Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 06:37 PM EDT

PDB ID	:	3IS8
Title	:	Structure of mineralized Bfrb soaked with FeSO4 from Pseudomonas aeruginosa to 2.25A Resolution
Authors	:	Lovell, S.; Weeratunga, S.K.; Battaile, K.P.; Rivera, M.
Deposited on	:	2009-08-25
Resolution	:	2.25 Å(reported)

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

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

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

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

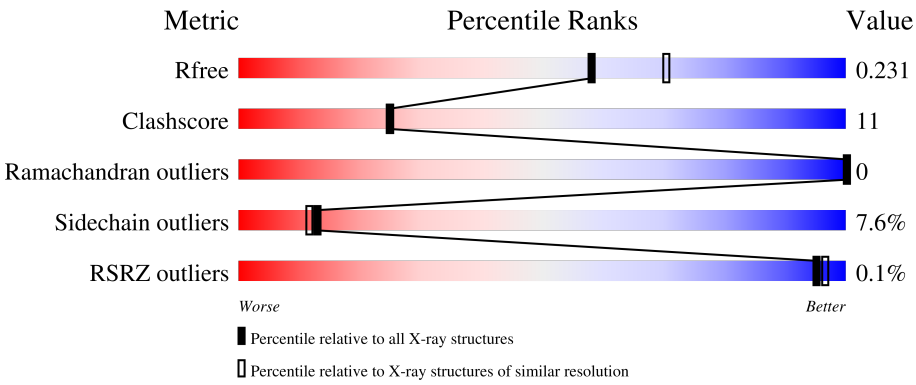
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	77% 18% • •
1	C	158	78% 17% • •
1	D	158	% 80% 15% • •
1	E	158	77% 18% • •

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Mol	Chain	Length	Quality of chain
1	F	158	78% 16%
1	G	158	80% 15%
1	H	158	% 81% 13%
1	I	158	77% 17%
1	J	158	80% 15%
1	K	158	84% 11%
1	L	158	79% 16%
1	M	158	78% 16%
1	N	158	82% 15%
1	O	158	78% 17%
1	P	158	77% 17%
1	Q	158	77% 18%
1	R	158	79% 16%
1	S	158	78% 18%
1	T	158	82% 14%
1	U	158	78% 15%
1	V	158	75% 20%
1	W	158	% 80% 15%
1	X	158	75% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	D	163	-	-	X	-
5	SO4	O	163	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 32963 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
			Total	C	N	O	S			
1	A	155	1289	816	224	243	6	0	2	0
1	B	155	1287	815	223	243	6	0	2	0
1	C	155	1288	816	223	243	6	0	2	0
1	D	154	1280	810	222	242	6	0	2	0
1	E	155	1286	814	223	243	6	0	2	0
1	F	155	1285	813	223	243	6	0	2	0
1	G	155	1286	814	223	243	6	0	2	0
1	H	154	1280	810	222	242	6	0	2	0
1	I	154	1280	810	222	242	6	0	2	0
1	J	155	1286	814	223	243	6	0	2	0
1	K	155	1289	816	224	243	6	0	2	0
1	L	155	1286	814	223	243	6	0	2	0
1	M	155	1280	810	221	243	6	0	2	0
1	N	155	1280	810	221	243	6	0	2	0
1	O	155	1285	814	222	243	6	0	2	0
1	P	155	1282	811	222	243	6	0	2	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	155	1289	816	224	243	6	0	2	0
			Total	C	N	O	S			
1	R	155	1284	813	222	243	6	0	2	0
			Total	C	N	O	S			
1	S	155	1284	813	222	243	6	0	2	0
			Total	C	N	O	S			
1	T	155	1281	811	221	243	6	0	2	0
			Total	C	N	O	S			
1	U	154	1276	808	220	242	6	0	2	0
			Total	C	N	O	S			
1	V	155	1281	811	221	243	6	0	2	0
			Total	C	N	O	S			
1	W	155	1279	809	221	243	6	0	2	0
			Total	C	N	O	S			
1	X	155	1282	811	222	243	6	0	2	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	5	5	5	0	0
			Total	Fe		
2	B	5	5	5	0	0
			Total	Fe		
2	C	5	5	5	0	0
			Total	Fe		
2	D	4	4	4	0	0
			Total	Fe		
2	E	5	5	5	0	0
			Total	Fe		
2	F	4	4	4	0	0
			Total	Fe		
2	G	5	5	5	0	0
			Total	Fe		
2	H	3	3	3	0	0
			Total	Fe		
2	I	4	4	4	0	0
			Total	Fe		
2	J	4	4	4	0	0
			Total	Fe		
2	K	4	4	4	0	0

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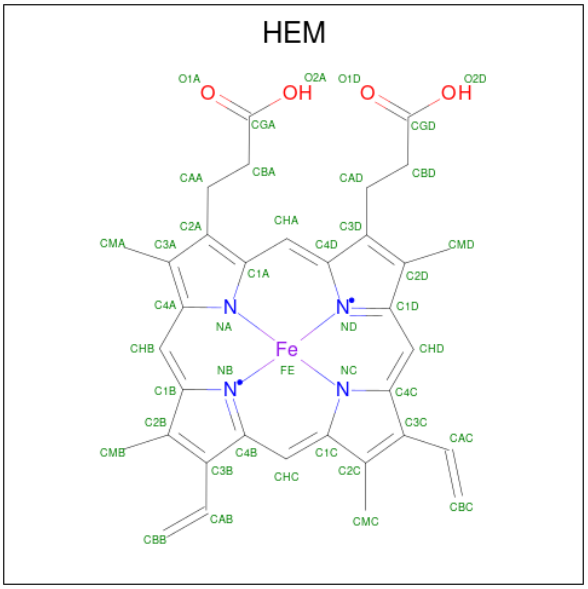
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	L	4	4	4	0	0
2	M	4	4	4	0	0
2	N	5	5	5	0	0
2	O	4	4	4	0	0
2	P	4	4	4	0	0
2	Q	4	4	4	0	0
2	R	4	4	4	0	0
2	S	4	4	4	0	0
2	T	3	3	3	0	0
2	U	3	3	3	0	0
2	V	3	3	3	0	0
2	W	3	3	3	0	0
2	X	3	3	3	0	0

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

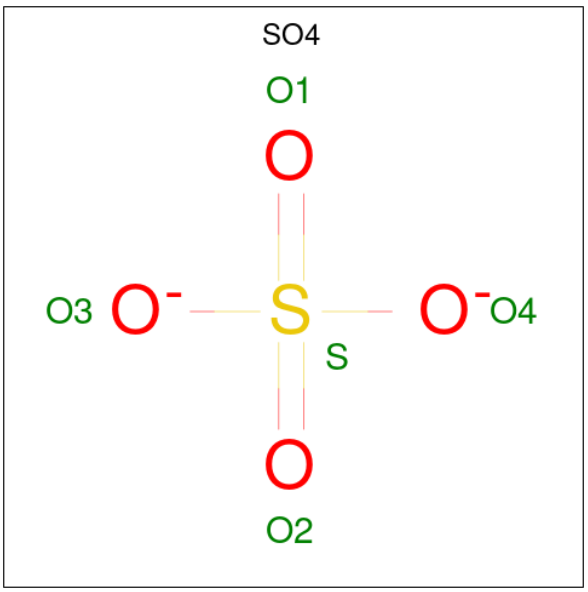
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	E	1	1	1	0	0
3	G	1	1	1	0	0
3	N	1	1	1	0	0

- 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
			Total	C	Fe	N	O		
4	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	F	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	H	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	I	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	L	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	N	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	P	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	Q	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	S	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	U	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	X	1	43	34	1	4	4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	M	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	R	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	61	Total O 61 61	0	0
6	B	56	Total O 56 56	0	0
6	C	65	Total O 65 65	0	0

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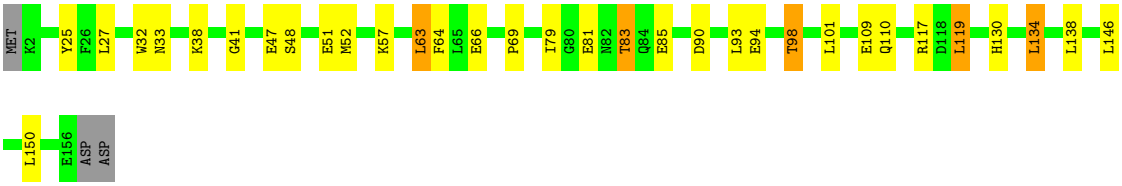
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	62	Total O 62 62	0	0
6	E	69	Total O 69 69	0	0
6	F	62	Total O 62 62	0	0
6	G	70	Total O 70 70	0	0
6	H	73	Total O 73 73	0	0
6	I	61	Total O 61 61	0	0
6	J	58	Total O 58 58	0	0
6	K	67	Total O 67 67	0	0
6	L	59	Total O 59 59	0	0
6	M	57	Total O 57 57	0	0
6	N	51	Total O 51 51	0	0
6	O	68	Total O 68 68	0	0
6	P	52	Total O 52 52	0	0
6	Q	70	Total O 70 70	0	0
6	R	72	Total O 72 72	0	0
6	S	64	Total O 64 64	0	0
6	T	51	Total O 51 51	0	0
6	U	69	Total O 69 69	0	0
6	V	68	Total O 68 68	0	0
6	W	65	Total O 65 65	0	0
6	X	50	Total O 50 50	0	0

3 Residue-property plots (i)

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

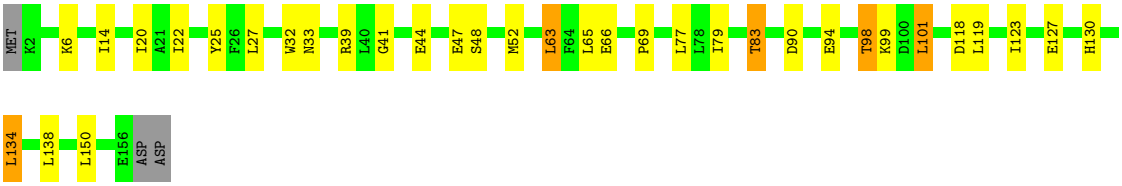
• Molecule 1: Bacterioferritin

Chain A:



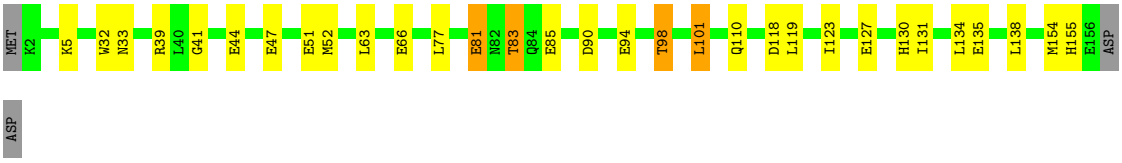
• Molecule 1: Bacterioferritin

Chain B:



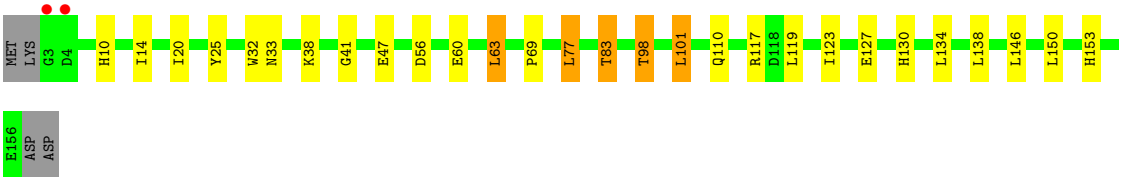
• Molecule 1: Bacterioferritin

Chain C:



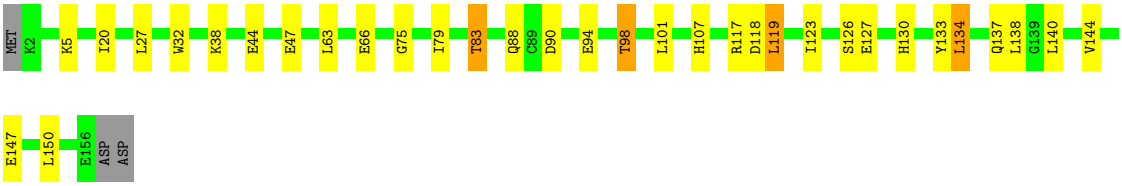
• Molecule 1: Bacterioferritin

Chain D:



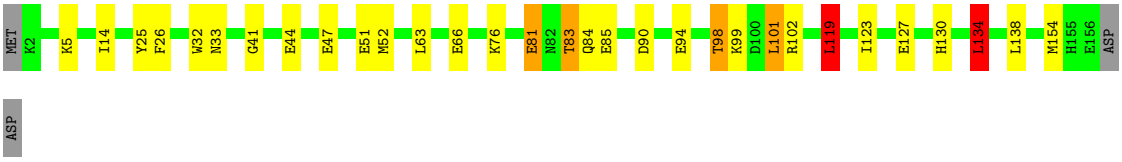
• Molecule 1: Bacterioferritin

Chain E:



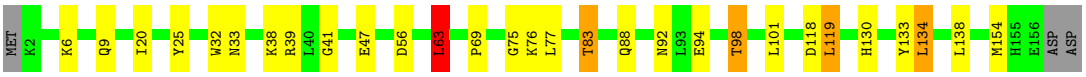
• Molecule 1: Bacterioferritin

Chain F:



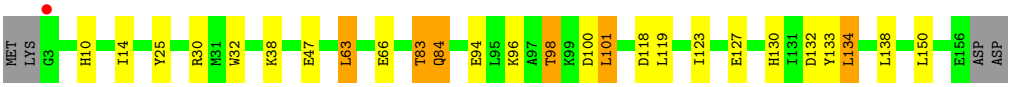
• Molecule 1: Bacterioferritin

Chain G:



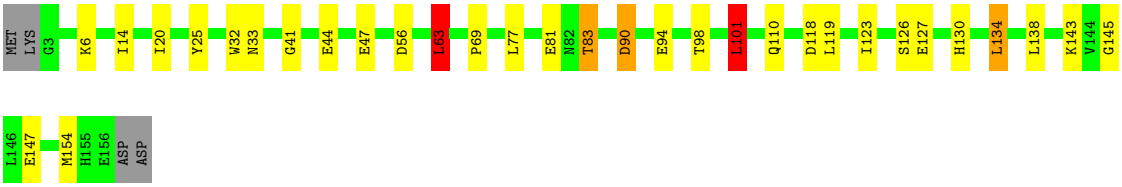
• Molecule 1: Bacterioferritin

Chain H:



• Molecule 1: Bacterioferritin

Chain I:



• Molecule 1: Bacterioferritin

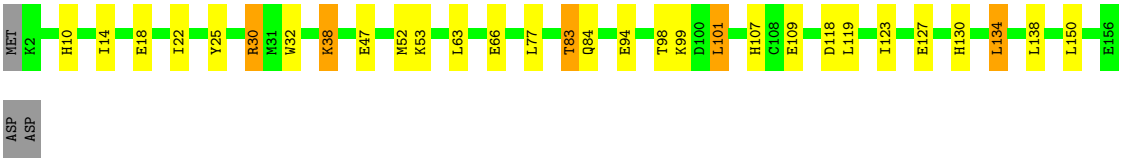
Chain J:

• Molecule 1: Bacterioferritin

Chain K:

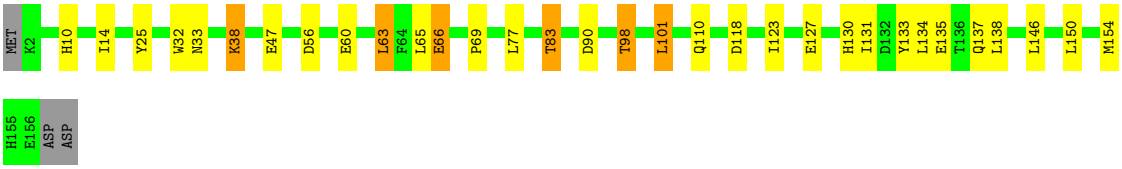
• Molecule 1: Bacterioferritin

Chain L:



• Molecule 1: Bacterioferritin

Chain M:

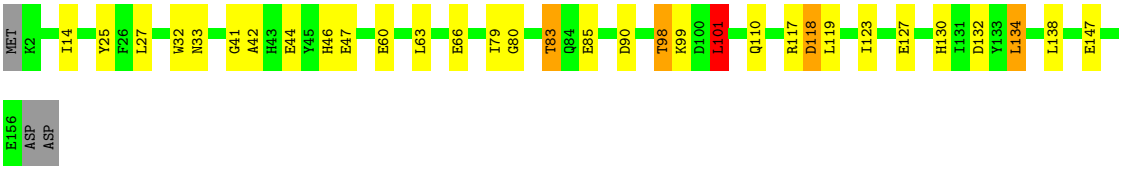


• Molecule 1: Bacterioferritin

Chain N:

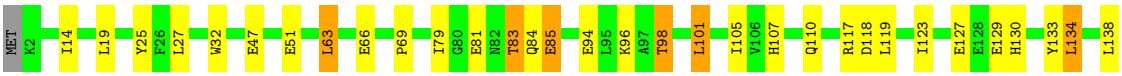
• Molecule 1: Bacterioferritin

Chain O:



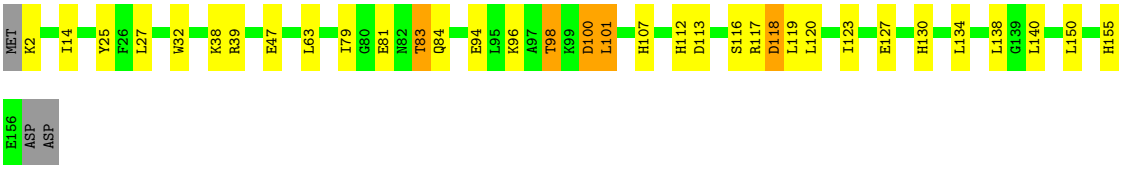
• Molecule 1: Bacterioferritin

Chain P:



