Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 11:28 AM EDT

PDB ID	:	3ISE
Title	:	Structure of mineralized Bfrb (double soak) from Pseudomonas aeruginosa to 2.8A Resolution
Authors	:	Lovell, S.; Weeratunga, S.K.; Battaile, K.P.; Rivera, M.
Deposited on	:	2009-08-25
Resolution	:	2.80 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 ⓘ 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 ⓘ) were used in the production of this report:

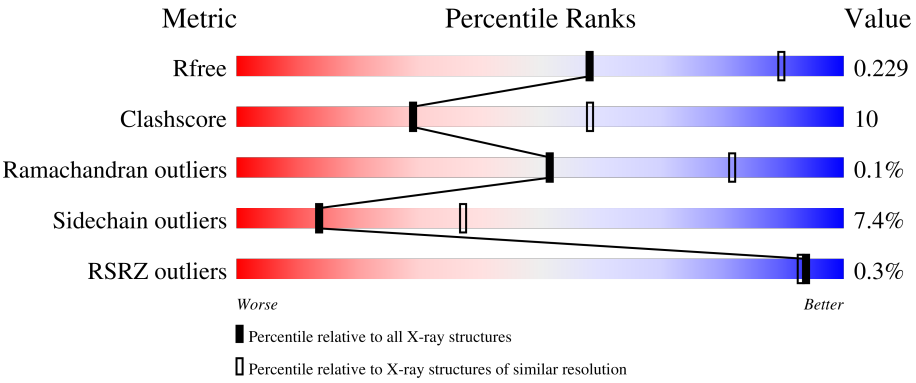
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.80 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.



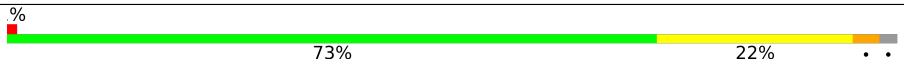
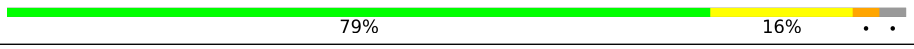
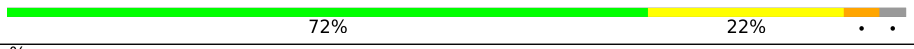
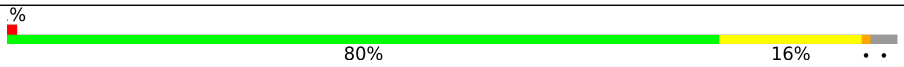
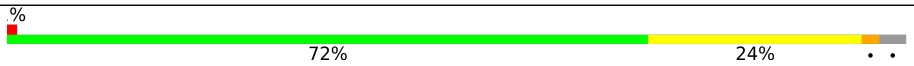
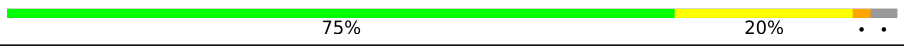
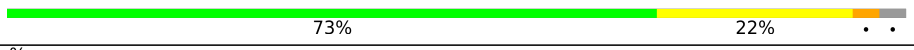
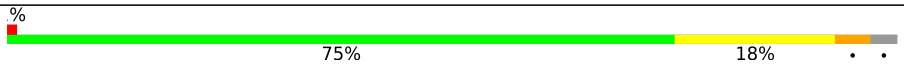
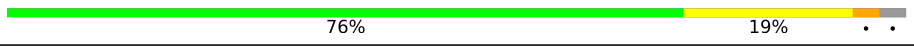
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	77% 18%
1	B	158	72% 22%
1	C	158	78% 18%
1	D	158	77% 20%
1	E	158	77% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	158	
1	G	158	
1	H	158	
1	I	158	
1	J	158	
1	K	158	
1	L	158	
1	M	158	
1	N	158	
1	O	158	
1	P	158	
1	Q	158	
1	R	158	
1	S	158	
1	T	158	
1	U	158	
1	V	158	
1	W	158	
1	X	158	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30960 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1267	801	218	242	6			
1	B	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	C	154	Total	C	N	O	S	0	0	0
			1265	799	218	242	6			
1	D	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	E	154	Total	C	N	O	S	0	0	0
			1265	799	218	242	6			
1	F	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	G	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	H	155	Total	C	N	O	S	0	0	0
			1275	806	220	243	6			
1	I	154	Total	C	N	O	S	0	0	0
			1265	799	218	242	6			
1	J	154	Total	C	N	O	S	0	0	0
			1265	799	218	242	6			
1	K	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	L	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	M	154	Total	C	N	O	S	0	0	0
			1265	799	218	242	6			
1	N	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	O	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	P	154	Total	C	N	O	S	0	0	0
			1267	801	218	242	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	R	155	Total	C	N	O	S	0	0	0
			1275	806	220	243	6			
1	S	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	T	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	U	154	Total	C	N	O	S	0	0	0
			1265	799	218	242	6			
1	V	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			
1	W	156	Total	C	N	O	S	0	0	0
			1282	810	221	244	7			
1	X	154	Total	C	N	O	S	0	0	0
			1266	800	218	242	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		
2	G	2	Total	Fe	0	0
			2	2		
2	I	1	Total	Fe	0	0
			1	1		
2	K	2	Total	Fe	0	0
			2	2		
2	L	1	Total	Fe	0	0
			1	1		
2	M	1	Total	Fe	0	0
			1	1		

Continued on next page...

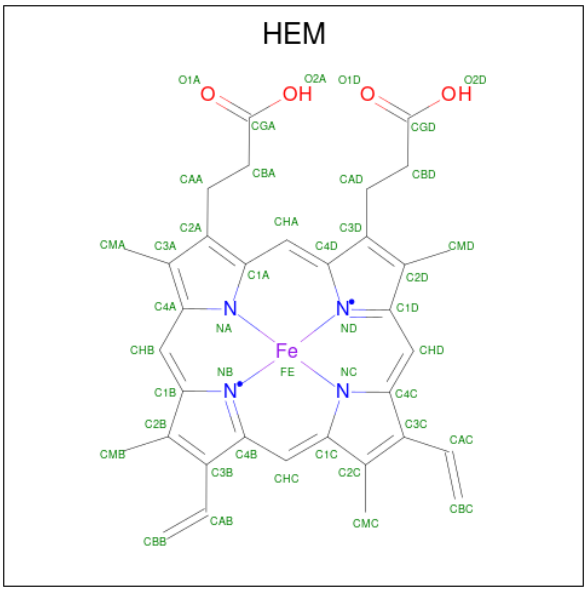
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	1	Total Fe 1 1	0	0
2	P	2	Total Fe 2 2	0	0
2	Q	1	Total Fe 1 1	0	0
2	T	1	Total Fe 1 1	0	0
2	U	1	Total Fe 1 1	0	0
2	V	2	Total Fe 2 2	0	0
2	W	1	Total Fe 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0
3	C	1	Total K 1 1	0	0
3	G	1	Total K 1 1	0	0
3	N	1	Total K 1 1	0	0
3	V	1	Total K 1 1	0	0

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



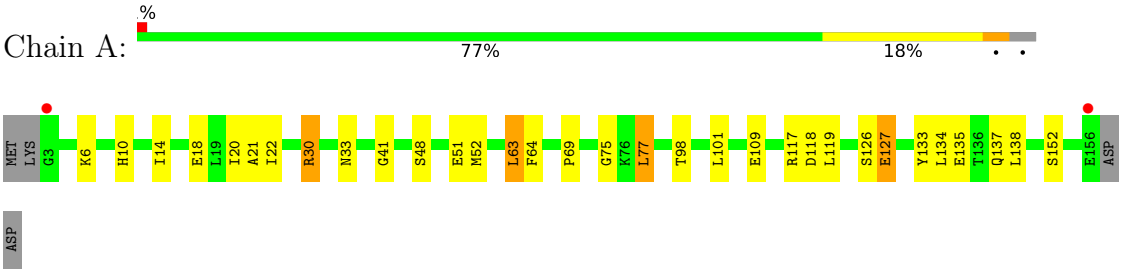
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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.

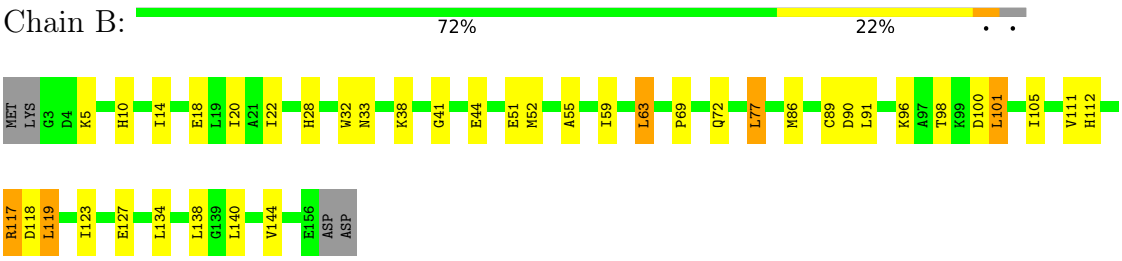
• Molecule 1: Bacterioferritin

Chain A:



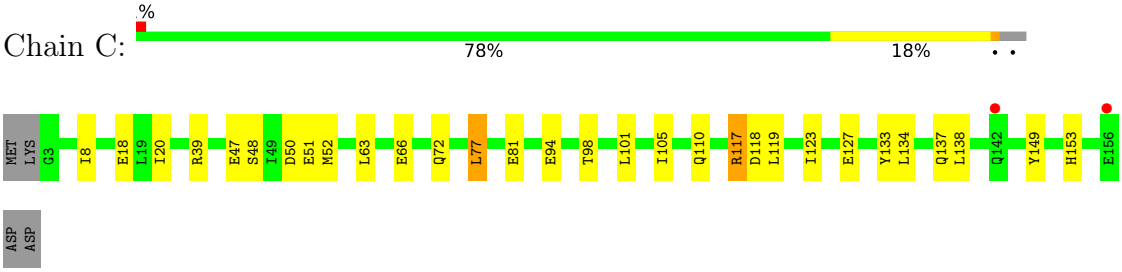
• Molecule 1: Bacterioferritin

Chain B:



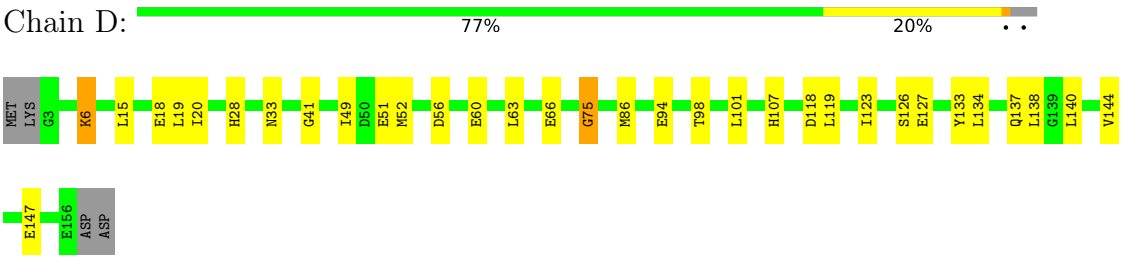
• Molecule 1: Bacterioferritin

Chain C:



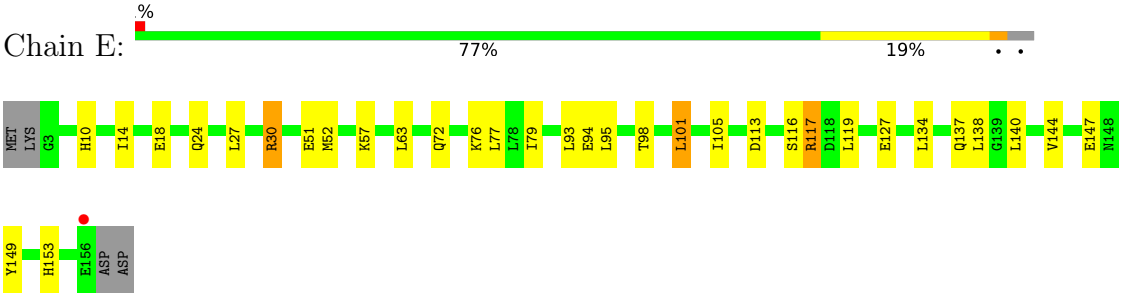
• Molecule 1: Bacterioferritin

Chain D:



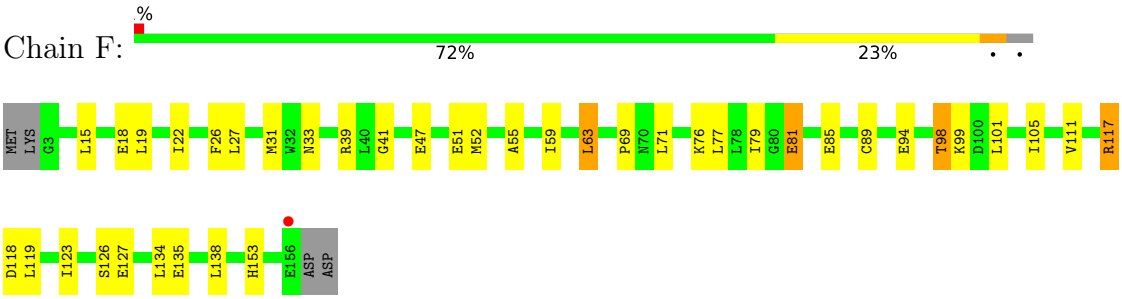
• Molecule 1: Bacterioferritin

Chain E:



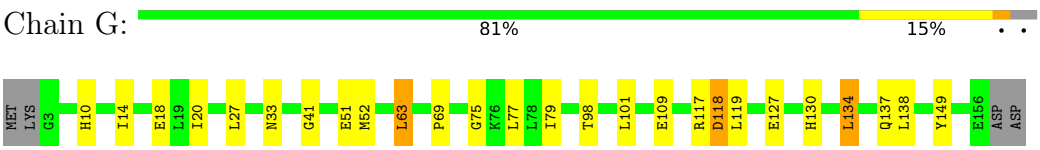
• Molecule 1: Bacterioferritin

Chain F:



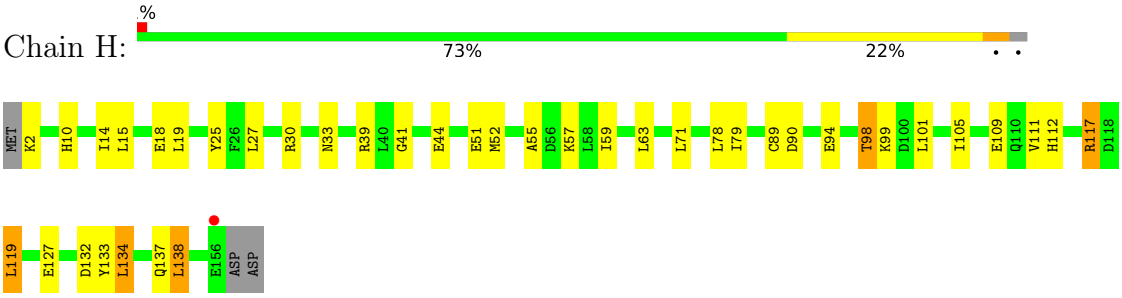
• Molecule 1: Bacterioferritin

Chain G:



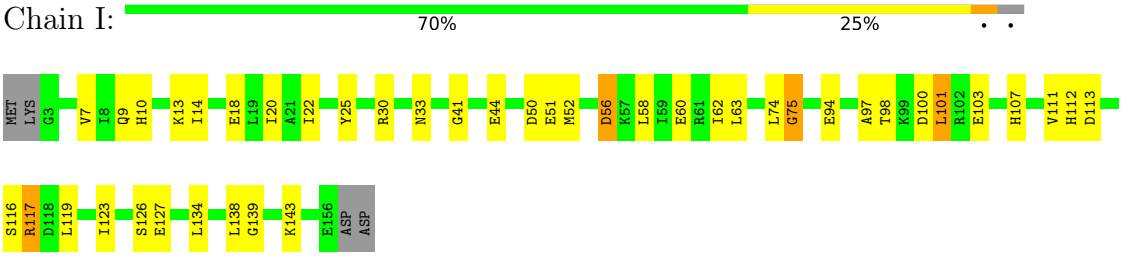
• Molecule 1: Bacterioferritin

Chain H:



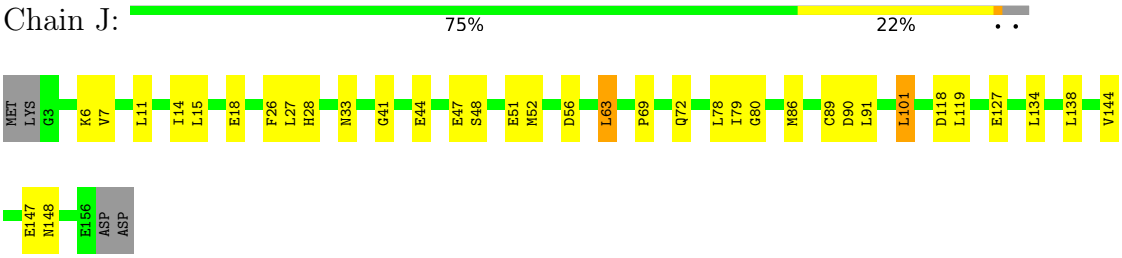
• Molecule 1: Bacterioferritin

Chain I:



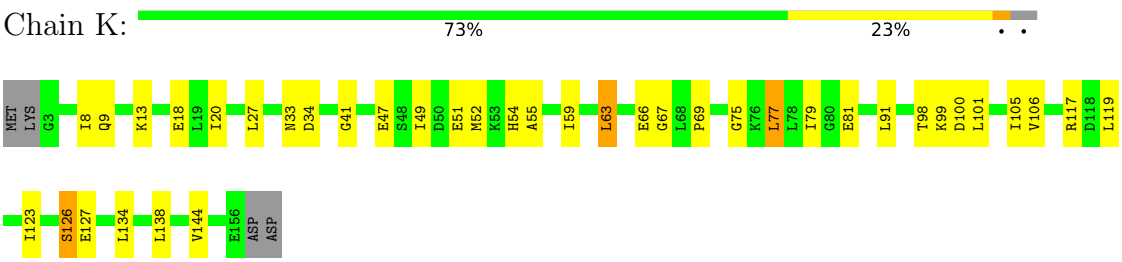
• Molecule 1: Bacterioferritin

Chain J:



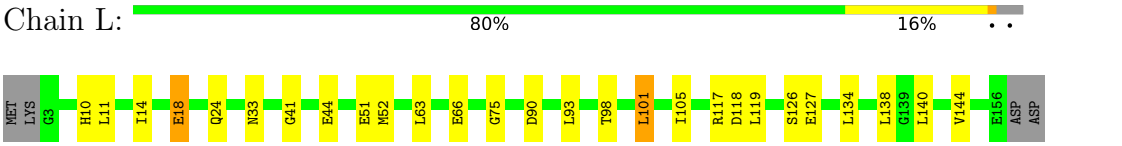
• Molecule 1: Bacterioferritin

Chain K:



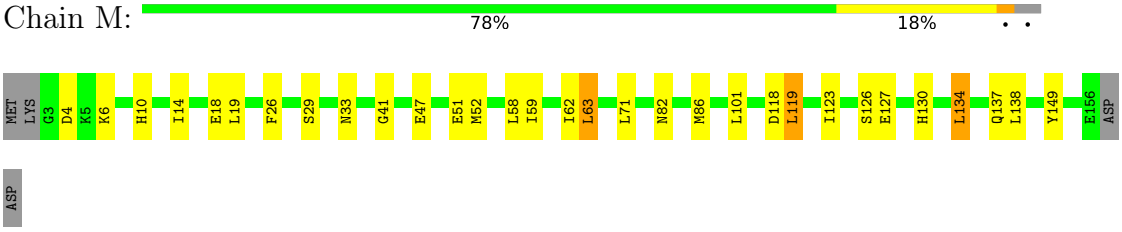
• Molecule 1: Bacterioferritin

Chain L:



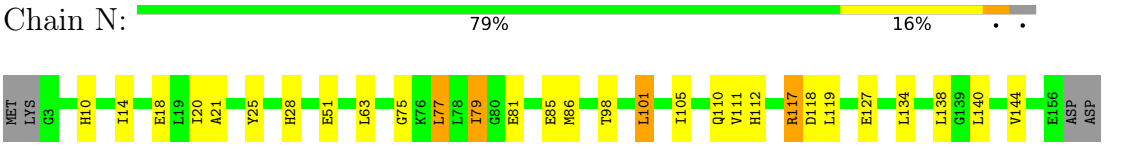
• Molecule 1: Bacterioferritin

Chain M:



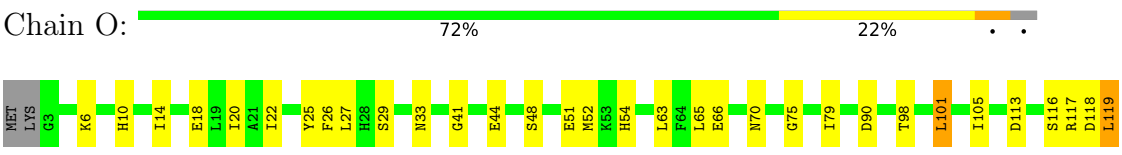
• Molecule 1: Bacterioferritin

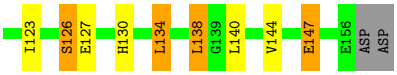
Chain N:



• Molecule 1: Bacterioferritin

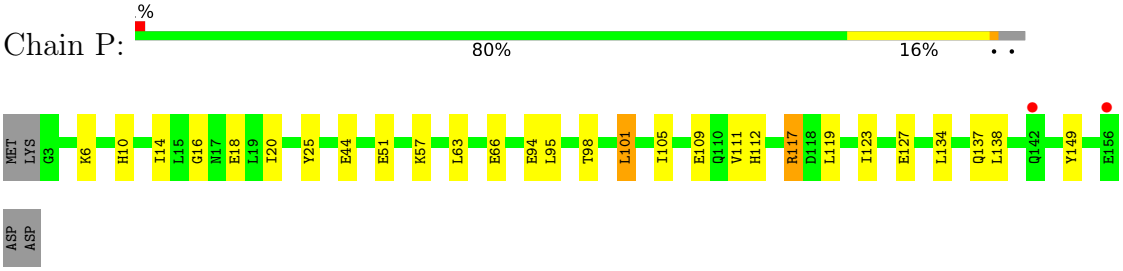
Chain O:





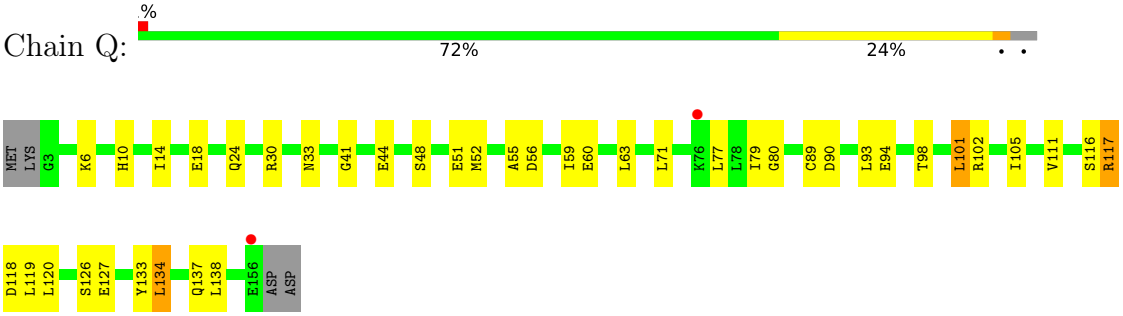
• Molecule 1: Bacterioferritin

Chain P:



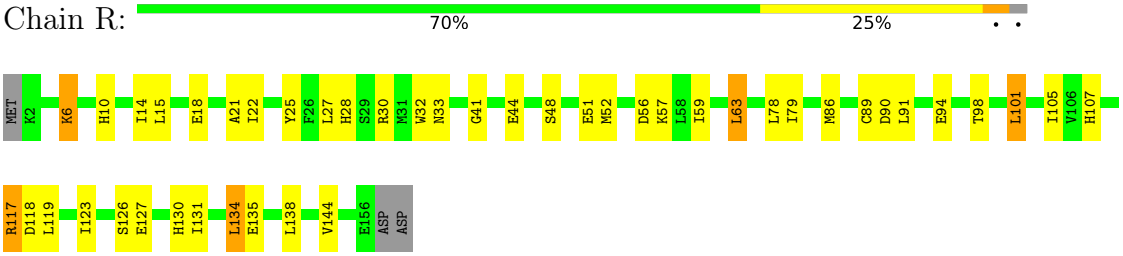
• Molecule 1: Bacterioferritin

Chain Q:



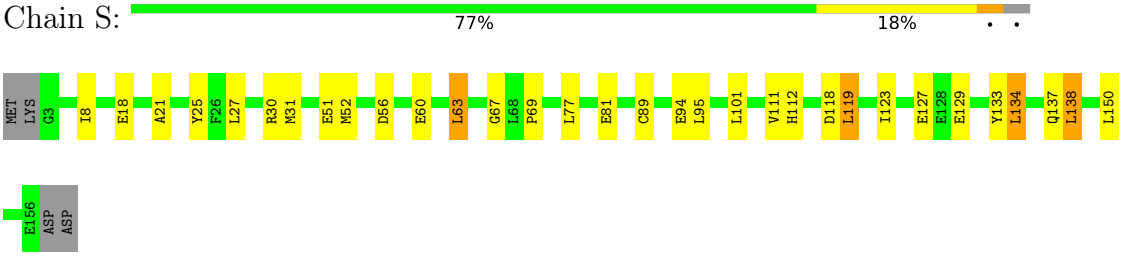
• Molecule 1: Bacterioferritin

Chain R:



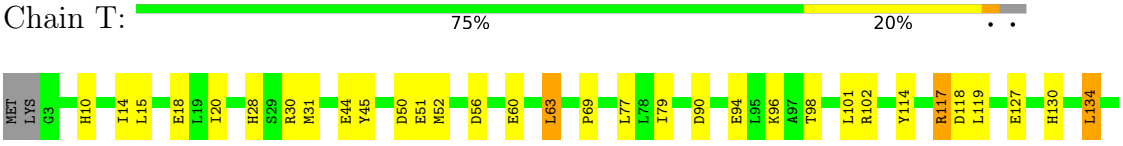
• Molecule 1: Bacterioferritin

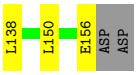
Chain S:



• Molecule 1: Bacterioferritin

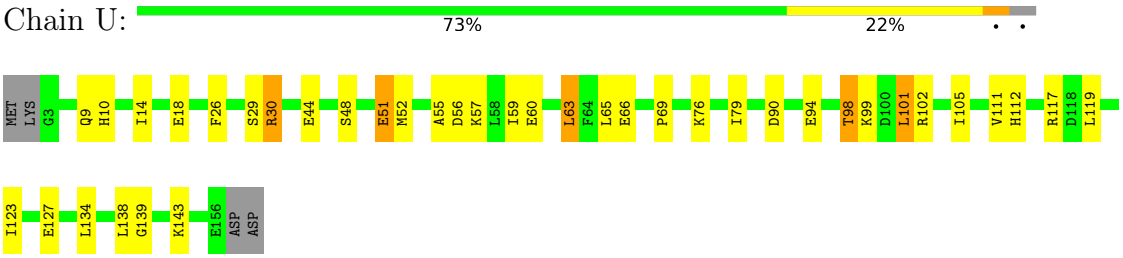
Chain T:





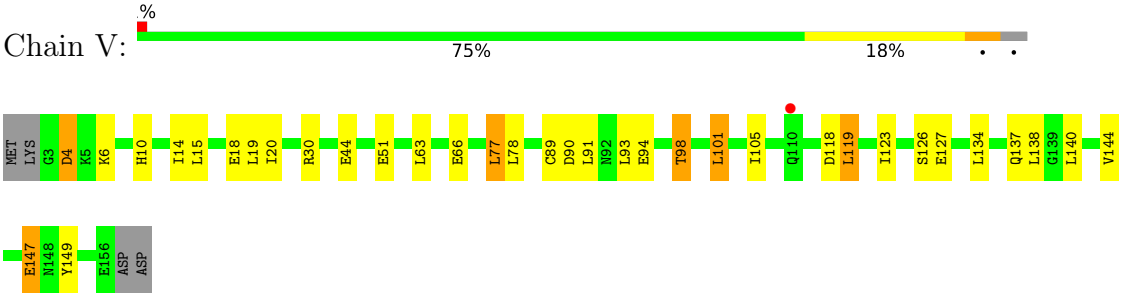
• Molecule 1: Bacterioferritin

Chain U:



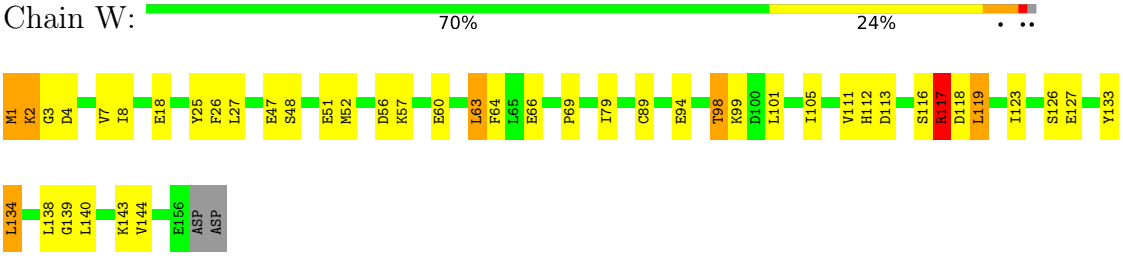
• Molecule 1: Bacterioferritin

Chain V:



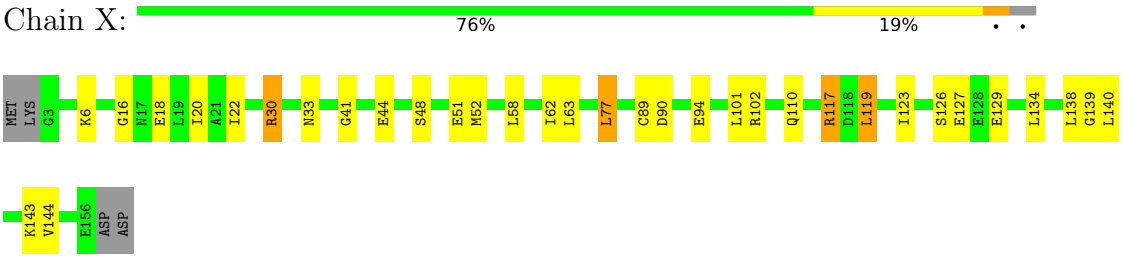
• Molecule 1: Bacterioferritin

Chain W:



• Molecule 1: Bacterioferritin

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.71Å 203.21Å 207.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 2.80 47.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.51-2.80) 99.9 (47.54-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.81Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0066	Depositor
R, R_{free}	0.195 , 0.237 0.194 , 0.229	Depositor DCC
R_{free} test set	6599 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 16.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	30960	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: K, HEM, FE

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	0.78	1/1288 (0.1%)	0.77	0/1734
1	B	0.82	1/1287 (0.1%)	0.78	1/1733 (0.1%)
1	C	0.80	0/1286	0.78	0/1732
1	D	0.82	1/1287 (0.1%)	0.79	0/1733
1	E	0.82	1/1286 (0.1%)	0.78	0/1732
1	F	0.82	1/1287 (0.1%)	0.77	0/1733
1	G	0.80	0/1287	0.82	1/1733 (0.1%)
1	H	0.84	0/1296	0.81	0/1744
1	I	0.82	2/1286 (0.2%)	0.81	1/1732 (0.1%)
1	J	0.78	0/1286	0.79	1/1732 (0.1%)
1	K	0.79	0/1287	0.79	0/1733
1	L	0.80	2/1287 (0.2%)	0.79	1/1733 (0.1%)
1	M	0.78	0/1286	0.77	0/1732
1	N	0.79	0/1287	0.78	1/1733 (0.1%)
1	O	0.77	0/1287	0.78	0/1733
1	P	0.78	0/1288	0.79	0/1734
1	Q	0.80	1/1287 (0.1%)	0.78	0/1733
1	R	0.83	0/1296	0.78	0/1744
1	S	0.80	2/1287 (0.2%)	0.78	0/1733
1	T	0.80	0/1287	0.82	0/1733
1	U	0.75	1/1286 (0.1%)	0.76	0/1732
1	V	0.78	0/1287	0.79	0/1733
1	W	0.76	1/1303 (0.1%)	0.78	1/1753 (0.1%)
1	X	0.75	1/1287 (0.1%)	0.76	1/1733 (0.1%)
All	All	0.79	15/30918 (0.0%)	0.79	8/41630 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	103	GLU	CG-CD	7.11	1.62	1.51
1	Q	89	CYS	CB-SG	-7.04	1.70	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	CYS	CB-SG	-7.03	1.70	1.82
1	E	147	GLU	CG-CD	6.71	1.62	1.51
1	S	89	CYS	CB-SG	-6.51	1.71	1.82
1	X	89	CYS	CB-SG	-6.50	1.71	1.82
1	F	89	CYS	CB-SG	-6.46	1.71	1.82
1	L	18	GLU	CG-CD	5.76	1.60	1.51
1	L	18	GLU	CB-CG	5.71	1.63	1.52
1	I	103	GLU	CB-CG	5.70	1.62	1.52
1	D	147	GLU	CG-CD	5.34	1.59	1.51
1	A	127	GLU	CB-CG	5.34	1.62	1.52
1	W	89	CYS	CB-SG	-5.28	1.73	1.81
1	U	51	GLU	CG-CD	5.15	1.59	1.51
1	S	129	GLU	CG-CD	5.15	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	117	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	L	18	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	I	56	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	101	LEU	CA-CB-CG	5.72	128.45	115.30
1	X	117	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	118	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	J	56	ASP	CB-CG-OD1	5.01	122.81	118.30
1	N	79	ILE	CB-CA-C	-5.00	101.59	111.60

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	1267	0	1250	17	0
1	B	1266	0	1248	32	0
1	C	1265	0	1246	18	0
1	D	1266	0	1248	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1265	0	1246	20	0
1	F	1266	0	1248	25	0
1	G	1266	0	1248	14	0
1	H	1275	0	1261	29	0
1	I	1265	0	1246	26	0
1	J	1265	0	1246	25	0
1	K	1266	0	1248	22	0
1	L	1266	0	1248	16	0
1	M	1265	0	1246	19	0
1	N	1266	0	1248	14	0
1	O	1266	0	1248	24	0
1	P	1267	0	1250	14	0
1	Q	1266	0	1248	23	0
1	R	1275	0	1261	30	0
1	S	1266	0	1248	20	0
1	T	1266	0	1248	26	0
1	U	1265	0	1246	36	0
1	V	1266	0	1248	25	0
1	W	1282	0	1271	30	0
1	X	1266	0	1248	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	2	0	0	0	0
2	I	1	0	0	0	0
2	K	2	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	P	2	0	0	0	0
2	Q	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	2	0	0	0	0
2	W	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1	0	0	0	0
3	V	1	0	0	0	0
4	B	43	0	30	10	0
4	D	43	0	30	6	0
4	E	43	0	30	6	0
4	H	43	0	30	9	0
4	J	43	0	30	10	0
4	L	43	0	30	8	0
4	M	43	0	30	9	0
4	P	43	0	30	8	0
4	R	43	0	30	6	0
4	S	43	0	30	7	0
4	U	43	0	30	1	0
4	W	43	0	30	3	0
All	All	30960	0	30353	586	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 10.

