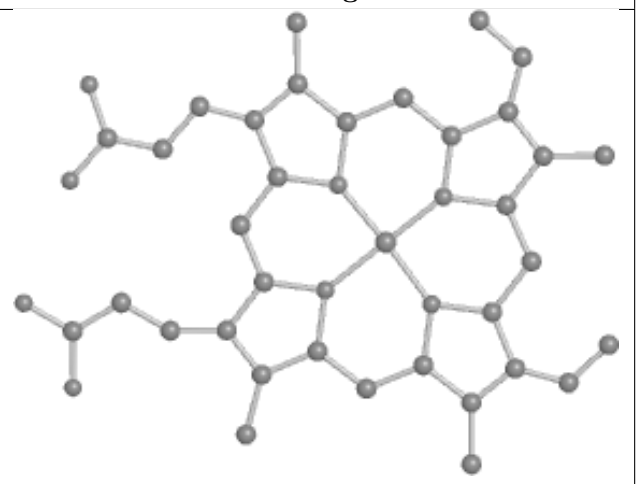
Bond lengths



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 (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	156/158 (98%)	-0.78	0	100	100	16, 22, 33, 49	0
1	B	156/158 (98%)	-0.85	0	100	100	17, 23, 35, 54	0
1	C	156/158 (98%)	-0.88	0	100	100	19, 25, 38, 49	0
1	D	156/158 (98%)	-0.89	0	100	100	18, 23, 35, 48	0
1	E	156/158 (98%)	-0.85	0	100	100	19, 25, 37, 52	0
1	F	156/158 (98%)	-0.87	0	100	100	19, 26, 38, 51	0
1	G	156/158 (98%)	-0.84	0	100	100	19, 26, 39, 54	0
1	H	156/158 (98%)	-0.87	0	100	100	19, 25, 38, 51	0
1	I	156/158 (98%)	-0.87	0	100	100	20, 26, 37, 55	0
1	J	156/158 (98%)	-0.85	0	100	100	20, 26, 36, 50	0
1	K	156/158 (98%)	-0.85	0	100	100	20, 26, 38, 48	0
1	L	156/158 (98%)	-0.86	0	100	100	18, 25, 39, 53	0
1	M	156/158 (98%)	-0.76	0	100	100	18, 22, 34, 50	0
1	N	156/158 (98%)	-0.86	0	100	100	18, 24, 36, 49	0
1	O	156/158 (98%)	-0.85	0	100	100	21, 27, 39, 56	0
1	P	156/158 (98%)	-0.90	0	100	100	20, 26, 37, 50	0
1	Q	156/158 (98%)	-0.93	0	100	100	18, 23, 35, 49	0
1	R	156/158 (98%)	-0.89	0	100	100	19, 24, 36, 51	0
1	S	156/158 (98%)	-0.87	0	100	100	17, 22, 34, 51	0
1	T	156/158 (98%)	-0.88	0	100	100	18, 23, 36, 54	0
1	U	156/158 (98%)	-0.86	0	100	100	19, 25, 37, 51	0
1	V	156/158 (98%)	-0.86	0	100	100	20, 26, 38, 48	0
1	W	156/158 (98%)	-0.87	0	100	100	19, 26, 37, 51	0
1	X	156/158 (98%)	-0.88	0	100	100	19, 25, 36, 49	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3744/3792 (98%)	-0.86	0 100 100	16, 25, 37, 56	0

There are no RSRZ outliers to report.