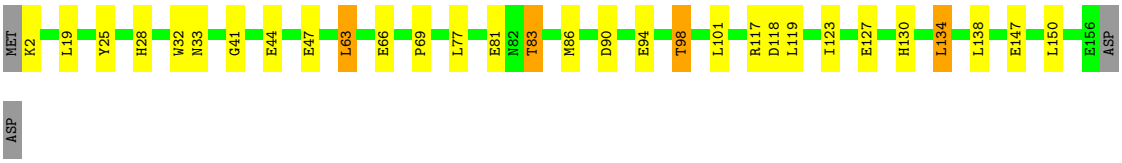
• Molecule 1: Bacterioferritin

Chain Q:



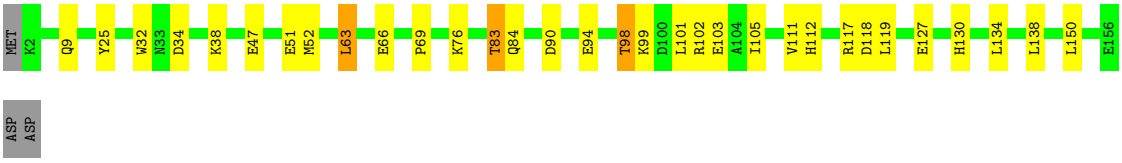
• Molecule 1: Bacterioferritin

Chain R:



• Molecule 1: Bacterioferritin

Chain S:

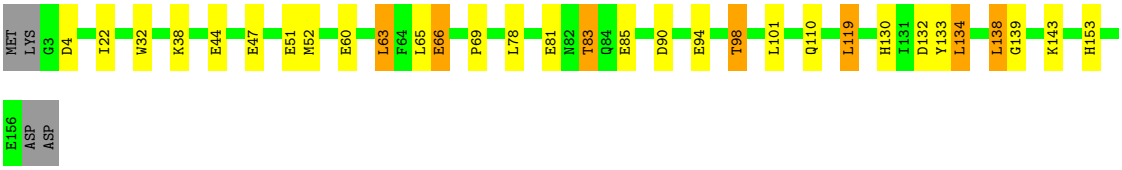


• Molecule 1: Bacterioferritin

Chain T:

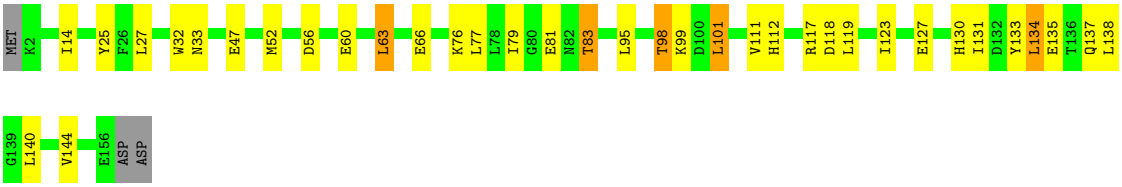
• Molecule 1: Bacterioferritin

Chain U:



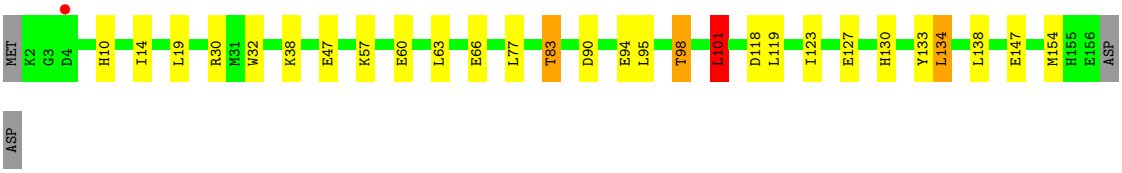
• Molecule 1: Bacterioferritin

Chain V:



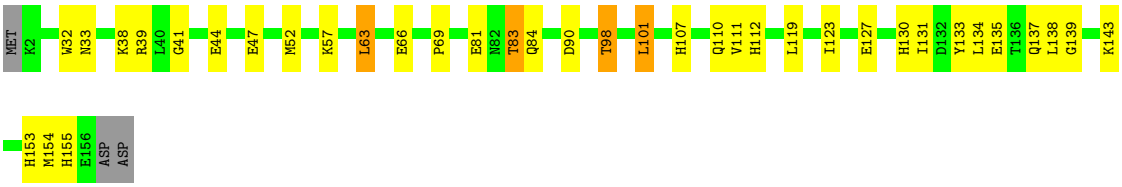
• Molecule 1: Bacterioferritin

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	125.72Å 203.28Å 207.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 49.36 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.25) 99.7 (49.36-2.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.25Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0066	Depositor
R, R_{free}	0.177 , 0.226 0.185 , 0.231	Depositor DCC
R_{free} test set	12585 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32963	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, K, SO4, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.97	2/1318 (0.2%)	0.83	0/1774
1	B	0.92	0/1316	0.82	1/1772 (0.1%)
1	C	0.90	1/1317 (0.1%)	0.81	1/1773 (0.1%)
1	D	0.94	0/1309	0.84	0/1763
1	E	0.87	0/1315	0.82	1/1771 (0.1%)
1	F	0.92	2/1314 (0.2%)	0.82	2/1770 (0.1%)
1	G	0.89	0/1315	0.87	5/1771 (0.3%)
1	H	0.90	0/1309	0.86	2/1763 (0.1%)
1	I	0.88	1/1309 (0.1%)	0.90	6/1763 (0.3%)
1	J	0.92	1/1315 (0.1%)	0.85	1/1771 (0.1%)
1	K	0.87	0/1318	0.86	4/1774 (0.2%)
1	L	0.89	1/1315 (0.1%)	0.84	1/1771 (0.1%)
1	M	0.86	0/1309	0.80	1/1765 (0.1%)
1	N	0.82	0/1309	0.79	1/1765 (0.1%)
1	O	0.87	1/1314 (0.1%)	0.80	2/1770 (0.1%)
1	P	0.88	2/1311 (0.2%)	0.83	0/1767
1	Q	0.91	0/1318	0.88	4/1774 (0.2%)
1	R	0.87	0/1313	0.81	0/1769
1	S	0.90	0/1313	0.84	2/1769 (0.1%)
1	T	0.86	0/1310	0.83	0/1766
1	U	0.93	1/1305 (0.1%)	0.87	2/1759 (0.1%)
1	V	0.91	0/1310	0.86	2/1766 (0.1%)
1	W	0.90	2/1308 (0.2%)	0.83	3/1764 (0.2%)
1	X	0.86	0/1311	0.79	1/1767 (0.1%)
All	All	0.89	14/31501 (0.0%)	0.84	42/42437 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GLU	CB-CG	7.83	1.67	1.52
1	F	66	GLU	CB-CG	7.68	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GLU	CG-CD	6.27	1.61	1.51
1	L	99	LYS	CD-CE	5.96	1.66	1.51
1	U	60	GLU	CG-CD	5.75	1.60	1.51
1	W	66	GLU	CG-CD	5.75	1.60	1.51
1	C	81	GLU	CG-CD	5.73	1.60	1.51
1	P	85	GLU	CG-CD	5.56	1.60	1.51
1	J	60	GLU	CG-CD	5.45	1.60	1.51
1	P	129	GLU	CG-CD	5.29	1.59	1.51
1	O	60	GLU	CG-CD	5.29	1.59	1.51
1	I	81	GLU	CG-CD	5.26	1.59	1.51
1	W	66	GLU	CB-CG	5.24	1.62	1.52
1	F	66	GLU	CG-CD	5.18	1.59	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	56	ASP	CB-CG-OD1	7.74	125.27	118.30
1	Q	101	LEU	CA-CB-CG	7.72	133.07	115.30
1	Q	118	ASP	CB-CG-OD1	-7.02	111.99	118.30
1	C	101	LEU	CA-CB-CG	7.00	131.41	115.30
1	I	90	ASP	CB-CG-OD1	6.79	124.41	118.30
1	W	90	ASP	CB-CG-OD1	6.72	124.35	118.30
1	V	63	LEU	CA-CB-CG	6.62	130.52	115.30
1	G	56	ASP	CB-CG-OD1	6.46	124.11	118.30
1	E	134	LEU	CA-CB-CG	6.21	129.59	115.30
1	K	30	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	H	63	LEU	CA-CB-CG	5.85	128.75	115.30
1	J	101	LEU	CA-CB-CG	5.79	128.63	115.30
1	Q	100	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	N	101	LEU	CA-CB-CG	5.64	128.26	115.30
1	G	63	LEU	CA-CB-CG	5.62	128.21	115.30
1	G	39	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	K	56	ASP	CB-CG-OD1	5.56	123.30	118.30
1	S	90	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	39	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	V	63	LEU	CB-CG-CD1	5.49	120.34	111.00
1	U	138	LEU	CB-CG-CD1	5.48	120.32	111.00
1	M	90	ASP	CB-CG-OD1	5.47	123.22	118.30
1	K	30	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	I	56	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	U	78	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	S	102	ARG	NE-CZ-NH1	5.39	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	63	LEU	CB-CG-CD1	5.36	120.11	111.00
1	W	101	LEU	CA-CB-CG	5.36	127.63	115.30
1	I	134	LEU	CA-CB-CG	5.32	127.53	115.30
1	H	30	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	G	63	LEU	CB-CG-CD1	5.29	119.98	111.00
1	F	119	LEU	CB-CG-CD2	-5.28	102.03	111.00
1	Q	100	ASP	CB-CG-OD2	5.24	123.02	118.30
1	W	90	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	I	101	LEU	CA-CB-CG	5.20	127.26	115.30
1	F	134	LEU	CA-CB-CG	5.18	127.20	115.30
1	G	56	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	O	101	LEU	CA-CB-CG	5.13	127.11	115.30
1	K	63	LEU	CA-CB-CG	5.10	127.03	115.30
1	O	134	LEU	CB-CG-CD1	5.09	119.65	111.00
1	L	30	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	X	101	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1289	0	1275	31	0
1	B	1287	0	1268	29	0
1	C	1288	0	1270	25	0
1	D	1280	0	1262	25	0
1	E	1286	0	1266	26	0
1	F	1285	0	1264	32	0
1	G	1286	0	1266	24	0
1	H	1280	0	1262	23	0
1	I	1280	0	1262	20	0
1	J	1286	0	1266	23	0
1	K	1289	0	1275	20	0
1	L	1286	0	1266	23	0
1	M	1280	0	1248	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1280	0	1248	19	0
1	O	1285	0	1261	22	0
1	P	1282	0	1255	26	0
1	Q	1289	0	1275	22	0
1	R	1284	0	1259	22	0
1	S	1284	0	1259	25	0
1	T	1281	0	1250	25	0
1	U	1276	0	1248	29	0
1	V	1281	0	1250	30	0
1	W	1279	0	1246	25	0
1	X	1282	0	1255	31	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
2	E	5	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	3	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
2	M	4	0	0	0	0
2	N	5	0	0	0	0
2	O	4	0	0	0	0
2	P	4	0	0	0	0
2	Q	4	0	0	0	0
2	R	4	0	0	0	0
2	S	4	0	0	0	0
2	T	3	0	0	0	0
2	U	3	0	0	0	0
2	V	3	0	0	0	0
2	W	3	0	0	0	0
2	X	3	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	E	1	0	0	0	0
3	G	1	0	0	0	0
3	N	1	0	0	0	0
4	A	43	0	30	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	43	0	30	6	0
4	F	43	0	30	11	0
4	H	43	0	30	9	0
4	I	43	0	30	7	0
4	L	43	0	30	6	0
4	N	43	0	30	8	0
4	P	43	0	30	6	0
4	Q	43	0	30	0	0
4	S	43	0	30	7	0
4	U	43	0	30	9	0
4	X	43	0	30	13	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	2	0
5	F	5	0	0	0	0
5	I	5	0	0	1	0
5	M	5	0	0	1	0
5	O	5	0	0	2	0
5	R	5	0	0	1	0
6	A	61	0	0	6	0
6	B	56	0	0	9	0
6	C	65	0	0	5	0
6	D	62	0	0	5	0
6	E	69	0	0	8	0
6	F	62	0	0	5	0
6	G	70	0	0	6	0
6	H	73	0	0	8	0
6	I	61	0	0	6	0
6	J	58	0	0	5	0
6	K	67	0	0	7	0
6	L	59	0	0	8	0
6	M	57	0	0	6	0
6	N	51	0	0	5	0
6	O	68	0	0	8	0
6	P	52	0	0	5	0
6	Q	70	0	0	4	0
6	R	72	0	0	6	0
6	S	64	0	0	8	0
6	T	51	0	0	5	0
6	U	69	0	0	7	0
6	V	68	0	0	7	0
6	W	65	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	X	50	0	0	10	0
All	All	32963	0	30616	669	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 11.