All (586) 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)
4:H:159:HEM:HBB2	4:H:159:HEM:CMB	1.79	1.11
4:E:159:HEM:HHD	4:E:159:HEM:HBC2	1.36	1.08
4:W:159:HEM:HBC2	4:W:159:HEM:HHD	1.34	1.07
4:M:159:HEM:HBC2	4:M:159:HEM:CMC	1.80	1.06
4:S:159:HEM:HBC2	4:S:159:HEM:CMC	1.81	1.06
4:D:159:HEM:HMB1	4:D:159:HEM:HBB2	1.38	1.06
4:H:159:HEM:HMC1	4:H:159:HEM:HBC2	1.35	1.06
4:S:159:HEM:HBC2	4:S:159:HEM:HMC1	1.14	1.06
4:J:159:HEM:HHD	4:J:159:HEM:HBC2	1.34	1.04
4:D:159:HEM:HBC2	4:D:159:HEM:HHD	1.38	1.02
1:G:18:GLU:OE1	1:G:51:GLU:OE1	1.79	1.00
4:H:159:HEM:HMB2	4:H:159:HEM:CBB	1.93	0.98
4:M:159:HEM:HBC2	4:M:159:HEM:HMC1	1.02	0.98
1:H:18:GLU:OE1	1:H:51:GLU:OE1	1.81	0.98
4:H:159:HEM:HBC2	4:H:159:HEM:CMC	1.90	0.97
4:H:159:HEM:HBB2	4:H:159:HEM:HMB2	0.98	0.96
4:M:159:HEM:HMB1	4:M:159:HEM:HBB2	1.49	0.94
1:P:18:GLU:OE1	1:P:51:GLU:OE1	1.85	0.94
4:M:159:HEM:HBB2	4:M:159:HEM:CMB	1.98	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:159:HEM:HMC2	4:R:159:HEM:HBC2	1.49	0.92
4:M:159:HEM:HMC1	4:M:159:HEM:CBC	1.97	0.92
1:V:137:GLN:NE2	1:V:149:TYR:OH	2.03	0.89
4:P:159:HEM:CMB	4:P:159:HEM:HBB2	2.01	0.88
4:J:159:HEM:HHC	4:J:159:HEM:HBB2	1.56	0.88
1:J:44:GLU:OE2	1:J:90:ASP:OD2	1.93	0.87
4:S:159:HEM:HMC1	4:S:159:HEM:CBC	2.04	0.86
1:C:18:GLU:OE1	1:C:51:GLU:OE1	1.96	0.83
4:R:159:HEM:HBC2	4:R:159:HEM:CMC	2.09	0.83
1:R:18:GLU:OE1	1:R:51:GLU:OE1	1.97	0.82
1:U:44:GLU:OE2	1:U:90:ASP:OD2	1.98	0.81
1:Q:18:GLU:OE1	1:Q:51:GLU:OE1	1.98	0.80
4:D:159:HEM:HBB2	4:D:159:HEM:CMB	2.13	0.79
1:J:18:GLU:OE1	1:J:51:GLU:OE1	2.01	0.78
4:P:159:HEM:HBC2	4:P:159:HEM:HHD	1.65	0.77
4:H:159:HEM:HMC1	4:H:159:HEM:CBC	2.14	0.76
1:T:56:ASP:O	1:T:60:GLU:HG3	1.87	0.75
1:W:18:GLU:OE1	1:W:51:GLU:OE1	2.05	0.74
1:V:20:ILE:HG23	1:V:77:LEU:HD12	1.70	0.73
4:P:159:HEM:CMB	4:P:159:HEM:CBB	2.64	0.73
1:I:56:ASP:O	1:I:60:GLU:HG3	1.90	0.72
1:L:52:MET:HB3	4:L:159:HEM:CHB	2.19	0.72
1:V:14:ILE:HD12	1:V:101:LEU:HD13	1.71	0.72
1:E:105:ILE:HG23	1:E:117:ARG:HG3	1.71	0.72
1:K:105:ILE:HG23	1:K:117:ARG:HG3	1.71	0.72
1:D:51:GLU:OE1	1:D:127:GLU:OE2	2.07	0.71
1:G:20:ILE:HD11	1:G:75:GLY:HA3	1.72	0.71
1:O:18:GLU:OE1	1:O:51:GLU:OE1	2.09	0.71
1:U:18:GLU:OE1	1:U:51:GLU:OE1	2.07	0.71
1:W:25:TYR:OH	1:W:94:GLU:OE2	2.09	0.71
1:G:137:GLN:NE2	1:G:149:TYR:OH	2.15	0.71
1:S:18:GLU:OE1	1:S:51:GLU:OE1	2.09	0.70
1:K:55:ALA:O	1:K:59:ILE:HG13	1.92	0.70
4:R:159:HEM:HMC2	4:R:159:HEM:CBC	2.22	0.70
1:B:111:VAL:O	1:B:112:HIS:HB2	1.91	0.70
4:M:159:HEM:HMB1	4:M:159:HEM:CBB	2.22	0.69
1:N:18:GLU:OE1	1:N:51:GLU:OE1	2.10	0.69
1:B:10:HIS:O	1:B:14:ILE:HG12	1.92	0.68
4:P:159:HEM:HBB2	4:P:159:HEM:HMB3	1.76	0.68
4:P:159:HEM:CBB	4:P:159:HEM:HMB1	2.22	0.68
1:U:48:SER:O	1:U:52:MET:HG3	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:159:HEM:HHC	4:J:159:HEM:CBB	2.24	0.68
1:E:140:LEU:O	1:E:144:VAL:HG22	1.93	0.68
1:T:18:GLU:OE1	1:T:51:GLU:OE1	2.12	0.68
1:U:29:SER:OG	1:U:30:ARG:NH1	2.27	0.67
1:X:119:LEU:C	1:X:119:LEU:CD2	2.62	0.67
1:N:111:VAL:O	1:N:112:HIS:HB2	1.95	0.67
1:V:140:LEU:O	1:V:144:VAL:HG22	1.95	0.67
4:B:159:HEM:CMB	4:B:159:HEM:HBB2	2.24	0.66
1:I:18:GLU:OE2	1:I:127:GLU:OE2	2.13	0.66
1:M:18:GLU:OE1	1:M:51:GLU:OE1	2.14	0.66
1:W:2:LYS:NZ	1:W:64:PHE:O	2.28	0.65
1:X:51:GLU:OE1	1:X:127:GLU:OE2	2.14	0.65
1:X:119:LEU:HD23	1:X:119:LEU:O	1.97	0.65
4:B:159:HEM:HBC2	4:B:159:HEM:CMC	2.26	0.65
1:K:91:LEU:HD12	1:K:91:LEU:O	1.97	0.65
1:P:94:GLU:OE1	1:P:127:GLU:HB3	1.97	0.65
1:T:18:GLU:OE2	1:T:127:GLU:OE2	2.15	0.65
4:E:159:HEM:HHD	4:E:159:HEM:CBC	2.20	0.64
1:E:18:GLU:OE1	1:E:51:GLU:OE1	2.16	0.64
1:L:52:MET:HB3	4:L:159:HEM:C1B	2.32	0.64
1:N:51:GLU:OE1	1:N:127:GLU:OE2	2.15	0.64
1:O:52:MET:HB3	4:P:159:HEM:CHD	2.27	0.64
1:K:27:LEU:HD23	1:K:79:ILE:HD12	1.80	0.64
1:K:18:GLU:OE1	1:K:51:GLU:OE1	2.16	0.64
1:Q:33:ASN:ND2	1:Q:41:GLY:HA3	2.13	0.63
4:J:159:HEM:HBC2	4:J:159:HEM:CHD	2.08	0.63
1:W:94:GLU:O	1:W:98:THR:HB	1.99	0.63
1:X:119:LEU:C	1:X:119:LEU:HD23	2.18	0.63
1:L:44:GLU:OE2	1:L:90:ASP:OD2	2.16	0.63
1:O:65:LEU:O	1:O:66:GLU:HB2	1.98	0.63
1:O:51:GLU:OE1	1:O:127:GLU:OE2	2.17	0.62
1:V:123:ILE:O	1:V:127:GLU:HG2	1.99	0.62
1:W:140:LEU:O	1:W:144:VAL:HG22	1.99	0.62
4:J:159:HEM:HBB2	4:J:159:HEM:CHC	2.27	0.62
1:F:33:ASN:ND2	1:F:41:GLY:HA3	2.14	0.61
4:L:159:HEM:CMB	4:L:159:HEM:HBB2	2.30	0.61
1:Q:18:GLU:OE2	1:Q:127:GLU:OE2	2.19	0.61
1:I:123:ILE:O	1:I:127:GLU:HG2	2.00	0.61
1:M:10:HIS:O	1:M:14:ILE:HG12	2.01	0.61
1:Q:116:SER:O	1:Q:120:LEU:HG	2.01	0.61
1:J:27:LEU:HD23	1:J:79:ILE:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:ILE:HG23	1:L:117:ARG:HG3	1.81	0.60
1:N:105:ILE:HG23	1:N:117:ARG:HG3	1.83	0.60
1:U:56:ASP:O	1:U:60:GLU:HG3	2.01	0.60
1:F:63:LEU:HD13	1:F:69:PRO:CG	2.31	0.60
4:S:159:HEM:CHB	1:T:52:MET:HB3	2.31	0.60
1:P:137:GLN:NE2	1:P:149:TYR:OH	2.24	0.60
1:B:18:GLU:OE2	1:B:127:GLU:OE2	2.19	0.60
1:F:27:LEU:HD23	1:F:79:ILE:HD12	1.84	0.60
1:Q:14:ILE:HD12	1:Q:101:LEU:HD13	1.83	0.60
1:E:137:GLN:NE2	1:E:149:TYR:OH	2.33	0.59
1:U:51:GLU:OE1	1:U:127:GLU:OE2	2.19	0.59
4:L:159:HEM:CMB	4:L:159:HEM:CBB	2.80	0.59
1:R:51:GLU:OE1	1:R:127:GLU:OE2	2.20	0.59
1:S:51:GLU:OE1	1:S:127:GLU:OE2	2.21	0.59
1:F:55:ALA:O	1:F:59:ILE:HG13	2.03	0.59
1:B:119:LEU:O	1:B:123:ILE:HG13	2.03	0.59
1:U:14:ILE:HD12	1:U:101:LEU:HD13	1.84	0.59
1:F:51:GLU:OE1	1:F:127:GLU:OE2	2.21	0.58
1:X:16:GLY:O	1:X:20:ILE:HG13	2.02	0.58
1:R:18:GLU:O	1:R:22:ILE:HG13	2.03	0.58
1:W:27:LEU:HD23	1:W:79:ILE:HD12	1.85	0.58
1:P:10:HIS:O	1:P:14:ILE:HG12	2.04	0.58
4:H:159:HEM:CMB	4:H:159:HEM:CBB	2.61	0.58
1:H:105:ILE:HG23	1:H:117:ARG:HG3	1.86	0.58
1:L:33:ASN:ND2	1:L:41:GLY:HA3	2.19	0.58
1:K:8:ILE:HD13	1:K:67:GLY:HA3	1.86	0.57
1:N:110:GLN:O	1:N:110:GLN:HG3	2.02	0.57
1:W:123:ILE:O	1:W:127:GLU:HG2	2.04	0.57
1:B:20:ILE:HG23	1:B:77:LEU:HD12	1.85	0.57
1:R:52:MET:HB3	4:R:159:HEM:C1B	2.39	0.57
1:T:51:GLU:OE1	1:T:127:GLU:OE2	2.22	0.57
1:D:18:GLU:OE1	1:D:51:GLU:OE1	2.23	0.57
1:Q:94:GLU:OE1	1:Q:127:GLU:HB3	2.05	0.57
1:R:27:LEU:HD23	1:R:79:ILE:HD12	1.85	0.57
1:R:44:GLU:OE2	1:R:90:ASP:OD2	2.22	0.57
1:U:102:ARG:HG2	1:U:102:ARG:HH11	1.69	0.57
1:T:15:LEU:HD12	1:T:15:LEU:O	2.04	0.57
1:L:140:LEU:O	1:L:144:VAL:HG22	2.05	0.56
1:U:10:HIS:O	1:U:14:ILE:HG12	2.05	0.56
1:W:139:GLY:O	1:W:143:LYS:HG3	2.05	0.56
4:M:159:HEM:CMC	4:M:159:HEM:CBC	2.63	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:18:GLU:OE1	1:U:51:GLU:CD	2.44	0.56
1:X:102:ARG:HG2	1:X:102:ARG:HH11	1.70	0.56
1:F:33:ASN:HD21	1:F:41:GLY:HA3	1.71	0.56
1:I:113:ASP:CG	1:I:116:SER:HB2	2.25	0.56
1:J:15:LEU:HD12	1:J:15:LEU:O	2.06	0.56
1:J:63:LEU:HD13	1:J:69:PRO:HD3	1.87	0.56
1:D:20:ILE:HD11	1:D:75:GLY:HA3	1.86	0.56
1:R:52:MET:HB3	4:R:159:HEM:CHB	2.34	0.56
1:T:98:THR:HG23	1:T:102:ARG:HH21	1.70	0.56
1:U:18:GLU:OE2	1:U:51:GLU:OE1	2.24	0.56
1:V:94:GLU:OE1	1:V:127:GLU:OE1	2.23	0.56
1:J:26:PHE:CE1	4:J:159:HEM:HBC1	2.41	0.56
1:X:123:ILE:O	1:X:127:GLU:HG2	2.06	0.56
1:A:18:GLU:OE1	1:A:51:GLU:CD	2.43	0.56
1:D:18:GLU:OE2	1:D:127:GLU:OE2	2.24	0.56
1:E:10:HIS:O	1:E:14:ILE:HG12	2.06	0.56
1:K:20:ILE:HD11	1:K:75:GLY:HA3	1.88	0.56
1:P:14:ILE:HD12	1:P:101:LEU:HD13	1.87	0.56
1:R:131:ILE:O	1:R:135:GLU:HG3	2.05	0.56
1:A:20:ILE:HG23	1:A:77:LEU:HD12	1.87	0.56
1:B:96:LYS:NZ	1:B:100:ASP:OD2	2.38	0.56
1:J:27:LEU:HD23	1:J:79:ILE:CD1	2.35	0.56
4:B:159:HEM:HBC2	4:B:159:HEM:HMC2	1.86	0.55
1:E:94:GLU:OE1	1:E:127:GLU:HB3	2.06	0.55
1:M:47:GLU:HA	1:M:47:GLU:OE1	2.06	0.55
1:R:6:LYS:HB3	1:R:107:HIS:NE2	2.21	0.55
1:R:10:HIS:O	1:R:14:ILE:HG12	2.05	0.55
1:E:52:MET:HB3	4:E:159:HEM:CHD	2.36	0.55
4:P:159:HEM:HBC2	4:P:159:HEM:CHD	2.32	0.55
1:T:20:ILE:HG23	1:T:77:LEU:HD12	1.88	0.55
1:G:51:GLU:OE1	1:G:127:GLU:OE2	2.24	0.55
1:S:119:LEU:O	1:S:119:LEU:HD22	2.06	0.55
1:I:101:LEU:HD21	1:I:123:ILE:HG22	1.87	0.55
1:V:147:GLU:CD	1:V:147:GLU:H	2.07	0.55
1:Q:137:GLN:NE2	1:Q:137:GLN:HA	2.21	0.55
1:T:156:GLU:OE2	1:T:156:GLU:HA	2.06	0.55
1:R:33:ASN:ND2	1:R:41:GLY:HA3	2.20	0.55
1:S:94:GLU:OE1	1:S:127:GLU:HB3	2.05	0.55
1:I:52:MET:HB3	4:J:159:HEM:CHD	2.37	0.55
1:N:28:HIS:CD2	1:N:86:MET:HG2	2.41	0.55
1:V:18:GLU:OE1	1:V:51:GLU:OE1	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:GLU:OE2	1:F:127:GLU:OE2	2.24	0.55
1:J:33:ASN:ND2	1:J:41:GLY:HA3	2.23	0.54
1:M:82:ASN:O	1:M:86:MET:HG3	2.07	0.54
1:Q:105:ILE:HG23	1:Q:117:ARG:HG3	1.89	0.54
1:R:28:HIS:CD2	1:R:86:MET:HG2	2.43	0.54
1:B:28:HIS:CD2	1:B:86:MET:HG2	2.43	0.54
1:A:18:GLU:OE1	1:A:51:GLU:OE1	2.25	0.54
1:K:49:ILE:HA	1:K:52:MET:HG3	1.88	0.54
1:F:94:GLU:OE1	1:F:127:GLU:HB3	2.08	0.54
1:V:18:GLU:OE2	1:V:127:GLU:OE2	2.26	0.54
1:I:33:ASN:ND2	1:I:41:GLY:HA3	2.23	0.54
1:X:18:GLU:OE1	1:X:51:GLU:OE1	2.26	0.54
1:N:20:ILE:HD11	1:N:75:GLY:HA3	1.90	0.53
1:P:109:GLU:HB2	1:P:117:ARG:HE	1.73	0.53
1:J:14:ILE:HD12	1:J:101:LEU:HD13	1.89	0.53
1:I:58:LEU:O	1:I:62:ILE:HG13	2.09	0.53
1:U:63:LEU:HD13	1:U:69:PRO:CG	2.37	0.53
1:F:123:ILE:O	1:F:127:GLU:HG2	2.08	0.53
1:V:44:GLU:OE2	1:V:90:ASP:OD2	2.26	0.53
1:V:119:LEU:HD22	1:V:123:ILE:CD1	2.38	0.53
1:O:123:ILE:O	1:O:127:GLU:HG2	2.09	0.53
1:U:63:LEU:CD1	1:U:69:PRO:HD3	2.38	0.53
1:H:33:ASN:ND2	1:H:41:GLY:HA3	2.23	0.53
1:U:18:GLU:OE2	1:U:127:GLU:OE2	2.27	0.53
1:V:10:HIS:O	1:V:14:ILE:HG12	2.08	0.53
1:S:18:GLU:OE1	1:S:51:GLU:CD	2.48	0.53
1:Q:24:GLN:OE1	1:Q:93:LEU:HD22	2.09	0.53
1:J:44:GLU:OE1	1:J:44:GLU:HA	2.09	0.52
1:Q:33:ASN:HD21	1:Q:41:GLY:HA3	1.73	0.52
4:L:159:HEM:CBB	4:L:159:HEM:HMB1	2.40	0.52
1:J:47:GLU:HA	1:J:47:GLU:OE1	2.10	0.52
1:N:10:HIS:O	1:N:14:ILE:HG12	2.10	0.52
1:H:10:HIS:O	1:H:14:ILE:HG12	2.09	0.52
1:S:111:VAL:O	1:S:112:HIS:HB2	2.09	0.52
1:F:105:ILE:HG23	1:F:117:ARG:HG3	1.92	0.52
1:A:51:GLU:OE1	1:A:127:GLU:OE2	2.27	0.52
1:A:135:GLU:OE1	1:W:2:LYS:HE2	2.10	0.52
1:I:18:GLU:O	1:I:22:ILE:HG13	2.09	0.52
1:V:94:GLU:O	1:V:98:THR:HB	2.10	0.52
1:A:48:SER:O	1:A:52:MET:HG3	2.10	0.52
1:U:30:ARG:CD	1:U:30:ARG:N	2.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:GLY:O	1:I:143:LYS:HG3	2.11	0.52
1:U:105:ILE:HG23	1:U:117:ARG:HG3	1.92	0.52
1:B:33:ASN:ND2	1:B:41:GLY:HA3	2.25	0.51
1:C:137:GLN:NE2	1:C:149:TYR:OH	2.28	0.51
1:T:117:ARG:HG2	1:T:117:ARG:O	2.08	0.51
1:A:52:MET:HB3	4:B:159:HEM:CHD	2.40	0.51
1:G:18:GLU:OE2	1:G:127:GLU:OE2	2.29	0.51
1:M:52:MET:HB3	4:M:159:HEM:CHD	2.39	0.51
1:R:59:ILE:O	1:R:63:LEU:HD22	2.11	0.51
4:E:159:HEM:CMB	4:E:159:HEM:HBB2	2.40	0.51
1:D:94:GLU:OE1	1:D:127:GLU:HB3	2.11	0.51
1:E:72:GLN:O	1:E:72:GLN:HG3	2.11	0.51
1:O:147:GLU:CD	1:O:147:GLU:H	2.14	0.51
1:V:4:ASP:OD2	1:V:6:LYS:N	2.43	0.51
4:E:159:HEM:HBC2	4:E:159:HEM:CHD	2.14	0.51
1:Q:52:MET:HB3	4:R:159:HEM:CHD	2.40	0.51
1:U:123:ILE:O	1:U:127:GLU:HG2	2.11	0.51
1:R:21:ALA:HB1	1:R:25:TYR:CE2	2.46	0.51
1:D:123:ILE:O	1:D:127:GLU:HG2	2.12	0.50
1:T:98:THR:HG23	1:T:102:ARG:NH2	2.26	0.50
4:B:159:HEM:HBB2	4:B:159:HEM:HMB1	1.93	0.50
1:X:140:LEU:O	1:X:144:VAL:HG22	2.11	0.50
1:I:75:GLY:O	1:J:72:GLN:NE2	2.45	0.50
1:T:44:GLU:OE2	1:T:90:ASP:OD2	2.29	0.50
1:U:18:GLU:CD	1:U:51:GLU:OE1	2.50	0.50
4:B:159:HEM:CMB	4:B:159:HEM:CBB	2.89	0.50
1:I:20:ILE:HD11	1:I:75:GLY:HA3	1.93	0.50
1:O:44:GLU:OE2	1:O:90:ASP:OD2	2.29	0.50
1:V:51:GLU:OE1	1:V:127:GLU:OE2	2.29	0.50
1:F:22:ILE:HD11	1:F:52:MET:HA	1.93	0.50
1:J:7:VAL:O	1:J:11:LEU:HG	2.12	0.50
1:O:113:ASP:OD2	1:O:116:SER:OG	2.25	0.50
1:T:79:ILE:HD13	1:T:79:ILE:N	2.27	0.50
1:B:91:LEU:HD12	1:B:91:LEU:O	2.11	0.50
1:W:105:ILE:HG23	1:W:117:ARG:HG3	1.94	0.50
1:C:48:SER:O	1:C:52:MET:HG3	2.10	0.50
1:H:44:GLU:OE2	1:H:90:ASP:OD2	2.30	0.50
1:A:133:TYR:O	1:A:137:GLN:HG2	2.12	0.50
1:B:18:GLU:OE2	1:B:51:GLU:OE1	2.28	0.50
1:C:20:ILE:HG23	1:C:77:LEU:HD12	1.94	0.50
1:H:78:LEU:HB2	1:H:89:CYS:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:58:LEU:O	1:M:62:ILE:HG13	2.12	0.50
1:J:26:PHE:CZ	4:J:159:HEM:CBC	2.95	0.50
1:S:27:LEU:O	1:S:31:MET:HG3	2.12	0.50
1:G:33:ASN:ND2	1:G:41:GLY:HA3	2.27	0.49
1:K:47:GLU:OE1	1:K:47:GLU:HA	2.12	0.49
1:L:119:LEU:HD23	1:L:119:LEU:O	2.13	0.49
1:M:123:ILE:O	1:M:127:GLU:HG2	2.12	0.49
1:Q:55:ALA:O	1:Q:59:ILE:HG13	2.12	0.49
1:U:30:ARG:N	1:U:30:ARG:HD2	2.24	0.49
1:G:27:LEU:HD23	1:G:79:ILE:HD12	1.95	0.49
1:D:140:LEU:O	1:D:144:VAL:HG22	2.12	0.49
1:C:105:ILE:HG23	1:C:117:ARG:HG3	1.95	0.49
1:A:64:PHE:CE1	1:H:132:ASP:HB2	2.47	0.49
1:B:18:GLU:OE1	1:B:18:GLU:HA	2.12	0.49
1:B:18:GLU:OE1	1:B:51:GLU:CD	2.51	0.49
1:E:27:LEU:HD23	1:E:79:ILE:HD12	1.95	0.49
1:K:27:LEU:HD23	1:K:79:ILE:CD1	2.41	0.49
1:O:14:ILE:HD12	1:O:101:LEU:HD13	1.94	0.49
4:P:159:HEM:HHD	4:P:159:HEM:CBC	2.37	0.49
1:S:8:ILE:HD13	1:S:67:GLY:HA3	1.94	0.49
1:B:52:MET:HB3	4:B:159:HEM:CHB	2.43	0.49
1:Q:44:GLU:OE2	1:Q:90:ASP:OD2	2.31	0.49
1:R:94:GLU:OE1	1:R:127:GLU:HB3	2.13	0.49
4:B:159:HEM:HMB1	4:B:159:HEM:CBB	2.43	0.49
1:D:33:ASN:ND2	1:D:41:GLY:HA3	2.27	0.49
1:L:51:GLU:OE1	1:L:127:GLU:OE2	2.30	0.49
1:B:18:GLU:O	1:B:22:ILE:HG13	2.13	0.49
1:D:28:HIS:CD2	1:D:86:MET:HG2	2.48	0.49
1:E:14:ILE:HD12	1:E:101:LEU:HD13	1.95	0.49
1:I:25:TYR:O	1:I:44:GLU:HG3	2.13	0.49
4:J:159:HEM:HHD	4:J:159:HEM:CBC	2.24	0.49
1:V:44:GLU:OE1	1:V:44:GLU:HA	2.12	0.49
1:V:119:LEU:HD22	1:V:123:ILE:HD11	1.95	0.49
1:B:44:GLU:OE2	1:B:90:ASP:OD2	2.31	0.48
1:B:123:ILE:O	1:B:127:GLU:HG2	2.13	0.48
1:S:133:TYR:O	1:S:137:GLN:HG2	2.13	0.48
1:C:39:ARG:HD3	1:C:153:HIS:CD2	2.48	0.48
1:H:52:MET:HB3	4:H:159:HEM:CHB	2.43	0.48
1:K:63:LEU:HD13	1:K:69:PRO:HD3	1.94	0.48
1:W:1:MET:HB3	1:W:66:GLU:OE2	2.13	0.48
1:O:140:LEU:O	1:O:144:VAL:HG22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HD13	1:B:69:PRO:HD3	1.96	0.48
1:C:133:TYR:O	1:C:137:GLN:HG2	2.14	0.48
1:H:15:LEU:O	1:H:19:LEU:HG	2.14	0.48
1:B:63:LEU:HD13	1:B:69:PRO:CG	2.44	0.48
1:A:33:ASN:ND2	1:A:41:GLY:HA3	2.28	0.48
1:B:18:GLU:OE1	1:B:51:GLU:OE1	2.30	0.48
1:U:55:ALA:O	1:U:59:ILE:HG13	2.14	0.48
1:A:10:HIS:O	1:A:14:ILE:HG12	2.14	0.48
1:C:18:GLU:OE2	1:C:127:GLU:OE2	2.32	0.48
1:R:51:GLU:OE2	1:R:127:GLU:OE1	2.32	0.48
1:B:51:GLU:OE1	1:B:127:GLU:OE2	2.32	0.48
1:J:28:HIS:CD2	1:J:86:MET:HG2	2.48	0.48
1:O:130:HIS:CD2	1:O:134:LEU:HD22	2.49	0.48
1:V:78:LEU:HB2	1:V:89:CYS:HB3	1.96	0.48
1:L:14:ILE:HD12	1:L:101:LEU:HD13	1.96	0.48
1:R:105:ILE:HG23	1:R:117:ARG:HG3	1.96	0.48
1:Q:30:ARG:HH21	1:R:56:ASP:CG	2.18	0.47
1:W:119:LEU:O	1:W:119:LEU:HD23	2.15	0.47
1:B:38:LYS:HE2	1:B:38:LYS:HB2	1.58	0.47
1:J:18:GLU:OE1	1:J:51:GLU:CD	2.53	0.47
1:K:13:LYS:HE2	1:K:100:ASP:OD2	2.14	0.47
1:K:52:MET:HB3	4:L:159:HEM:CHD	2.44	0.47
1:M:130:HIS:O	1:M:134:LEU:HD22	2.14	0.47
1:F:63:LEU:HD13	1:F:69:PRO:CD	2.44	0.47
1:P:16:GLY:O	1:P:20:ILE:HG13	2.14	0.47
1:U:94:GLU:OE1	1:U:127:GLU:OE1	2.33	0.47
1:J:78:LEU:HB2	1:J:89:CYS:HB3	1.97	0.47
1:Q:10:HIS:O	1:Q:14:ILE:HG12	2.15	0.47
1:X:30:ARG:HD2	1:X:30:ARG:N	2.27	0.47
1:D:94:GLU:OE1	1:D:127:GLU:OE1	2.33	0.47
1:D:133:TYR:O	1:D:137:GLN:HG2	2.15	0.47
4:D:159:HEM:HBC2	4:D:159:HEM:CHD	2.12	0.47
1:H:55:ALA:O	1:H:59:ILE:HG13	2.14	0.47
1:R:27:LEU:HD23	1:R:79:ILE:CD1	2.45	0.47
1:C:47:GLU:HA	1:C:47:GLU:OE1	2.13	0.47
1:D:15:LEU:O	1:D:19:LEU:HG	2.14	0.47
1:K:144:VAL:HG12	1:S:150:LEU:HB2	1.96	0.47
1:L:24:GLN:OE1	1:L:93:LEU:HD22	2.14	0.47
1:M:33:ASN:ND2	1:M:41:GLY:HA3	2.30	0.47
1:O:27:LEU:HD23	1:O:79:ILE:HD12	1.96	0.47
1:W:51:GLU:OE1	1:W:127:GLU:OE2	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:119:LEU:C	1:W:119:LEU:CD2	2.83	0.47
1:F:15:LEU:HD12	1:F:15:LEU:O	2.14	0.47
1:T:94:GLU:OE1	1:T:127:GLU:HB3	2.14	0.47
1:A:30:ARG:N	1:A:30:ARG:HD2	2.29	0.47
1:K:91:LEU:HD12	1:K:91:LEU:C	2.33	0.47
1:L:119:LEU:HD23	1:L:119:LEU:C	2.36	0.47
1:M:137:GLN:NE2	1:M:149:TYR:OH	2.34	0.47
1:R:33:ASN:HD21	1:R:41:GLY:HA3	1.80	0.47
1:U:26:PHE:O	1:U:29:SER:HB3	2.14	0.47
1:E:30:ARG:HA	1:E:30:ARG:HD2	1.76	0.46
1:N:20:ILE:HG23	1:N:77:LEU:HD12	1.97	0.46
1:R:30:ARG:HA	1:R:30:ARG:HD2	1.72	0.46
1:B:72:GLN:O	1:B:72:GLN:HG3	2.15	0.46
1:H:98:THR:HG22	1:H:99:LYS:N	2.30	0.46
1:W:63:LEU:HD13	1:W:69:PRO:CD	2.46	0.46
1:B:32:TRP:CE2	1:B:86:MET:HE1	2.51	0.46
1:P:25:TYR:HA	1:P:44:GLU:OE2	2.16	0.46
4:S:159:HEM:C1B	1:T:52:MET:HB3	2.49	0.46
1:E:24:GLN:OE1	1:E:93:LEU:HD22	2.16	0.46
1:P:51:GLU:OE1	1:P:127:GLU:OE2	2.33	0.46
1:U:63:LEU:HD13	1:U:69:PRO:HD3	1.98	0.46
1:U:65:LEU:O	1:U:66:GLU:HB2	2.16	0.46
1:A:63:LEU:HD13	1:A:69:PRO:HD3	1.96	0.46
1:C:94:GLU:OE1	1:C:127:GLU:OE1	2.33	0.46
1:I:14:ILE:HD12	1:I:101:LEU:HD13	1.98	0.46
1:P:105:ILE:HG23	1:P:117:ARG:HG3	1.97	0.46
1:V:4:ASP:OD2	1:V:4:ASP:C	2.54	0.46
1:G:63:LEU:HD13	1:G:69:PRO:CG	2.46	0.46
1:M:119:LEU:O	1:M:123:ILE:HG13	2.16	0.46
1:N:14:ILE:HD12	1:N:101:LEU:HD13	1.98	0.46
1:A:63:LEU:HD13	1:A:69:PRO:CD	2.46	0.46
1:C:18:GLU:OE1	1:C:51:GLU:CD	2.53	0.46
1:X:44:GLU:OE2	1:X:90:ASP:OD2	2.34	0.46
1:H:51:GLU:OE1	1:H:127:GLU:OE2	2.34	0.45
1:W:47:GLU:OE1	1:W:47:GLU:HA	2.16	0.45
1:G:20:ILE:HG23	1:G:77:LEU:HD12	1.98	0.45
1:U:139:GLY:O	1:U:143:LYS:HG3	2.16	0.45
4:B:159:HEM:HMC2	4:B:159:HEM:CBC	2.47	0.45
1:C:110:GLN:O	1:C:110:GLN:HG2	2.17	0.45
1:E:95:LEU:HD23	1:E:95:LEU:HA	1.86	0.45
1:Q:56:ASP:O	1:Q:60:GLU:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:111:VAL:O	1:P:112:HIS:HB2	2.17	0.45
1:P:123:ILE:O	1:P:127:GLU:HG2	2.16	0.45
1:R:48:SER:O	1:R:52:MET:HG3	2.17	0.45
1:W:57:LYS:HA	1:W:57:LYS:HD3	1.56	0.45
1:X:94:GLU:OE1	1:X:127:GLU:OE1	2.35	0.45
1:H:109:GLU:OE1	1:W:117:ARG:NH2	2.50	0.45
1:U:52:MET:HB3	4:U:159:HEM:CHD	2.47	0.45
1:X:18:GLU:O	1:X:22:ILE:HG13	2.17	0.45
1:H:133:TYR:O	1:H:137:GLN:HG2	2.17	0.45
1:F:81:GLU:HG2	1:F:85:GLU:OE2	2.17	0.45
1:M:26:PHE:O	1:M:29:SER:HB3	2.16	0.45
1:O:48:SER:O	1:O:52:MET:HG3	2.16	0.45
1:P:18:GLU:OE1	1:P:51:GLU:CD	2.54	0.45
1:R:15:LEU:HD12	1:R:15:LEU:O	2.17	0.45
1:V:91:LEU:HD12	1:V:91:LEU:O	2.16	0.45
1:I:97:ALA:O	1:I:101:LEU:HB2	2.17	0.44
4:M:159:HEM:HHA	4:M:159:HEM:CBD	2.47	0.44
1:J:79:ILE:HG22	1:J:80:GLY:O	2.17	0.44
1:B:105:ILE:HG23	1:B:117:ARG:HG3	1.98	0.44
1:D:18:GLU:OE1	1:D:51:GLU:CD	2.56	0.44
1:I:94:GLU:OE1	1:I:127:GLU:HB3	2.18	0.44
1:O:54:HIS:HE1	1:O:126:SER:OG	2.00	0.44
1:O:119:LEU:C	1:O:119:LEU:CD2	2.86	0.44
1:E:51:GLU:OE1	1:E:127:GLU:OE2	2.36	0.44
1:E:57:LYS:HD3	1:E:57:LYS:HA	1.45	0.44
1:H:117:ARG:O	1:H:117:ARG:HG2	2.17	0.44
1:J:51:GLU:OE1	1:J:127:GLU:OE2	2.35	0.44
1:J:91:LEU:HD12	1:J:91:LEU:O	2.18	0.44
1:N:81:GLU:HG2	1:N:85:GLU:OE2	2.17	0.44
1:S:21:ALA:HB1	1:S:25:TYR:CE2	2.52	0.44
1:T:30:ARG:N	1:T:30:ARG:HD2	2.32	0.44
1:V:147:GLU:CD	1:V:147:GLU:N	2.71	0.44
1:W:63:LEU:HD13	1:W:69:PRO:HD3	1.99	0.44
1:A:109:GLU:CD	1:H:117:ARG:HH22	2.21	0.44
1:M:130:HIS:CD2	1:M:134:LEU:HD22	2.52	0.44
1:R:144:VAL:HG12	1:T:150:LEU:HB2	2.00	0.44
1:S:30:ARG:N	1:S:30:ARG:HD2	2.33	0.44
1:S:119:LEU:O	1:S:119:LEU:CD2	2.65	0.44
1:X:20:ILE:HG23	1:X:77:LEU:HD12	2.00	0.44
1:X:102:ARG:HH11	1:X:102:ARG:CG	2.30	0.44
1:F:63:LEU:HD13	1:F:69:PRO:HG2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:LEU:C	1:H:119:LEU:CD2	2.87	0.44
1:K:20:ILE:HG23	1:K:77:LEU:HD12	1.99	0.44
1:X:139:GLY:O	1:X:143:LYS:HG3	2.18	0.44
1:K:18:GLU:OE1	1:K:51:GLU:CD	2.57	0.44
1:S:95:LEU:HD23	1:S:95:LEU:HA	1.89	0.44
1:H:25:TYR:N	1:H:25:TYR:CD1	2.84	0.43
1:H:71:LEU:HD12	1:H:71:LEU:N	2.33	0.43
1:O:70:ASN:C	1:O:70:ASN:OD1	2.54	0.43
1:U:102:ARG:HH11	1:U:102:ARG:CG	2.29	0.43
4:L:159:HEM:HBB2	4:L:159:HEM:HMB3	2.00	0.43
1:C:123:ILE:O	1:C:127:GLU:HG2	2.17	0.43
1:L:33:ASN:HD21	1:L:41:GLY:HA3	1.84	0.43
1:X:30:ARG:N	1:X:30:ARG:CD	2.81	0.43
1:E:30:ARG:HD2	1:E:30:ARG:N	2.30	0.43
1:H:133:TYR:CD2	1:H:134:LEU:HD13	2.53	0.43
1:J:48:SER:O	1:J:52:MET:HG3	2.18	0.43
1:O:105:ILE:HG23	1:O:117:ARG:HG3	1.99	0.43
1:T:98:THR:CG2	1:T:102:ARG:HH21	2.32	0.43
1:T:28:HIS:O	1:T:31:MET:HB2	2.19	0.43
1:L:11:LEU:HD23	1:L:11:LEU:HA	1.85	0.43
1:M:59:ILE:O	1:M:63:LEU:HD22	2.18	0.43
1:F:111:VAL:O	1:F:111:VAL:HG23	2.19	0.43
1:K:54:HIS:HE1	1:K:126:SER:OG	2.01	0.43
1:G:10:HIS:O	1:G:14:ILE:HG12	2.18	0.43
1:W:3:GLY:HA3	1:W:8:ILE:HD11	2.01	0.43
1:F:94:GLU:O	1:F:98:THR:HB	2.19	0.43
1:G:130:HIS:CD2	1:G:134:LEU:HD22	2.53	0.43
1:I:117:ARG:O	1:I:117:ARG:HG2	2.19	0.43
1:V:93:LEU:HD12	1:V:93:LEU:HA	1.87	0.43
1:W:26:PHE:CZ	4:W:159:HEM:CBC	3.02	0.43
1:J:72:GLN:O	1:J:72:GLN:HG3	2.18	0.43
1:W:113:ASP:CG	1:W:116:SER:HB2	2.40	0.43
1:B:32:TRP:CE2	1:B:86:MET:CE	3.02	0.42
1:F:19:LEU:HD11	1:F:71:LEU:HA	2.00	0.42
1:I:30:ARG:HA	1:I:30:ARG:HD2	1.84	0.42
1:M:18:GLU:OE2	1:M:127:GLU:OE2	2.37	0.42
1:O:138:LEU:HD12	1:O:138:LEU:HA	1.91	0.42
1:Q:71:LEU:HD13	1:R:27:LEU:HD22	2.00	0.42
1:S:56:ASP:O	1:S:60:GLU:HG3	2.19	0.42
1:K:52:MET:HB3	4:L:159:HEM:C1D	2.54	0.42
1:T:28:HIS:CE1	1:T:90:ASP:OD1	2.71	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:51:GLU:OE1	1:M:127:GLU:OE2	2.36	0.42
1:N:77:LEU:HB3	1:N:79:ILE:HD11	2.02	0.42
1:Q:71:LEU:N	1:Q:71:LEU:HD12	2.34	0.42
1:U:98:THR:HG23	1:U:102:ARG:HE	1.85	0.42
1:V:101:LEU:O	1:V:105:ILE:HG13	2.19	0.42
1:C:72:GLN:NE2	1:D:75:GLY:O	2.47	0.42
1:Q:79:ILE:HG22	1:Q:80:GLY:O	2.19	0.42
1:S:63:LEU:HD13	1:S:69:PRO:CG	2.49	0.42
1:W:4:ASP:HB3	1:W:7:VAL:HB	2.02	0.42
1:W:56:ASP:O	1:W:60:GLU:HG3	2.19	0.42
1:C:51:GLU:OE1	1:C:127:GLU:OE2	2.38	0.42
1:H:30:ARG:N	1:H:30:ARG:HD2	2.34	0.42
1:H:33:ASN:HD21	1:H:41:GLY:HA3	1.85	0.42
1:R:130:HIS:CD2	1:R:134:LEU:HD22	2.53	0.42
1:S:138:LEU:HD12	1:S:138:LEU:HA	1.91	0.42
1:U:57:LYS:HA	1:U:57:LYS:HE2	2.02	0.42
1:O:20:ILE:HD11	1:O:75:GLY:HA3	2.02	0.42
1:P:95:LEU:HD23	1:P:95:LEU:HA	1.81	0.42
1:S:52:MET:HB3	4:S:159:HEM:CHD	2.49	0.42
1:T:10:HIS:O	1:T:14:ILE:HG12	2.20	0.42
1:U:98:THR:HG22	1:U:99:LYS:N	2.35	0.42
1:H:119:LEU:O	1:H:119:LEU:HD23	2.20	0.42
1:H:133:TYR:HD2	1:H:134:LEU:HD13	1.83	0.42
1:L:119:LEU:C	1:L:119:LEU:CD2	2.87	0.42
4:S:159:HEM:CMC	4:S:159:HEM:CBC	2.65	0.42
1:U:30:ARG:HD2	1:U:30:ARG:HA	1.84	0.42
1:X:119:LEU:CD2	1:X:119:LEU:O	2.66	0.42
1:F:39:ARG:HD3	1:F:153:HIS:CD2	2.55	0.42
1:F:117:ARG:HH22	1:G:109:GLU:CD	2.23	0.42
1:R:101:LEU:HD21	1:R:123:ILE:HG22	2.01	0.42
1:T:63:LEU:HD13	1:T:69:PRO:CG	2.50	0.42
1:T:130:HIS:O	1:T:134:LEU:HD22	2.19	0.42
1:U:111:VAL:O	1:U:112:HIS:HB2	2.19	0.42
1:B:111:VAL:O	1:B:112:HIS:CB	2.61	0.42
1:W:48:SER:O	1:W:52:MET:HG3	2.20	0.42
1:B:18:GLU:CD	1:B:51:GLU:OE1	2.58	0.42
1:B:55:ALA:O	1:B:59:ILE:HG13	2.20	0.42
1:C:52:MET:HB3	4:D:159:HEM:C1D	2.55	0.42
1:I:51:GLU:OE1	1:I:51:GLU:HA	2.20	0.42
1:M:71:LEU:HD12	1:M:71:LEU:N	2.35	0.42
1:X:33:ASN:ND2	1:X:41:GLY:HA3	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:MET:HB3	4:H:159:HEM:CHD	2.50	0.41
1:W:133:TYR:CD2	1:W:134:LEU:HD13	2.55	0.41
1:S:123:ILE:O	1:S:127:GLU:HG2	2.19	0.41
1:S:134:LEU:HD12	1:S:134:LEU:HA	1.97	0.41
1:B:140:LEU:O	1:B:144:VAL:HG22	2.20	0.41
1:D:56:ASP:O	1:D:60:GLU:HG3	2.20	0.41
1:H:111:VAL:O	1:H:112:HIS:HB2	2.21	0.41
1:I:18:GLU:OE1	1:I:51:GLU:OE1	2.38	0.41
1:J:26:PHE:CE1	4:J:159:HEM:CBC	3.03	0.41
1:L:10:HIS:O	1:L:14:ILE:HG12	2.21	0.41
1:O:33:ASN:ND2	1:O:41:GLY:HA3	2.34	0.41
1:R:32:TRP:CE2	1:R:86:MET:CE	3.03	0.41
1:U:63:LEU:HD13	1:U:69:PRO:CD	2.50	0.41
1:V:30:ARG:HA	1:V:30:ARG:HD2	1.79	0.41
1:D:6:LYS:HB2	1:D:107:HIS:NE2	2.35	0.41
1:I:13:LYS:HE2	1:I:100:ASP:OD2	2.20	0.41
1:K:106:VAL:HG23	1:T:114:TYR:OH	2.21	0.41
1:K:123:ILE:O	1:K:127:GLU:HG2	2.21	0.41
1:W:111:VAL:O	1:W:112:HIS:HB2	2.19	0.41
1:N:21:ALA:HB1	1:N:25:TYR:CE2	2.55	0.41
1:A:21:ALA:O	1:A:22:ILE:C	2.59	0.41
1:C:8:ILE:O	1:C:8:ILE:HG22	2.19	0.41
1:E:30:ARG:N	1:E:30:ARG:CD	2.83	0.41
1:J:144:VAL:O	1:J:148:ASN:HB2	2.19	0.41
4:E:159:HEM:HBC1	1:F:26:PHE:CE1	2.56	0.41
1:I:107:HIS:O	1:I:111:VAL:HG22	2.21	0.41
1:J:63:LEU:HD13	1:J:69:PRO:CD	2.48	0.41
1:L:18:GLU:OE2	1:L:51:GLU:OE1	2.38	0.41
1:M:137:GLN:NE2	1:M:137:GLN:HA	2.34	0.41
1:O:26:PHE:O	1:O:29:SER:HB3	2.21	0.41
1:F:27:LEU:O	1:F:31:MET:HG3	2.21	0.41
1:F:81:GLU:HG2	1:F:81:GLU:H	1.76	0.41
1:I:10:HIS:O	1:I:14:ILE:HG12	2.20	0.41
1:O:10:HIS:O	1:O:14:ILE:HG12	2.20	0.41
1:F:47:GLU:OE1	1:F:47:GLU:HA	2.20	0.41
1:H:27:LEU:HD23	1:H:79:ILE:HD12	2.02	0.41
1:I:7:VAL:O	1:I:10:HIS:HB2	2.20	0.41
1:K:33:ASN:ND2	1:K:41:GLY:HA3	2.36	0.41
1:R:78:LEU:HB2	1:R:89:CYS:HB3	2.03	0.41
1:R:91:LEU:HD12	1:R:91:LEU:O	2.21	0.41
1:A:20:ILE:HD11	1:A:75:GLY:HA3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:44:GLU:HA	1:T:44:GLU:OE1	2.21	0.41
1:U:102:ARG:CG	1:U:102:ARG:NH1	2.83	0.41
1:V:15:LEU:O	1:V:19:LEU:HG	2.21	0.41
1:W:26:PHE:CE1	4:W:159:HEM:HBC1	2.55	0.41
1:W:94:GLU:OE1	1:W:127:GLU:OE1	2.39	0.41
1:X:48:SER:O	1:X:52:MET:HG3	2.21	0.41
1:B:33:ASN:HD21	1:B:41:GLY:HA3	1.86	0.40
1:D:52:MET:HB3	4:D:159:HEM:CHB	2.50	0.40
1:E:113:ASP:CG	1:E:116:SER:HB2	2.42	0.40
1:N:140:LEU:O	1:N:144:VAL:HG22	2.21	0.40
1:D:49:ILE:HG23	1:D:49:ILE:HD12	1.73	0.40
1:B:63:LEU:HD13	1:B:69:PRO:CD	2.51	0.40
1:B:119:LEU:O	1:B:119:LEU:HD23	2.20	0.40
1:E:18:GLU:OE2	1:E:127:GLU:OE2	2.38	0.40
1:E:149:TYR:CE1	1:E:153:HIS:CE1	3.09	0.40
1:H:94:GLU:OE1	1:H:127:GLU:OE1	2.38	0.40
1:H:138:LEU:HD12	1:H:138:LEU:HA	1.82	0.40
1:M:19:LEU:HA	1:M:19:LEU:HD23	1.85	0.40
1:Q:48:SER:O	1:Q:52:MET:HG3	2.22	0.40
1:Q:133:TYR:HD2	1:Q:134:LEU:HD13	1.87	0.40
1:T:45:TYR:CD2	1:T:45:TYR:C	2.93	0.40
1:U:79:ILE:N	1:U:79:ILE:HD13	2.36	0.40
1:C:117:ARG:O	1:C:117:ARG:HG2	2.20	0.40
1:Q:111:VAL:O	1:Q:111:VAL:HG23	2.20	0.40
1:U:63:LEU:HD13	1:U:69:PRO:HG3	2.04	0.40
4:B:159:HEM:CMC	4:B:159:HEM:CBC	2.96	0.40
1:F:117:ARG:NH2	1:G:109:GLU:OE1	2.55	0.40
1:H:30:ARG:N	1:H:30:ARG:CD	2.84	0.40
1:I:74:LEU:O	1:I:75:GLY:O	2.39	0.40
1:I:112:HIS:O	1:Q:102:ARG:NH1	2.51	0.40
1:O:22:ILE:HD11	1:O:52:MET:HA	2.04	0.40
1:O:25:TYR:O	1:O:26:PHE:C	2.59	0.40
1:W:18:GLU:CD	1:W:51:GLU:OE1	2.60	0.40
1:X:58:LEU:O	1:X:62:ILE:HG13	2.21	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	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
1	B	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
1	C	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
1	D	152/158 (96%)	148 (97%)	3 (2%)	1 (1%)	22	53
1	E	152/158 (96%)	146 (96%)	6 (4%)	0	100	100
1	F	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	G	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	H	153/158 (97%)	150 (98%)	3 (2%)	0	100	100
1	I	152/158 (96%)	149 (98%)	2 (1%)	1 (1%)	22	53
1	J	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	K	152/158 (96%)	147 (97%)	5 (3%)	0	100	100
1	L	152/158 (96%)	151 (99%)	0	1 (1%)	22	53
1	M	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	N	152/158 (96%)	147 (97%)	5 (3%)	0	100	100
1	O	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	P	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	Q	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
1	R	153/158 (97%)	149 (97%)	4 (3%)	0	100	100
1	S	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
1	T	152/158 (96%)	146 (96%)	6 (4%)	0	100	100
1	U	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
1	V	152/158 (96%)	148 (97%)	3 (2%)	1 (1%)	22	53
1	W	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
1	X	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
All	All	3652/3792 (96%)	3575 (98%)	73 (2%)	4 (0%)	51	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	75	GLY
1	I	75	GLY
1	V	4	ASP
1	L	75	GLY