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
2	FE2	F	205	1/1	0.20	0.12	101,101,101,101	0
2	FE2	N	206	1/1	0.29	0.15	103,103,103,103	0
2	FE2	W	204	1/1	0.39	0.14	99,99,99,99	0
2	FE2	P	206	1/1	0.49	0.14	105,105,105,105	0
2	FE2	A	208	1/1	0.50	0.09	95,95,95,95	0
2	FE2	I	206	1/1	0.53	0.14	98,98,98,98	0
2	FE2	D	207	1/1	0.55	0.09	96,96,96,96	0
2	FE2	C	206	1/1	0.57	0.09	103,103,103,103	0
2	FE2	H	206	1/1	0.58	0.08	98,98,98,98	0
2	FE2	R	207	1/1	0.63	0.10	106,106,106,106	0
2	FE2	U	206	1/1	0.64	0.09	101,101,101,101	0
2	FE2	K	206	1/1	0.65	0.10	98,98,98,98	0
2	FE2	Q	204	1/1	0.67	0.11	99,99,99,99	0
2	FE2	G	207	1/1	0.67	0.11	99,99,99,99	0
2	FE2	E	207	1/1	0.68	0.09	89,89,89,89	0
2	FE2	S	205	1/1	0.68	0.07	97,97,97,97	0
2	FE2	X	205	1/1	0.72	0.12	98,98,98,98	0
2	FE2	T	206	1/1	0.73	0.13	97,97,97,97	0
2	FE2	V	205	1/1	0.73	0.09	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	J	206	1/1	0.74	0.18	104,104,104,104	0
2	FE2	L	208	1/1	0.74	0.07	98,98,98,98	0
2	FE2	O	204	1/1	0.76	0.08	89,89,89,89	0
2	FE2	B	207	1/1	0.85	0.08	95,95,95,95	0
3	ACT	F	206	4/4	0.88	0.18	33,37,40,43	0
2	FE2	M	207	1/1	0.89	0.11	99,99,99,99	0
3	ACT	O	205	4/4	0.90	0.19	35,38,39,40	0
3	ACT	C	207	4/4	0.91	0.18	38,38,39,45	0
2	FE2	R	206	1/1	0.91	0.04	63,63,63,63	0
2	FE2	G	206	1/1	0.91	0.06	67,67,67,67	0
3	ACT	G	209	4/4	0.92	0.16	33,39,42,45	0
3	ACT	H	207	4/4	0.92	0.12	39,42,42,42	0
3	ACT	D	209	4/4	0.92	0.22	32,38,38,41	0
2	FE2	N	205	1/1	0.93	0.04	69,69,69,69	0
3	ACT	M	209	4/4	0.93	0.15	32,33,39,42	0
2	FE2	R	205	1/1	0.93	0.03	65,65,65,65	0
3	ACT	W	206	4/4	0.93	0.13	37,41,44,44	0
5	HEM	D	208	43/43	0.93	0.11	24,32,47,51	0
5	HEM	E	208	43/43	0.93	0.12	24,31,51,57	0
3	ACT	L	209	4/4	0.94	0.17	32,37,39,39	0
2	FE2	Q	203	1/1	0.94	0.05	54,54,54,54	0
3	ACT	K	208	4/4	0.94	0.15	35,38,39,40	0
5	HEM	G	208	43/43	0.94	0.10	23,34,48,55	0
5	HEM	P	207	43/43	0.94	0.10	25,34,50,59	0
5	HEM	R	208	43/43	0.94	0.09	21,29,45,52	0
5	HEM	U	207	43/43	0.94	0.10	23,31,50,56	0
5	HEM	W	205	43/43	0.94	0.10	25,32,47,48	0
5	HEM	I	207	43/43	0.95	0.08	24,31,47,59	0
5	HEM	K	207	43/43	0.95	0.11	23,33,45,50	0
3	ACT	B	209	4/4	0.95	0.21	27,32,35,36	0
2	FE2	D	206	1/1	0.95	0.09	65,65,65,65	0
5	HEM	S	206	43/43	0.95	0.08	18,29,44,50	0
3	ACT	A	209	4/4	0.95	0.12	30,32,35,36	0
3	ACT	I	208	4/4	0.95	0.12	33,36,37,37	0
2	FE2	O	203	1/1	0.96	0.03	52,52,52,52	0
5	HEM	B	208	43/43	0.96	0.08	21,29,44,49	0
2	FE2	R	203	1/1	0.96	0.04	56,56,56,56	0
2	FE2	N	201	1/1	0.96	0.06	51,51,51,51	0
2	FE2	P	204	1/1	0.96	0.03	68,68,68,68	0
2	FE2	P	205	1/1	0.96	0.03	69,69,69,69	0
2	FE2	I	205	1/1	0.96	0.04	69,69,69,69	0
5	HEM	M	208	43/43	0.96	0.08	18,29,47,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	C	203	1/1	0.96	0.04	56,56,56,56	0
2	FE2	U	204	1/1	0.96	0.05	55,55,55,55	0
3	ACT	Q	205	4/4	0.96	0.06	33,35,36,37	0
3	ACT	S	207	4/4	0.96	0.16	32,36,36,37	0
3	ACT	U	208	4/4	0.96	0.13	26,37,37,40	0
2	FE2	K	203	1/1	0.97	0.04	51,51,51,51	0
2	FE2	A	206	1/1	0.97	0.06	60,60,60,60	0
2	FE2	S	203	1/1	0.97	0.04	51,51,51,51	0
3	ACT	V	206	4/4	0.97	0.08	35,36,42,43	0
2	FE2	L	206	1/1	0.97	0.05	70,70,70,70	0
3	ACT	X	206	4/4	0.97	0.17	35,39,40,45	0
3	ACT	E	209	4/4	0.97	0.08	33,35,39,42	0
2	FE2	I	204	1/1	0.97	0.07	52,52,52,52	0
2	FE2	M	206	1/1	0.97	0.03	57,57,57,57	0
2	FE2	U	205	1/1	0.97	0.04	59,59,59,59	0
2	FE2	A	207	1/1	0.97	0.05	62,62,62,62	0
3	ACT	J	207	4/4	0.97	0.15	34,36,37,40	0
2	FE2	D	205	1/1	0.97	0.03	52,52,52,52	0
2	FE2	J	204	1/1	0.97	0.04	52,52,52,52	0
2	FE2	X	204	1/1	0.97	0.03	60,60,60,60	0
3	ACT	N	207	4/4	0.97	0.15	27,37,37,39	0
2	FE2	H	204	1/1	0.97	0.04	64,64,64,64	0
3	ACT	P	208	4/4	0.97	0.10	28,35,37,41	0
2	FE2	J	201	1/1	0.98	0.04	42,42,42,42	0
2	FE2	R	204	1/1	0.98	0.03	36,36,36,36	0
3	ACT	T	207	4/4	0.98	0.14	32,36,36,37	0
2	FE2	B	206	1/1	0.98	0.04	60,60,60,60	0
2	FE2	J	205	1/1	0.98	0.04	61,61,61,61	0
2	FE2	F	201	1/1	0.98	0.04	37,37,37,37	0
2	FE2	H	205	1/1	0.98	0.03	60,60,60,60	0
2	FE2	K	205	1/1	0.98	0.03	61,61,61,61	0
2	FE2	T	203	1/1	0.98	0.05	50,50,50,50	0
2	FE2	P	203	1/1	0.98	0.04	55,55,55,55	0
2	FE2	U	203	1/1	0.98	0.04	45,45,45,45	0
2	FE2	F	204	1/1	0.98	0.04	53,53,53,53	0
2	FE2	C	205	1/1	0.98	0.04	62,62,62,62	0
2	FE2	L	207	1/1	0.98	0.05	56,56,56,56	0
2	FE2	V	202	1/1	0.98	0.03	41,41,41,41	0
2	FE2	V	204	1/1	0.98	0.06	62,62,62,62	0
2	FE2	G	205	1/1	0.98	0.03	53,53,53,53	0
2	FE2	W	203	1/1	0.98	0.05	55,55,55,55	0
2	FE2	B	205	1/1	0.98	0.04	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	T	205	1/1	0.99	0.04	59,59,59,59	0
2	FE2	C	201	1/1	0.99	0.03	34,34,34,34	0
2	FE2	U	201	1/1	0.99	0.04	35,35,35,35	0
2	FE2	K	201	1/1	0.99	0.04	33,33,33,33	0
2	FE2	K	202	1/1	0.99	0.03	41,41,41,41	0
2	FE2	C	202	1/1	0.99	0.04	39,39,39,39	0
2	FE2	K	204	1/1	0.99	0.03	43,43,43,43	0
2	FE2	V	201	1/1	0.99	0.04	35,35,35,35	0
2	FE2	F	202	1/1	0.99	0.03	37,37,37,37	0
2	FE2	V	203	1/1	0.99	0.07	54,54,54,54	0
2	FE2	F	203	1/1	0.99	0.02	42,42,42,42	0
2	FE2	L	201	1/1	0.99	0.04	40,40,40,40	0
2	FE2	W	201	1/1	0.99	0.04	33,33,33,33	0
2	FE2	W	202	1/1	0.99	0.03	40,40,40,40	0
2	FE2	L	203	1/1	0.99	0.03	34,34,34,34	0
2	FE2	L	204	1/1	0.99	0.05	55,55,55,55	0
2	FE2	X	202	1/1	0.99	0.03	38,38,38,38	0
2	FE2	X	203	1/1	0.99	0.03	57,57,57,57	0
2	FE2	B	201	1/1	0.99	0.04	41,41,41,41	0
2	FE2	C	204	1/1	0.99	0.03	41,41,41,41	0
2	FE2	G	202	1/1	0.99	0.04	38,38,38,38	0
2	FE2	M	201	1/1	0.99	0.04	38,38,38,38	0
2	FE2	M	204	1/1	0.99	0.06	45,45,45,45	0
2	FE2	G	203	1/1	0.99	0.05	40,40,40,40	0
2	FE2	G	204	1/1	0.99	0.04	43,43,43,43	0
2	FE2	B	203	1/1	0.99	0.03	31,31,31,31	0
2	FE2	N	202	1/1	0.99	0.05	39,39,39,39	0
2	FE2	N	204	1/1	0.99	0.03	36,36,36,36	0
2	FE2	B	204	1/1	0.99	0.03	33,33,33,33	0
2	FE2	D	201	1/1	0.99	0.04	38,38,38,38	0
2	FE2	O	202	1/1	0.99	0.03	41,41,41,41	0
2	FE2	H	202	1/1	0.99	0.04	35,35,35,35	0
2	FE2	H	203	1/1	0.99	0.02	39,39,39,39	0
2	FE2	P	202	1/1	0.99	0.03	37,37,37,37	0
2	FE2	D	202	1/1	0.99	0.03	37,37,37,37	0
2	FE2	D	204	1/1	0.99	0.03	40,40,40,40	0
2	FE2	A	201	1/1	0.99	0.03	37,37,37,37	0
3	ACT	R	209	4/4	0.99	0.09	29,30,37,41	0
2	FE2	I	201	1/1	0.99	0.03	36,36,36,36	0
2	FE2	Q	202	1/1	0.99	0.03	37,37,37,37	0
2	FE2	I	202	1/1	0.99	0.04	41,41,41,41	0
2	FE2	I	203	1/1	0.99	0.03	44,44,44,44	0