All (669) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:GLU:OE1	1:E:130[B]:HIS:CD2	1.81	1.32
1:P:47:GLU:OE1	1:P:130[B]:HIS:CD2	1.83	1.30
1:P:96:LYS:HD2	6:P:854:HOH:O	1.34	1.22
1:L:47:GLU:OE1	1:L:130[B]:HIS:CD2	1.93	1.21
1:O:98:THR:HG21	6:O:1032:HOH:O	1.40	1.18
4:X:162:HEM:CMB	4:X:162:HEM:HBB2	1.66	1.17
4:X:162:HEM:HBC2	4:X:162:HEM:CMC	1.62	1.16
1:A:47:GLU:OE2	1:A:130[B]:HIS:CD2	2.00	1.14
4:N:165:HEM:HBC2	4:N:165:HEM:CMC	1.72	1.14
1:A:98:THR:HG21	6:A:638:HOH:O	1.46	1.12
4:P:163:HEM:HBB2	4:P:163:HEM:HMB2	1.32	1.09
1:Q:38:LYS:HD3	6:Q:522:HOH:O	1.53	1.09
4:X:162:HEM:HBB2	4:X:162:HEM:HMB2	1.09	1.07
1:V:83:THR:HG23	6:V:166:HOH:O	1.53	1.05
1:R:98:THR:HG21	6:R:616:HOH:O	1.55	1.05
1:G:47:GLU:OE1	1:G:130[B]:HIS:CD2	2.11	1.04
4:X:162:HEM:HMC1	4:X:162:HEM:CBC	1.85	1.02
4:U:162:HEM:HMB1	4:U:162:HEM:HBB2	1.41	1.02
1:H:98:THR:HG21	6:H:517:HOH:O	1.62	1.00
4:U:162:HEM:HBB2	4:U:162:HEM:CMB	1.88	0.99
1:G:38:LYS:HD2	6:W:323:HOH:O	1.62	0.99
1:F:119:LEU:C	1:F:119:LEU:HD23	1.83	0.99
1:B:98:THR:HG21	6:B:254:HOH:O	1.61	0.98
1:F:83:THR:HG23	6:F:427:HOH:O	1.63	0.98
1:T:98:THR:HG21	6:T:164:HOH:O	1.65	0.96
4:P:163:HEM:HBB2	4:P:163:HEM:CMB	1.92	0.96
4:S:163:HEM:HBB2	4:S:163:HEM:HHC	1.49	0.95
4:S:163:HEM:HBC2	4:S:163:HEM:HHD	1.47	0.95
1:X:83:THR:HG23	6:X:367:HOH:O	1.67	0.95
1:I:32:TRP:HE1	1:I:83:THR:HB	1.31	0.94
1:E:27:LEU:HD23	1:E:79:ILE:HD12	1.49	0.94
1:E:147:GLU:HG3	6:E:430:HOH:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:163:HEM:HBC2	4:F:163:HEM:HHD	1.50	0.94
4:X:162:HEM:HMB2	4:X:162:HEM:CBB	1.94	0.93
1:M:98:THR:HG21	6:M:960:HOH:O	1.67	0.93
1:O:83:THR:HG23	6:O:248:HOH:O	1.67	0.93
1:S:98:THR:HG21	6:S:734:HOH:O	1.68	0.92
1:C:98:THR:HG21	6:C:545:HOH:O	1.70	0.91
1:L:83:THR:CG2	6:L:756:HOH:O	2.18	0.90
4:N:165:HEM:CMC	4:N:165:HEM:CBC	2.50	0.90
1:D:83:THR:HG23	6:D:184:HOH:O	1.70	0.90
1:V:98:THR:HG21	6:V:567:HOH:O	1.69	0.90
1:C:32:TRP:HE1	1:C:83:THR:HB	1.34	0.90
1:H:83:THR:HG23	6:H:167:HOH:O	1.71	0.90
4:A:165:HEM:HBB2	4:A:165:HEM:CMB	2.01	0.89
1:E:98:THR:HG21	6:E:368:HOH:O	1.72	0.89
1:N:47:GLU:OE1	1:N:130[B]:HIS:CD2	2.25	0.89
4:N:165:HEM:HBC2	4:N:165:HEM:HMC2	1.52	0.89
1:T:32:TRP:HE1	1:T:83:THR:HB	1.37	0.88
1:X:98:THR:HG21	6:X:1336:HOH:O	1.72	0.88
1:M:32:TRP:HE1	1:M:83:THR:HB	1.37	0.88
4:F:163:HEM:CMB	4:F:163:HEM:HBB2	2.03	0.88
1:B:32:TRP:HE1	1:B:83:THR:HB	1.39	0.87
4:X:162:HEM:HBC2	4:X:162:HEM:HMC1	0.89	0.87
1:K:130[B]:HIS:CE1	6:K:257:HOH:O	2.26	0.87
1:H:25:TYR:CE2	1:H:130[B]:HIS:HE1	1.93	0.87
1:N:83:THR:HG23	6:N:166:HOH:O	1.74	0.87
1:V:47:GLU:OE1	1:V:130[B]:HIS:CD2	2.28	0.87
1:J:83:THR:HG23	6:J:165:HOH:O	1.73	0.86
1:A:25:TYR:CE2	1:A:130[B]:HIS:HE1	1.93	0.86
1:F:119:LEU:HD23	1:F:119:LEU:O	1.73	0.86
1:U:130[B]:HIS:CE1	6:U:166:HOH:O	2.29	0.86
1:S:32:TRP:HE1	1:S:83:THR:HB	1.40	0.86
1:C:81:GLU:HG2	1:C:85:GLU:OE2	1.76	0.85
1:T:14:ILE:HD12	1:T:101:LEU:HD13	1.59	0.85
1:W:130[B]:HIS:CE1	6:W:164:HOH:O	2.28	0.84
4:I:163:HEM:HBC2	4:I:163:HEM:HHD	1.59	0.84
4:N:165:HEM:CBC	4:N:165:HEM:HMC2	2.06	0.84
1:A:98:THR:CG2	6:A:638:HOH:O	2.13	0.84
1:S:83:THR:HG22	6:S:166:HOH:O	1.77	0.84
1:A:47:GLU:OE2	1:A:130[B]:HIS:NE2	2.09	0.83
1:T:94:GLU:OE2	1:T:130[B]:HIS:ND1	2.10	0.83
4:N:165:HEM:HBC2	4:N:165:HEM:HMC3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:GLU:OE1	1:G:130[B]:HIS:NE2	2.11	0.83
4:U:162:HEM:HMB1	4:U:162:HEM:CBB	2.09	0.83
1:G:98:THR:HG21	6:G:445:HOH:O	1.78	0.82
4:L:163:HEM:CMB	4:L:163:HEM:HBB2	2.09	0.82
1:C:47:GLU:OE2	1:C:130[B]:HIS:CD2	2.33	0.82
1:A:32:TRP:HE1	1:A:83:THR:HB	1.43	0.82
1:W:98:THR:HG21	6:W:513:HOH:O	1.79	0.82
1:K:32:TRP:HE1	1:K:83:THR:HB	1.42	0.81
1:S:83:THR:CG2	6:S:166:HOH:O	2.27	0.81
1:A:83:THR:HG23	6:A:173:HOH:O	1.81	0.80
1:F:119:LEU:C	1:F:119:LEU:CD2	2.49	0.80
1:K:83:THR:HG23	6:K:337:HOH:O	1.82	0.80
1:L:83:THR:HG23	6:L:756:HOH:O	1.79	0.79
1:U:81:GLU:HG2	1:U:85:GLU:OE2	1.83	0.79
1:P:47:GLU:OE1	1:P:130[B]:HIS:NE2	2.15	0.79
1:U:83:THR:HG23	6:U:165:HOH:O	1.82	0.79
1:X:32:TRP:HE1	1:X:83:THR:HB	1.47	0.78
4:C:165:HEM:HBB2	4:C:165:HEM:CMB	2.13	0.78
4:H:162:HEM:HBC2	4:H:162:HEM:CMC	2.13	0.78
1:R:130[B]:HIS:CD2	1:R:134:LEU:HD22	2.19	0.78
1:P:47:GLU:OE1	1:P:130[B]:HIS:CG	2.36	0.78
1:K:47:GLU:OE2	1:K:130[B]:HIS:CD2	2.36	0.78
1:N:94:GLU:OE2	1:N:130[B]:HIS:ND1	2.15	0.78
1:G:32:TRP:HE1	1:G:83:THR:HB	1.48	0.77
1:F:47:GLU:OE1	1:F:130[B]:HIS:CD2	2.36	0.77
1:C:83:THR:CG2	6:C:170:HOH:O	2.33	0.77
1:H:130[B]:HIS:CE1	6:H:164:HOH:O	2.38	0.76
1:Q:32:TRP:HE1	1:Q:83:THR:HB	1.51	0.76
1:S:98:THR:CG2	6:S:734:HOH:O	2.30	0.76
1:H:130[B]:HIS:NE2	6:H:164:HOH:O	2.19	0.76
1:L:47:GLU:OE1	1:L:130[B]:HIS:CG	2.40	0.75
1:L:32:TRP:HE1	1:L:83:THR:HB	1.51	0.75
4:C:165:HEM:HBB2	4:C:165:HEM:HMB1	1.69	0.74
4:P:163:HEM:HMB2	4:P:163:HEM:CBB	2.13	0.74
1:S:84:GLN:NE2	6:S:894:HOH:O	2.21	0.74
1:C:83:THR:HG23	6:C:170:HOH:O	1.86	0.74
1:J:25:TYR:CE2	1:J:130[B]:HIS:HE1	2.05	0.74
1:D:98:THR:HG21	6:D:750:HOH:O	1.87	0.74
4:F:163:HEM:HBB2	4:F:163:HEM:HMB1	1.70	0.74
1:H:47:GLU:HA	1:H:47:GLU:OE1	1.87	0.74
1:F:32:TRP:HE1	1:F:83:THR:HB	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:THR:CG2	6:F:427:HOH:O	2.26	0.73
1:Q:84:GLN:NE2	6:Q:165:HOH:O	2.22	0.72
1:L:83:THR:HG22	6:L:756:HOH:O	1.84	0.72
4:I:163:HEM:CMB	4:I:163:HEM:HBB2	2.19	0.72
1:R:32:TRP:HE1	1:R:83:THR:HB	1.54	0.72
6:S:1361:HOH:O	1:T:76:LYS:HE2	1.90	0.72
4:A:165:HEM:HBB2	4:A:165:HEM:HMB1	1.71	0.71
1:B:27:LEU:HD23	1:B:79:ILE:HD12	1.73	0.71
1:H:25:TYR:CE2	1:H:130[B]:HIS:CE1	2.79	0.71
1:O:27:LEU:HD23	1:O:79:ILE:HD12	1.72	0.71
1:R:83:THR:HG23	6:R:187:HOH:O	1.88	0.71
1:W:32:TRP:HE1	1:W:83:THR:HB	1.54	0.71
1:K:130[B]:HIS:HE1	6:K:257:HOH:O	1.70	0.71
1:I:47:GLU:OE1	1:I:130[A]:HIS:CD2	2.44	0.70
1:R:47:GLU:OE1	1:R:130[A]:HIS:CD2	2.44	0.70
1:H:94:GLU:OE2	1:H:130[B]:HIS:ND1	2.25	0.70
1:S:47:GLU:CD	1:S:130[B]:HIS:CD2	2.65	0.70
1:B:83:THR:HG22	6:B:173:HOH:O	1.91	0.70
1:E:47:GLU:OE1	1:E:130[B]:HIS:NE2	2.25	0.70
1:B:118:ASP:OD2	6:B:902:HOH:O	2.09	0.69
1:E:83:THR:HG23	6:E:172:HOH:O	1.92	0.69
4:P:163:HEM:HBC2	4:P:163:HEM:HHD	1.73	0.69
1:B:83:THR:CG2	6:B:173:HOH:O	2.40	0.69
1:D:32:TRP:HE1	1:D:83:THR:HB	1.57	0.69
1:S:99:LYS:NZ	1:S:103:GLU:OE1	2.26	0.69
1:R:147:GLU:HG3	6:R:166:HOH:O	1.94	0.68
1:X:38:LYS:HD2	6:X:312:HOH:O	1.94	0.68
4:X:162:HEM:CMC	4:X:162:HEM:CBC	2.49	0.68
1:T:14:ILE:CD1	1:T:101:LEU:HD13	2.23	0.68
1:W:19:LEU:CD2	4:X:162:HEM:HBB1	2.24	0.68
4:A:165:HEM:HMB1	4:A:165:HEM:CBB	2.24	0.68
1:W:123:ILE:O	1:W:127:GLU:HG2	1.94	0.68
4:I:163:HEM:HBC2	4:I:163:HEM:CHD	2.23	0.67
4:A:165:HEM:CMB	4:A:165:HEM:CBB	2.72	0.67
1:C:47:GLU:CD	1:C:130[B]:HIS:CD2	2.68	0.67
1:I:83:THR:CG2	6:I:279:HOH:O	2.42	0.67
1:B:47:GLU:OE2	1:B:130[B]:HIS:CD2	2.47	0.67
1:H:83:THR:CG2	6:H:167:HOH:O	2.33	0.67
1:O:83:THR:CG2	6:O:248:HOH:O	2.33	0.67
1:O:147:GLU:HG3	6:O:164:HOH:O	1.94	0.67
4:H:162:HEM:CMB	4:H:162:HEM:HBB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:25:TYR:CE2	1:T:130[B]:HIS:HE1	2.13	0.67
1:P:32:TRP:HE1	1:P:83:THR:HB	1.59	0.67
1:Q:14:ILE:HD13	1:Q:120:LEU:HD22	1.77	0.67
1:T:60:GLU:OE1	6:T:1157:HOH:O	2.12	0.67
1:I:32:TRP:NE1	1:I:83:THR:HB	2.07	0.67
1:O:32:TRP:HE1	1:O:83:THR:HB	1.60	0.66
1:M:98:THR:CG2	6:M:960:HOH:O	2.35	0.66
1:P:81:GLU:HG2	1:P:85:GLU:OE2	1.96	0.66
1:Q:47:GLU:OE1	1:Q:130[A]:HIS:CD2	2.49	0.66
1:C:32:TRP:NE1	1:C:83:THR:HB	2.09	0.66
1:C:81:GLU:HG2	1:C:85:GLU:CD	2.16	0.66
1:G:83:THR:HG23	6:G:229:HOH:O	1.95	0.66
1:V:32:TRP:HE1	1:V:83:THR:HB	1.61	0.66
1:O:132:ASP:OD2	6:O:319:HOH:O	2.12	0.66
1:T:32:TRP:NE1	1:T:83:THR:HB	2.10	0.66
1:X:47:GLU:OE1	1:X:130[A]:HIS:CD2	2.49	0.66
1:D:153:HIS:HE1	1:F:154:MET:HE1	1.60	0.65
1:A:25:TYR:CE2	1:A:130[B]:HIS:CE1	2.82	0.65
1:X:83:THR:CG2	6:X:367:HOH:O	2.35	0.65
1:K:32:TRP:NE1	1:K:83:THR:HB	2.11	0.65
1:V:47:GLU:OE1	1:V:130[B]:HIS:NE2	2.29	0.65
1:M:56:ASP:O	1:M:60:GLU:HG3	1.97	0.64
1:U:119:LEU:C	1:U:119:LEU:HD22	2.17	0.64
1:U:130[B]:HIS:NE2	6:U:166:HOH:O	2.30	0.64
1:L:47:GLU:OE1	1:L:130[B]:HIS:NE2	2.31	0.64
1:I:44:GLU:OE2	1:I:90:ASP:OD2	2.16	0.64
1:M:47:GLU:OE1	1:M:130[A]:HIS:CD2	2.50	0.64
1:E:27:LEU:HD23	1:E:79:ILE:CD1	2.26	0.64
1:G:47:GLU:OE1	1:G:130[B]:HIS:CG	2.50	0.64
4:N:165:HEM:CMB	4:N:165:HEM:HBB2	2.28	0.64
1:R:83:THR:CG2	6:R:187:HOH:O	2.46	0.64
4:F:163:HEM:CMB	4:F:163:HEM:CBB	2.76	0.64
1:S:47:GLU:OE1	1:S:130[A]:HIS:CD2	2.51	0.64
1:G:47:GLU:OE1	1:G:130[B]:HIS:CE1	2.50	0.63
1:P:147:GLU:HG3	6:P:288:HOH:O	1.97	0.63
1:E:32:TRP:HE1	1:E:83:THR:HB	1.63	0.63
1:J:147:GLU:HG3	6:J:166:HOH:O	1.98	0.63
1:W:47:GLU:OE1	1:W:47:GLU:HA	2.00	0.62
4:F:163:HEM:HMB1	4:F:163:HEM:CBB	2.27	0.62
1:W:60:GLU:OE1	6:W:1016:HOH:O	2.15	0.62
1:E:83:THR:CG2	6:E:172:HOH:O	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:119:LEU:C	1:U:119:LEU:CD2	2.67	0.62
4:L:163:HEM:HBB2	4:L:163:HEM:HMB1	1.81	0.61
1:J:94:GLU:OE2	1:J:130[B]:HIS:ND1	2.33	0.61
1:G:83:THR:CG2	6:G:229:HOH:O	2.47	0.61
1:D:10:HIS:O	1:D:14:ILE:HG12	2.00	0.61
1:E:47:GLU:OE1	1:E:130[B]:HIS:CG	2.49	0.61
1:U:32:TRP:HE1	1:U:83:THR:HB	1.65	0.61
1:I:83:THR:HG23	6:I:279:HOH:O	1.99	0.61
4:I:163:HEM:CMB	4:I:163:HEM:CBB	2.78	0.61
1:Q:27:LEU:HD23	1:Q:79:ILE:HD12	1.82	0.61
1:R:63:LEU:HD13	1:R:69:PRO:HD3	1.83	0.60
4:L:163:HEM:CMB	4:L:163:HEM:CBB	2.80	0.60
1:D:14:ILE:HD12	1:D:101:LEU:HD13	1.83	0.60
1:E:88:GLN:OE1	6:E:1159:HOH:O	2.15	0.60
1:N:44:GLU:OE2	1:N:90:ASP:OD2	2.20	0.60
1:P:32:TRP:HE1	1:P:83:THR:CG2	2.14	0.60
1:G:98:THR:CG2	6:G:445:HOH:O	2.40	0.59
4:I:163:HEM:HHD	4:I:163:HEM:CBC	2.32	0.59
1:F:26:PHE:CE1	4:F:163:HEM:HBC1	2.37	0.59
1:F:14:ILE:HD13	1:F:101:LEU:CD1	2.32	0.59
1:M:154:MET:HE1	1:X:153:HIS:HE1	1.67	0.59
1:T:14:ILE:HD12	1:T:101:LEU:CD1	2.31	0.59
1:F:130[B]:HIS:CD2	1:F:134:LEU:HD22	2.38	0.59
5:M:163:SO4:O2	1:T:117:ARG:NH2	2.34	0.59
1:N:47:GLU:OE1	1:N:130[B]:HIS:CG	2.55	0.59
1:W:19:LEU:HD21	4:X:162:HEM:HBB1	1.83	0.59
1:S:32:TRP:NE1	1:S:83:THR:HB	2.15	0.59
1:D:123:ILE:O	1:D:127:GLU:HG2	2.03	0.59
1:L:109:GLU:OE1	6:L:1051:HOH:O	2.17	0.59
1:X:32:TRP:NE1	1:X:83:THR:HB	2.16	0.59
1:E:94:GLU:OE2	1:E:130[B]:HIS:ND1	2.32	0.59
1:O:117:ARG:NE	5:O:163:SO4:O2	2.35	0.59
1:U:32:TRP:HE1	1:U:83:THR:CG2	2.16	0.59
1:X:107:HIS:HB2	6:X:1021:HOH:O	2.02	0.59
1:F:98:THR:HG22	6:F:167:HOH:O	2.01	0.58
1:B:130[B]:HIS:NE2	6:B:171:HOH:O	2.32	0.58
1:H:14:ILE:HD12	1:H:101:LEU:HD13	1.85	0.58
1:V:77:LEU:HD23	1:V:79:ILE:HD11	1.85	0.58
1:E:98:THR:CG2	6:E:368:HOH:O	2.40	0.58
4:H:162:HEM:CMC	4:H:162:HEM:CBC	2.79	0.58
4:U:162:HEM:HBC2	4:U:162:HEM:HHD	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:105:ILE:HG23	1:P:117:ARG:HG3	1.85	0.58
1:B:20:ILE:HG23	1:B:77:LEU:HD12	1.86	0.58
1:N:84:GLN:HB2	6:N:404:HOH:O	2.04	0.58
1:A:32:TRP:NE1	1:A:83:THR:HB	2.18	0.58
1:D:56:ASP:O	1:D:60:GLU:HG3	2.04	0.58
6:N:890:HOH:O	1:O:118:ASP:HB3	2.03	0.58
1:B:44:GLU:OE2	1:B:90:ASP:OD2	2.22	0.57
1:M:47:GLU:HG3	1:M:130[B]:HIS:NE2	2.19	0.57
1:K:32:TRP:HE1	1:K:83:THR:CB	2.14	0.57
1:D:33:ASN:ND2	1:D:41:GLY:HA3	2.20	0.57
1:D:98:THR:CG2	6:D:750:HOH:O	2.48	0.57
1:C:47:GLU:OE1	1:C:130[A]:HIS:CD2	2.58	0.57
1:E:119:LEU:HD22	1:E:119:LEU:O	2.03	0.57
1:F:98:THR:CG2	6:F:167:HOH:O	2.52	0.57
4:H:162:HEM:CBC	4:H:162:HEM:HMC1	2.35	0.57
1:M:33:ASN:O	1:M:38:LYS:NZ	2.37	0.57
1:X:32:TRP:HE1	1:X:83:THR:CB	2.16	0.57
1:J:38:LYS:HD2	6:J:345:HOH:O	2.03	0.57
1:F:123:ILE:O	1:F:127:GLU:HG2	2.05	0.57
1:R:94:GLU:OE2	1:R:130[B]:HIS:ND1	2.38	0.57
1:D:47:GLU:OE1	1:D:130[A]:HIS:CD2	2.58	0.56
1:F:25:TYR:CE2	1:F:130[B]:HIS:HE1	2.23	0.56
4:L:163:HEM:HMB1	4:L:163:HEM:CBB	2.34	0.56
1:N:32:TRP:HE1	1:N:83:THR:HB	1.69	0.56
1:V:47:GLU:OE1	1:V:130[B]:HIS:CE1	2.58	0.56
1:F:26:PHE:CE1	4:F:163:HEM:CBC	2.88	0.56
1:K:98:THR:HG22	6:K:426:HOH:O	2.04	0.56
1:M:32:TRP:NE1	1:M:83:THR:HB	2.15	0.56
1:V:47:GLU:OE1	1:V:130[B]:HIS:CG	2.58	0.56
1:W:32:TRP:NE1	1:W:83:THR:HB	2.20	0.56
4:I:163:HEM:CBB	4:I:163:HEM:HMB1	2.36	0.56
1:Q:94:GLU:OE2	1:Q:130[B]:HIS:ND1	2.37	0.56
1:X:38:LYS:HE2	6:X:312:HOH:O	2.06	0.56
1:N:47:GLU:CD	1:N:130[B]:HIS:CD2	2.79	0.56
1:W:147:GLU:HG3	6:W:163:HOH:O	2.06	0.56
1:L:98:THR:HG21	6:L:659:HOH:O	2.06	0.56
1:E:123:ILE:O	1:E:127:GLU:HG2	2.06	0.56
1:B:32:TRP:NE1	1:B:83:THR:HB	2.15	0.56
4:H:162:HEM:HBC2	4:H:162:HEM:HMC1	1.88	0.55
5:D:163:SO4:O3	1:E:117:ARG:NE	2.38	0.55
1:N:65:LEU:O	1:N:66:GLU:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:165:HEM:HBB2	4:A:165:HEM:HMB3	1.86	0.55
1:X:63:LEU:HD13	1:X:69:PRO:HD3	1.87	0.55
1:L:123:ILE:O	1:L:127:GLU:HG2	2.06	0.55
1:V:117:ARG:HG2	6:V:954:HOH:O	2.06	0.55
1:B:83:THR:HG21	1:B:150:LEU:CD2	2.36	0.55
1:M:146:LEU:O	1:M:150:LEU:HG	2.07	0.55
1:F:81:GLU:HG2	1:F:85:GLU:OE2	2.07	0.55
4:H:162:HEM:CMB	4:H:162:HEM:CBB	2.82	0.55
1:G:32:TRP:NE1	1:G:83:THR:HB	2.19	0.55
1:I:83:THR:HG22	6:I:279:HOH:O	2.07	0.55
1:P:98:THR:HG22	6:P:292:HOH:O	2.07	0.55
1:H:98:THR:HG22	6:H:541:HOH:O	2.06	0.54
1:L:38:LYS:HG3	6:L:1406:HOH:O	2.07	0.54
1:V:14:ILE:HD12	1:V:101:LEU:HD13	1.89	0.54
1:H:32:TRP:HE1	1:H:83:THR:HB	1.72	0.54
1:S:47:GLU:OE2	1:S:130[B]:HIS:CD2	2.59	0.54
4:C:165:HEM:HBC2	4:C:165:HEM:HHD	1.88	0.54
1:T:77:LEU:CD1	1:T:77:LEU:N	2.70	0.54
1:M:131:ILE:O	1:M:135:GLU:HG3	2.08	0.54
1:O:33:ASN:ND2	1:O:41:GLY:HA3	2.23	0.54
1:R:19:LEU:HD13	6:R:585:HOH:O	2.07	0.54
1:I:14:ILE:HD12	1:I:101:LEU:HD13	1.89	0.54
1:A:48:SER:O	1:A:52:MET:HG3	2.08	0.54
1:J:81:GLU:HG2	1:J:85:GLU:OE2	2.08	0.53
1:G:25:TYR:CE2	1:G:130[B]:HIS:HE1	2.26	0.53
1:L:107:HIS:CE1	6:L:1184:HOH:O	2.61	0.53
1:P:19:LEU:CD2	4:P:163:HEM:HBB1	2.38	0.53
1:A:32:TRP:HE1	1:A:83:THR:CB	2.17	0.53
1:P:25:TYR:CE2	1:P:130[B]:HIS:HE1	2.27	0.53
1:P:94:GLU:OE2	1:P:130[B]:HIS:ND1	2.40	0.53
1:F:26:PHE:CZ	4:F:163:HEM:CBC	2.91	0.53
1:M:98:THR:HG23	6:M:572:HOH:O	2.07	0.53
1:W:47:GLU:OE1	1:W:130[A]:HIS:CD2	2.62	0.53
1:P:123:ILE:O	1:P:127:GLU:HG2	2.07	0.53
1:H:84:GLN:HB2	6:H:201:HOH:O	2.07	0.53
1:K:119:LEU:HD23	1:K:119:LEU:O	2.09	0.53
1:S:52:MET:HB3	4:S:163:HEM:CHD	2.39	0.52
1:Q:94:GLU:O	1:Q:98:THR:HB	2.09	0.52
1:A:130[B]:HIS:CD2	1:A:134:LEU:HD22	2.44	0.52
1:P:32:TRP:HE1	1:P:83:THR:CB	2.21	0.52
1:T:147:GLU:HG3	6:T:432:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:162:HEM:HBC2	4:U:162:HEM:CHD	2.38	0.52
4:U:162:HEM:HBB2	4:U:162:HEM:HMB3	1.87	0.52
4:X:162:HEM:HBB2	4:X:162:HEM:HMB3	1.81	0.52
1:W:47:GLU:HG3	1:W:130[B]:HIS:NE2	2.25	0.52
1:M:10:HIS:ND1	6:M:521:HOH:O	2.32	0.52
1:Q:32:TRP:NE1	1:Q:83:THR:HB	2.22	0.52
1:C:83:THR:HG22	6:C:170:HOH:O	2.06	0.52
1:T:98:THR:CG2	6:T:164:HOH:O	2.39	0.52
4:U:162:HEM:HHD	4:U:162:HEM:CBC	2.39	0.52
1:A:27:LEU:HD23	1:A:79:ILE:HD12	1.91	0.52
1:B:83:THR:HG21	1:B:150:LEU:HD21	1.91	0.51
1:V:98:THR:CG2	6:V:567:HOH:O	2.38	0.51
1:X:139:GLY:O	1:X:143:LYS:HG3	2.09	0.51
1:K:33:ASN:ND2	1:K:41:GLY:HA3	2.25	0.51
1:M:47:GLU:CD	1:M:130[B]:HIS:CD2	2.84	0.51
1:V:123:ILE:O	1:V:127:GLU:HG2	2.09	0.51
1:S:47:GLU:HG3	1:S:130[B]:HIS:NE2	2.25	0.51
1:J:44:GLU:OE2	1:J:90:ASP:OD2	2.27	0.51
1:F:33:ASN:ND2	1:F:41:GLY:HA3	2.26	0.51
1:X:130[A]:HIS:HD2	6:X:554:HOH:O	1.93	0.51
1:L:130[B]:HIS:CD2	1:L:134:LEU:HD22	2.46	0.51
1:P:32:TRP:HE1	1:P:83:THR:HG22	1.76	0.51
1:S:83:THR:HG21	1:S:150:LEU:CD2	2.41	0.51
1:C:154:MET:HE1	1:U:153:HIS:HE1	1.75	0.51
1:F:32:TRP:NE1	1:F:83:THR:HB	2.24	0.51
1:R:117:ARG:NE	5:R:163:SO4:O3	2.44	0.51
1:D:32:TRP:HE1	1:D:83:THR:CB	2.24	0.50
1:Q:38:LYS:CD	6:Q:522:HOH:O	2.29	0.50
1:F:94:GLU:OE2	1:F:130[B]:HIS:ND1	2.44	0.50
1:P:27:LEU:HD23	1:P:79:ILE:HD12	1.93	0.50
1:H:10:HIS:O	1:H:14:ILE:HG12	2.11	0.50
1:K:130[A]:HIS:HD2	6:K:1099:HOH:O	1.93	0.50
1:N:112:HIS:HE1	6:N:917:HOH:O	1.93	0.50
1:W:98:THR:CG2	6:W:513:HOH:O	2.49	0.50
1:U:32:TRP:HE1	1:U:83:THR:HG22	1.77	0.50
4:N:165:HEM:CMB	4:N:165:HEM:CBB	2.88	0.50
1:J:47:GLU:OE1	1:J:130[A]:HIS:CD2	2.64	0.50
1:V:111:VAL:O	1:V:112:HIS:HB2	2.11	0.50
1:A:83:THR:CG2	6:A:173:HOH:O	2.47	0.49
1:F:84:GLN:HB2	6:F:320:HOH:O	2.11	0.49
1:H:123:ILE:O	1:H:127:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:14:ILE:HG12	1:O:101:LEU:HD13	1.93	0.49