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	139/144 (96%)	126 (91%)	13 (9%)	8 26
1	B	139/144 (96%)	129 (93%)	10 (7%)	14 38
1	C	139/144 (96%)	127 (91%)	12 (9%)	10 30
1	D	139/144 (96%)	129 (93%)	10 (7%)	14 38
1	E	139/144 (96%)	129 (93%)	10 (7%)	14 38
1	F	139/144 (96%)	125 (90%)	14 (10%)	7 22
1	G	139/144 (96%)	131 (94%)	8 (6%)	20 50
1	H	140/144 (97%)	130 (93%)	10 (7%)	14 39
1	I	139/144 (96%)	129 (93%)	10 (7%)	14 38
1	J	139/144 (96%)	131 (94%)	8 (6%)	20 50
1	K	139/144 (96%)	126 (91%)	13 (9%)	8 26
1	L	139/144 (96%)	131 (94%)	8 (6%)	20 50
1	M	139/144 (96%)	130 (94%)	9 (6%)	17 44
1	N	139/144 (96%)	130 (94%)	9 (6%)	17 44
1	O	139/144 (96%)	129 (93%)	10 (7%)	14 38
1	P	139/144 (96%)	129 (93%)	10 (7%)	14 38
1	Q	139/144 (96%)	128 (92%)	11 (8%)	12 34
1	R	140/144 (97%)	129 (92%)	11 (8%)	12 34
1	S	139/144 (96%)	131 (94%)	8 (6%)	20 50
1	T	139/144 (96%)	130 (94%)	9 (6%)	17 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	U	139/144 (96%)	130 (94%)	9 (6%)	17 44
1	V	139/144 (96%)	128 (92%)	11 (8%)	12 34
1	W	141/144 (98%)	129 (92%)	12 (8%)	10 31
1	X	139/144 (96%)	127 (91%)	12 (9%)	10 30
All	All	3340/3456 (97%)	3093 (93%)	247 (7%)	13 37

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	30	ARG
1	A	63	LEU
1	A	77	LEU
1	A	98	THR
1	A	101	LEU
1	A	117	ARG
1	A	118	ASP
1	A	119	LEU
1	A	126	SER
1	A	134	LEU
1	A	138	LEU
1	A	152	SER
1	B	5	LYS
1	B	63	LEU
1	B	77	LEU
1	B	98	THR
1	B	101	LEU
1	B	117	ARG
1	B	118	ASP
1	B	119	LEU
1	B	134	LEU
1	B	138	LEU
1	C	50	ASP
1	C	63	LEU
1	C	66	GLU
1	C	77	LEU
1	C	81	GLU
1	C	98	THR
1	C	101	LEU
1	C	117	ARG
1	C	118	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	119	LEU
1	C	134	LEU
1	C	138	LEU
1	D	6	LYS
1	D	63	LEU
1	D	66	GLU
1	D	98	THR
1	D	101	LEU
1	D	118	ASP
1	D	119	LEU
1	D	126	SER
1	D	134	LEU
1	D	138	LEU
1	E	30	ARG
1	E	63	LEU
1	E	76	LYS
1	E	77	LEU
1	E	98	THR
1	E	101	LEU
1	E	117	ARG
1	E	119	LEU
1	E	134	LEU
1	E	138	LEU
1	F	63	LEU
1	F	76	LYS
1	F	77	LEU
1	F	81	GLU
1	F	98	THR
1	F	99	LYS
1	F	101	LEU
1	F	117	ARG
1	F	118	ASP
1	F	119	LEU
1	F	126	SER
1	F	134	LEU
1	F	135	GLU
1	F	138	LEU
1	G	63	LEU
1	G	98	THR
1	G	101	LEU
1	G	117	ARG
1	G	118	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	119	LEU
1	G	134	LEU
1	G	138	LEU
1	H	2	LYS
1	H	39	ARG
1	H	57	LYS
1	H	63	LEU
1	H	98	THR
1	H	101	LEU
1	H	117	ARG
1	H	119	LEU
1	H	134	LEU
1	H	138	LEU
1	I	9	GLN
1	I	50	ASP
1	I	63	LEU
1	I	98	THR
1	I	101	LEU
1	I	117	ARG
1	I	119	LEU
1	I	126	SER
1	I	134	LEU
1	I	138	LEU
1	J	6	LYS
1	J	63	LEU
1	J	101	LEU
1	J	118	ASP
1	J	119	LEU
1	J	134	LEU
1	J	138	LEU
1	J	147	GLU
1	K	9	GLN
1	K	34	ASP
1	K	63	LEU
1	K	66	GLU
1	K	77	LEU
1	K	81	GLU
1	K	98	THR
1	K	99	LYS
1	K	101	LEU
1	K	119	LEU
1	K	126	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	134	LEU
1	K	138	LEU
1	L	63	LEU
1	L	66	GLU
1	L	98	THR
1	L	101	LEU
1	L	118	ASP
1	L	126	SER
1	L	134	LEU
1	L	138	LEU
1	M	4	ASP
1	M	6	LYS
1	M	63	LEU
1	M	101	LEU
1	M	118	ASP
1	M	119	LEU
1	M	126	SER
1	M	134	LEU
1	M	138	LEU
1	N	63	LEU
1	N	77	LEU
1	N	98	THR
1	N	101	LEU
1	N	117	ARG
1	N	118	ASP
1	N	119	LEU
1	N	134	LEU
1	N	138	LEU
1	O	6	LYS
1	O	63	LEU
1	O	98	THR
1	O	101	LEU
1	O	118	ASP
1	O	119	LEU
1	O	126	SER
1	O	134	LEU
1	O	138	LEU
1	O	147	GLU
1	P	6	LYS
1	P	57	LYS
1	P	63	LEU
1	P	66	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	98	THR
1	P	101	LEU
1	P	117	ARG
1	P	119	LEU
1	P	134	LEU
1	P	138	LEU
1	Q	6	LYS
1	Q	63	LEU
1	Q	77	LEU
1	Q	98	THR
1	Q	101	LEU
1	Q	117	ARG
1	Q	118	ASP
1	Q	119	LEU
1	Q	126	SER
1	Q	134	LEU
1	Q	138	LEU
1	R	6	LYS
1	R	57	LYS
1	R	63	LEU
1	R	98	THR
1	R	101	LEU
1	R	117	ARG
1	R	118	ASP
1	R	119	LEU
1	R	126	SER
1	R	134	LEU
1	R	138	LEU
1	S	63	LEU
1	S	77	LEU
1	S	81	GLU
1	S	101	LEU
1	S	118	ASP
1	S	119	LEU
1	S	134	LEU
1	S	138	LEU
1	T	50	ASP
1	T	63	LEU
1	T	96	LYS
1	T	101	LEU
1	T	117	ARG
1	T	118	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	119	LEU
1	T	134	LEU
1	T	138	LEU
1	U	9	GLN
1	U	30	ARG
1	U	63	LEU
1	U	76	LYS
1	U	98	THR
1	U	101	LEU
1	U	119	LEU
1	U	134	LEU
1	U	138	LEU
1	V	63	LEU
1	V	66	GLU
1	V	77	LEU
1	V	98	THR
1	V	101	LEU
1	V	118	ASP
1	V	119	LEU
1	V	126	SER
1	V	134	LEU
1	V	138	LEU
1	V	147	GLU
1	W	1	MET
1	W	2	LYS
1	W	63	LEU
1	W	98	THR
1	W	99	LYS
1	W	101	LEU
1	W	117	ARG
1	W	118	ASP
1	W	119	LEU
1	W	126	SER
1	W	134	LEU
1	W	138	LEU
1	X	6	LYS
1	X	30	ARG
1	X	63	LEU
1	X	77	LEU
1	X	101	LEU
1	X	110	GLN
1	X	117	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	119	LEU
1	X	126	SER
1	X	129	GLU
1	X	134	LEU
1	X	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	43	HIS
1	B	33	ASN
1	B	137	GLN
1	C	33	ASN
1	C	112	HIS
1	C	137	GLN
1	D	33	ASN
1	E	33	ASN
1	E	43	HIS
1	E	84	GLN
1	E	130	HIS
1	E	137	GLN
1	F	33	ASN
1	F	43	HIS
1	F	112	HIS
1	G	33	ASN
1	G	54	HIS
1	G	130	HIS
1	G	137	GLN
1	H	33	ASN
1	H	54	HIS
1	H	84	GLN
1	H	137	GLN
1	I	33	ASN
1	I	54	HIS
1	I	112	HIS
1	I	137	GLN
1	J	33	ASN
1	J	43	HIS
1	J	112	HIS
1	K	33	ASN
1	K	54	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	110	GLN
1	L	9	GLN
1	L	33	ASN
1	M	33	ASN
1	M	112	HIS
1	M	137	GLN
1	M	155	HIS
1	N	33	ASN
1	N	112	HIS
1	N	130	HIS
1	O	33	ASN
1	O	43	HIS
1	O	54	HIS
1	O	130	HIS
1	P	33	ASN
1	P	43	HIS
1	P	137	GLN
1	Q	33	ASN
1	Q	137	GLN
1	R	33	ASN
1	R	54	HIS
1	R	112	HIS
1	R	130	HIS
1	S	33	ASN
1	S	112	HIS
1	T	33	ASN
1	T	43	HIS
1	U	33	ASN
1	U	137	GLN
1	V	33	ASN
1	V	130	HIS
1	V	137	GLN
1	W	33	ASN
1	W	54	HIS
1	X	33	ASN
1	X	112	HIS

5.3.3 RNA

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 42 ligands modelled in this entry, 30 are monoatomic - leaving 12 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	D	159	1	41,50,50	2.08	7 (17%)	45,82,82	2.29	14 (31%)
4	HEM	U	159	1	41,50,50	2.02	8 (19%)	45,82,82	2.06	15 (33%)
4	HEM	R	159	1	41,50,50	1.88	6 (14%)	45,82,82	1.82	11 (24%)
4	HEM	P	159	1	41,50,50	2.01	5 (12%)	45,82,82	2.28	17 (37%)
4	HEM	E	159	1	41,50,50	2.07	8 (19%)	45,82,82	2.24	15 (33%)
4	HEM	J	159	1	41,50,50	2.04	7 (17%)	45,82,82	2.26	17 (37%)
4	HEM	L	159	1	41,50,50	1.98	10 (24%)	45,82,82	2.23	17 (37%)
4	HEM	S	159	1	41,50,50	1.92	8 (19%)	45,82,82	2.08	14 (31%)
4	HEM	B	159	1	41,50,50	1.73	6 (14%)	45,82,82	2.28	16 (35%)
4	HEM	M	159	1	41,50,50	1.94	7 (17%)	45,82,82	1.97	13 (28%)
4	HEM	W	159	1	41,50,50	2.11	7 (17%)	45,82,82	2.12	11 (24%)
4	HEM	H	159	1	41,50,50	1.83	7 (17%)	45,82,82	2.53	17 (37%)

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	D	159	1	-	6/12/54/54	-
4	HEM	U	159	1	-	4/12/54/54	-
4	HEM	R	159	1	-	6/12/54/54	-
4	HEM	P	159	1	-	4/12/54/54	-
4	HEM	E	159	1	-	4/12/54/54	-
4	HEM	J	159	1	-	4/12/54/54	-
4	HEM	L	159	1	-	4/12/54/54	-
4	HEM	S	159	1	-	2/12/54/54	-
4	HEM	B	159	1	-	4/12/54/54	-
4	HEM	M	159	1	-	6/12/54/54	-
4	HEM	W	159	1	-	6/12/54/54	-
4	HEM	H	159	1	-	4/12/54/54	-

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	159	HEM	C3D-C2D	8.24	1.54	1.36
4	W	159	HEM	C3D-C2D	8.17	1.54	1.36
4	J	159	HEM	C3D-C2D	7.89	1.53	1.36
4	E	159	HEM	C3D-C2D	7.85	1.53	1.36
4	P	159	HEM	C3D-C2D	7.66	1.53	1.36
4	U	159	HEM	C3D-C2D	7.50	1.52	1.36
4	H	159	HEM	C3D-C2D	7.45	1.52	1.36
4	L	159	HEM	C3D-C2D	7.43	1.52	1.36
4	R	159	HEM	C3D-C2D	7.05	1.51	1.36
4	M	159	HEM	C3D-C2D	7.04	1.51	1.36
4	S	159	HEM	C3D-C2D	6.87	1.51	1.36
4	B	159	HEM	C3D-C2D	6.84	1.51	1.36
4	W	159	HEM	C3C-C2C	-6.31	1.31	1.40
4	P	159	HEM	C3C-C2C	-6.29	1.31	1.40
4	E	159	HEM	C3C-C2C	-6.22	1.31	1.40
4	D	159	HEM	C3C-C2C	-6.18	1.31	1.40
4	M	159	HEM	C3C-C2C	-6.04	1.32	1.40
4	J	159	HEM	C3C-C2C	-5.87	1.32	1.40
4	U	159	HEM	C3C-C2C	-5.28	1.33	1.40
4	R	159	HEM	C3C-C2C	-5.11	1.33	1.40
4	S	159	HEM	C3C-C2C	-4.82	1.33	1.40
4	L	159	HEM	FE-NB	4.33	2.18	1.96
4	B	159	HEM	C3C-C2C	-4.23	1.34	1.40
4	R	159	HEM	C3C-CAC	3.80	1.55	1.47
4	J	159	HEM	FE-NB	3.77	2.15	1.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	159	HEM	C3C-C2C	-3.70	1.35	1.40
4	L	159	HEM	C3C-C2C	-3.65	1.35	1.40
4	U	159	HEM	CAA-C2A	3.36	1.57	1.52
4	L	159	HEM	C3C-CAC	3.36	1.54	1.47
4	S	159	HEM	CAA-C2A	3.30	1.56	1.52
4	E	159	HEM	FE-ND	3.28	2.13	1.96
4	R	159	HEM	FE-ND	3.28	2.13	1.96
4	D	159	HEM	FE-ND	3.21	2.12	1.96
4	W	159	HEM	FE-ND	3.12	2.12	1.96
4	S	159	HEM	FE-ND	3.11	2.12	1.96
4	U	159	HEM	C3C-CAC	2.95	1.53	1.47
4	P	159	HEM	C3B-C2B	-2.82	1.31	1.37
4	H	159	HEM	C3C-CAC	2.82	1.53	1.47
4	M	159	HEM	FE-ND	2.75	2.10	1.96
4	J	159	HEM	C1A-NA	2.69	1.41	1.36
4	B	159	HEM	C3C-CAC	2.67	1.53	1.47
4	E	159	HEM	CAA-C2A	2.63	1.55	1.52
4	J	159	HEM	CAB-C3B	2.60	1.54	1.47
4	U	159	HEM	FE-ND	2.57	2.09	1.96
4	H	159	HEM	FE-NB	2.57	2.09	1.96
4	U	159	HEM	CMB-C2B	2.55	1.56	1.50
4	M	159	HEM	C3C-CAC	2.52	1.53	1.47
4	P	159	HEM	CHA-C4D	2.52	1.41	1.35
4	S	159	HEM	CHA-C4D	2.52	1.41	1.35
4	W	159	HEM	C3B-C2B	-2.49	1.32	1.37
4	S	159	HEM	CAB-C3B	2.48	1.54	1.47
4	J	159	HEM	C3B-C2B	-2.44	1.32	1.37
4	H	159	HEM	C3B-C2B	-2.41	1.32	1.37
4	D	159	HEM	C3C-CAC	2.39	1.52	1.47
4	W	159	HEM	FE-NB	2.35	2.08	1.96
4	L	159	HEM	CMA-C3A	2.35	1.56	1.51
4	D	159	HEM	CMD-C2D	2.35	1.55	1.50
4	E	159	HEM	CHA-C4D	2.35	1.41	1.35
4	M	159	HEM	CHA-C4D	2.34	1.41	1.35
4	E	159	HEM	C3C-CAC	2.32	1.52	1.47
4	P	159	HEM	FE-ND	2.31	2.08	1.96
4	E	159	HEM	FE-NB	2.29	2.08	1.96
4	L	159	HEM	CAA-C2A	2.25	1.55	1.52
4	L	159	HEM	CMC-C2C	2.23	1.56	1.51
4	R	159	HEM	CAA-C2A	2.19	1.55	1.52
4	W	159	HEM	CHA-C4D	2.19	1.40	1.35
4	L	159	HEM	CHA-C4D	2.19	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	159	HEM	FE-ND	2.18	2.07	1.96
4	B	159	HEM	FE-NB	2.16	2.07	1.96
4	B	159	HEM	CHA-C4D	2.14	1.40	1.35
4	M	159	HEM	C3B-C2B	-2.14	1.32	1.37
4	W	159	HEM	CAB-C3B	2.13	1.53	1.47
4	H	159	HEM	CHA-C4D	2.13	1.40	1.35
4	M	159	HEM	FE-NB	2.12	2.07	1.96
4	R	159	HEM	C3B-C2B	-2.12	1.33	1.37
4	L	159	HEM	C3B-C2B	-2.12	1.33	1.37
4	S	159	HEM	C3C-CAC	2.11	1.52	1.47
4	B	159	HEM	CAB-C3B	2.11	1.53	1.47
4	D	159	HEM	CHA-C4D	2.10	1.40	1.35
4	U	159	HEM	FE-NB	2.09	2.07	1.96
4	S	159	HEM	FE-NB	2.07	2.07	1.96
4	D	159	HEM	CAB-C3B	2.07	1.53	1.47
4	L	159	HEM	CAB-C3B	2.07	1.53	1.47
4	E	159	HEM	CMB-C2B	2.04	1.55	1.50
4	U	159	HEM	CAB-C3B	2.02	1.52	1.47
4	J	159	HEM	CHA-C4D	2.01	1.40	1.35