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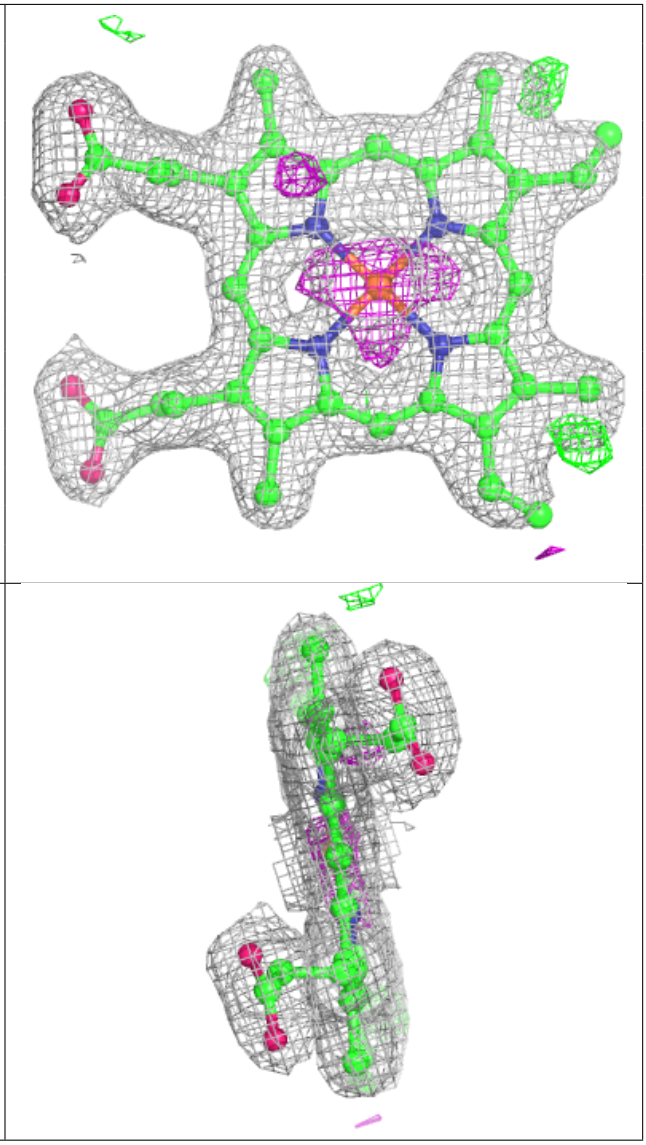
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	R	201	1/1	0.99	0.04	43,43,43,43	0
2	FE2	A	203	1/1	0.99	0.03	33,33,33,33	0
4	K	D	210	1/1	0.99	0.04	32,32,32,32	0
4	K	L	210	1/1	0.99	0.04	30,30,30,30	0
2	FE2	A	204	1/1	0.99	0.06	45,45,45,45	0
2	FE2	E	201	1/1	0.99	0.06	34,34,34,34	0
2	FE2	E	204	1/1	0.99	0.03	47,47,47,47	0
2	FE2	J	202	1/1	0.99	0.05	34,34,34,34	0
2	FE2	S	201	1/1	0.99	0.04	33,33,33,33	0
2	FE2	S	202	1/1	0.99	0.04	39,39,39,39	0
2	FE2	J	203	1/1	0.99	0.03	43,43,43,43	0
2	FE2	S	204	1/1	0.99	0.03	39,39,39,39	0
2	FE2	E	205	1/1	0.99	0.03	37,37,37,37	0
2	FE2	T	201	1/1	0.99	0.02	39,39,39,39	0
2	FE2	T	202	1/1	0.99	0.04	32,32,32,32	0
2	FE2	E	206	1/1	0.99	0.05	59,59,59,59	0
2	FE2	L	202	1/1	1.00	0.04	38,38,38,38	0
2	FE2	Q	201	1/1	1.00	0.03	33,33,33,33	0
2	FE2	T	204	1/1	1.00	0.04	38,38,38,38	0
2	FE2	G	201	1/1	1.00	0.05	35,35,35,35	0
2	FE2	A	205	1/1	1.00	0.04	39,39,39,39	0
2	FE2	N	203	1/1	1.00	0.04	32,32,32,32	0
2	FE2	U	202	1/1	1.00	0.03	39,39,39,39	0
4	K	A	210	1/1	1.00	0.06	26,26,26,26	0
4	K	B	210	1/1	1.00	0.05	35,35,35,35	0
2	FE2	L	205	1/1	1.00	0.04	40,40,40,40	0
4	K	E	210	1/1	1.00	0.06	38,38,38,38	0
4	K	G	210	1/1	1.00	0.04	31,31,31,31	0
2	FE2	R	202	1/1	1.00	0.03	33,33,33,33	0
2	FE2	E	202	1/1	1.00	0.04	40,40,40,40	0
2	FE2	E	203	1/1	1.00	0.05	44,44,44,44	0
2	FE2	O	201	1/1	1.00	0.03	36,36,36,36	0
2	FE2	B	202	1/1	1.00	0.05	39,39,39,39	0
2	FE2	A	202	1/1	1.00	0.05	36,36,36,36	0
2	FE2	M	202	1/1	1.00	0.05	41,41,41,41	0
2	FE2	P	201	1/1	1.00	0.04	34,34,34,34	0
2	FE2	M	203	1/1	1.00	0.03	32,32,32,32	0
2	FE2	D	203	1/1	1.00	0.04	33,33,33,33	0
2	FE2	M	205	1/1	1.00	0.05	36,36,36,36	0
2	FE2	H	201	1/1	1.00	0.05	42,42,42,42	0
2	FE2	X	201	1/1	1.00	0.03	33,33,33,33	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.