1:B:130[B]:HIS:CD2	1:B:134:LEU:HD22	2.47	0.49
1:L:52:MET:HB3	4:L:163:HEM:CHB	2.43	0.49
1:U:47:GLU:OE1	1:U:47:GLU:HA	2.12	0.49
1:V:130[B]:HIS:CD2	1:V:134:LEU:HD13	2.47	0.49
1:F:52:MET:HB3	4:F:163:HEM:CHB	2.43	0.49
1:N:47:GLU:OE1	1:N:130[A]:HIS:CD2	2.66	0.49
1:K:83:THR:CG2	6:K:337:HOH:O	2.48	0.49
1:K:119:LEU:HD23	1:K:119:LEU:C	2.33	0.49
1:V:27:LEU:HD23	1:V:79:ILE:HD12	1.94	0.49
1:E:133:TYR:O	1:E:137:GLN:HG2	2.13	0.49
1:J:32:TRP:HE1	1:J:83:THR:CG2	2.26	0.49
1:R:25:TYR:CE2	1:R:130[B]:HIS:HE1	2.30	0.49
1:E:20:ILE:HD11	1:E:75:GLY:HA3	1.94	0.49
1:I:94:GLU:OE2	1:I:130[B]:HIS:ND1	2.44	0.49
1:L:25:TYR:CE2	1:L:130[B]:HIS:HE1	2.31	0.49
1:P:84:GLN:HB2	6:P:482:HOH:O	2.12	0.49
1:Q:47:GLU:OE1	1:Q:130[A]:HIS:NE2	2.45	0.49
1:V:133:TYR:HD2	1:V:134:LEU:HD13	1.78	0.49
5:I:164:SO4:O4	1:Q:117:ARG:NE	2.40	0.49
1:J:14:ILE:HD13	1:J:101:LEU:HD13	1.93	0.49
1:M:123:ILE:O	1:M:127:GLU:HG2	2.12	0.49
1:P:47:GLU:O	1:P:51:GLU:HG2	2.13	0.49
1:X:131:ILE:O	1:X:135:GLU:HG3	2.12	0.49
4:H:162:HEM:CBB	4:H:162:HEM:HMB1	2.42	0.48
1:W:130[B]:HIS:NE2	6:W:164:HOH:O	2.34	0.48
1:G:20:ILE:HD11	1:G:75:GLY:HA3	1.96	0.48
1:B:25:TYR:CE2	1:B:130[B]:HIS:HE1	2.31	0.48
1:V:56:ASP:O	1:V:60:GLU:HG3	2.13	0.48
1:K:32:TRP:HE1	1:K:83:THR:CG2	2.25	0.48
1:X:98:THR:HG23	6:X:239:HOH:O	2.12	0.48
1:R:98:THR:HG22	6:R:1163:HOH:O	2.13	0.48
1:N:32:TRP:HE1	1:N:83:THR:CG2	2.27	0.48
1:P:32:TRP:NE1	1:P:83:THR:HB	2.26	0.48
1:S:105:ILE:HG23	1:S:117:ARG:HG3	1.96	0.48
1:X:33:ASN:ND2	1:X:41:GLY:HA3	2.29	0.48
1:A:119:LEU:C	1:A:119:LEU:CD2	2.81	0.48
1:B:130[B]:HIS:CE1	6:B:171:HOH:O	2.65	0.48
1:R:83:THR:HG21	1:R:150:LEU:HD21	1.94	0.48
1:T:77:LEU:N	1:T:77:LEU:HD12	2.29	0.48
1:B:33:ASN:ND2	1:B:41:GLY:HA3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:GLU:HG3	1:C:130[B]:HIS:NE2	2.27	0.48
1:D:83:THR:CG2	6:D:184:HOH:O	2.45	0.48
4:I:163:HEM:HBB2	4:I:163:HEM:HMB3	1.94	0.48
1:L:25:TYR:CD1	1:L:25:TYR:N	2.79	0.48
1:M:110:GLN:NE2	6:M:1415:HOH:O	2.38	0.48
1:W:57:LYS:NZ	6:W:713:HOH:O	2.41	0.48
1:Q:25:TYR:CE2	1:Q:130[B]:HIS:HE1	2.32	0.48
1:A:64:PHE:CE1	1:H:132:ASP:HB2	2.49	0.47
1:J:25:TYR:CE2	1:J:130[B]:HIS:CE1	2.93	0.47
4:S:163:HEM:HHD	4:S:163:HEM:CBC	2.33	0.47
1:P:14:ILE:HD13	1:P:101:LEU:HD13	1.96	0.47
1:D:32:TRP:HE1	1:D:83:THR:CG2	2.27	0.47
1:G:119:LEU:HD22	1:G:119:LEU:O	2.13	0.47
1:S:47:GLU:OE2	1:S:130[B]:HIS:HD2	1.97	0.47
1:C:47:GLU:O	1:C:51:GLU:HG2	2.15	0.47
1:E:119:LEU:HD22	1:E:119:LEU:C	2.34	0.47
1:I:33:ASN:ND2	1:I:41:GLY:HA3	2.28	0.47
1:Q:2:LYS:HA	1:Q:2:LYS:HE3	1.97	0.47
1:W:14:ILE:HD12	1:W:101:LEU:HD13	1.97	0.47
1:B:33:ASN:ND2	6:B:454:HOH:O	2.42	0.47
1:G:33:ASN:ND2	1:G:41:GLY:HA3	2.30	0.47
1:J:32:TRP:HE1	1:J:83:THR:HB	1.77	0.47
1:B:14:ILE:HD12	1:B:101:LEU:HD13	1.96	0.47
1:J:25:TYR:CZ	1:J:130[B]:HIS:HE1	2.32	0.47
1:W:10:HIS:O	1:W:14:ILE:HG12	2.14	0.47
1:I:147:GLU:HG3	6:I:170:HOH:O	2.14	0.47
1:A:94:GLU:OE2	1:A:130[B]:HIS:ND1	2.48	0.47
1:T:19:LEU:HD13	6:T:188:HOH:O	2.14	0.47
1:C:52:MET:HB3	4:C:165:HEM:CHD	2.45	0.47
1:H:96:LYS:NZ	1:H:100:ASP:OD2	2.48	0.47
1:S:127:GLU:HA	1:S:127:GLU:OE1	2.14	0.47
1:A:146:LEU:O	1:A:150:LEU:HG	2.15	0.46
1:J:14:ILE:HD13	1:J:101:LEU:CD1	2.45	0.46
1:L:32:TRP:NE1	1:L:83:THR:HB	2.25	0.46
1:T:32:TRP:HE1	1:T:83:THR:CB	2.17	0.46
1:P:25:TYR:CE2	1:P:130[B]:HIS:CE1	3.03	0.46
1:Q:83:THR:HG21	1:Q:150:LEU:CD2	2.46	0.46
4:A:165:HEM:HMC1	4:A:165:HEM:HBC2	1.98	0.46
1:C:33:ASN:ND2	1:C:41:GLY:HA3	2.31	0.46
1:T:94:GLU:OE2	1:T:130[B]:HIS:CE1	2.68	0.46
1:M:14:ILE:HD12	1:M:101:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:113:ASP:CG	1:Q:116:SER:HB2	2.36	0.46
1:C:47:GLU:OE2	1:C:130[B]:HIS:HD2	1.93	0.46
1:E:118:ASP:OD2	6:E:1372:HOH:O	2.21	0.46
1:E:140:LEU:O	1:E:144:VAL:HG22	2.16	0.46
1:R:32:TRP:NE1	1:R:83:THR:HB	2.26	0.46
1:A:81:GLU:HG2	1:A:85:GLU:OE2	2.15	0.46
1:B:65:LEU:O	1:B:66:GLU:HB2	2.15	0.46
1:I:123:ILE:O	1:I:127:GLU:HG2	2.15	0.46
1:J:83:THR:CG2	6:J:165:HOH:O	2.48	0.46
1:R:33:ASN:ND2	1:R:41:GLY:HA3	2.31	0.46
1:U:133:TYR:CD2	1:U:134:LEU:HD13	2.51	0.46
1:B:83:THR:HG23	6:B:173:HOH:O	2.13	0.46
1:V:95:LEU:O	1:V:98:THR:HG22	2.16	0.46
1:A:110:GLN:HB2	6:A:1143:HOH:O	2.16	0.46
1:B:48:SER:O	1:B:52:MET:HG3	2.16	0.46
1:I:20:ILE:HG23	1:I:77:LEU:HD12	1.98	0.46
1:Q:123:ILE:O	1:Q:127:GLU:HG2	2.16	0.46
1:U:47:GLU:OE2	1:U:130[B]:HIS:CD2	2.69	0.46
1:W:47:GLU:CD	1:W:130[B]:HIS:CD2	2.89	0.46
1:G:6:LYS:NZ	1:G:9:GLN:OE1	2.42	0.45
1:O:44:GLU:OE2	1:O:90:ASP:OD2	2.34	0.45
1:A:57:LYS:HE3	6:A:351:HOH:O	2.16	0.45
1:G:130[B]:HIS:CD2	1:G:134:LEU:HD22	2.51	0.45
1:I:145:GLY:HA3	6:I:450:HOH:O	2.15	0.45
1:O:42:ALA:O	1:O:46[B]:HIS:HD2	1.98	0.45
1:V:117:ARG:CG	6:V:954:HOH:O	2.61	0.45
1:W:95:LEU:O	1:W:98:THR:HG22	2.17	0.45
1:D:47:GLU:OE1	1:D:130[A]:HIS:NE2	2.49	0.45
1:J:133:TYR:HD2	1:J:134:LEU:HD13	1.81	0.45
1:L:94:GLU:OE2	1:L:130[B]:HIS:ND1	2.48	0.45
1:X:133:TYR:O	1:X:137:GLN:HG2	2.16	0.45
4:X:162:HEM:CMB	4:X:162:HEM:CBB	2.52	0.45
1:G:33:ASN:ND2	6:G:1033:HOH:O	2.47	0.45
1:H:133:TYR:CD2	1:H:134:LEU:HD13	2.51	0.45
1:R:123:ILE:O	1:R:127:GLU:HG2	2.17	0.45
1:B:98:THR:CG2	6:B:254:HOH:O	2.38	0.45
1:I:63:LEU:HD13	1:I:69:PRO:HD3	1.98	0.45
1:V:83:THR:CG2	6:V:166:HOH:O	2.31	0.45
1:V:130[B]:HIS:CD2	1:V:134:LEU:HD22	2.52	0.45
1:A:33:ASN:ND2	1:A:41:GLY:HA3	2.31	0.45
1:Q:112:HIS:HE1	6:Q:457:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:TYR:CE2	1:F:130[B]:HIS:CE1	3.04	0.45
1:K:133:TYR:O	1:K:137:GLN:HG2	2.17	0.45
4:C:165:HEM:CMB	4:C:165:HEM:CBB	2.92	0.45
1:H:83:THR:HG21	1:H:150:LEU:HD21	1.98	0.45
1:L:53:LYS:HB2	6:L:317:HOH:O	2.15	0.45
1:N:42:ALA:O	1:N:46[B]:HIS:CD2	2.70	0.45
1:Q:39:ARG:HD2	1:Q:155:HIS:O	2.16	0.45
1:E:32:TRP:NE1	1:E:83:THR:HB	2.30	0.45
1:H:130[B]:HIS:CD2	1:H:134:LEU:HD22	2.52	0.45
1:I:143:LYS:HE2	6:O:505:HOH:O	2.16	0.45
1:U:98:THR:HG22	6:U:1134:HOH:O	2.16	0.45
1:U:132:ASP:OD2	6:U:598:HOH:O	2.20	0.45
1:J:47:GLU:OE1	1:J:47:GLU:HA	2.17	0.45
1:M:154:MET:CE	1:X:153:HIS:HE1	2.29	0.45
1:U:94:GLU:O	1:U:98:THR:HB	2.17	0.45
4:H:162:HEM:HBC2	4:H:162:HEM:HMC3	1.96	0.44
1:C:98:THR:CG2	6:C:545:HOH:O	2.45	0.44
1:F:102:ARG:HG2	1:F:102:ARG:HH11	1.82	0.44
1:U:44:GLU:OE2	1:U:90:ASP:OD2	2.35	0.44
1:V:33:ASN:ND2	6:V:939:HOH:O	2.51	0.44
1:F:14:ILE:HD13	1:F:101:LEU:HD13	1.99	0.44
1:H:83:THR:HG21	1:H:150:LEU:CD2	2.47	0.44
1:A:63:LEU:HD13	1:A:69:PRO:CG	2.47	0.44
4:F:163:HEM:HBB2	4:F:163:HEM:HMB3	1.93	0.44
4:H:162:HEM:HBB2	4:H:162:HEM:HMB3	1.98	0.44
1:N:25:TYR:CE2	1:N:130[B]:HIS:HE1	2.36	0.44
1:W:133:TYR:HD2	1:W:134:LEU:HD13	1.82	0.44
1:S:130[A]:HIS:HD2	6:S:1255:HOH:O	1.99	0.44
1:A:47:GLU:O	1:A:51:GLU:HG2	2.17	0.44
1:G:130[A]:HIS:CD2	6:G:523:HOH:O	2.70	0.44
1:Q:140:LEU:HD23	1:Q:140:LEU:HA	1.86	0.44
1:U:32:TRP:NE1	1:U:83:THR:HB	2.32	0.44
1:L:10:HIS:O	1:L:14:ILE:HG12	2.17	0.44
1:R:28:HIS:CD2	1:R:86:MET:HG2	2.53	0.44
1:U:139:GLY:O	1:U:143:LYS:HG3	2.18	0.44
4:A:165:HEM:HBC2	4:A:165:HEM:CMC	2.48	0.44
1:D:47:GLU:OE2	1:D:130[B]:HIS:CD2	2.71	0.44
1:E:83:THR:HG21	1:E:150:LEU:HD21	1.99	0.44
1:O:80:GLY:CA	1:O:85:GLU:HG2	2.48	0.44
1:P:63:LEU:HD13	1:P:69:PRO:HD3	2.00	0.44
1:P:81:GLU:HG2	1:P:85:GLU:CD	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:97:ALA:O	1:T:101:LEU:HD22	2.17	0.44
1:V:32:TRP:HE1	1:V:83:THR:CG2	2.31	0.44
1:B:123:ILE:O	1:B:127:GLU:HG2	2.17	0.43
1:D:32:TRP:NE1	1:D:83:THR:HB	2.27	0.43
1:H:98:THR:CG2	6:H:541:HOH:O	2.64	0.43
1:O:123:ILE:O	1:O:127:GLU:HG2	2.18	0.43
1:G:88:GLN:NE2	1:G:92:ASN:OD1	2.44	0.43
1:N:10:HIS:CE1	6:N:1330:HOH:O	2.71	0.43
1:U:65:LEU:O	1:U:66:GLU:HB2	2.18	0.43
1:E:44:GLU:OE2	1:E:90:ASP:OD2	2.36	0.43
4:C:165:HEM:HMB1	4:C:165:HEM:CBB	2.42	0.43
1:D:25:TYR:CD1	1:D:25:TYR:N	2.85	0.43
1:D:47:GLU:CD	1:D:130[B]:HIS:CD2	2.91	0.43
1:D:117:ARG:HD3	6:D:893:HOH:O	2.17	0.43
1:K:63:LEU:HD13	1:K:69:PRO:HD3	2.01	0.43
1:U:65:LEU:O	1:U:66:GLU:CB	2.65	0.43
1:X:52:MET:HE1	4:X:162:HEM:C4A	2.54	0.43
1:A:25:TYR:CZ	1:A:130[B]:HIS:HE1	2.34	0.43
1:O:25:TYR:CE2	1:O:130[B]:HIS:HE1	2.36	0.43
1:F:44:GLU:OE2	1:F:90:ASP:OD2	2.37	0.43
1:G:133:TYR:CD2	1:G:134:LEU:HD13	2.54	0.43
1:M:63:LEU:HD13	1:M:69:PRO:CD	2.49	0.43
1:R:83:THR:HG21	1:R:150:LEU:CD2	2.48	0.43
1:V:32:TRP:HE1	1:V:83:THR:CB	2.29	0.43
1:X:47:GLU:OE1	1:X:130[A]:HIS:NE2	2.52	0.43
1:K:88:GLN:NE2	1:K:92:ASN:OD1	2.51	0.43
1:O:42:ALA:O	1:O:46[B]:HIS:CD2	2.71	0.43
1:S:94:GLU:O	1:S:98:THR:HB	2.19	0.43
1:S:111:VAL:O	1:S:112:HIS:HB2	2.19	0.43
1:T:25:TYR:CE2	1:T:130[B]:HIS:CE1	3.01	0.43
1:B:63:LEU:HD13	1:B:69:PRO:HD3	2.00	0.43
1:L:14:ILE:HD12	1:L:101:LEU:HD13	2.00	0.43
1:M:33:ASN:ND2	6:M:1291:HOH:O	2.51	0.43
4:F:163:HEM:HBC2	4:F:163:HEM:CHD	2.25	0.43
1:M:65:LEU:O	1:M:66:GLU:CB	2.66	0.43
1:R:44:GLU:OE2	1:R:90:ASP:OD2	2.37	0.43
1:S:83:THR:HG23	6:S:166:HOH:O	2.03	0.43
1:V:131:ILE:O	1:V:135:GLU:HG3	2.19	0.43
1:D:20:ILE:HG23	1:D:77:LEU:HD12	2.01	0.43
4:L:163:HEM:HBB2	4:L:163:HEM:HMB3	1.95	0.43
1:X:84:GLN:NE2	6:X:634:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TYR:N	1:B:25:TYR:CD1	2.86	0.42
1:V:130[B]:HIS:HD2	1:V:134:LEU:HD13	1.84	0.42
1:X:39:ARG:HD2	1:X:155:HIS:O	2.19	0.42
1:J:133:TYR:CD2	1:J:134:LEU:HD13	2.53	0.42
1:N:47:GLU:OE1	1:N:130[B]:HIS:NE2	2.51	0.42
1:O:98:THR:CG2	6:O:1032:HOH:O	2.25	0.42
1:Q:96:LYS:NZ	1:Q:100:ASP:OD2	2.44	0.42
1:X:47:GLU:OE2	1:X:130[B]:HIS:CD2	2.72	0.42
1:C:44:GLU:OE2	1:C:90:ASP:OD2	2.37	0.42
1:I:25:TYR:CE2	1:I:130[B]:HIS:HE1	2.37	0.42
1:J:98:THR:HG22	6:J:315:HOH:O	2.18	0.42
1:O:47:GLU:OE1	1:O:130[A]:HIS:CD2	2.73	0.42
4:U:162:HEM:CHB	1:V:52:MET:HB3	2.50	0.42
1:X:123:ILE:O	1:X:127:GLU:HG2	2.19	0.42
1:J:25:TYR:N	1:J:25:TYR:CD1	2.83	0.42
1:S:25:TYR:N	1:S:25:TYR:CD1	2.86	0.42
1:X:47:GLU:CD	1:X:130[B]:HIS:CD2	2.92	0.42
1:D:117:ARG:NE	5:D:163:SO4:O4	2.52	0.42
1:G:94:GLU:OE2	1:G:130[B]:HIS:ND1	2.53	0.42
1:N:117:ARG:NE	5:O:163:SO4:O1	2.52	0.42
1:V:133:TYR:O	1:V:137:GLN:HG2	2.19	0.42
1:W:38:LYS:HG3	6:W:1088:HOH:O	2.20	0.42
1:M:133:TYR:O	1:M:137:GLN:HG2	2.20	0.42
1:I:130[B]:HIS:CE1	6:I:166:HOH:O	2.72	0.42
1:B:22:ILE:HD11	1:B:52:MET:HA	2.02	0.42
1:C:123:ILE:O	1:C:127:GLU:HG2	2.19	0.42
1:E:44:GLU:HB2	6:E:1137:HOH:O	2.19	0.42
1:S:83:THR:HG21	1:S:150:LEU:HD21	2.00	0.42
1:V:140:LEU:O	1:V:144:VAL:HG22	2.20	0.42
1:M:25:TYR:N	1:M:25:TYR:CD1	2.84	0.42
4:N:165:HEM:CBB	4:N:165:HEM:HMB1	2.49	0.42
1:W:32:TRP:HE1	1:W:83:THR:CB	2.29	0.42
1:W:133:TYR:CD2	1:W:134:LEU:HD13	2.53	0.42
1:X:32:TRP:HE1	1:X:83:THR:CG2	2.33	0.42
1:X:44:GLU:OE2	1:X:90:ASP:OD2	2.37	0.42
1:J:140:LEU:O	1:J:144:VAL:HG22	2.20	0.42
1:L:83:THR:HG21	1:L:150:LEU:CD2	2.50	0.42
1:T:47:GLU:OE1	1:T:130[A]:HIS:CD2	2.73	0.42
1:V:25:TYR:CE2	1:V:130[B]:HIS:HE1	2.37	0.42
1:C:154:MET:HE1	1:U:153:HIS:CE1	2.54	0.41
1:D:146:LEU:O	1:D:150:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:TYR:CZ	1:H:130[B]:HIS:HE1	2.35	0.41
1:K:33:ASN:ND2	6:K:207:HOH:O	2.48	0.41
1:G:25:TYR:CE2	1:G:130[B]:HIS:CE1	3.08	0.41
1:I:143:LYS:CE	6:O:505:HOH:O	2.67	0.41
1:U:47:GLU:OE1	1:U:130[A]:HIS:CD2	2.73	0.41
1:A:32:TRP:HE1	1:A:83:THR:CG2	2.33	0.41
1:B:94:GLU:OE2	1:B:130[B]:HIS:ND1	2.53	0.41
1:E:119:LEU:C	1:E:119:LEU:CD2	2.88	0.41
1:F:47:GLU:OE1	1:F:130[B]:HIS:CG	2.74	0.41
1:U:32:TRP:HE1	1:U:83:THR:CB	2.31	0.41
1:M:65:LEU:O	1:M:66:GLU:HB2	2.21	0.41
4:P:163:HEM:HBC2	4:P:163:HEM:CHD	2.43	0.41
1:Q:83:THR:HG21	1:Q:150:LEU:HD22	2.02	0.41
4:S:163:HEM:HBC2	4:S:163:HEM:CHD	2.24	0.41
1:I:47:GLU:OE2	1:I:130[B]:HIS:CD2	2.73	0.41
1:R:130[B]:HIS:CD2	1:R:134:LEU:CD2	2.96	0.41
1:T:25:TYR:CZ	1:T:130[B]:HIS:HE1	2.38	0.41
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.20	0.41
1:C:127:GLU:OE1	1:C:127:GLU:HA	2.20	0.41
1:F:5:LYS:HE3	1:F:5:LYS:HB3	1.91	0.41
1:W:94:GLU:CD	1:W:130[B]:HIS:HD1	2.24	0.41
1:X:52:MET:CE	4:X:162:HEM:NB	2.83	0.41
1:C:131:ILE:O	1:C:135:GLU:HG3	2.21	0.41
1:L:18:GLU:O	1:L:22:ILE:HG13	2.20	0.41
1:O:32:TRP:NE1	1:O:83:THR:HB	2.30	0.41
1:O:99:LYS:HE3	1:O:99:LYS:HB2	1.66	0.41
1:T:33:ASN:ND2	1:T:41:GLY:HA3	2.36	0.41
1:D:38:LYS:HZ2	1:D:38:LYS:HG2	1.72	0.41
1:N:123:ILE:O	1:N:127:GLU:HG2	2.20	0.41
4:S:163:HEM:CBC	1:T:26:PHE:CE1	3.03	0.41
1:U:83:THR:CG2	6:U:165:HOH:O	2.56	0.41
1:W:130[B]:HIS:HE1	6:W:164:HOH:O	1.85	0.41
1:X:111:VAL:O	1:X:112:HIS:HB2	2.21	0.41
1:A:25:TYR:CD1	1:A:25:TYR:N	2.87	0.41
1:A:109:GLU:HB2	1:A:117:ARG:HH11	1.85	0.41
1:B:127:GLU:HA	1:B:127:GLU:OE1	2.21	0.41
1:C:39:ARG:HD2	1:C:155:HIS:O	2.21	0.41
1:A:90:ASP:HB3	1:A:134:LEU:HD21	2.03	0.40
1:F:76:LYS:HA	1:F:76:LYS:HD2	1.81	0.40
1:K:130[B]:HIS:CD2	1:K:134:LEU:HD22	2.55	0.40
1:A:93:LEU:HD12	1:A:93:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:MET:HE3	1:F:154:MET:HB3	1.91	0.40
1:M:77:LEU:N	1:M:77:LEU:CD1	2.84	0.40
1:O:127:GLU:OE1	1:O:127:GLU:HA	2.20	0.40
1:R:47:GLU:OE1	1:R:130[A]:HIS:NE2	2.53	0.40
1:S:47:GLU:O	1:S:51:GLU:HG2	2.21	0.40
4:S:163:HEM:CHB	1:T:52:MET:HB3	2.51	0.40
1:U:63:LEU:HD13	1:U:69:PRO:HD3	2.03	0.40
1:K:63:LEU:HD13	1:K:69:PRO:CD	2.52	0.40
1:U:52:MET:CE	4:U:162:HEM:NB	2.83	0.40
1:C:94:GLU:O	1:C:98:THR:HB	2.22	0.40
1:G:63:LEU:HD13	1:G:69:PRO:CD	2.52	0.40
1:P:133:TYR:CD2	1:P:134:LEU:HD13	2.57	0.40
1:S:63:LEU:HD13	1:S:69:PRO:CG	2.52	0.40
1:U:130[B]:HIS:HE1	6:U:166:HOH:O	1.87	0.40
1:X:38:LYS:CE	6:X:312:HOH:O	2.67	0.40
1:D:63:LEU:HD13	1:D:69:PRO:HD3	2.03	0.40
1:F:47:GLU:O	1:F:51:GLU:HG2	2.22	0.40
1:J:32:TRP:HE1	1:J:83:THR:HG22	1.86	0.40
1:J:109:GLU:HB2	1:J:117:ARG:HH11	1.87	0.40
1:N:47:GLU:OE1	1:N:130[A]:HIS:CG	2.74	0.40
1:P:107:HIS:CE1	6:P:338:HOH:O	2.74	0.40
1:U:22:ILE:HG13	1:U:51:GLU:HB2	2.03	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	155/158 (98%)	155 (100%)	0	0	100	100
1	B	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	C	155/158 (98%)	154 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	154/158 (98%)	150 (97%)	4 (3%)	0	100	100
1	E	155/158 (98%)	155 (100%)	0	0	100	100
1	F	155/158 (98%)	155 (100%)	0	0	100	100
1	G	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	H	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
1	I	154/158 (98%)	154 (100%)	0	0	100	100
1	J	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	K	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	L	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	M	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	N	155/158 (98%)	152 (98%)	3 (2%)	0	100	100
1	O	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	P	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	Q	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	R	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	S	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	T	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	U	154/158 (98%)	153 (99%)	1 (1%)	0	100	100
1	V	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
1	W	155/158 (98%)	155 (100%)	0	0	100	100
1	X	155/158 (98%)	154 (99%)	1 (1%)	0	100	100
All	All	3716/3792 (98%)	3687 (99%)	29 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/144 (99%)	134 (94%)	8 (6%)	21	21
1	B	141/144 (98%)	132 (94%)	9 (6%)	17	16
1	C	141/144 (98%)	129 (92%)	12 (8%)	10	9
1	D	141/144 (98%)	132 (94%)	9 (6%)	17	16
1	E	141/144 (98%)	129 (92%)	12 (8%)	10	9
1	F	141/144 (98%)	132 (94%)	9 (6%)	17	16
1	G	141/144 (98%)	130 (92%)	11 (8%)	12	11
1	H	141/144 (98%)	130 (92%)	11 (8%)	12	11
1	I	141/144 (98%)	129 (92%)	12 (8%)	10	9
1	J	141/144 (98%)	131 (93%)	10 (7%)	14	13
1	K	142/144 (99%)	133 (94%)	9 (6%)	18	17
1	L	141/144 (98%)	129 (92%)	12 (8%)	10	9
1	M	139/144 (96%)	130 (94%)	9 (6%)	17	16
1	N	139/144 (96%)	129 (93%)	10 (7%)	14	12
1	O	140/144 (97%)	130 (93%)	10 (7%)	14	13
1	P	140/144 (97%)	130 (93%)	10 (7%)	14	13
1	Q	142/144 (99%)	132 (93%)	10 (7%)	15	13
1	R	140/144 (97%)	128 (91%)	12 (9%)	10	9
1	S	140/144 (97%)	127 (91%)	13 (9%)	9	6
1	T	139/144 (96%)	129 (93%)	10 (7%)	14	12
1	U	139/144 (96%)	128 (92%)	11 (8%)	12	10
1	V	139/144 (96%)	127 (91%)	12 (9%)	10	9
1	W	139/144 (96%)	128 (92%)	11 (8%)	12	10
1	X	140/144 (97%)	128 (91%)	12 (9%)	10	9
All	All	3370/3456 (98%)	3116 (92%)	254 (8%)	13	12