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	159	HEM	C4D-ND-C1D	7.83	113.16	105.07
4	H	159	HEM	C4D-ND-C1D	7.60	112.92	105.07
4	W	159	HEM	C4D-ND-C1D	7.23	112.54	105.07
4	P	159	HEM	C4D-ND-C1D	7.16	112.47	105.07
4	J	159	HEM	C4D-ND-C1D	7.15	112.46	105.07
4	L	159	HEM	C4D-ND-C1D	6.98	112.28	105.07
4	E	159	HEM	C4D-ND-C1D	6.95	112.25	105.07
4	U	159	HEM	C4D-ND-C1D	6.90	112.20	105.07
4	S	159	HEM	C4D-ND-C1D	6.60	111.89	105.07
4	B	159	HEM	CHC-C4B-NB	6.36	131.34	124.43
4	M	159	HEM	C4D-ND-C1D	6.34	111.63	105.07
4	B	159	HEM	C4D-ND-C1D	6.03	111.30	105.07
4	J	159	HEM	C2C-C3C-C4C	6.00	111.09	106.90
4	P	159	HEM	C2C-C3C-C4C	5.91	111.03	106.90
4	R	159	HEM	C4D-ND-C1D	5.76	111.02	105.07
4	W	159	HEM	C2C-C3C-C4C	5.70	110.88	106.90
4	E	159	HEM	C2C-C3C-C4C	5.36	110.64	106.90
4	H	159	HEM	C2C-C3C-C4C	5.18	110.52	106.90
4	E	159	HEM	CHC-C4B-NB	5.17	130.04	124.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	159	HEM	C2C-C3C-C4C	5.15	110.50	106.90
4	U	159	HEM	C4C-CHD-C1D	4.98	129.12	122.56
4	H	159	HEM	CBA-CAA-C2A	-4.88	104.28	112.62
4	H	159	HEM	CHC-C4B-NB	4.87	129.72	124.43
4	D	159	HEM	CHC-C4B-NB	4.68	129.51	124.43
4	B	159	HEM	C2C-C3C-C4C	4.52	110.05	106.90
4	D	159	HEM	CBA-CAA-C2A	-4.49	104.96	112.62
4	L	159	HEM	C2C-C3C-C4C	4.38	109.96	106.90
4	P	159	HEM	C4B-C3B-C2B	4.27	110.51	107.11
4	S	159	HEM	C2C-C3C-C4C	4.26	109.88	106.90
4	H	159	HEM	C4B-C3B-C2B	4.18	110.44	107.11
4	M	159	HEM	C4C-CHD-C1D	4.07	127.92	122.56
4	M	159	HEM	C2C-C3C-C4C	4.06	109.74	106.90
4	W	159	HEM	C4C-CHD-C1D	4.03	127.88	122.56
4	U	159	HEM	CMD-C2D-C1D	4.01	131.15	125.04
4	U	159	HEM	C2C-C3C-C4C	3.96	109.67	106.90
4	E	159	HEM	C1B-NB-C4B	3.86	109.06	105.07
4	E	159	HEM	C4B-C3B-C2B	3.86	110.18	107.11
4	S	159	HEM	C4C-CHD-C1D	3.80	127.57	122.56
4	B	159	HEM	C4B-C3B-C2B	3.77	110.11	107.11
4	J	159	HEM	CMA-C3A-C4A	-3.76	122.69	128.46
4	P	159	HEM	CHC-C4B-NB	3.75	128.51	124.43
4	L	159	HEM	C4C-CHD-C1D	3.74	127.49	122.56
4	R	159	HEM	C4C-CHD-C1D	3.73	127.47	122.56
4	B	159	HEM	C4C-CHD-C1D	3.67	127.41	122.56
4	L	159	HEM	CHC-C4B-NB	3.60	128.35	124.43
4	S	159	HEM	CHC-C4B-NB	3.59	128.34	124.43
4	B	159	HEM	CMA-C3A-C4A	-3.58	122.97	128.46
4	L	159	HEM	CAD-C3D-C4D	3.57	130.89	124.66
4	B	159	HEM	C4A-C3A-C2A	3.56	109.47	107.00
4	J	159	HEM	C4C-CHD-C1D	3.50	127.18	122.56
4	D	159	HEM	CMA-C3A-C4A	-3.48	123.12	128.46
4	S	159	HEM	CMD-C2D-C1D	3.43	130.27	125.04
4	H	159	HEM	C3D-C4D-ND	-3.38	106.41	110.17
4	L	159	HEM	CBA-CAA-C2A	-3.35	106.89	112.62
4	W	159	HEM	C3B-C2B-C1B	3.35	108.97	106.49
4	J	159	HEM	CHC-C4B-NB	3.31	128.02	124.43
4	E	159	HEM	C4C-CHD-C1D	3.30	126.92	122.56
4	R	159	HEM	C4B-C3B-C2B	3.26	109.71	107.11
4	S	159	HEM	C1B-NB-C4B	3.26	108.44	105.07
4	H	159	HEM	C1B-NB-C4B	3.25	108.44	105.07
4	H	159	HEM	CAD-CBD-CGD	-3.23	106.65	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	159	HEM	CMB-C2B-C1B	3.23	129.95	125.04
4	H	159	HEM	C4C-CHD-C1D	3.20	126.79	122.56
4	H	159	HEM	CBD-CAD-C3D	-3.19	103.77	112.63
4	D	159	HEM	C4C-CHD-C1D	3.16	126.73	122.56
4	P	159	HEM	CHA-C4D-ND	3.16	128.28	124.38
4	L	159	HEM	CBB-CAB-C3B	-3.11	112.13	127.62
4	P	159	HEM	CBB-CAB-C3B	-3.09	112.25	127.62
4	P	159	HEM	C4B-CHC-C1C	3.04	126.57	122.56
4	W	159	HEM	C1B-NB-C4B	3.03	108.20	105.07
4	B	159	HEM	C1B-NB-C4B	3.01	108.18	105.07
4	H	159	HEM	CMD-C2D-C1D	2.98	129.58	125.04
4	H	159	HEM	CBB-CAB-C3B	-2.97	112.82	127.62
4	M	159	HEM	CAD-C3D-C4D	2.97	129.85	124.66
4	J	159	HEM	C3C-C4C-NC	-2.96	105.36	110.94
4	M	159	HEM	C4B-C3B-C2B	2.92	109.44	107.11
4	D	159	HEM	C4B-CHC-C1C	2.89	126.38	122.56
4	W	159	HEM	CHC-C4B-NB	2.87	127.55	124.43
4	J	159	HEM	CBD-CAD-C3D	-2.87	104.65	112.63
4	R	159	HEM	CBB-CAB-C3B	-2.84	113.48	127.62
4	E	159	HEM	CBB-CAB-C3B	-2.78	113.79	127.62
4	R	159	HEM	CBA-CAA-C2A	-2.78	107.88	112.62
4	W	159	HEM	C3C-C4C-NC	-2.75	105.76	110.94
4	R	159	HEM	CMD-C2D-C1D	2.74	129.21	125.04
4	H	159	HEM	CHA-C4D-ND	2.72	127.74	124.38
4	W	159	HEM	CBA-CAA-C2A	-2.71	107.99	112.62
4	U	159	HEM	C1B-NB-C4B	2.71	107.87	105.07
4	J	159	HEM	CMB-C2B-C1B	2.70	129.15	125.04
4	D	159	HEM	C4B-C3B-C2B	2.67	109.24	107.11
4	J	159	HEM	CHA-C4D-ND	2.67	127.68	124.38
4	L	159	HEM	CBD-CAD-C3D	-2.66	105.23	112.63
4	P	159	HEM	CMD-C2D-C1D	2.65	129.08	125.04
4	S	159	HEM	C3C-C4C-NC	-2.65	105.94	110.94
4	U	159	HEM	CAD-CBD-CGD	-2.64	107.93	113.60
4	J	159	HEM	CBA-CAA-C2A	-2.62	108.16	112.62
4	D	159	HEM	C3C-C4C-NC	-2.61	106.01	110.94
4	M	159	HEM	CBB-CAB-C3B	-2.61	114.64	127.62
4	L	159	HEM	C4B-C3B-C2B	2.60	109.18	107.11
4	W	159	HEM	C2B-C1B-NB	-2.60	106.76	109.84
4	R	159	HEM	CHB-C1B-NB	2.60	127.59	124.38
4	L	159	HEM	CMB-C2B-C3B	-2.60	121.95	128.30
4	P	159	HEM	CMA-C3A-C4A	-2.58	124.50	128.46
4	P	159	HEM	C3C-C4C-NC	-2.57	106.08	110.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	159	HEM	C4B-CHC-C1C	2.56	125.93	122.56
4	H	159	HEM	C3C-C4C-NC	-2.55	106.13	110.94
4	P	159	HEM	C1B-NB-C4B	2.54	107.69	105.07
4	S	159	HEM	C4B-C3B-C2B	2.53	109.13	107.11
4	E	159	HEM	O2A-CGA-CBA	2.53	122.17	114.03
4	B	159	HEM	CBA-CAA-C2A	-2.50	108.35	112.62
4	U	159	HEM	C4B-C3B-C2B	2.50	109.10	107.11
4	E	159	HEM	C2B-C1B-NB	-2.49	106.88	109.84
4	J	159	HEM	CMD-C2D-C1D	2.49	128.83	125.04
4	E	159	HEM	O1D-CGD-CBD	-2.49	115.09	123.08
4	B	159	HEM	CBB-CAB-C3B	-2.49	115.25	127.62
4	M	159	HEM	C3D-C4D-ND	-2.47	107.41	110.17
4	R	159	HEM	CAD-C3D-C4D	2.46	128.96	124.66
4	D	159	HEM	CBB-CAB-C3B	-2.46	115.40	127.62
4	H	159	HEM	C4A-C3A-C2A	2.45	108.70	107.00
4	S	159	HEM	C4A-C3A-C2A	2.45	108.70	107.00
4	L	159	HEM	CMD-C2D-C1D	2.42	128.73	125.04
4	R	159	HEM	CMA-C3A-C4A	-2.42	124.75	128.46
4	B	159	HEM	CAD-CBD-CGD	-2.41	108.41	113.60
4	R	159	HEM	CBD-CAD-C3D	-2.41	105.92	112.63
4	L	159	HEM	C1B-NB-C4B	2.39	107.55	105.07
4	L	159	HEM	C2B-C1B-NB	-2.38	107.02	109.84
4	D	159	HEM	C3D-C4D-ND	-2.38	107.52	110.17
4	U	159	HEM	CMA-C3A-C4A	-2.37	124.82	128.46
4	D	159	HEM	C2D-C1D-ND	-2.35	107.07	109.88
4	M	159	HEM	CMA-C3A-C4A	-2.32	124.89	128.46
4	P	159	HEM	C4C-CHD-C1D	2.32	125.62	122.56
4	J	159	HEM	C3D-C4D-ND	-2.31	107.59	110.17
4	E	159	HEM	CBD-CAD-C3D	-2.31	106.20	112.63
4	M	159	HEM	CBD-CAD-C3D	-2.30	106.23	112.63
4	D	159	HEM	CMA-C3A-C2A	2.30	129.28	124.94
4	W	159	HEM	C4B-C3B-C2B	2.27	108.92	107.11
4	S	159	HEM	C3D-C4D-ND	-2.26	107.65	110.17
4	S	159	HEM	CHA-C4D-ND	2.26	127.17	124.38
4	M	159	HEM	C1B-NB-C4B	2.25	107.40	105.07
4	B	159	HEM	CAD-C3D-C4D	2.22	128.54	124.66
4	L	159	HEM	C3C-C4C-NC	-2.22	106.75	110.94
4	E	159	HEM	C3D-C4D-ND	-2.22	107.70	110.17
4	E	159	HEM	CAD-CBD-CGD	-2.17	108.92	113.60
4	S	159	HEM	C3B-C2B-C1B	2.17	108.10	106.49
4	B	159	HEM	CBD-CAD-C3D	-2.17	106.60	112.63
4	S	159	HEM	C2B-C1B-NB	-2.17	107.27	109.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	159	HEM	CAD-C3D-C4D	2.15	128.42	124.66
4	L	159	HEM	C3B-C2B-C1B	2.15	108.08	106.49
4	U	159	HEM	CBB-CAB-C3B	-2.14	116.96	127.62
4	U	159	HEM	C2D-C1D-ND	-2.13	107.33	109.88
4	B	159	HEM	CMB-C2B-C1B	2.12	128.27	125.04
4	M	159	HEM	O1D-CGD-CBD	-2.12	116.27	123.08
4	H	159	HEM	CMB-C2B-C1B	2.11	128.25	125.04
4	J	159	HEM	CMB-C2B-C3B	-2.11	123.15	128.30
4	U	159	HEM	C4A-C3A-C2A	2.10	108.46	107.00
4	R	159	HEM	C1B-NB-C4B	2.09	107.24	105.07
4	E	159	HEM	C3C-C4C-NC	-2.09	106.99	110.94
4	B	159	HEM	CHD-C1D-ND	2.09	126.70	124.43
4	E	159	HEM	C4A-C3A-C2A	2.09	108.45	107.00
4	J	159	HEM	C4A-C3A-C2A	2.09	108.45	107.00
4	P	159	HEM	C2D-C1D-ND	-2.09	107.38	109.88
4	P	159	HEM	CMB-C2B-C1B	2.08	128.21	125.04
4	M	159	HEM	CAD-C3D-C2D	-2.08	124.00	127.88
4	L	159	HEM	CAD-C3D-C2D	-2.08	124.00	127.88
4	B	159	HEM	C3C-C4C-NC	-2.08	107.02	110.94
4	J	159	HEM	CMA-C3A-C2A	2.08	128.86	124.94
4	J	159	HEM	C4B-C3B-C2B	2.08	108.76	107.11
4	P	159	HEM	C3D-C4D-ND	-2.08	107.85	110.17
4	U	159	HEM	CHA-C4D-ND	2.07	126.94	124.38
4	D	159	HEM	CMD-C2D-C1D	2.07	128.18	125.04
4	H	159	HEM	CHD-C1D-ND	2.06	126.67	124.43
4	U	159	HEM	CHC-C4B-NB	2.05	126.66	124.43
4	U	159	HEM	C3C-C4C-NC	-2.05	107.08	110.94
4	P	159	HEM	CAB-C3B-C2B	-2.04	121.88	128.60
4	W	159	HEM	CBB-CAB-C3B	-2.04	117.49	127.62
4	P	159	HEM	CHB-C1B-NB	2.02	126.87	124.38
4	M	159	HEM	CHC-C4B-NB	2.01	126.62	124.43
4	U	159	HEM	CAD-C3D-C4D	2.01	128.17	124.66

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	159	HEM	C2B-C3B-CAB-CBB
4	R	159	HEM	C4B-C3B-CAB-CBB
4	M	159	HEM	C4D-C3D-CAD-CBD
4	M	159	HEM	C2D-C3D-CAD-CBD
4	D	159	HEM	C4D-C3D-CAD-CBD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	W	159	HEM	C2B-C3B-CAB-CBB
4	M	159	HEM	C3D-CAD-CBD-CGD
4	D	159	HEM	C2D-C3D-CAD-CBD
4	H	159	HEM	CAD-CBD-CGD-O1D
4	L	159	HEM	CAD-CBD-CGD-O2D
4	L	159	HEM	CAD-CBD-CGD-O1D
4	D	159	HEM	CAD-CBD-CGD-O1D
4	J	159	HEM	CAA-CBA-CGA-O2A
4	B	159	HEM	CAD-CBD-CGD-O1D
4	J	159	HEM	CAA-CBA-CGA-O1A
4	W	159	HEM	CAD-CBD-CGD-O1D
4	W	159	HEM	CAD-CBD-CGD-O2D
4	R	159	HEM	CAA-CBA-CGA-O1A
4	R	159	HEM	CAA-CBA-CGA-O2A
4	S	159	HEM	CAD-CBD-CGD-O1D
4	R	159	HEM	CAD-CBD-CGD-O1D
4	H	159	HEM	CAD-CBD-CGD-O2D
4	D	159	HEM	CAA-CBA-CGA-O1A
4	W	159	HEM	CAA-CBA-CGA-O2A
4	B	159	HEM	CAA-CBA-CGA-O2A
4	U	159	HEM	CAA-CBA-CGA-O2A
4	H	159	HEM	CAA-CBA-CGA-O2A
4	B	159	HEM	CAA-CBA-CGA-O1A
4	D	159	HEM	CAD-CBD-CGD-O2D
4	H	159	HEM	CAA-CBA-CGA-O1A
4	S	159	HEM	CAD-CBD-CGD-O2D
4	W	159	HEM	CAA-CBA-CGA-O1A
4	B	159	HEM	CAD-CBD-CGD-O2D
4	R	159	HEM	CAD-CBD-CGD-O2D
4	U	159	HEM	CAA-CBA-CGA-O1A
4	D	159	HEM	CAA-CBA-CGA-O2A
4	P	159	HEM	CAD-CBD-CGD-O2D
4	J	159	HEM	CAD-CBD-CGD-O2D
4	P	159	HEM	CAD-CBD-CGD-O1D
4	E	159	HEM	CAD-CBD-CGD-O2D
4	E	159	HEM	CAD-CBD-CGD-O1D
4	L	159	HEM	CAA-CBA-CGA-O2A
4	E	159	HEM	CAA-CBA-CGA-O2A
4	J	159	HEM	CAD-CBD-CGD-O1D
4	M	159	HEM	CAA-CBA-CGA-O2A
4	W	159	HEM	C4B-C3B-CAB-CBB
4	P	159	HEM	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	U	159	HEM	CAD-CBD-CGD-O1D
4	E	159	HEM	CAA-CBA-CGA-O1A
4	P	159	HEM	CAA-CBA-CGA-O1A
4	L	159	HEM	CAA-CBA-CGA-O1A
4	U	159	HEM	CAD-CBD-CGD-O2D
4	M	159	HEM	CAA-CBA-CGA-O1A
4	M	159	HEM	CAD-CBD-CGD-O2D

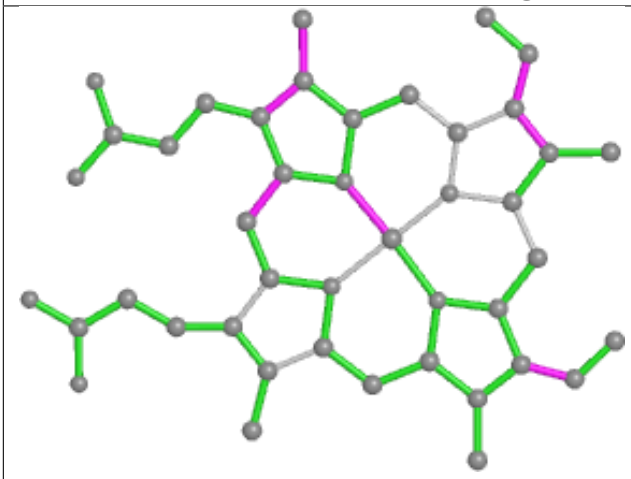
There are no ring outliers.

12 monomers are involved in 83 short contacts:

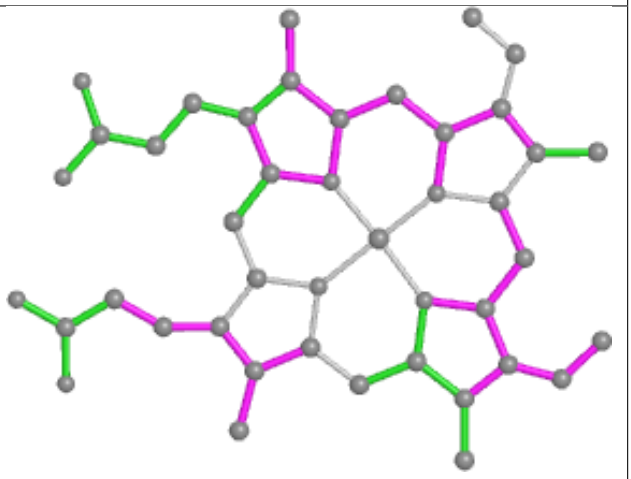
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	159	HEM	6	0
4	U	159	HEM	1	0
4	R	159	HEM	6	0
4	P	159	HEM	8	0
4	E	159	HEM	6	0
4	J	159	HEM	10	0
4	L	159	HEM	8	0
4	S	159	HEM	7	0
4	B	159	HEM	10	0
4	M	159	HEM	9	0
4	W	159	HEM	3	0
4	H	159	HEM	9	0

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.