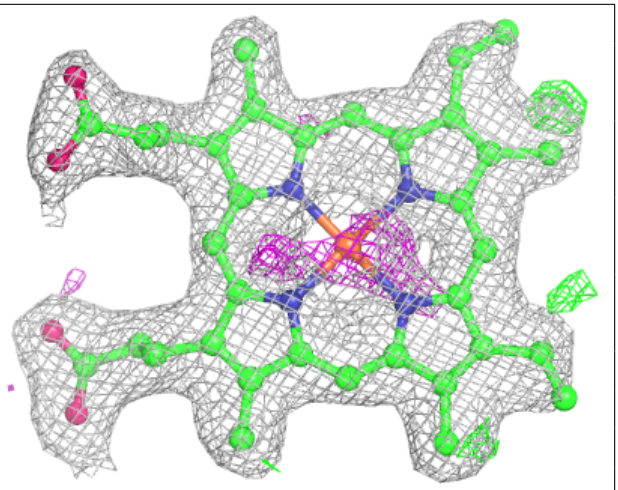
Electron density around HEM D 208:

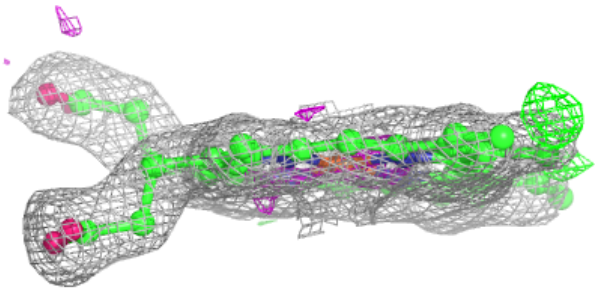
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