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	63	LEU
1	A	83	THR
1	A	98	THR
1	A	101	LEU
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	134	LEU
1	A	138	LEU
1	B	6	LYS
1	B	63	LEU
1	B	83	THR
1	B	98	THR
1	B	99	LYS
1	B	101	LEU
1	B	119	LEU
1	B	134	LEU
1	B	138	LEU
1	C	5	LYS
1	C	63	LEU
1	C	66	GLU
1	C	77	LEU
1	C	83	THR
1	C	98	THR
1	C	101	LEU
1	C	110	GLN
1	C	118	ASP
1	C	119	LEU
1	C	134	LEU
1	C	138	LEU
1	D	63	LEU
1	D	77	LEU
1	D	83	THR
1	D	98	THR
1	D	101	LEU
1	D	110	GLN
1	D	119	LEU
1	D	134	LEU
1	D	138	LEU
1	E	5	LYS
1	E	38	LYS
1	E	63	LEU
1	E	66	GLU
1	E	83	THR
1	E	98	THR
1	E	101	LEU
1	E	107	HIS
1	E	119	LEU
1	E	126	SER

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Mol	Chain	Res	Type
1	E	134	LEU
1	E	138	LEU
1	F	63	LEU
1	F	81	GLU
1	F	83	THR
1	F	98	THR
1	F	99	LYS
1	F	101	LEU
1	F	119	LEU
1	F	134	LEU
1	F	138	LEU
1	G	63	LEU
1	G	76	LYS
1	G	77	LEU
1	G	83	THR
1	G	98	THR
1	G	101	LEU
1	G	118	ASP
1	G	119	LEU
1	G	134	LEU
1	G	138	LEU
1	G	154	MET
1	H	38	LYS
1	H	63	LEU
1	H	66	GLU
1	H	83	THR
1	H	84	GLN
1	H	98	THR
1	H	101	LEU
1	H	118	ASP
1	H	119	LEU
1	H	134	LEU
1	H	138	LEU
1	I	6	LYS
1	I	63	LEU
1	I	83	THR
1	I	98	THR
1	I	101	LEU
1	I	110	GLN
1	I	118	ASP
1	I	119	LEU
1	I	126	SER