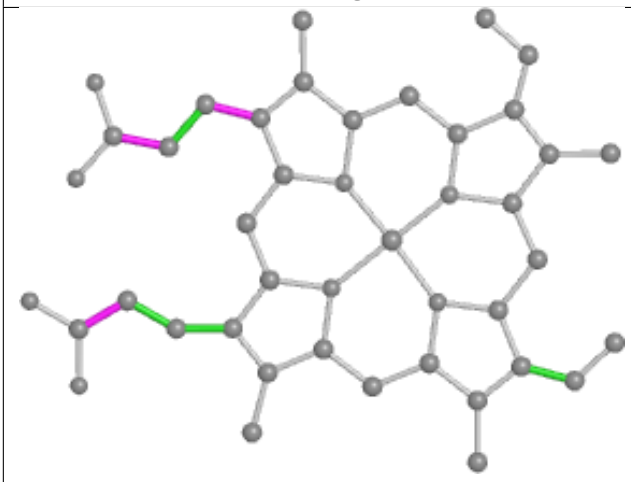
Ligand HEM D 159



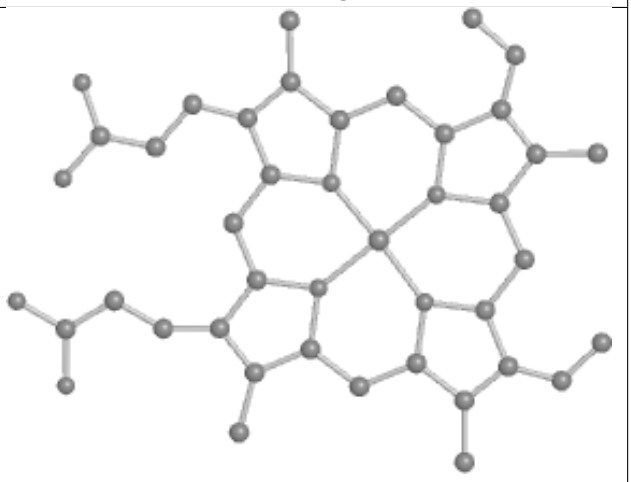
Bond lengths



Bond angles

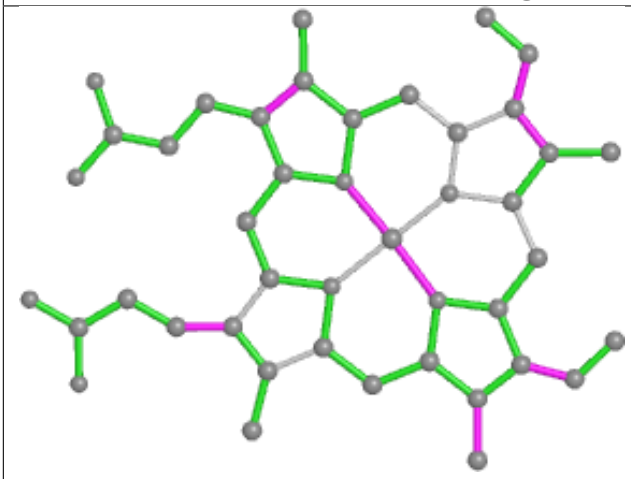


Torsions

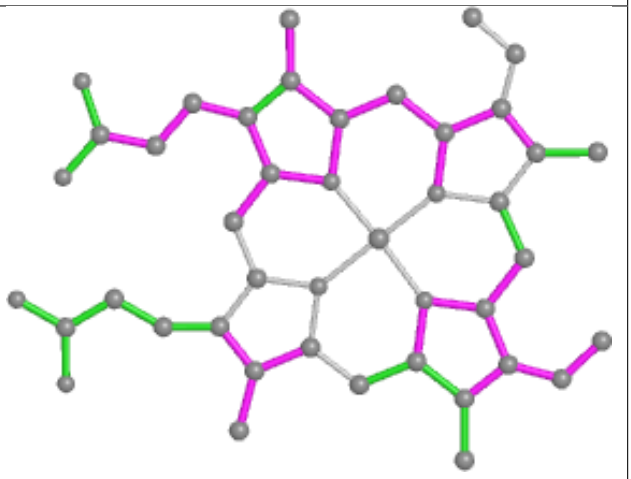


Rings

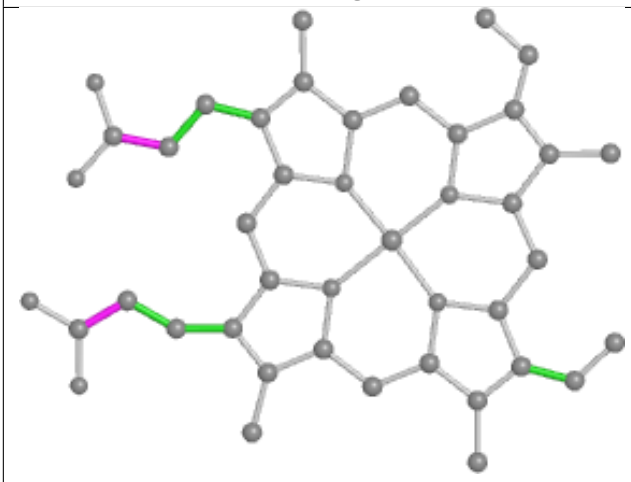
Ligand HEM U 159



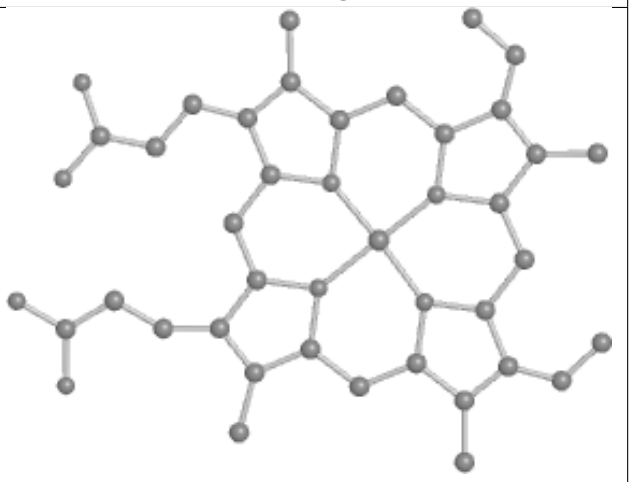
Bond lengths



Bond angles

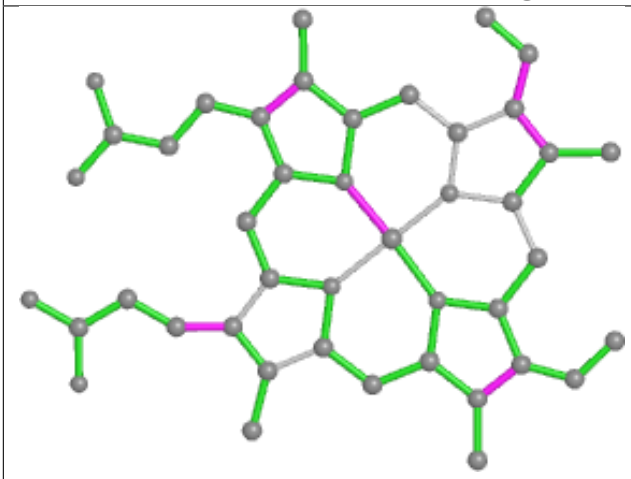


Torsions

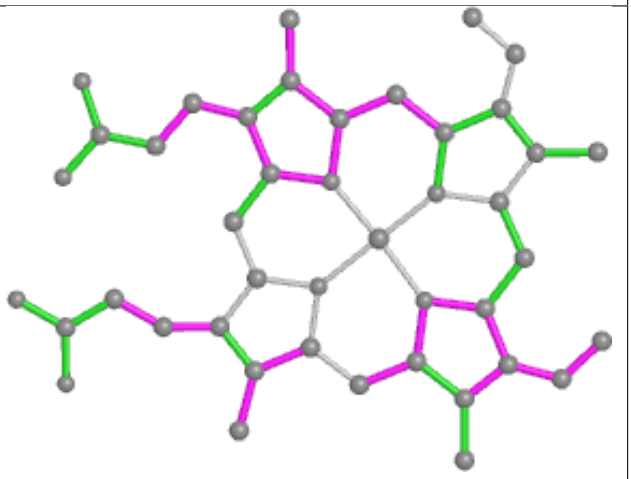


Rings

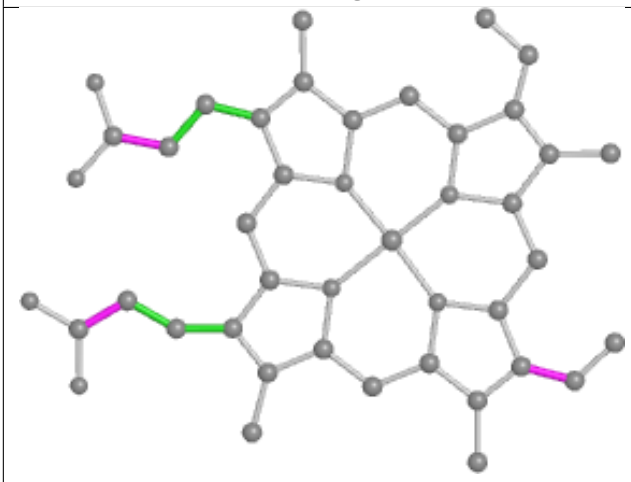
Ligand HEM R 159



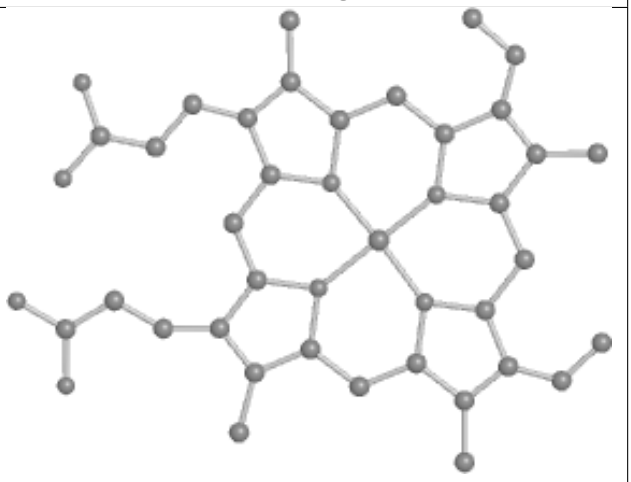
Bond lengths



Bond angles

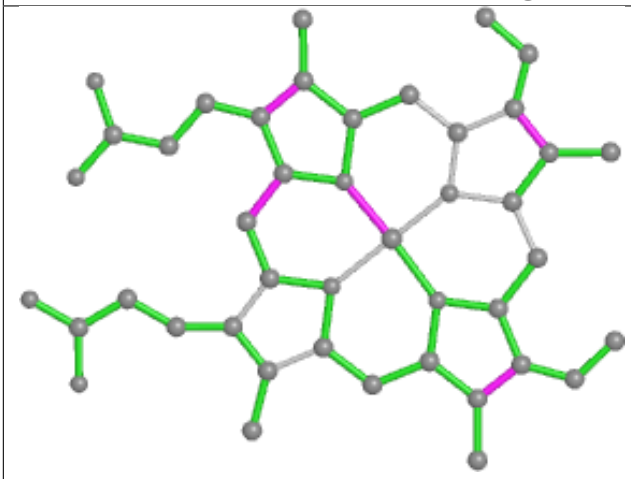


Torsions

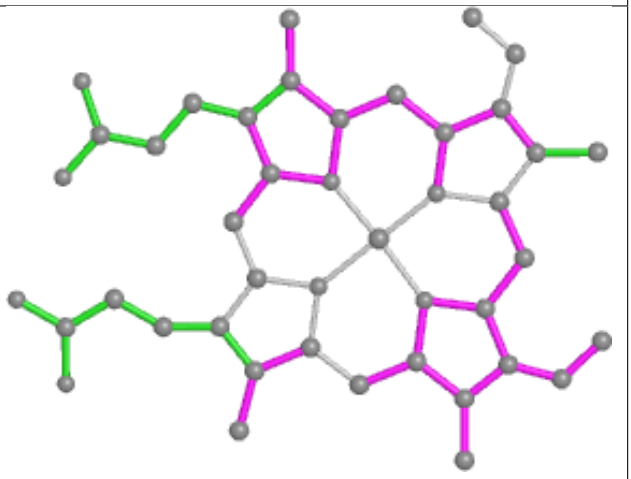


Rings

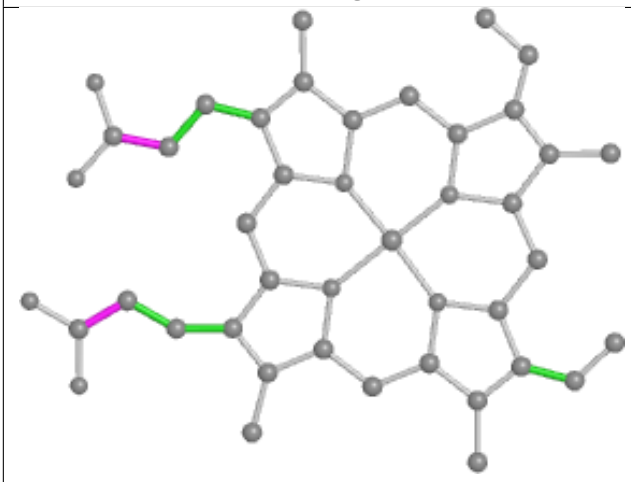
Ligand HEM P 159



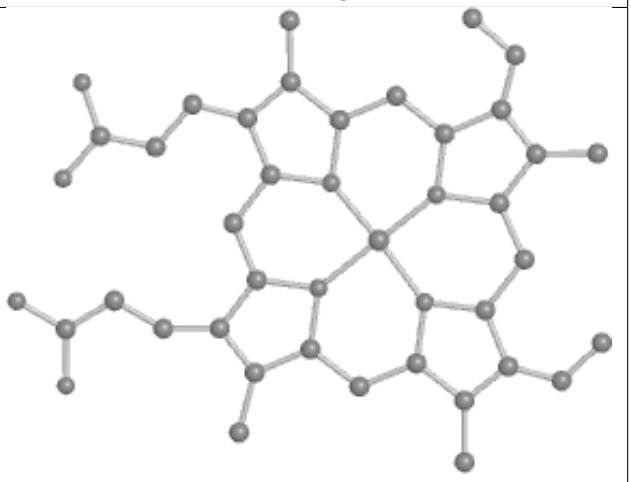
Bond lengths



Bond angles

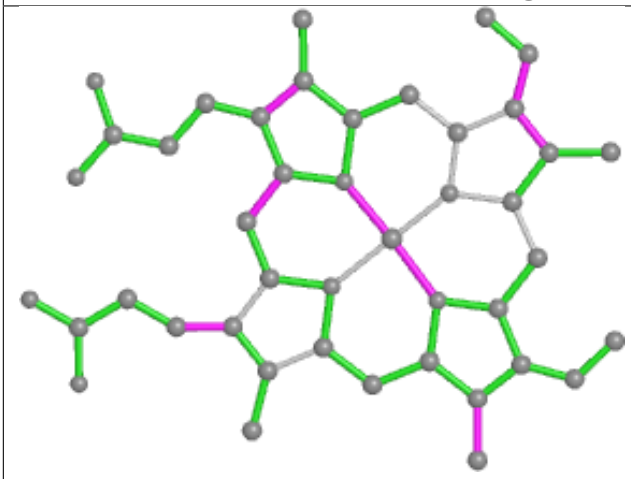


Torsions

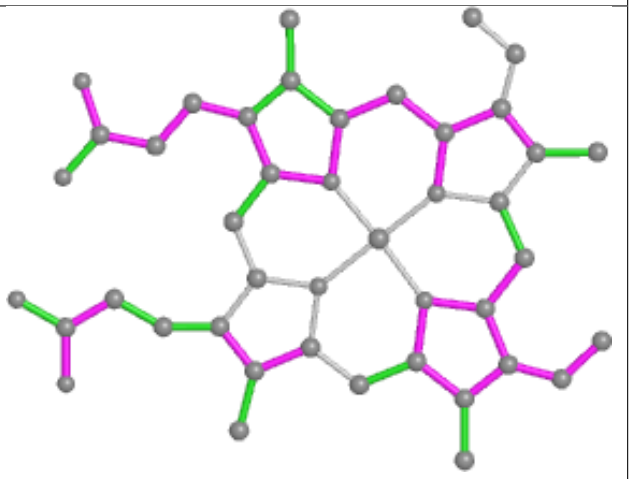


Rings

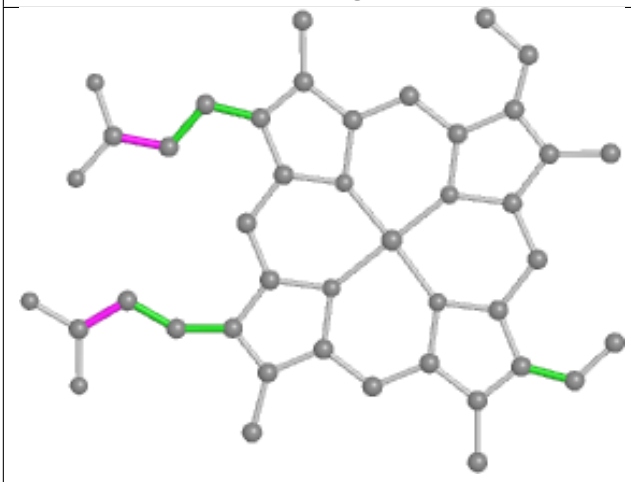
Ligand HEM E 159



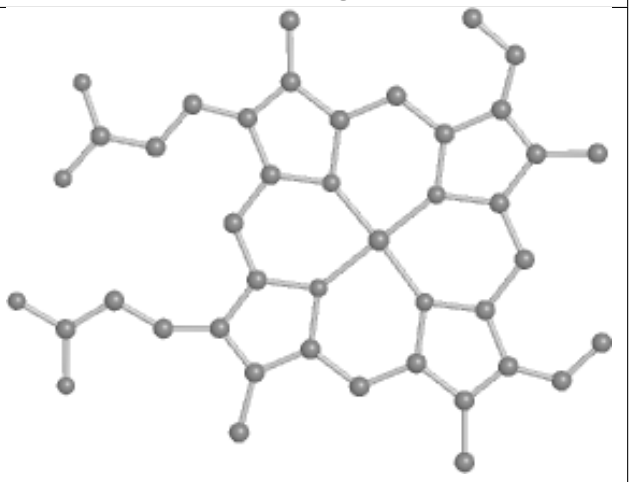
Bond lengths



Bond angles

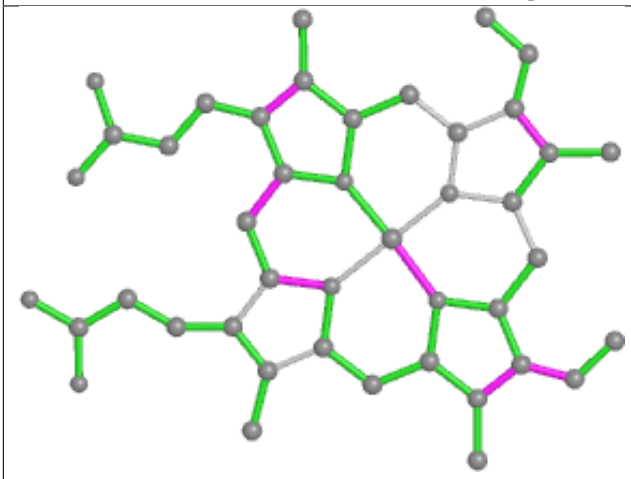


Torsions

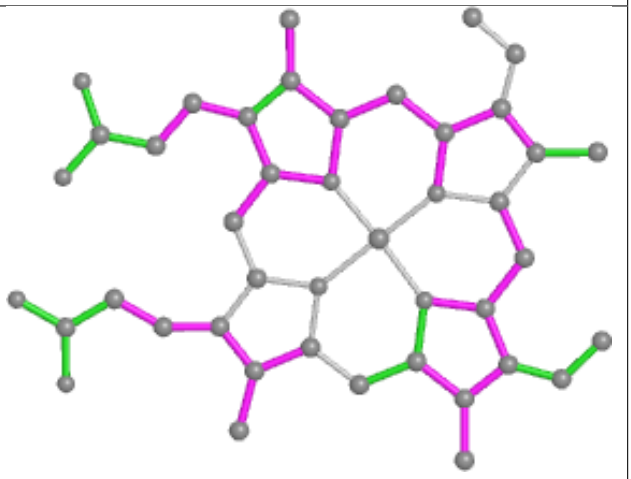


Rings

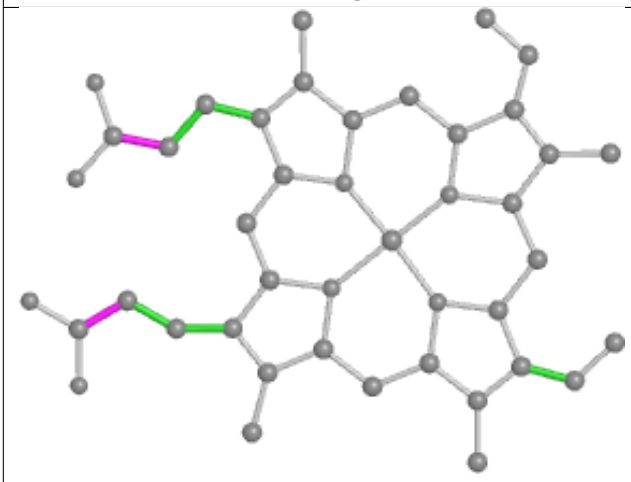
Ligand HEM J 159



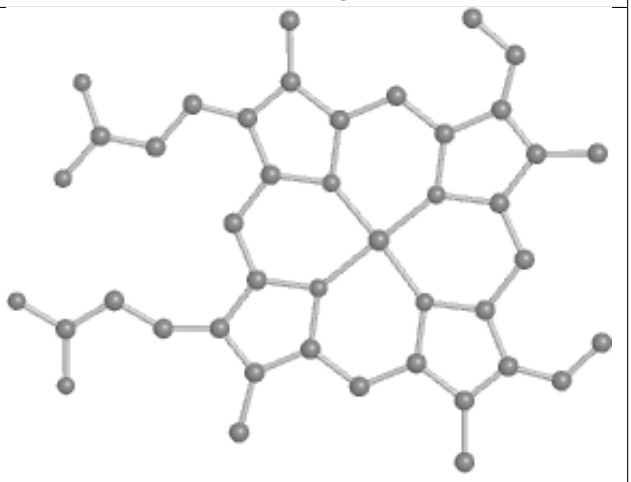
Bond lengths



Bond angles

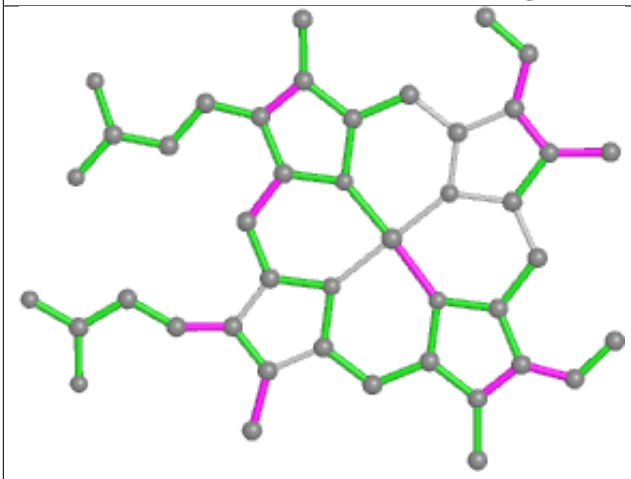


Torsions

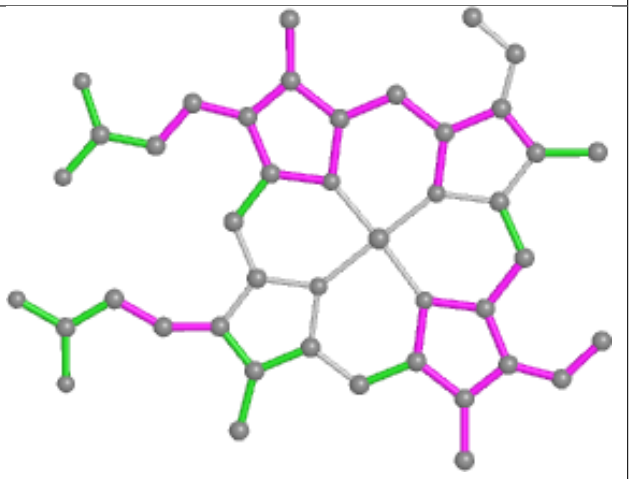


Rings

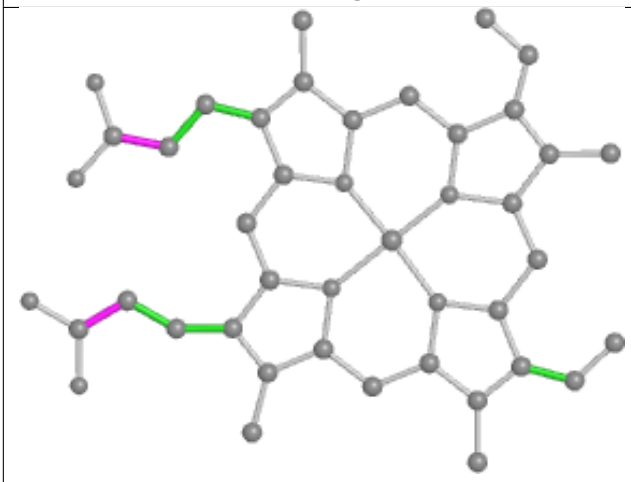
Ligand HEM L 159



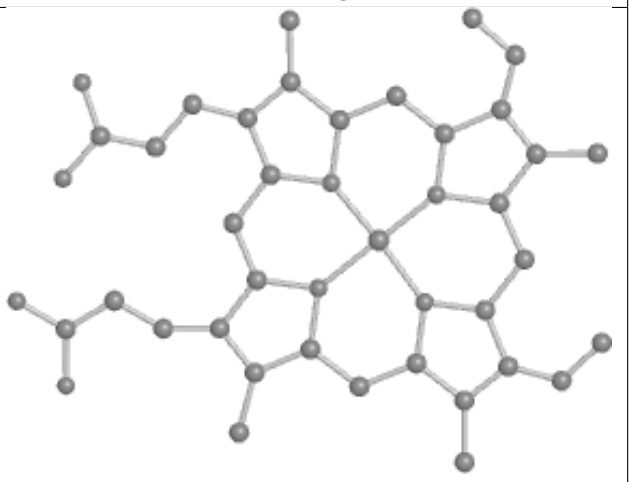
Bond lengths



Bond angles

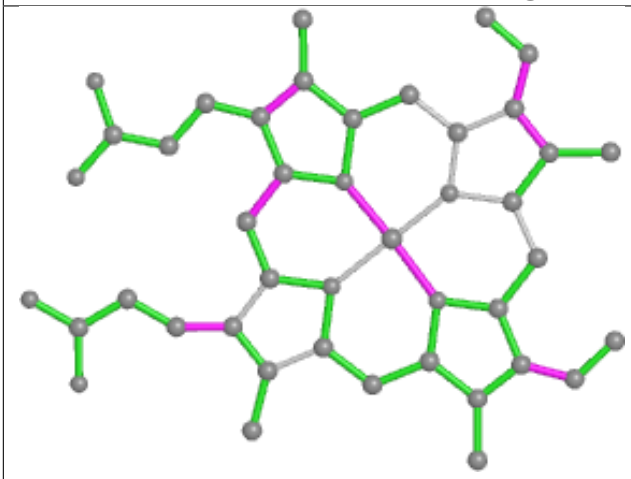


Torsions

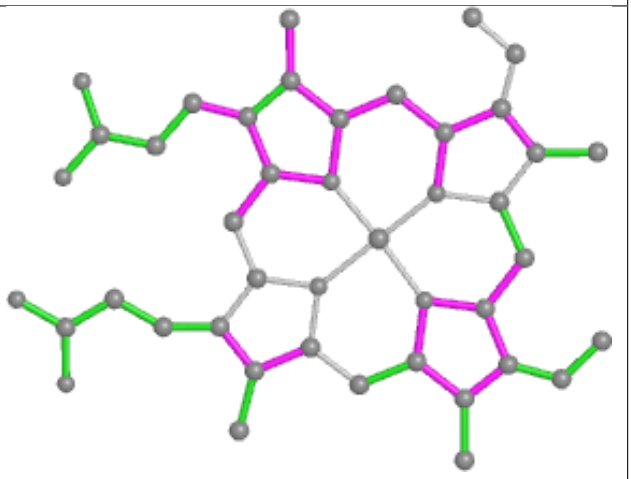


Rings

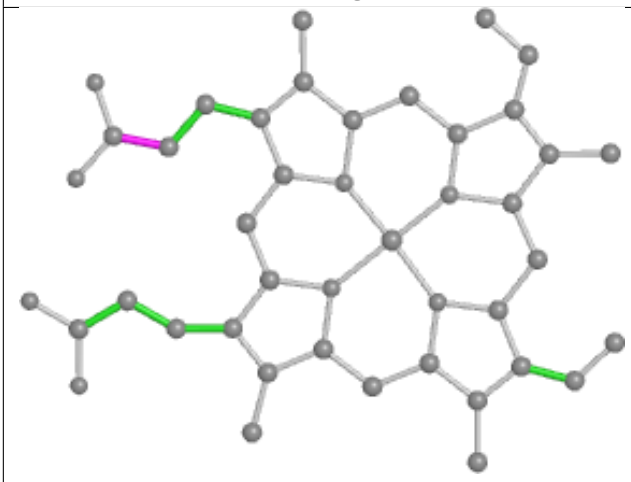
Ligand HEM S 159



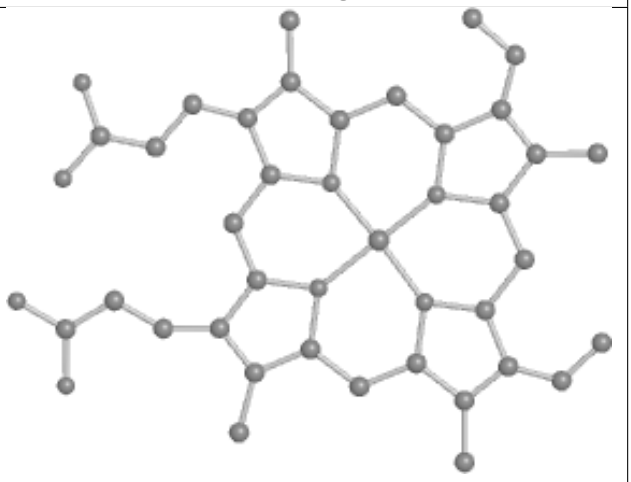
Bond lengths



Bond angles

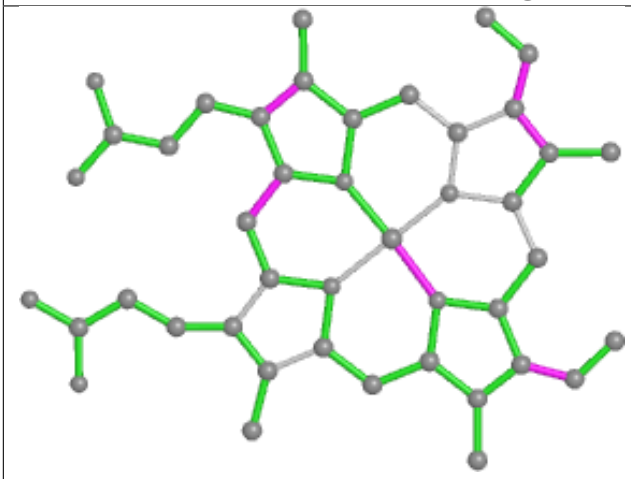


Torsions

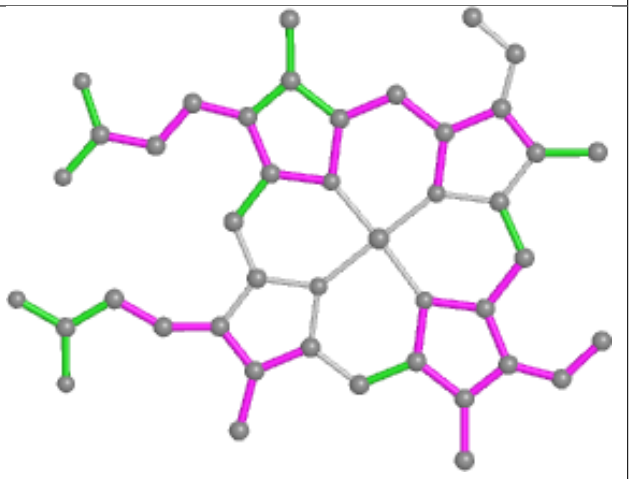


Rings

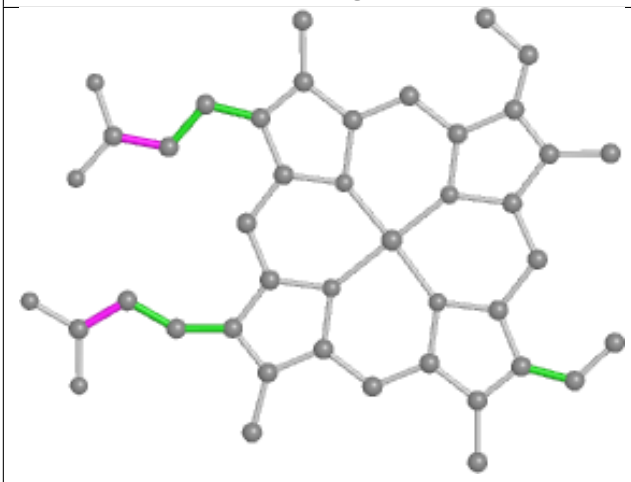
Ligand HEM B 159



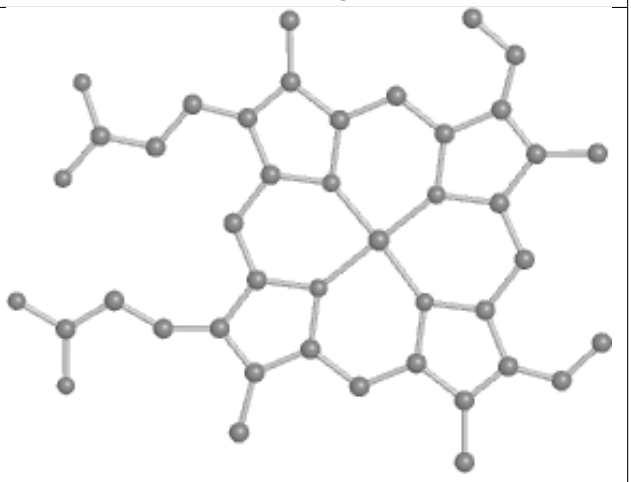
Bond lengths



Bond angles

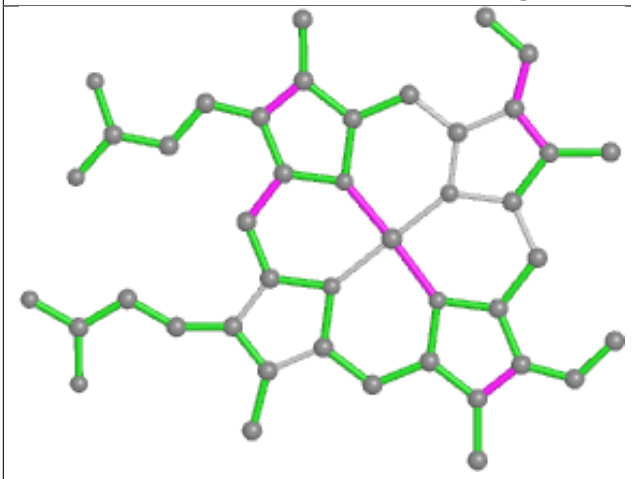


Torsions

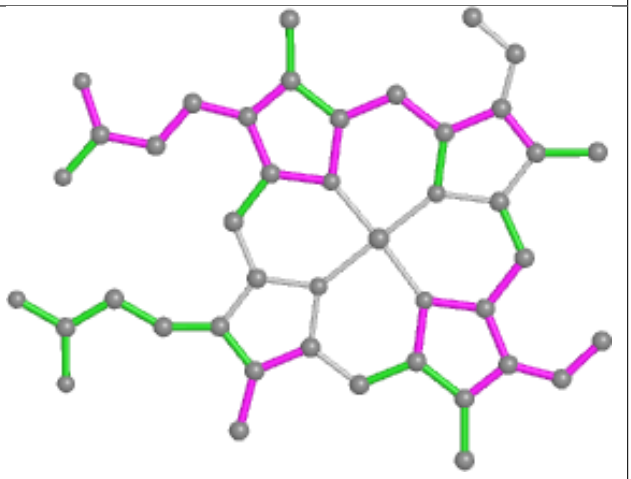


Rings

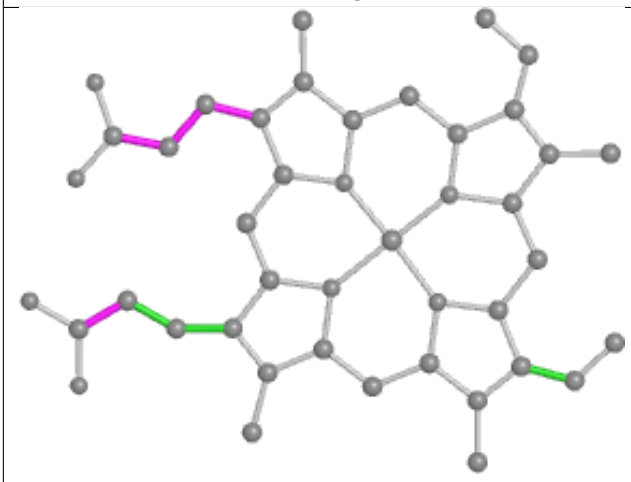
Ligand HEM M 159



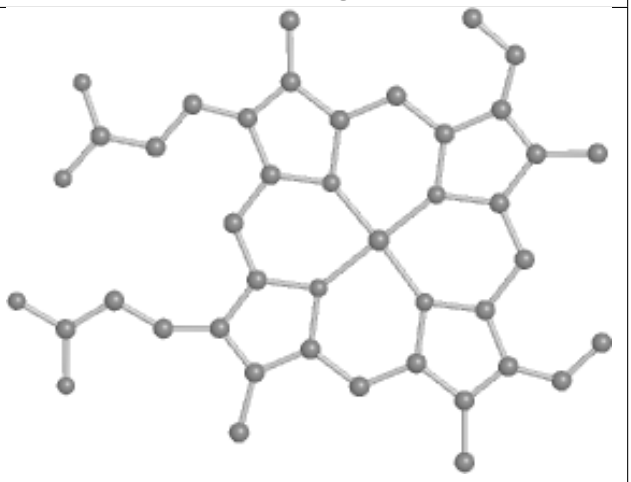
Bond lengths



Bond angles

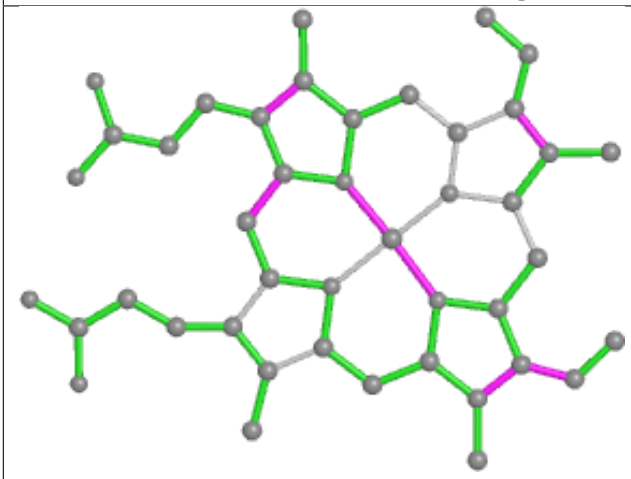