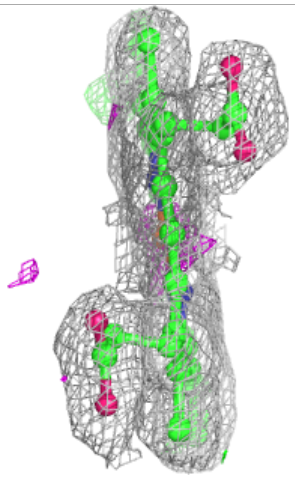


Electron density around HEM E 208:

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

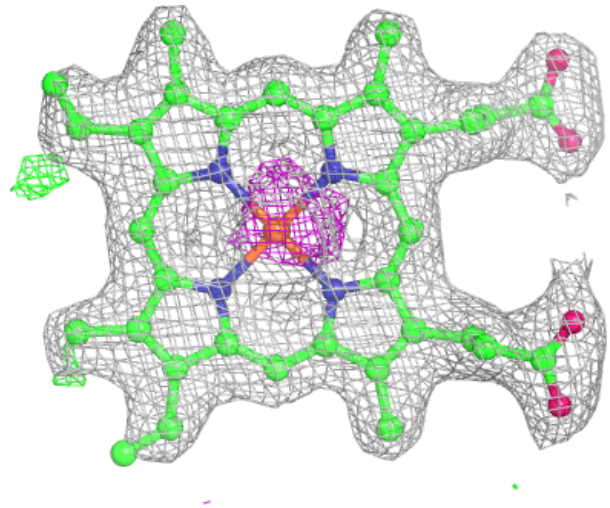


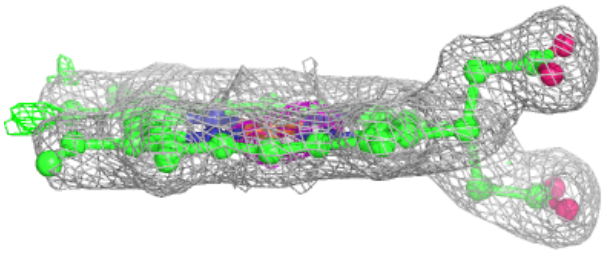


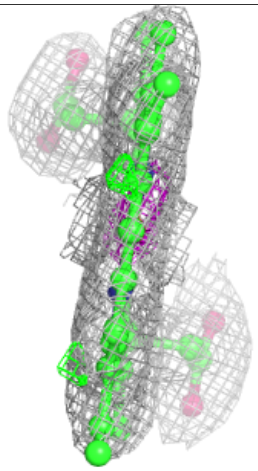


Electron density around HEM G 208:

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

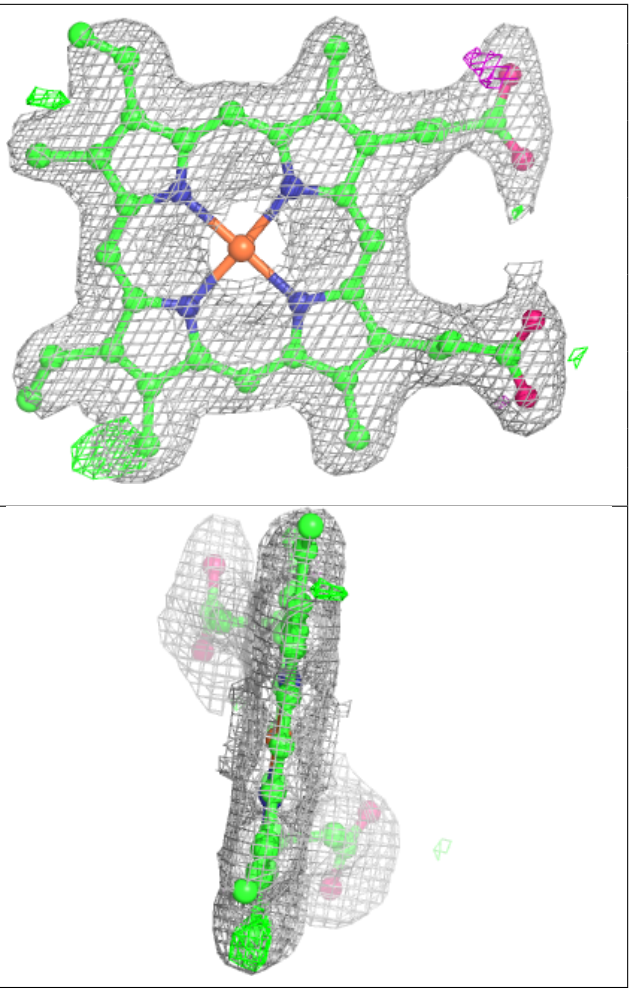






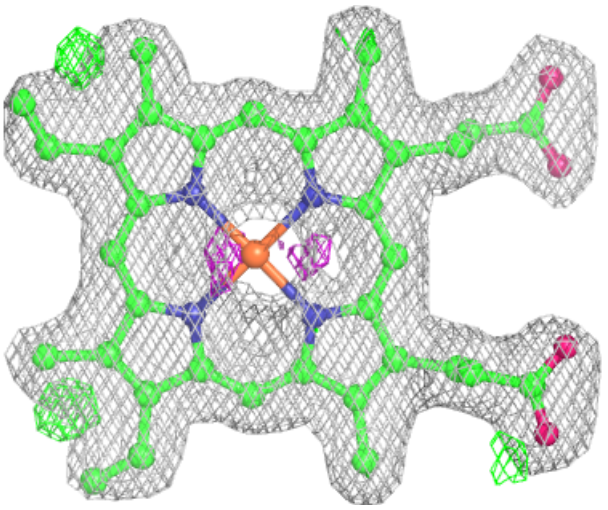
Electron density around HEM P 207:

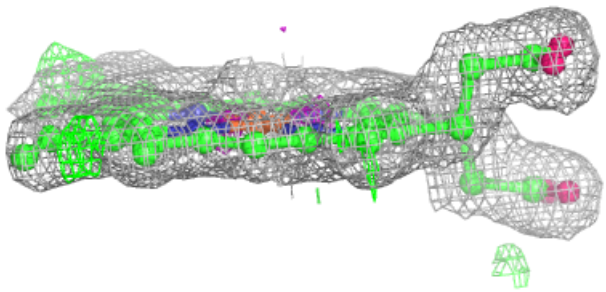
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

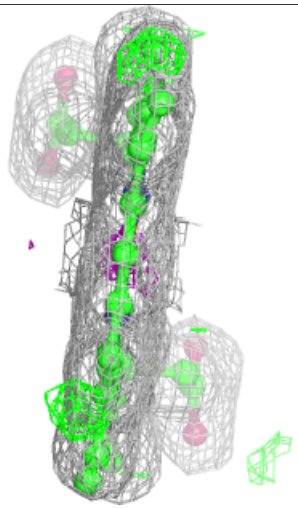


Electron density around HEM R 208:

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

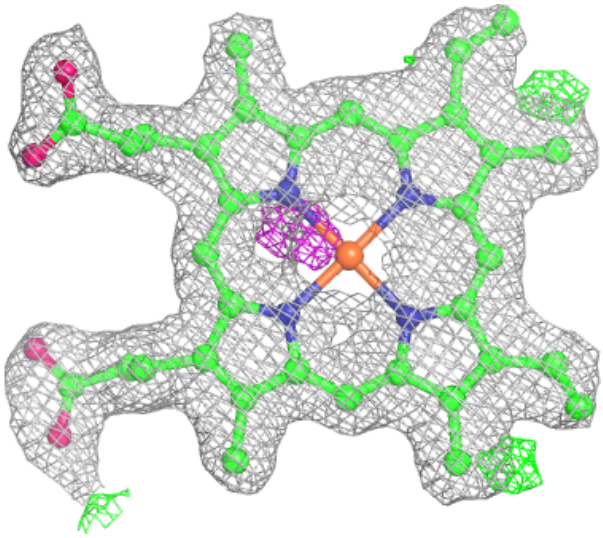


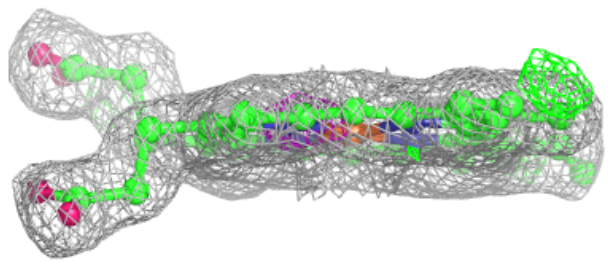


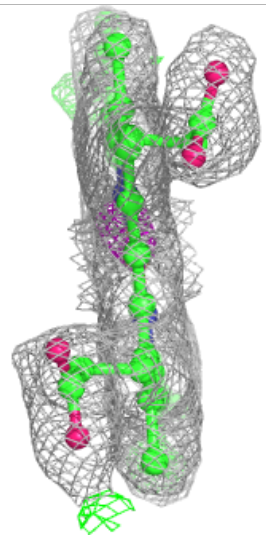


Electron density around HEM U 207:

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

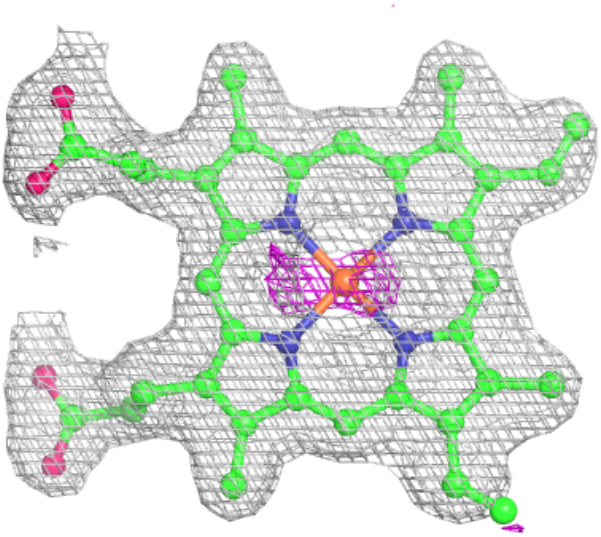


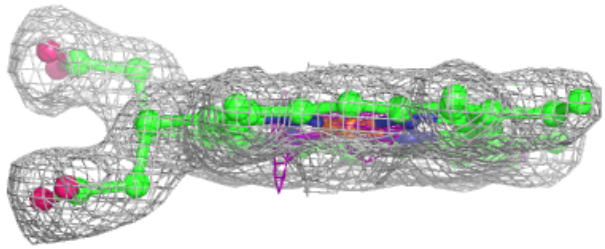


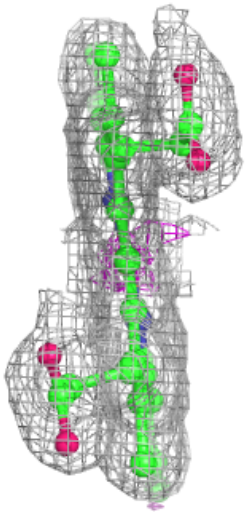


Electron density around HEM W 205:

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

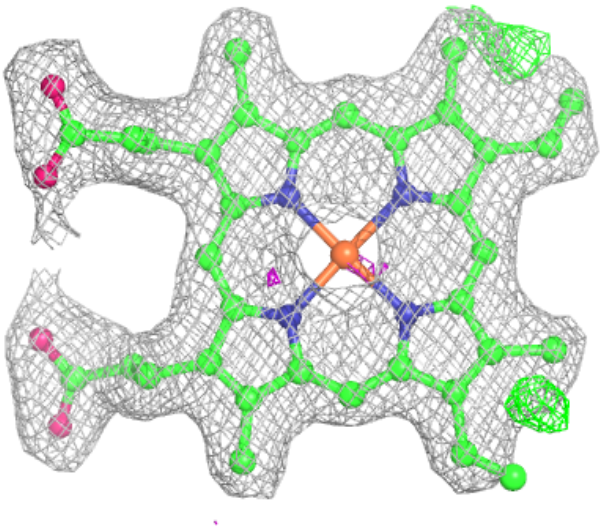


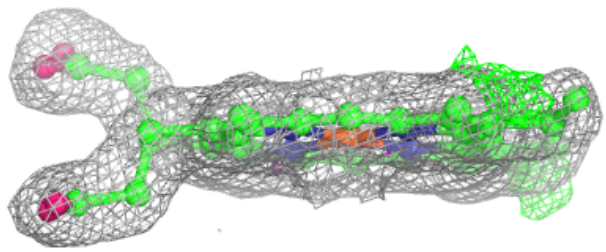


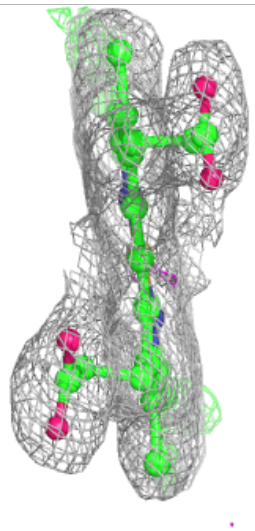


Electron density around HEM I 207:

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

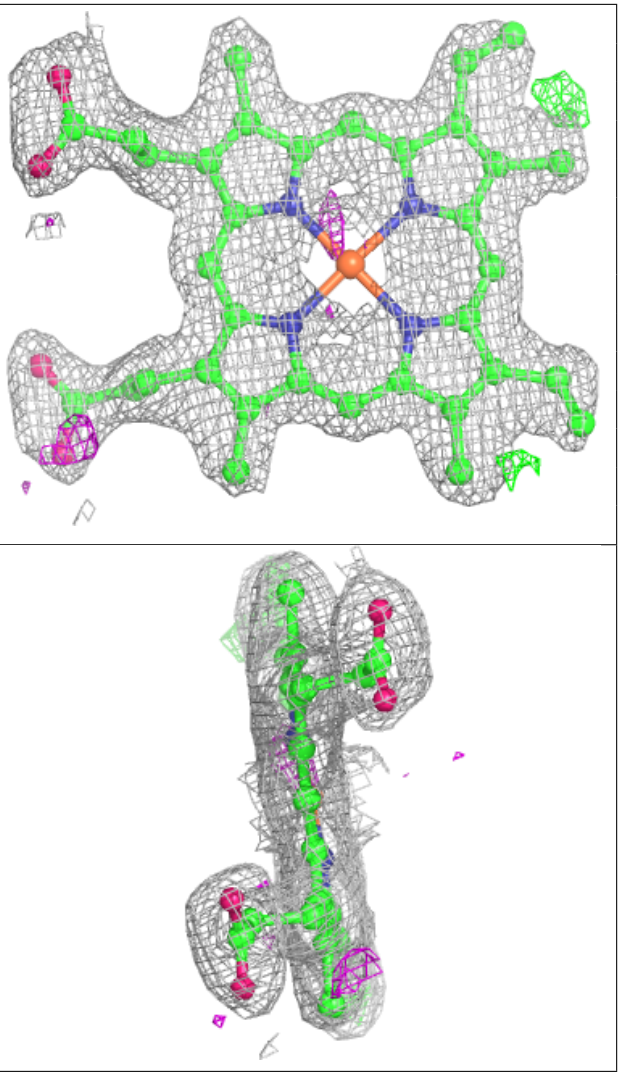


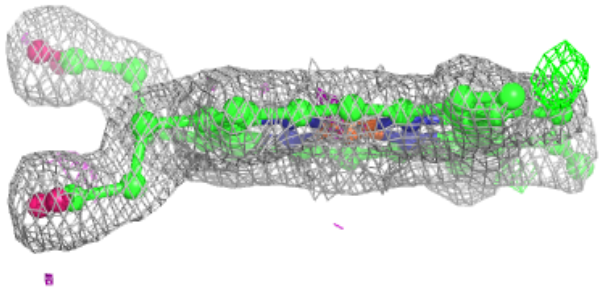




Electron density around HEM K 207:

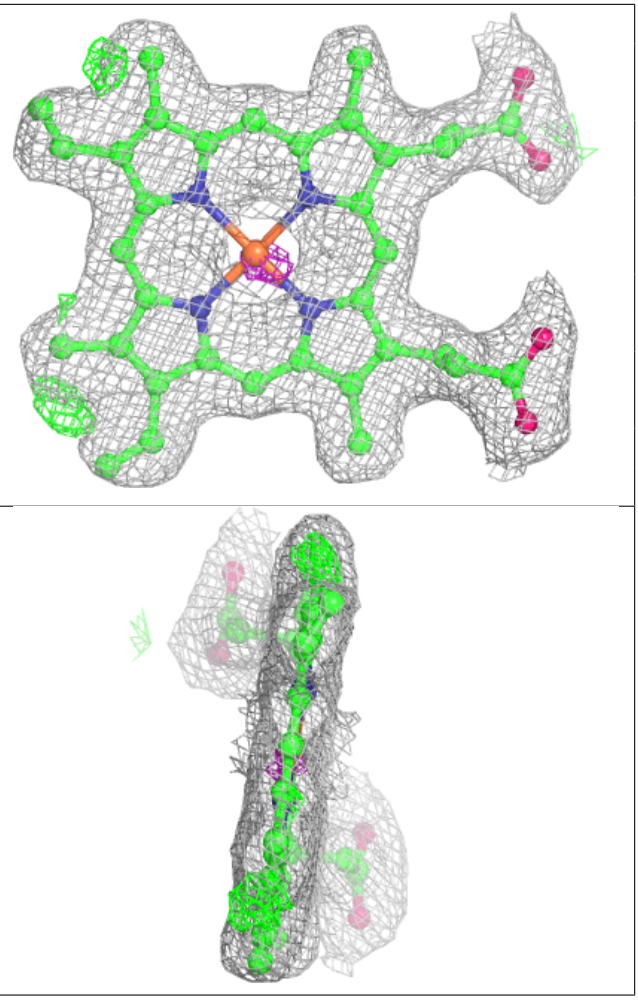
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





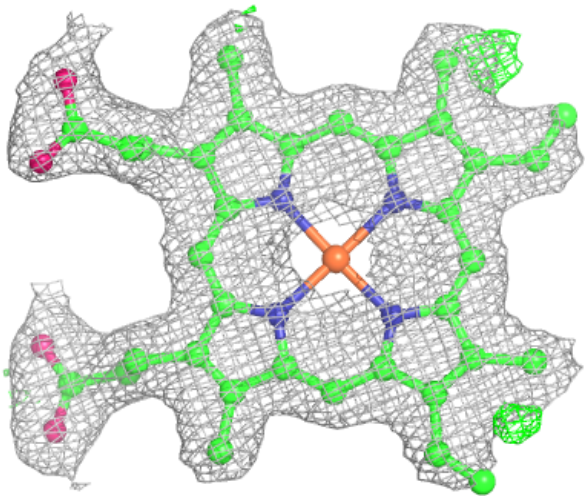
Electron density around HEM S 206:

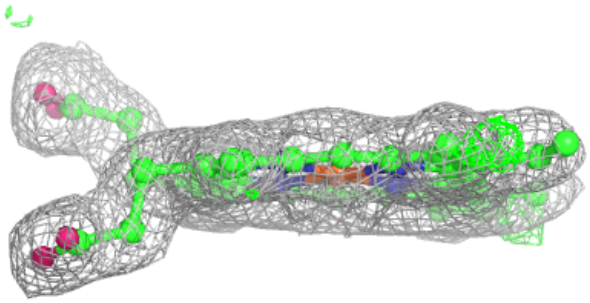
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

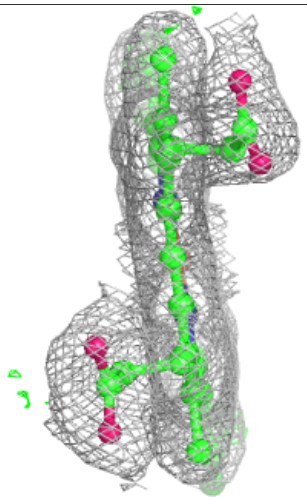


Electron density around HEM B 208:

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

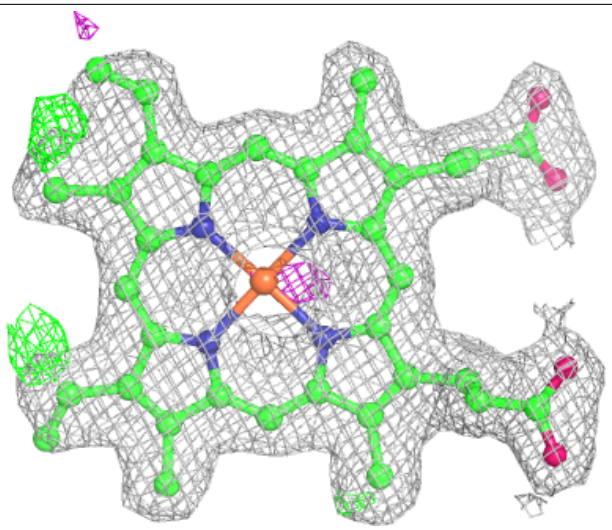


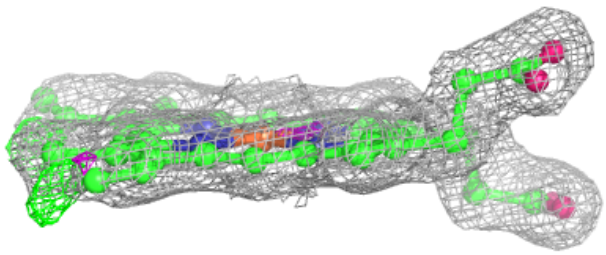


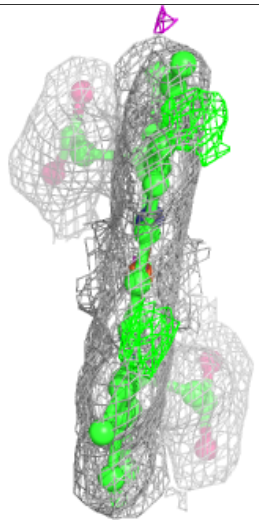


Electron density around HEM M 208:

$2mF_o$-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.