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Mol	Chain	Res	Type
1	I	134	LEU
1	I	138	LEU
1	I	154	MET
1	J	63	LEU
1	J	76	LYS
1	J	83	THR
1	J	98	THR
1	J	99	LYS
1	J	101	LEU
1	J	118	ASP
1	J	119	LEU
1	J	134	LEU
1	J	138	LEU
1	K	63	LEU
1	K	66	GLU
1	K	77	LEU
1	K	83	THR
1	K	98	THR
1	K	101	LEU
1	K	118	ASP
1	K	134	LEU
1	K	138	LEU
1	L	30	ARG
1	L	38	LYS
1	L	63	LEU
1	L	66	GLU
1	L	77	LEU
1	L	83	THR
1	L	84	GLN
1	L	101	LEU
1	L	118	ASP
1	L	119	LEU
1	L	134	LEU
1	L	138	LEU
1	M	38	LYS
1	M	63	LEU
1	M	66	GLU
1	M	83	THR
1	M	98	THR
1	M	101	LEU
1	M	118	ASP
1	M	134	LEU

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Mol	Chain	Res	Type
1	M	138	LEU
1	N	38	LYS
1	N	63	LEU
1	N	66	GLU
1	N	76	LYS
1	N	83	THR
1	N	101	LEU
1	N	118	ASP
1	N	119	LEU
1	N	134	LEU
1	N	138	LEU
1	O	63	LEU
1	O	66	GLU
1	O	83	THR
1	O	98	THR
1	O	101	LEU
1	O	110	GLN
1	O	118	ASP
1	O	119	LEU
1	O	134	LEU
1	O	138	LEU
1	P	63	LEU
1	P	66	GLU
1	P	83	THR
1	P	98	THR
1	P	101	LEU
1	P	110	GLN
1	P	118	ASP
1	P	119	LEU
1	P	134	LEU
1	P	138	LEU
1	Q	63	LEU
1	Q	81	GLU
1	Q	83	THR
1	Q	98	THR
1	Q	101	LEU
1	Q	107	HIS
1	Q	118	ASP
1	Q	119	LEU
1	Q	134	LEU
1	Q	138	LEU
1	R	2	LYS

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Mol	Chain	Res	Type
1	R	63	LEU
1	R	66	GLU
1	R	77	LEU
1	R	81	GLU
1	R	83	THR
1	R	98	THR
1	R	101	LEU
1	R	118	ASP
1	R	119	LEU
1	R	134	LEU
1	R	138	LEU
1	S	9	GLN
1	S	34	ASP
1	S	38	LYS
1	S	63	LEU
1	S	66	GLU
1	S	76	LYS
1	S	83	THR
1	S	98	THR
1	S	101	LEU
1	S	118	ASP
1	S	119	LEU
1	S	134	LEU
1	S	138	LEU
1	T	14	ILE
1	T	63	LEU
1	T	66	GLU
1	T	83	THR
1	T	98	THR
1	T	101	LEU
1	T	118	ASP
1	T	119	LEU
1	T	134	LEU
1	T	138	LEU
1	U	4	ASP
1	U	38	LYS
1	U	63	LEU
1	U	66	GLU
1	U	83	THR
1	U	98	THR
1	U	101	LEU
1	U	110	GLN

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Mol	Chain	Res	Type
1	U	119	LEU
1	U	134	LEU
1	U	138	LEU
1	V	63	LEU
1	V	66	GLU
1	V	76	LYS
1	V	81	GLU
1	V	83	THR
1	V	98	THR
1	V	99	LYS
1	V	101	LEU
1	V	118	ASP
1	V	119	LEU
1	V	134	LEU
1	V	138	LEU
1	W	30	ARG
1	W	63	LEU
1	W	77	LEU
1	W	83	THR
1	W	98	THR
1	W	101	LEU
1	W	118	ASP
1	W	119	LEU
1	W	134	LEU
1	W	138	LEU
1	W	154	MET
1	X	57	LYS
1	X	63	LEU
1	X	66	GLU
1	X	81	GLU
1	X	83	THR
1	X	98	THR
1	X	101	LEU
1	X	110	GLN
1	X	119	LEU
1	X	134	LEU
1	X	138	LEU
1	X	154	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	33	ASN
1	B	17	ASN
1	B	33	ASN
1	B	110	GLN
1	B	137	GLN
1	C	17	ASN
1	C	33	ASN
1	C	84	GLN
1	D	9	GLN
1	D	17	ASN
1	D	33	ASN
1	D	137	GLN
1	E	17	ASN
1	E	33	ASN
1	E	88	GLN
1	E	110	GLN
1	E	137	GLN
1	F	17	ASN
1	F	33	ASN
1	G	17	ASN
1	G	33	ASN
1	H	17	ASN
1	H	33	ASN
1	H	110	GLN
1	H	137	GLN
1	I	17	ASN
1	I	33	ASN
1	I	110	GLN
1	I	137	GLN
1	J	17	ASN
1	J	33	ASN
1	J	137	GLN
1	K	17	ASN
1	K	33	ASN
1	K	110	GLN
1	L	17	ASN
1	L	33	ASN
1	L	137	GLN
1	M	17	ASN
1	M	33	ASN
1	M	43	HIS
1	N	17	ASN

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Mol	Chain	Res	Type
1	N	33	ASN
1	O	17	ASN
1	O	33	ASN
1	O	84	GLN
1	O	110	GLN
1	O	137	GLN
1	O	142	GLN
1	P	17	ASN
1	P	33	ASN
1	P	137	GLN
1	Q	17	ASN
1	Q	33	ASN
1	Q	137	GLN
1	R	17	ASN
1	R	33	ASN
1	R	137	GLN
1	S	17	ASN
1	S	33	ASN
1	T	17	ASN
1	T	33	ASN
1	T	43	HIS
1	T	84	GLN
1	T	137	GLN
1	U	17	ASN
1	U	33	ASN
1	U	84	GLN
1	V	17	ASN
1	V	33	ASN
1	V	137	GLN
1	W	17	ASN
1	W	33	ASN
1	W	137	GLN
1	X	17	ASN
1	X	33	ASN
1	X	84	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 122 ligands modelled in this entry, 102 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
5	SO4	M	163	-	4,4,4	0.25	0	6,6,6	0.30	0
4	HEM	C	165	1	41,50,50	2.03	8 (19%)	45,82,82	1.89	15 (33%)
4	HEM	S	163	1	41,50,50	1.94	8 (19%)	45,82,82	2.18	16 (35%)
4	HEM	I	163	1	41,50,50	1.98	7 (17%)	45,82,82	2.23	15 (33%)
4	HEM	U	162	1	41,50,50	2.01	6 (14%)	45,82,82	2.41	18 (40%)
4	HEM	N	165	1	41,50,50	1.93	5 (12%)	45,82,82	2.25	16 (35%)
4	HEM	H	162	1	41,50,50	1.90	5 (12%)	45,82,82	2.12	14 (31%)
5	SO4	A	166	-	4,4,4	0.21	0	6,6,6	0.27	0
4	HEM	F	163	1	41,50,50	1.95	7 (17%)	45,82,82	2.29	15 (33%)
5	SO4	F	164	-	4,4,4	0.24	0	6,6,6	0.25	0
4	HEM	P	163	1	41,50,50	2.09	7 (17%)	45,82,82	2.15	14 (31%)
5	SO4	O	163	-	4,4,4	0.14	0	6,6,6	0.31	0
5	SO4	I	164	-	4,4,4	0.16	0	6,6,6	0.36	0
5	SO4	D	163	-	4,4,4	0.07	0	6,6,6	0.50	0
4	HEM	L	163	1	41,50,50	1.90	5 (12%)	45,82,82	2.23	14 (31%)
4	HEM	Q	163	1	41,50,50	1.95	6 (14%)	45,82,82	2.15	15 (33%)
4	HEM	X	162	1	41,50,50	1.90	5 (12%)	45,82,82	2.13	18 (40%)
4	HEM	A	165	1	41,50,50	1.99	5 (12%)	45,82,82	2.01	13 (28%)
5	SO4	R	163	-	4,4,4	0.08	0	6,6,6	0.58	0
5	SO4	B	165	-	4,4,4	0.17	0	6,6,6	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	H	162	1	-	4/12/54/54	-
4	HEM	C	165	1	-	4/12/54/54	-
4	HEM	S	163	1	-	5/12/54/54	-
4	HEM	F	163	1	-	4/12/54/54	-
4	HEM	L	163	1	-	4/12/54/54	-
4	HEM	Q	163	1	-	4/12/54/54	-
4	HEM	X	162	1	-	4/12/54/54	-
4	HEM	I	163	1	-	4/12/54/54	-
4	HEM	P	163	1	-	4/12/54/54	-
4	HEM	U	162	1	-	4/12/54/54	-
4	HEM	A	165	1	-	4/12/54/54	-
4	HEM	N	165	1	-	4/12/54/54	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	163	HEM	C3D-C2D	8.27	1.54	1.36
4	I	163	HEM	C3D-C2D	8.03	1.53	1.36
4	Q	163	HEM	C3D-C2D	7.48	1.52	1.36
4	A	165	HEM	C3D-C2D	7.47	1.52	1.36
4	L	163	HEM	C3D-C2D	7.25	1.52	1.36
4	S	163	HEM	C3D-C2D	7.17	1.52	1.36
4	U	162	HEM	C3C-C2C	-7.03	1.30	1.40
4	U	162	HEM	C3D-C2D	7.02	1.51	1.36
4	H	162	HEM	C3D-C2D	6.98	1.51	1.36
4	N	165	HEM	C3D-C2D	6.97	1.51	1.36
4	C	165	HEM	C3D-C2D	6.73	1.51	1.36
4	F	163	HEM	C3D-C2D	6.64	1.50	1.36
4	F	163	HEM	C3C-C2C	-6.59	1.31	1.40
4	X	162	HEM	C3D-C2D	6.59	1.50	1.36
4	H	162	HEM	C3C-C2C	-6.38	1.31	1.40
4	C	165	HEM	C3C-C2C	-6.19	1.31	1.40
4	L	163	HEM	C3C-C2C	-6.19	1.31	1.40
4	X	162	HEM	C3C-C2C	-6.13	1.31	1.40
4	Q	163	HEM	C3C-C2C	-6.07	1.31	1.40
4	N	165	HEM	C3C-C2C	-5.97	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	163	HEM	C3C-C2C	-5.93	1.32	1.40
4	S	163	HEM	C3C-C2C	-5.89	1.32	1.40
4	P	163	HEM	C3C-C2C	-5.67	1.32	1.40
4	A	165	HEM	C3C-C2C	-5.49	1.32	1.40
4	C	165	HEM	FE-NB	4.09	2.17	1.96
4	N	165	HEM	FE-ND	4.01	2.16	1.96
4	A	165	HEM	C3C-CAC	3.79	1.55	1.47
4	X	162	HEM	FE-ND	3.29	2.13	1.96
4	P	163	HEM	FE-NB	3.13	2.12	1.96
4	U	162	HEM	FE-ND	2.88	2.11	1.96
4	S	163	HEM	C3B-C2B	-2.85	1.31	1.37
4	S	163	HEM	FE-ND	2.77	2.10	1.96
4	F	163	HEM	C3B-C2B	-2.77	1.31	1.37
4	P	163	HEM	C3B-C2B	-2.77	1.31	1.37
4	H	162	HEM	C3B-C2B	-2.73	1.31	1.37
4	X	162	HEM	CAA-C2A	2.72	1.56	1.52
4	I	163	HEM	C3B-C2B	-2.67	1.31	1.37
4	X	162	HEM	C3B-C2B	-2.67	1.31	1.37
4	C	165	HEM	C1B-NB	-2.65	1.35	1.40
4	C	165	HEM	C3C-CAC	2.59	1.53	1.47
4	U	162	HEM	C3B-C2B	-2.57	1.32	1.37
4	C	165	HEM	FE-ND	2.54	2.09	1.96
4	Q	163	HEM	C3B-C2B	-2.50	1.32	1.37
4	I	163	HEM	CHA-C4D	2.46	1.41	1.35
4	P	163	HEM	CMB-C2B	2.41	1.55	1.50
4	A	165	HEM	C3B-C2B	-2.40	1.32	1.37
4	P	163	HEM	C3C-CAC	2.40	1.52	1.47
4	Q	163	HEM	CMD-C2D	2.37	1.55	1.50
4	A	165	HEM	CAB-C3B	2.35	1.53	1.47
4	F	163	HEM	CMB-C2B	2.35	1.55	1.50
4	S	163	HEM	C3C-CAC	2.32	1.52	1.47
4	I	163	HEM	C3C-CAC	2.31	1.52	1.47
4	P	163	HEM	CHB-C1B	2.28	1.40	1.35
4	N	165	HEM	CAA-C2A	2.28	1.55	1.52
4	S	163	HEM	O2D-CGD	-2.22	1.23	1.30
4	H	162	HEM	CMA-C3A	2.20	1.56	1.51
4	I	163	HEM	CMD-C2D	2.18	1.55	1.50
4	C	165	HEM	CAB-C3B	2.15	1.53	1.47
4	S	163	HEM	CAB-C3B	2.13	1.53	1.47
4	F	163	HEM	FE-ND	2.12	2.07	1.96
4	S	163	HEM	CMB-C2B	2.11	1.55	1.50
4	I	163	HEM	FE-NB	2.10	2.07	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	163	HEM	C3B-C2B	-2.10	1.33	1.37
4	Q	163	HEM	FE-ND	2.09	2.07	1.96
4	F	163	HEM	C1A-NA	2.09	1.40	1.36
4	Q	163	HEM	CMB-C2B	2.08	1.55	1.50
4	U	162	HEM	CAB-C3B	2.08	1.53	1.47
4	N	165	HEM	C3C-CAC	2.07	1.52	1.47
4	H	162	HEM	O2A-CGA	-2.07	1.23	1.30
4	C	165	HEM	CHC-C4B	-2.05	1.35	1.41
4	F	163	HEM	CAA-C2A	2.05	1.55	1.52
4	U	162	HEM	CMA-C3A	2.04	1.55	1.51
4	L	163	HEM	CAB-C3B	2.01	1.52	1.47
4	L	163	HEM	CAA-C2A	2.01	1.55	1.52