Torsions

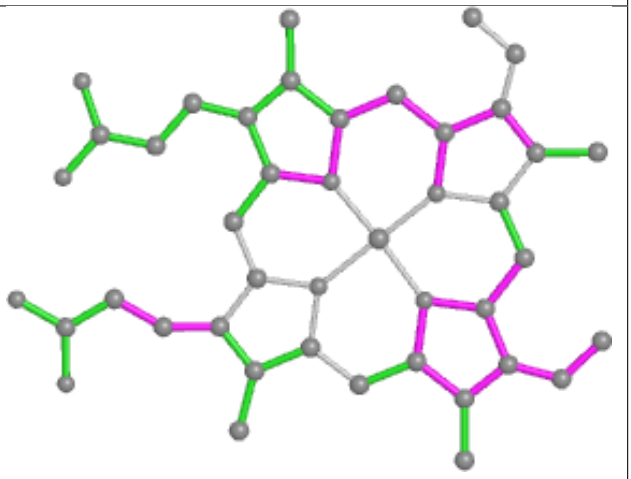


Rings

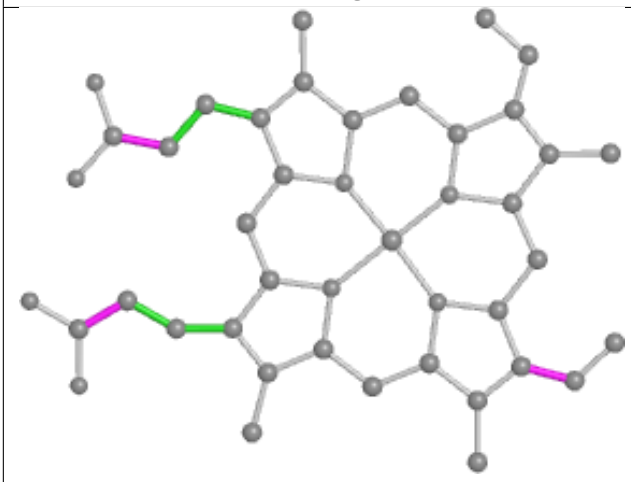
Ligand HEM W 159



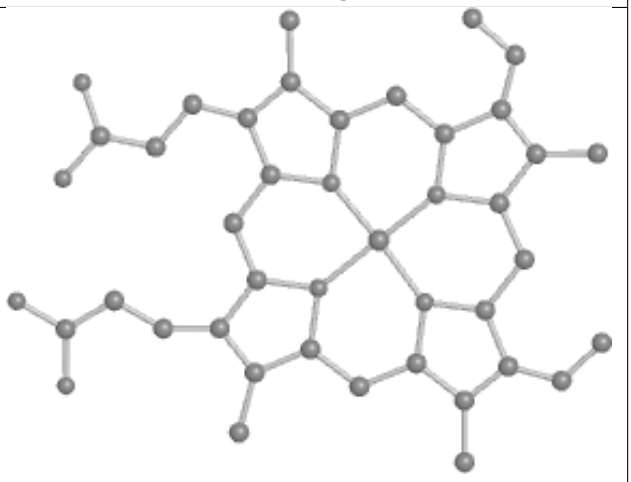
Bond lengths



Bond angles

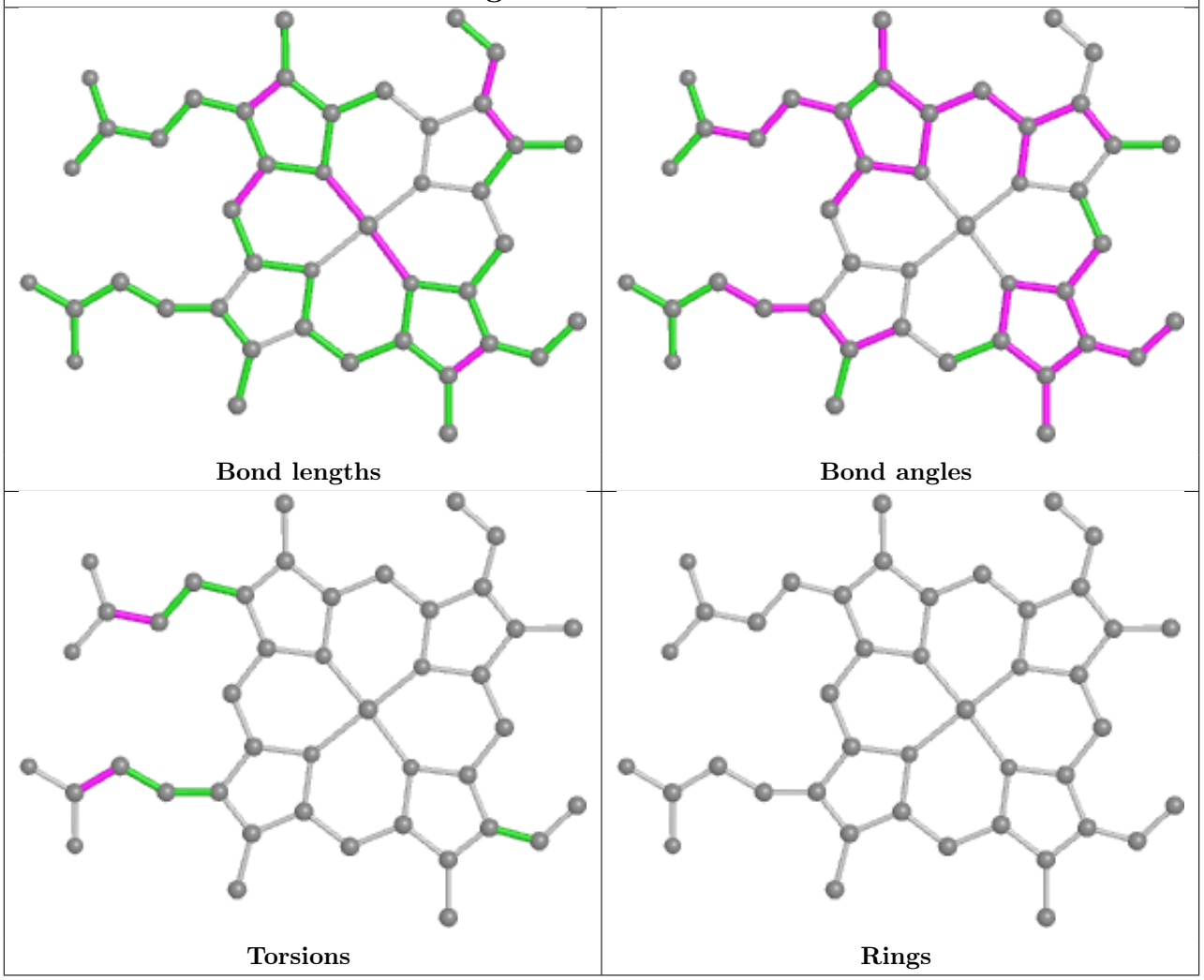


Torsions



Rings

Ligand HEM H 159



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	154/158 (97%)	-0.50	2 (1%) 77 72	32, 38, 47, 56	0
1	B	154/158 (97%)	-0.50	0 100 100	32, 38, 47, 55	0
1	C	154/158 (97%)	-0.51	2 (1%) 77 72	32, 39, 47, 55	0
1	D	154/158 (97%)	-0.50	0 100 100	32, 39, 47, 55	0
1	E	154/158 (97%)	-0.40	1 (0%) 89 86	32, 39, 47, 55	0
1	F	154/158 (97%)	-0.49	1 (0%) 89 86	31, 38, 47, 55	0
1	G	154/158 (97%)	-0.53	0 100 100	32, 38, 47, 55	0
1	H	155/158 (98%)	-0.42	1 (0%) 89 86	32, 38, 47, 57	0
1	I	154/158 (97%)	-0.56	0 100 100	32, 39, 47, 55	0
1	J	154/158 (97%)	-0.63	0 100 100	33, 39, 47, 55	0
1	K	154/158 (97%)	-0.58	0 100 100	32, 39, 47, 55	0
1	L	154/158 (97%)	-0.53	0 100 100	33, 39, 47, 56	0
1	M	154/158 (97%)	-0.51	0 100 100	32, 39, 47, 56	0
1	N	154/158 (97%)	-0.55	0 100 100	32, 39, 47, 55	0
1	O	154/158 (97%)	-0.43	0 100 100	32, 38, 47, 54	0
1	P	154/158 (97%)	-0.55	2 (1%) 77 72	32, 39, 47, 56	0
1	Q	154/158 (97%)	-0.57	2 (1%) 77 72	33, 39, 48, 56	0
1	R	155/158 (98%)	-0.60	0 100 100	33, 39, 48, 55	0
1	S	154/158 (97%)	-0.63	0 100 100	32, 39, 47, 55	0
1	T	154/158 (97%)	-0.58	0 100 100	32, 39, 48, 56	0
1	U	154/158 (97%)	-0.50	0 100 100	32, 39, 47, 55	0
1	V	154/158 (97%)	-0.58	1 (0%) 89 86	33, 39, 48, 56	0
1	W	156/158 (98%)	-0.53	0 100 100	32, 38, 48, 70	0
1	X	154/158 (97%)	-0.49	0 100 100	31, 38, 46, 55	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3700/3792 (97%)	-0.53	12 (0%)	94	93	31, 39, 47, 70	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	156	GLU	3.2
1	A	3	GLY	3.0
1	F	156	GLU	2.9
1	P	156	GLU	2.9
1	Q	76	LYS	2.6
1	Q	156	GLU	2.4
1	C	142	GLN	2.4
1	A	156	GLU	2.4
1	P	142	GLN	2.3
1	C	156	GLU	2.3
1	H	156	GLU	2.2
1	V	110	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	W	160	1/1	0.47	0.25	55,55,55,55	1
2	FE	K	159	1/1	0.53	0.20	44,44,44,44	1
2	FE	B	161	1/1	0.53	0.21	54,54,54,54	1
2	FE	I	159	1/1	0.57	0.23	45,45,45,45	1
2	FE	K	160	1/1	0.59	0.29	54,54,54,54	1

Continued on next page...

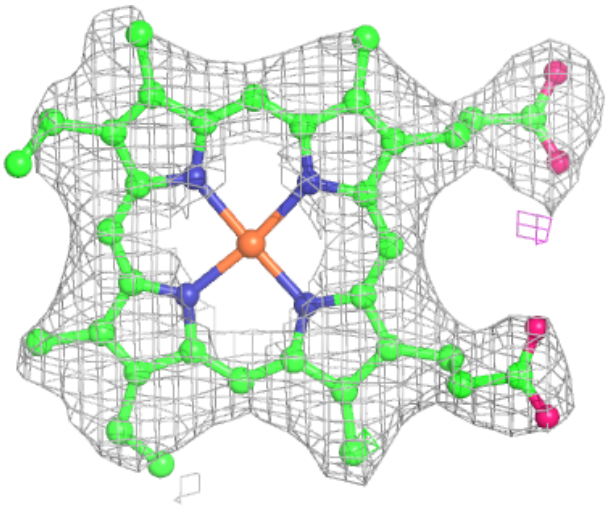
Continued from previous page...

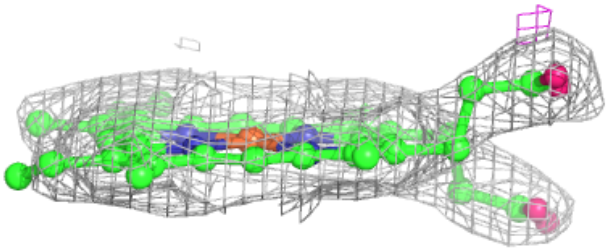
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	P	160	1/1	0.60	0.16	48,48,48,48	1
2	FE	D	160	1/1	0.60	0.21	59,59,59,59	1
2	FE	P	161	1/1	0.62	0.26	56,56,56,56	1
2	FE	T	159	1/1	0.66	0.23	46,46,46,46	1
3	K	C	160	1/1	0.67	0.20	35,35,35,35	1
2	FE	G	160	1/1	0.69	0.19	46,46,46,46	1
2	FE	F	159	1/1	0.72	0.15	42,42,42,42	1
2	FE	V	160	1/1	0.73	0.13	48,48,48,48	1
2	FE	E	160	1/1	0.76	0.18	45,45,45,45	1
2	FE	M	160	1/1	0.76	0.16	47,47,47,47	1
2	FE	U	160	1/1	0.77	0.21	57,57,57,57	1
2	FE	N	159	1/1	0.77	0.19	54,54,54,54	1
2	FE	Q	159	1/1	0.77	0.22	43,43,43,43	1
2	FE	L	160	1/1	0.77	0.13	57,57,57,57	1
2	FE	A	159	1/1	0.78	0.24	50,50,50,50	1
2	FE	V	159	1/1	0.79	0.20	50,50,50,50	1
2	FE	G	159	1/1	0.79	0.14	41,41,41,41	1
3	K	B	162	1/1	0.85	0.38	33,33,33,33	1
2	FE	C	159	1/1	0.86	0.18	56,56,56,56	1
3	K	N	160	1/1	0.88	0.14	29,29,29,29	1
2	FE	A	160	1/1	0.89	0.12	42,42,42,42	1
2	FE	B	160	1/1	0.89	0.21	36,36,36,36	1
3	K	V	161	1/1	0.89	0.15	37,37,37,37	1
4	HEM	J	159	43/43	0.95	0.16	44,48,51,53	0
4	HEM	E	159	43/43	0.96	0.15	40,44,52,53	0
4	HEM	H	159	43/43	0.96	0.18	37,40,48,49	0
4	HEM	D	159	43/43	0.96	0.17	39,43,50,53	0
4	HEM	P	159	43/43	0.96	0.18	43,46,51,56	0
4	HEM	R	159	43/43	0.96	0.18	47,52,55,58	0
4	HEM	S	159	43/43	0.96	0.19	40,43,49,52	0
4	HEM	U	159	43/43	0.96	0.26	45,50,55,59	0
4	HEM	W	159	43/43	0.96	0.17	38,42,49,54	0
4	HEM	B	159	43/43	0.97	0.16	36,40,46,49	0
4	HEM	L	159	43/43	0.97	0.14	44,47,51,54	0
4	HEM	M	159	43/43	0.97	0.16	45,50,56,58	0
3	K	A	161	1/1	0.97	0.16	27,27,27,27	1
3	K	G	161	1/1	0.98	0.13	24,24,24,24	1

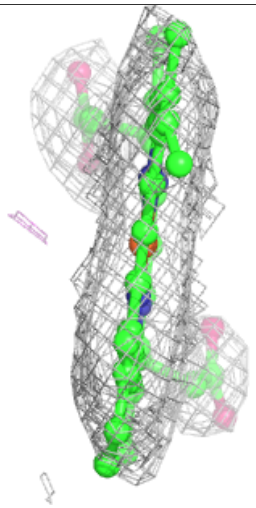
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM J 159:

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

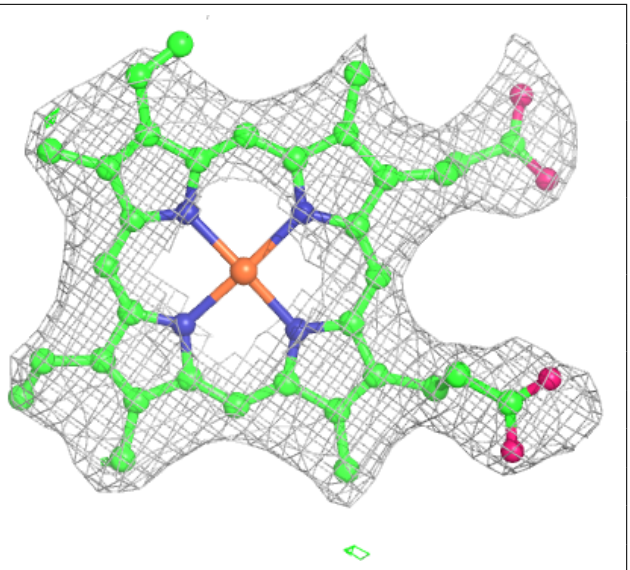


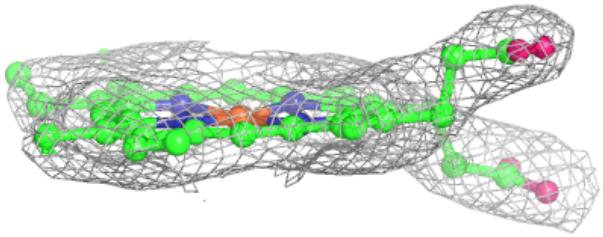


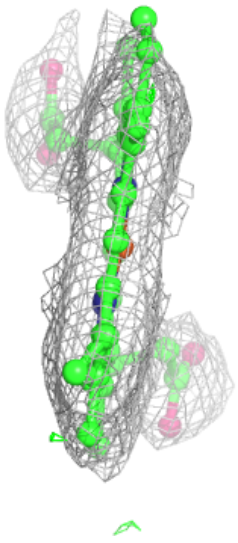


Electron density around HEM E 159:

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

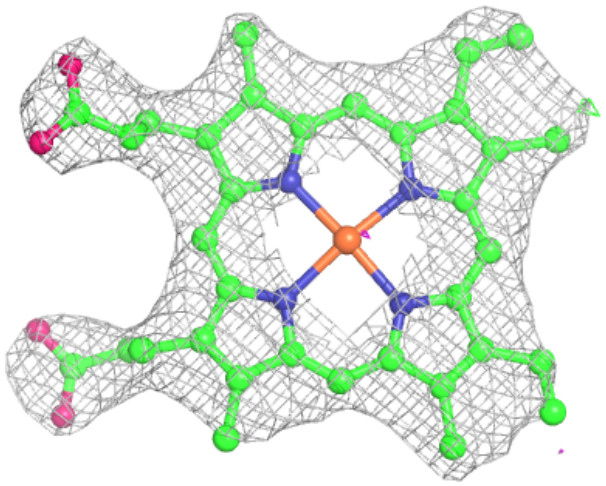


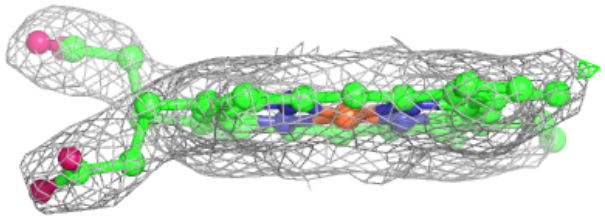


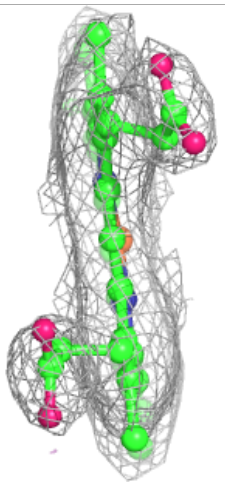


Electron density around HEM H 159:

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

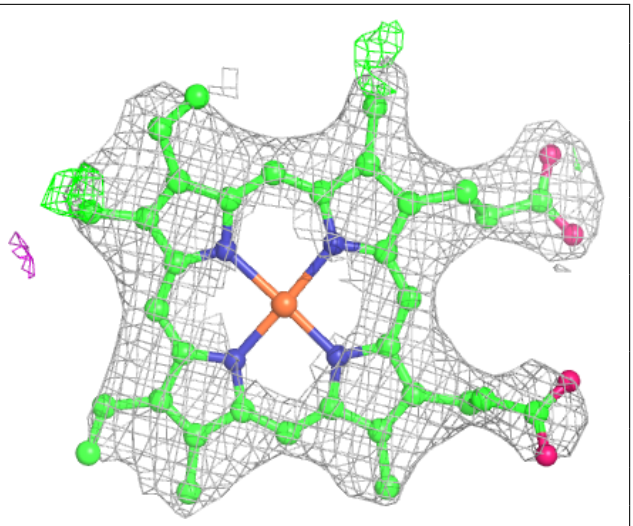


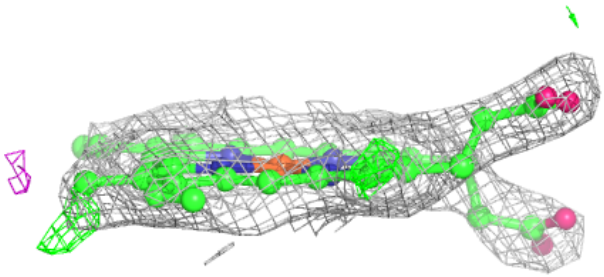


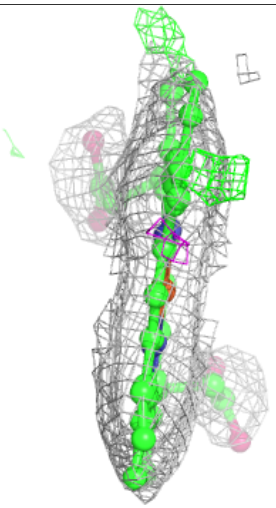


Electron density around HEM D 159:

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

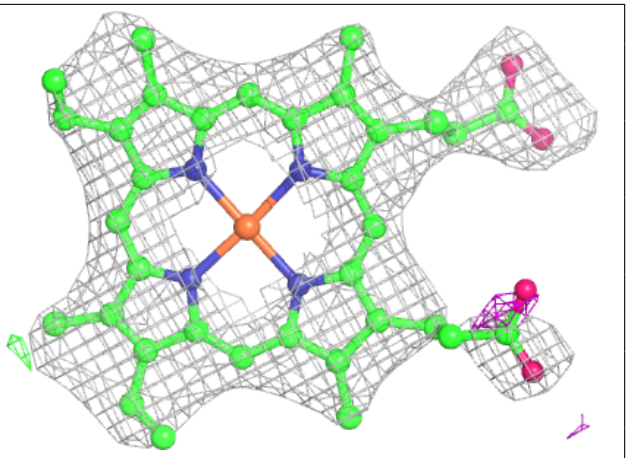


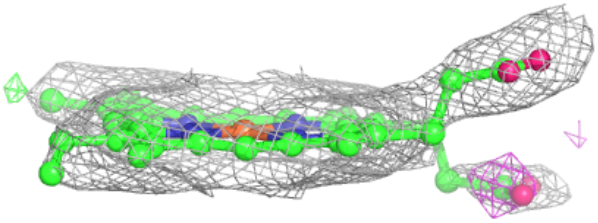


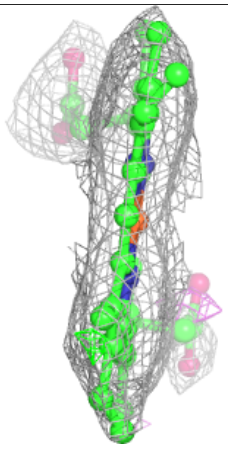


Electron density around HEM P 159:

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

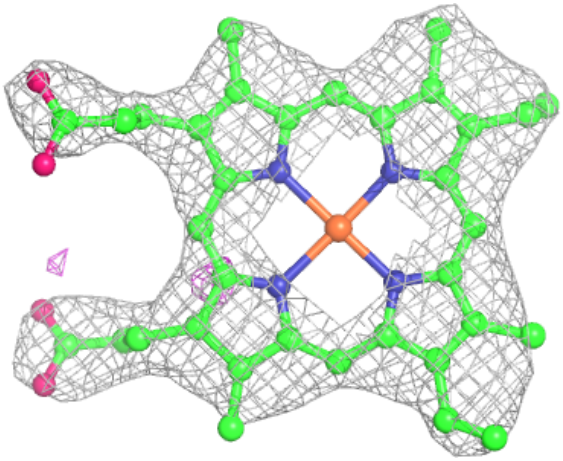


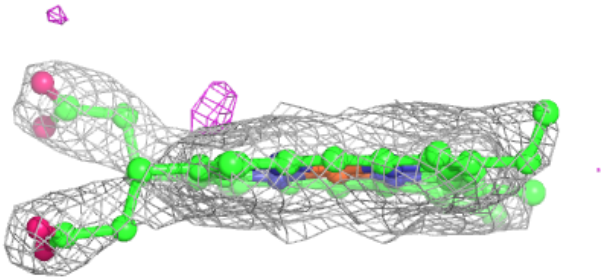


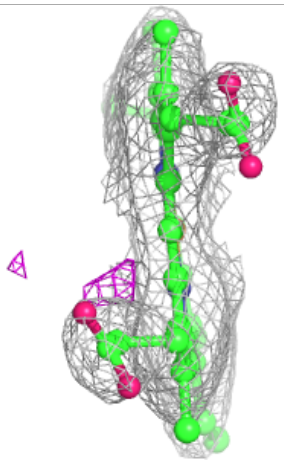


Electron density around HEM R 159:

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

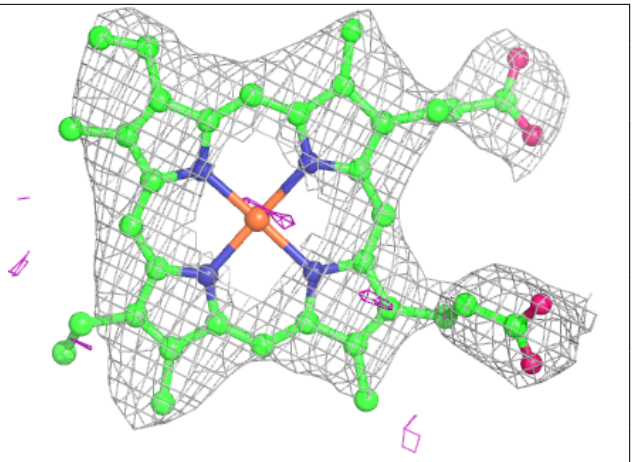


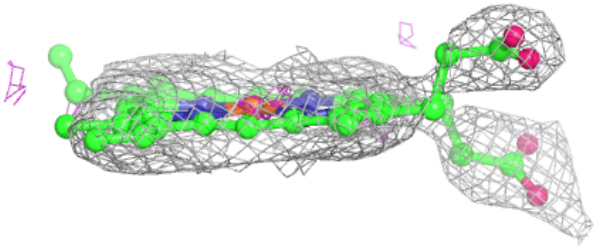


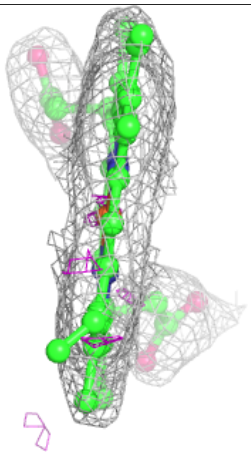


Electron density around HEM S 159:

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

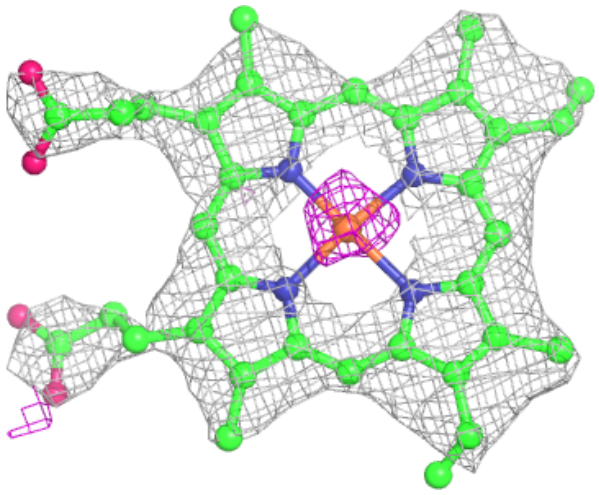


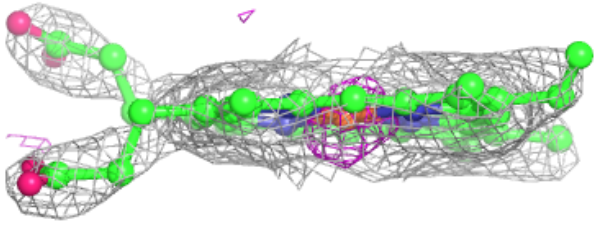


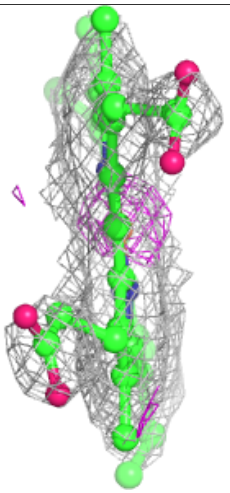


Electron density around HEM U 159:

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

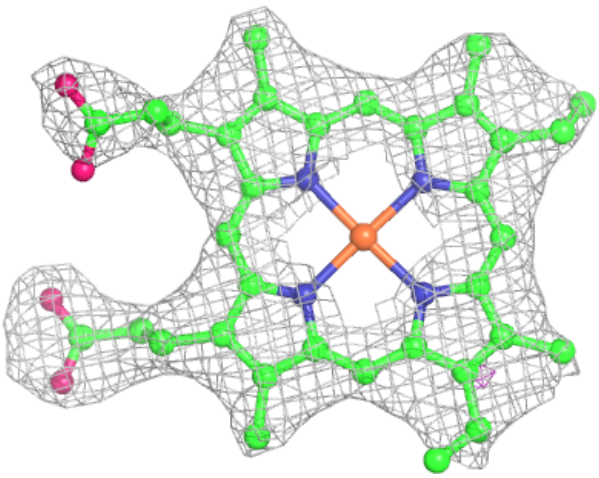


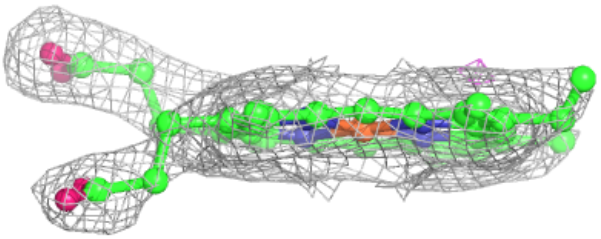


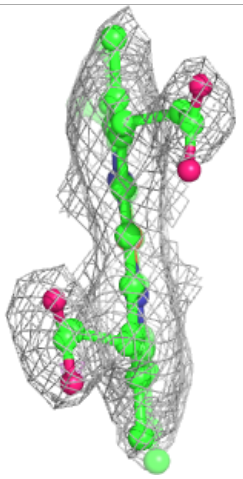


Electron density around HEM W 159:

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

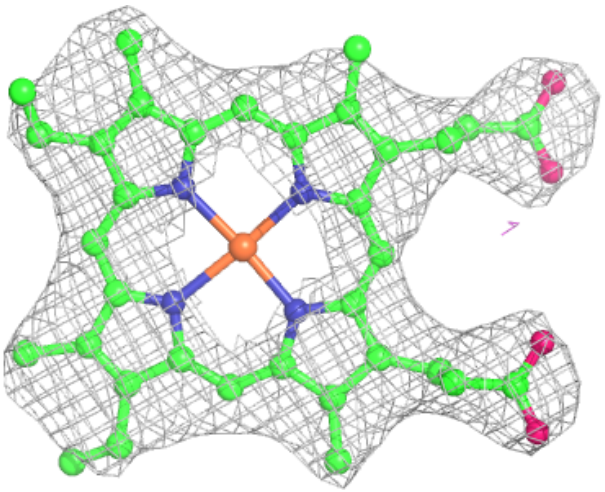


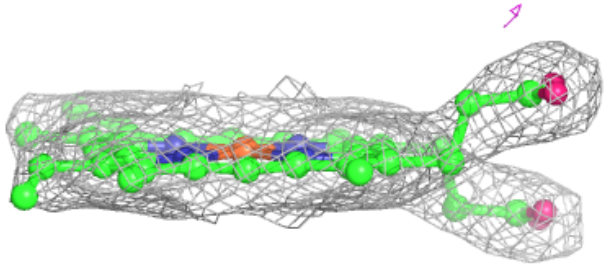


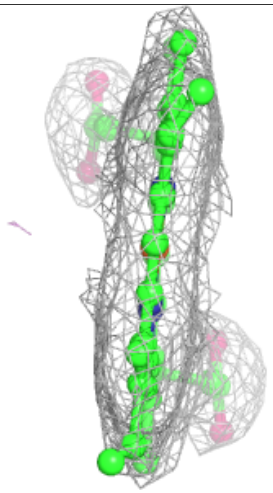


Electron density around HEM B 159:

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

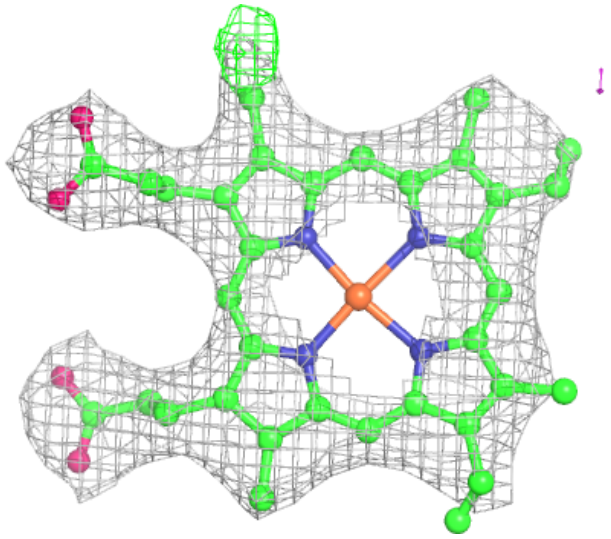


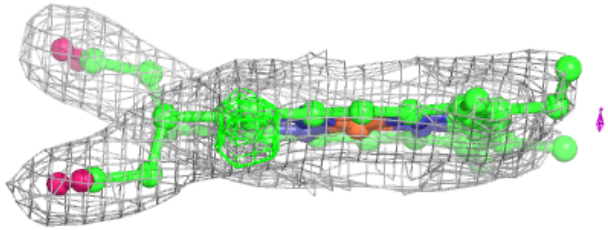


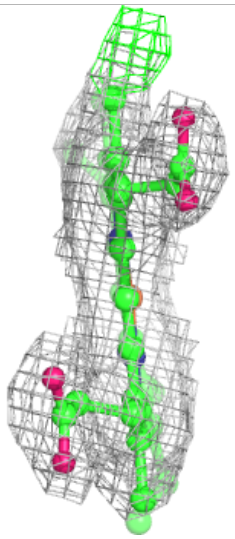


Electron density around HEM L 159:

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

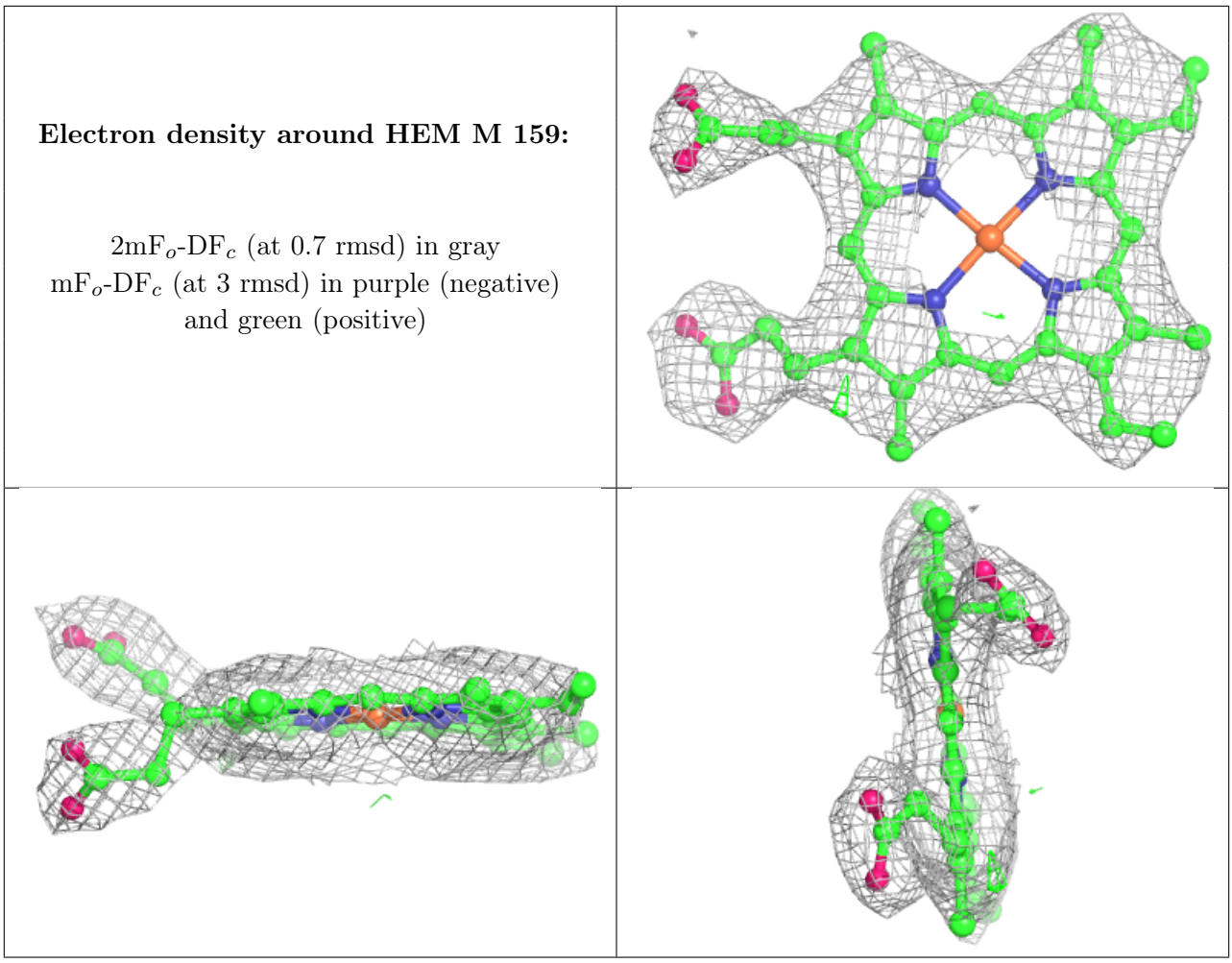






Electron density around HEM M 159:

$2mF_o$-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.