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	162	HEM	C4D-ND-C1D	7.76	113.09	105.07
4	I	163	HEM	C4D-ND-C1D	7.39	112.70	105.07
4	L	163	HEM	C4D-ND-C1D	6.93	112.23	105.07
4	P	163	HEM	C4D-ND-C1D	6.88	112.18	105.07
4	N	165	HEM	C4D-ND-C1D	6.74	112.03	105.07
4	S	163	HEM	C4D-ND-C1D	6.63	111.92	105.07
4	U	162	HEM	CBA-CAA-C2A	-6.36	101.76	112.62
4	F	163	HEM	C4D-ND-C1D	6.31	111.59	105.07
4	Q	163	HEM	C4D-ND-C1D	6.25	111.52	105.07
4	H	162	HEM	CBA-CAA-C2A	-5.80	102.73	112.62
4	L	163	HEM	CHC-C4B-NB	5.55	130.46	124.43
4	C	165	HEM	C4D-ND-C1D	5.49	110.75	105.07
4	H	162	HEM	C4D-ND-C1D	5.47	110.72	105.07
4	N	165	HEM	C2C-C3C-C4C	5.45	110.70	106.90
4	P	163	HEM	CBA-CAA-C2A	-5.21	103.73	112.62
4	A	165	HEM	C4D-ND-C1D	5.16	110.41	105.07
4	A	165	HEM	CHC-C4B-NB	5.12	130.00	124.43
4	U	162	HEM	C2C-C3C-C4C	4.90	110.32	106.90
4	Q	163	HEM	CHC-C4B-NB	4.88	129.74	124.43
4	I	163	HEM	CBA-CAA-C2A	-4.87	104.31	112.62
4	X	162	HEM	C4D-ND-C1D	4.83	110.06	105.07
4	F	163	HEM	C2C-C3C-C4C	4.69	110.17	106.90
4	U	162	HEM	CHC-C4B-NB	4.67	129.50	124.43
4	Q	163	HEM	CBA-CAA-C2A	-4.57	104.81	112.62
4	F	163	HEM	CHC-C4B-NB	4.53	129.35	124.43
4	H	162	HEM	C2C-C3C-C4C	4.39	109.96	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	163	HEM	C2C-C3C-C4C	4.28	109.89	106.90
4	I	163	HEM	CHC-C4B-NB	4.24	129.04	124.43
4	H	162	HEM	C4B-C3B-C2B	4.16	110.42	107.11
4	F	163	HEM	C4C-CHD-C1D	4.16	128.04	122.56
4	P	163	HEM	CHC-C4B-NB	4.15	128.94	124.43
4	C	165	HEM	CBA-CAA-C2A	-4.10	105.61	112.62
4	L	163	HEM	C2C-C3C-C4C	4.01	109.70	106.90
4	X	162	HEM	C4B-C3B-C2B	4.00	110.29	107.11
4	F	163	HEM	CBA-CAA-C2A	-3.94	105.89	112.62
4	N	165	HEM	CMD-C2D-C1D	3.93	131.03	125.04
4	I	163	HEM	C4B-C3B-C2B	3.91	110.22	107.11
4	X	162	HEM	C1D-C2D-C3D	-3.88	102.88	106.96
4	S	163	HEM	CBA-CAA-C2A	-3.87	106.01	112.62
4	I	163	HEM	C2C-C3C-C4C	3.83	109.57	106.90
4	Q	163	HEM	C4B-C3B-C2B	3.77	110.11	107.11
4	X	162	HEM	CMD-C2D-C1D	3.75	130.75	125.04
4	X	162	HEM	C2C-C3C-C4C	3.73	109.50	106.90
4	X	162	HEM	CHC-C4B-NB	3.69	128.44	124.43
4	N	165	HEM	CBA-CAA-C2A	-3.62	106.44	112.62
4	P	163	HEM	CHA-C4D-ND	3.62	128.85	124.38
4	S	163	HEM	C4B-CHC-C1C	3.61	127.32	122.56
4	H	162	HEM	CHC-C4B-NB	3.61	128.35	124.43
4	A	165	HEM	C4B-C3B-C2B	3.59	109.97	107.11
4	X	162	HEM	CBD-CAD-C3D	-3.54	102.79	112.63
4	F	163	HEM	C4B-C3B-C2B	3.49	109.89	107.11
4	F	163	HEM	CMB-C2B-C1B	3.48	130.34	125.04
4	F	163	HEM	CMD-C2D-C1D	3.47	130.33	125.04
4	L	163	HEM	CMD-C2D-C1D	3.47	130.32	125.04
4	A	165	HEM	CMB-C2B-C1B	3.46	130.31	125.04
4	L	163	HEM	CHA-C4D-ND	3.45	128.65	124.38
4	C	165	HEM	C2C-C3C-C4C	3.43	109.30	106.90
4	C	165	HEM	CBD-CAD-C3D	-3.41	103.15	112.63
4	L	163	HEM	CBA-CAA-C2A	-3.39	106.83	112.62
4	S	163	HEM	C4C-CHD-C1D	3.38	127.02	122.56
4	C	165	HEM	C1B-NB-C4B	3.37	108.56	105.07
4	N	165	HEM	CBB-CAB-C3B	-3.35	110.94	127.62
4	S	163	HEM	CMB-C2B-C1B	3.30	130.06	125.04
4	U	162	HEM	CMB-C2B-C1B	3.29	130.04	125.04
4	A	165	HEM	C4B-CHC-C1C	3.28	126.89	122.56
4	L	163	HEM	CBB-CAB-C3B	-3.25	111.47	127.62
4	X	162	HEM	CBA-CAA-C2A	-3.22	107.12	112.62
4	S	163	HEM	CMD-C2D-C1D	3.21	129.92	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	165	HEM	CBB-CAB-C3B	-3.17	111.83	127.62
4	I	163	HEM	CHA-C4D-ND	3.14	128.26	124.38
4	N	165	HEM	C3C-C4C-NC	-3.11	105.07	110.94
4	N	165	HEM	CHD-C1D-C2D	3.06	129.76	124.98
4	F	163	HEM	CBB-CAB-C3B	-3.02	112.57	127.62
4	H	162	HEM	CAD-CBD-CGD	-3.01	107.14	113.60
4	S	163	HEM	C2C-C3C-C4C	3.00	108.99	106.90
4	H	162	HEM	CBB-CAB-C3B	-2.99	112.73	127.62
4	A	165	HEM	CBB-CAB-C3B	-2.98	112.78	127.62
4	I	163	HEM	C4B-CHC-C1C	2.97	126.48	122.56
4	A	165	HEM	CBD-CAD-C3D	-2.96	104.41	112.63
4	N	165	HEM	CHC-C4B-NB	2.95	127.64	124.43
4	X	162	HEM	CBB-CAB-C3B	-2.95	112.95	127.62
4	N	165	HEM	C4B-C3B-C2B	2.90	109.42	107.11
4	S	163	HEM	C4B-C3B-C2B	2.89	109.41	107.11
4	L	163	HEM	CBD-CAD-C3D	-2.89	104.60	112.63
4	P	163	HEM	C4B-C3B-C2B	2.88	109.40	107.11
4	A	165	HEM	CMC-C2C-C3C	2.87	130.06	124.68
4	Q	163	HEM	CMD-C2D-C1D	2.86	129.39	125.04
4	U	162	HEM	CBD-CAD-C3D	-2.80	104.84	112.63
4	X	162	HEM	CMB-C2B-C1B	2.80	129.30	125.04
4	F	163	HEM	CBD-CAD-C3D	-2.79	104.89	112.63
4	P	163	HEM	CMD-C2D-C1D	2.78	129.27	125.04
4	I	163	HEM	CBB-CAB-C3B	-2.78	113.80	127.62
4	H	162	HEM	C1B-NB-C4B	2.76	107.92	105.07
4	N	165	HEM	C1B-NB-C4B	2.76	107.92	105.07
4	F	163	HEM	CHA-C4D-ND	2.74	127.77	124.38
4	A	165	HEM	C4C-CHD-C1D	2.73	126.16	122.56
4	P	163	HEM	C4C-CHD-C1D	2.72	126.15	122.56
4	X	162	HEM	CMA-C3A-C4A	-2.71	124.29	128.46
4	S	163	HEM	C1B-NB-C4B	2.71	107.87	105.07
4	U	162	HEM	C3D-C4D-ND	-2.71	107.15	110.17
4	F	163	HEM	CAD-CBD-CGD	-2.71	107.78	113.60
4	H	162	HEM	C1D-C2D-C3D	-2.70	104.11	106.96
4	C	165	HEM	CMD-C2D-C1D	2.69	129.14	125.04
4	C	165	HEM	C4B-CHC-C1C	2.67	126.08	122.56
4	L	163	HEM	C4B-C3B-C2B	2.67	109.23	107.11
4	U	162	HEM	O2D-CGD-CBD	2.67	122.60	114.03
4	Q	163	HEM	CBD-CAD-C3D	-2.66	105.24	112.63
4	N	165	HEM	CBD-CAD-C3D	-2.63	105.32	112.63
4	Q	163	HEM	CBB-CAB-C3B	-2.62	114.60	127.62
4	U	162	HEM	CBB-CAB-C3B	-2.60	114.67	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	165	HEM	CHA-C4D-ND	2.60	127.59	124.38
4	Q	163	HEM	C1D-C2D-C3D	-2.58	104.25	106.96
4	H	162	HEM	CHA-C4D-ND	2.57	127.56	124.38
4	H	162	HEM	CBD-CAD-C3D	-2.56	105.51	112.63
4	U	162	HEM	CAD-CBD-CGD	-2.53	108.17	113.60
4	U	162	HEM	O1D-CGD-CBD	-2.51	115.00	123.08
4	A	165	HEM	C1D-C2D-C3D	-2.51	104.32	106.96
4	X	162	HEM	CAD-CBD-CGD	-2.50	108.23	113.60
4	I	163	HEM	O1A-CGA-CBA	-2.48	115.10	123.08
4	X	162	HEM	CHA-C4D-ND	2.48	127.44	124.38
4	S	163	HEM	CAB-C3B-C2B	-2.47	120.48	128.60
4	X	162	HEM	CAD-C3D-C2D	-2.46	123.30	127.88
4	S	163	HEM	CAA-CBA-CGA	-2.46	106.87	113.76
4	F	163	HEM	O1A-CGA-CBA	-2.46	115.19	123.08
4	S	163	HEM	CBD-CAD-C3D	-2.45	105.83	112.63
4	F	163	HEM	C3C-C4C-NC	-2.42	106.37	110.94
4	L	163	HEM	C4B-CHC-C1C	2.41	125.73	122.56
4	C	165	HEM	O2A-CGA-CBA	2.41	121.76	114.03
4	I	163	HEM	C3D-C4D-ND	-2.41	107.49	110.17
4	P	163	HEM	C2C-C3C-C4C	2.40	108.57	106.90
4	S	163	HEM	CMB-C2B-C3B	-2.38	122.47	128.30
4	P	163	HEM	O2A-CGA-CBA	2.38	121.68	114.03
4	C	165	HEM	CHA-C4D-ND	2.37	127.31	124.38
4	I	163	HEM	C4C-CHD-C1D	2.37	125.68	122.56
4	U	162	HEM	CMB-C2B-C3B	-2.36	122.52	128.30
4	N	165	HEM	C4C-CHD-C1D	2.35	125.66	122.56
4	Q	163	HEM	C4B-CHC-C1C	2.35	125.66	122.56
4	P	163	HEM	C4B-CHC-C1C	2.35	125.65	122.56
4	Q	163	HEM	C3D-C4D-ND	-2.34	107.56	110.17
4	S	163	HEM	CBB-CAB-C3B	-2.34	115.99	127.62
4	U	162	HEM	CHA-C4D-ND	2.34	127.27	124.38
4	A	165	HEM	CBA-CAA-C2A	-2.32	108.66	112.62
4	L	163	HEM	C1B-NB-C4B	2.31	107.46	105.07
4	H	162	HEM	C2B-C1B-NB	-2.29	107.13	109.84
4	P	163	HEM	C3D-C4D-ND	-2.29	107.62	110.17
4	S	163	HEM	C3C-C4C-NC	-2.29	106.63	110.94
4	U	162	HEM	C3C-C4C-NC	-2.27	106.66	110.94
4	Q	163	HEM	CHA-C4D-ND	2.27	127.18	124.38
4	X	162	HEM	C3D-C4D-ND	-2.26	107.65	110.17
4	X	162	HEM	C1B-NB-C4B	2.26	107.41	105.07
4	C	165	HEM	C3C-C4C-NC	-2.25	106.69	110.94
4	P	163	HEM	CBB-CAB-C3B	-2.24	116.50	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	162	HEM	C4B-C3B-C2B	2.23	108.89	107.11
4	N	165	HEM	CMA-C3A-C4A	-2.23	125.04	128.46
4	F	163	HEM	CHC-C4B-C3B	-2.22	121.18	124.57
4	U	162	HEM	C4B-CHC-C1C	2.21	125.48	122.56
4	X	162	HEM	CAD-C3D-C4D	2.20	128.50	124.66
4	U	162	HEM	CHC-C4B-C3B	-2.19	121.22	124.57
4	C	165	HEM	O1D-CGD-CBD	-2.18	116.07	123.08
4	I	163	HEM	CBD-CAD-C3D	-2.18	106.58	112.63
4	L	163	HEM	C4C-CHD-C1D	2.17	125.42	122.56
4	S	163	HEM	CHC-C4B-C3B	2.16	127.88	124.57
4	P	163	HEM	CHD-C1D-ND	2.16	126.78	124.43
4	N	165	HEM	CHD-C1D-ND	-2.13	122.11	124.43
4	I	163	HEM	CMB-C2B-C1B	2.13	128.28	125.04
4	I	163	HEM	CMA-C3A-C4A	-2.13	125.20	128.46
4	L	163	HEM	C2D-C1D-ND	-2.11	107.35	109.88
4	H	162	HEM	CMB-C2B-C1B	2.11	128.25	125.04
4	A	165	HEM	CAD-C3D-C4D	2.10	128.32	124.66
4	N	165	HEM	CMA-C3A-C2A	2.09	128.88	124.94
4	L	163	HEM	C3C-C4C-NC	-2.08	107.01	110.94
4	U	162	HEM	C4C-CHD-C1D	2.07	125.30	122.56
4	Q	163	HEM	C1B-NB-C4B	2.07	107.21	105.07
4	A	165	HEM	CMB-C2B-C3B	-2.06	123.26	128.30
4	Q	163	HEM	CAD-C3D-C4D	2.05	128.24	124.66
4	C	165	HEM	C1D-C2D-C3D	-2.05	104.80	106.96
4	C	165	HEM	O1A-CGA-CBA	-2.04	116.53	123.08
4	H	162	HEM	C3D-C4D-ND	-2.04	107.90	110.17
4	X	162	HEM	C4B-CHC-C1C	2.03	125.23	122.56
4	Q	163	HEM	C3C-C4C-NC	-2.03	107.12	110.94
4	I	163	HEM	O2D-CGD-CBD	2.01	120.50	114.03
4	C	165	HEM	C2B-C1B-NB	-2.01	107.46	109.84
4	P	163	HEM	O2D-CGD-CBD	2.01	120.49	114.03

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	163	HEM	C4B-C3B-CAB-CBB
4	U	162	HEM	CAD-CBD-CGD-O2D
4	S	163	HEM	CAD-CBD-CGD-O2D
4	C	165	HEM	CAA-CBA-CGA-O1A
4	H	162	HEM	CAD-CBD-CGD-O2D
4	F	163	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
4	Q	163	HEM	CAD-CBD-CGD-O2D
4	A	165	HEM	CAD-CBD-CGD-O2D
4	H	162	HEM	CAD-CBD-CGD-O1D
4	S	163	HEM	CAD-CBD-CGD-O1D
4	N	165	HEM	CAA-CBA-CGA-O2A
4	S	163	HEM	CAA-CBA-CGA-O2A
4	X	162	HEM	CAD-CBD-CGD-O2D
4	A	165	HEM	CAD-CBD-CGD-O1D
4	C	165	HEM	CAA-CBA-CGA-O2A
4	I	163	HEM	CAD-CBD-CGD-O1D
4	N	165	HEM	CAD-CBD-CGD-O2D
4	P	163	HEM	CAD-CBD-CGD-O2D
4	H	162	HEM	CAA-CBA-CGA-O2A
4	I	163	HEM	CAA-CBA-CGA-O1A
4	H	162	HEM	CAA-CBA-CGA-O1A
4	N	165	HEM	CAD-CBD-CGD-O1D
4	P	163	HEM	CAD-CBD-CGD-O1D
4	S	163	HEM	CAA-CBA-CGA-O1A
4	X	162	HEM	CAD-CBD-CGD-O1D
4	Q	163	HEM	CAA-CBA-CGA-O2A
4	Q	163	HEM	CAD-CBD-CGD-O1D
4	N	165	HEM	CAA-CBA-CGA-O1A
4	X	162	HEM	CAA-CBA-CGA-O1A
4	C	165	HEM	CAD-CBD-CGD-O1D
4	C	165	HEM	CAD-CBD-CGD-O2D
4	I	163	HEM	CAA-CBA-CGA-O2A
4	Q	163	HEM	CAA-CBA-CGA-O1A
4	L	163	HEM	CAD-CBD-CGD-O1D
4	L	163	HEM	CAD-CBD-CGD-O2D
4	A	165	HEM	CAA-CBA-CGA-O2A
4	U	162	HEM	CAD-CBD-CGD-O1D
4	X	162	HEM	CAA-CBA-CGA-O2A
4	F	163	HEM	CAD-CBD-CGD-O2D
4	I	163	HEM	CAD-CBD-CGD-O2D
4	A	165	HEM	CAA-CBA-CGA-O1A
4	U	162	HEM	CAA-CBA-CGA-O2A
4	L	163	HEM	CAA-CBA-CGA-O2A
4	F	163	HEM	CAA-CBA-CGA-O2A
4	U	162	HEM	CAA-CBA-CGA-O1A
4	P	163	HEM	CAA-CBA-CGA-O1A
4	F	163	HEM	CAA-CBA-CGA-O1A
4	P	163	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
4	L	163	HEM	CAA-CBA-CGA-O1A

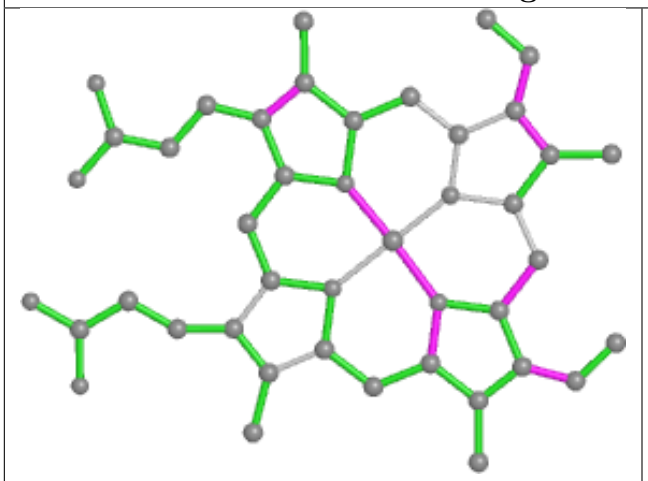
There are no ring outliers.

16 monomers are involved in 96 short contacts:

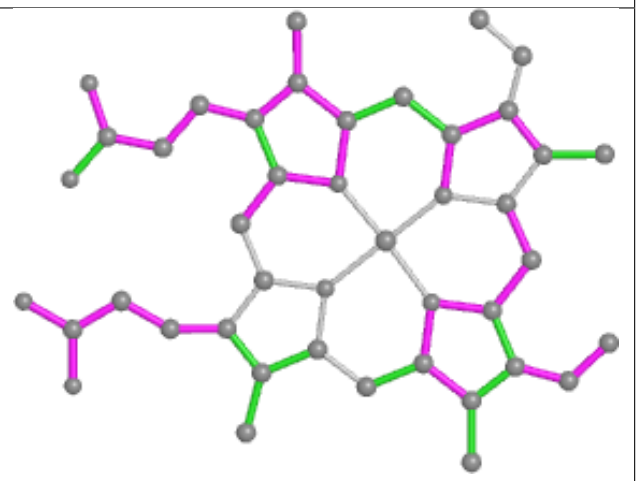
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	163	SO4	1	0
4	C	165	HEM	6	0
4	S	163	HEM	7	0
4	I	163	HEM	7	0
4	U	162	HEM	9	0
4	N	165	HEM	8	0
4	H	162	HEM	9	0
4	F	163	HEM	11	0
4	P	163	HEM	6	0
5	O	163	SO4	2	0
5	I	164	SO4	1	0
5	D	163	SO4	2	0
4	L	163	HEM	6	0
4	X	162	HEM	13	0
4	A	165	HEM	7	0
5	R	163	SO4	1	0

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

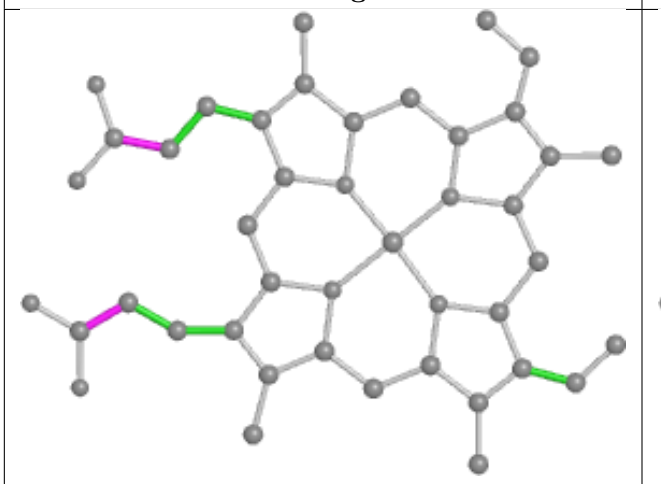
Ligand HEM C 165



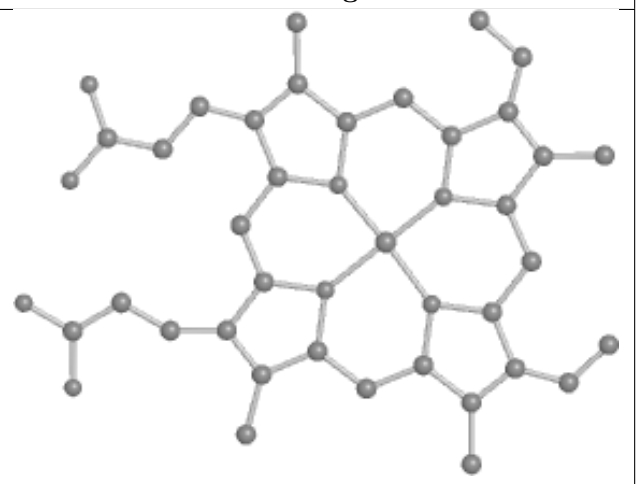
Bond lengths



Bond angles

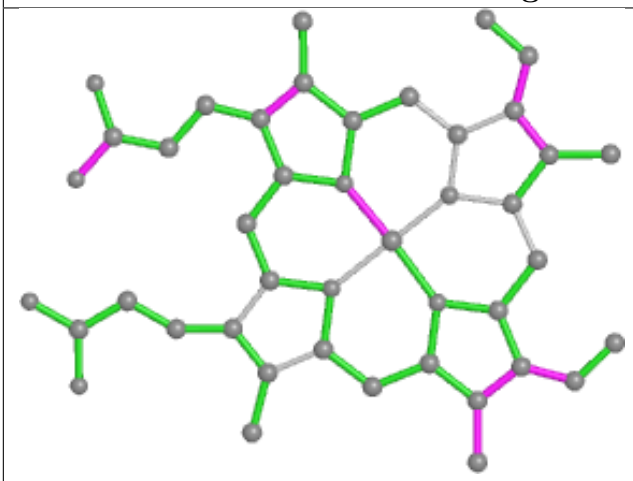


Torsions



Rings

Ligand HEM S 163



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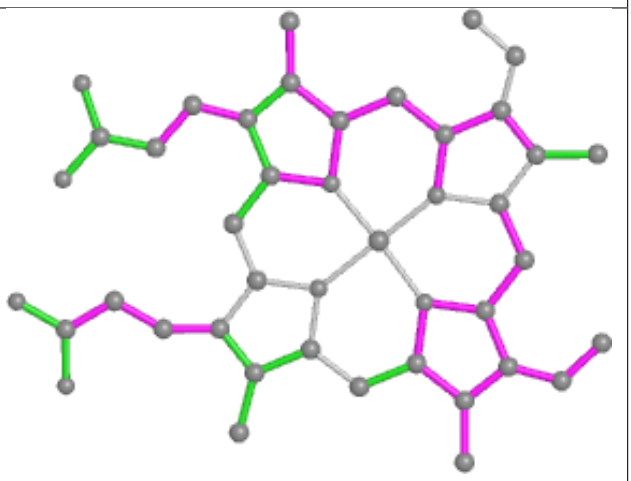

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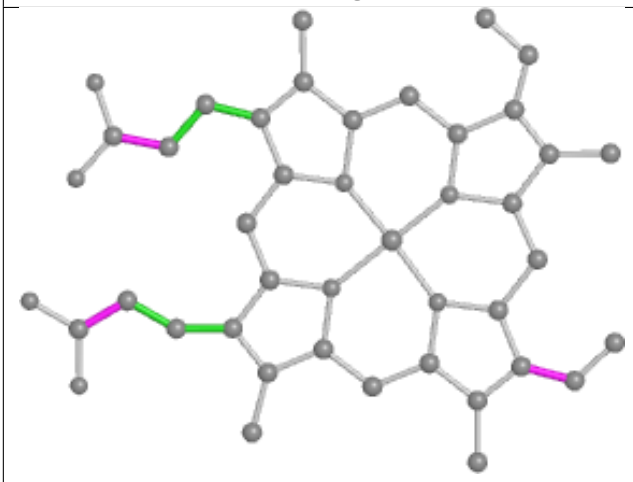
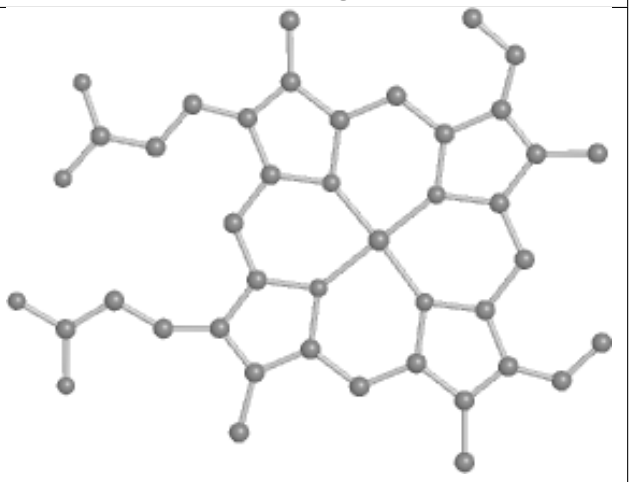
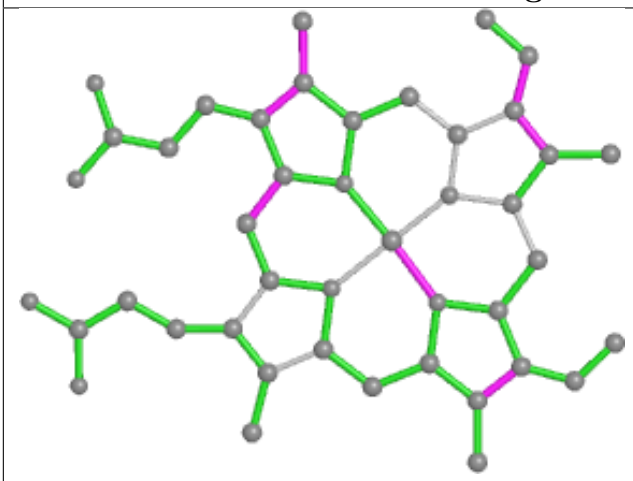


Torsions



Rings

Ligand HEM I 163



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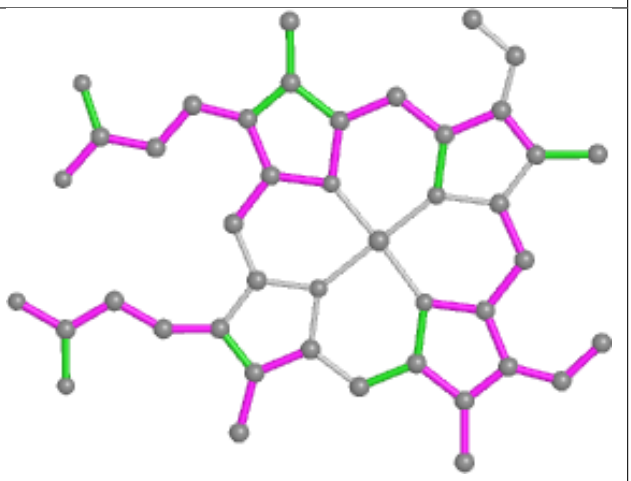
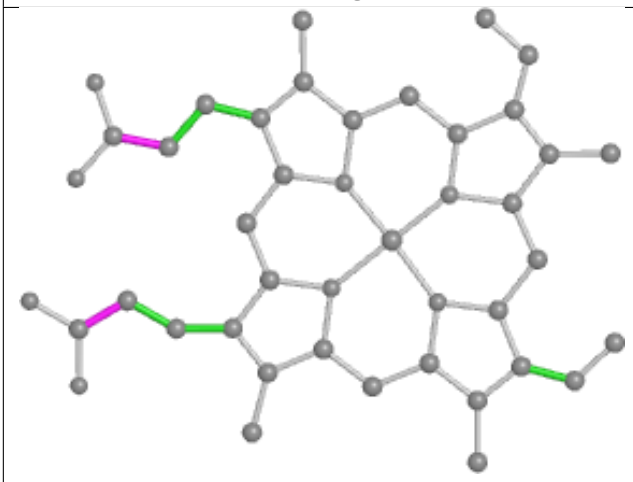


Bond angles



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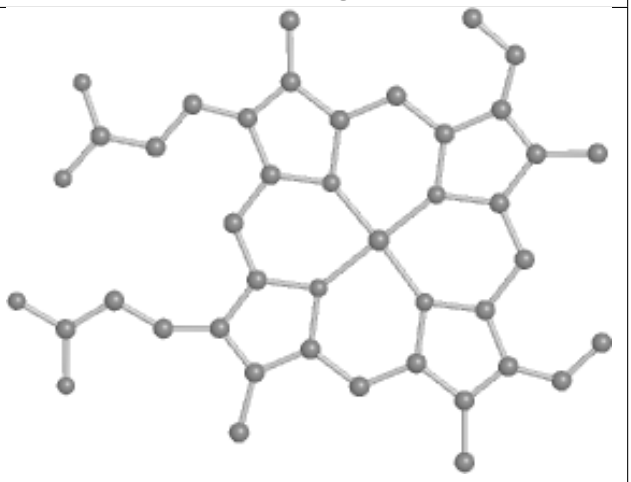
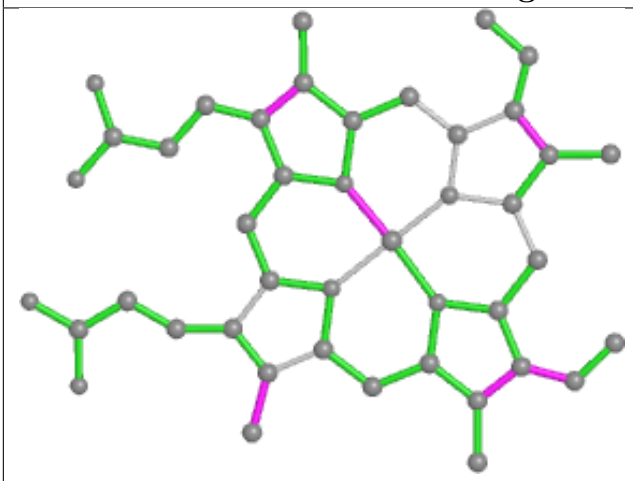


Rings

Ligand HEM U 162



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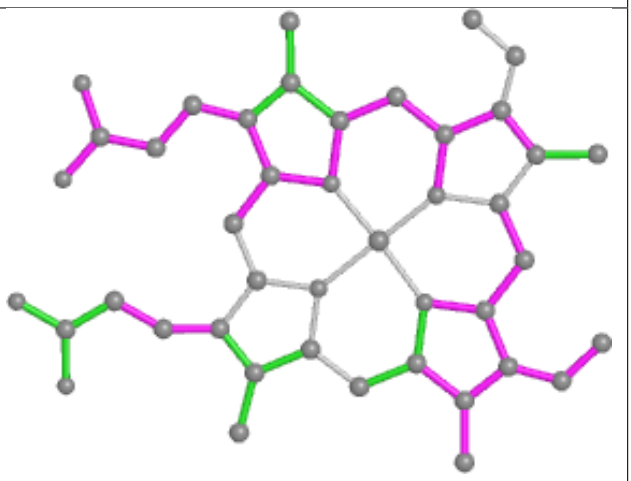
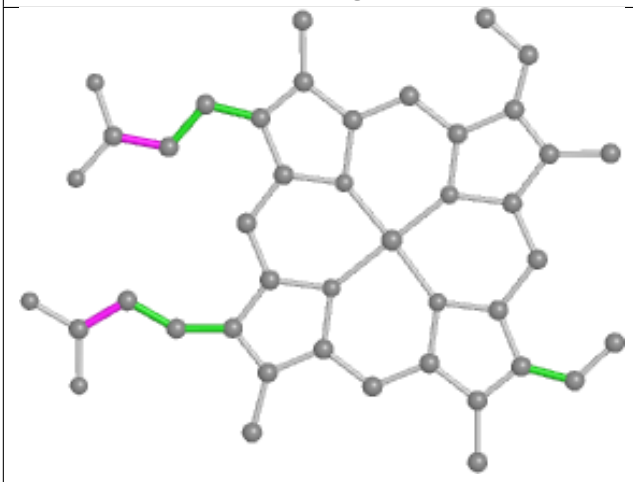
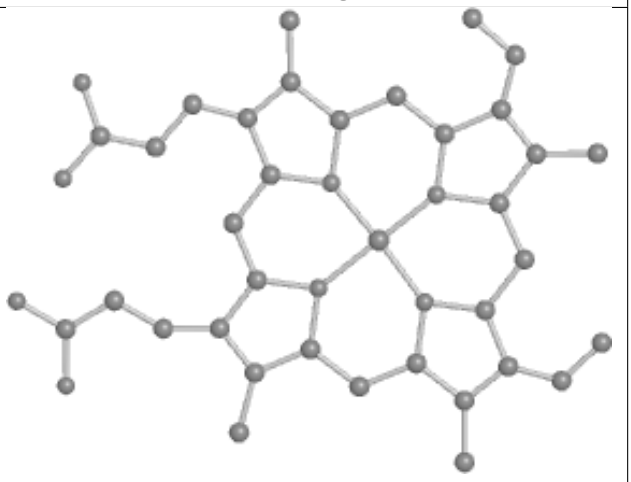


Bond angles

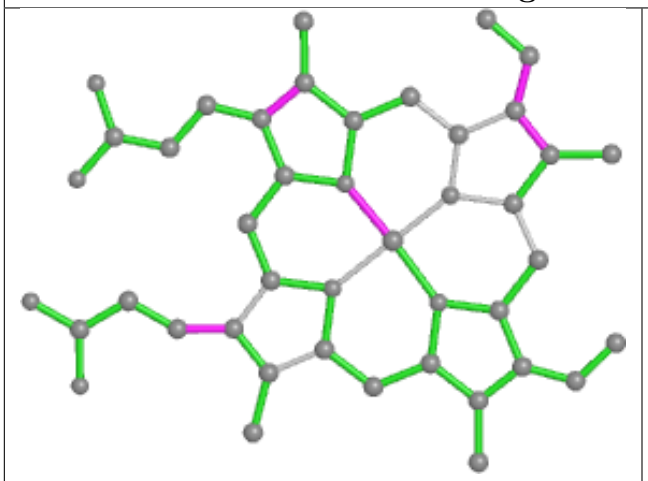


Torsions



Rings

Ligand HEM N 165



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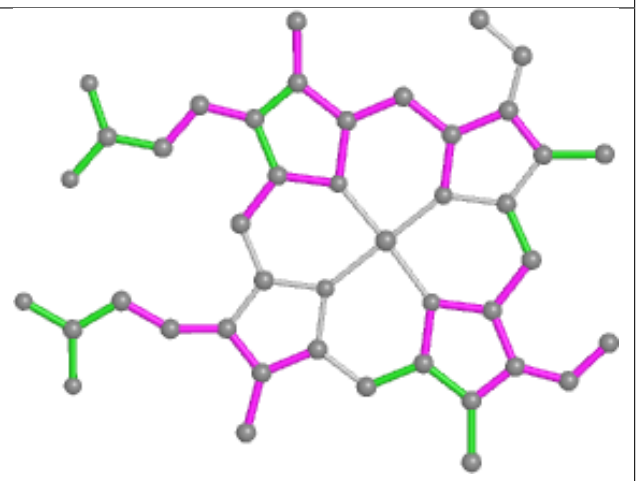
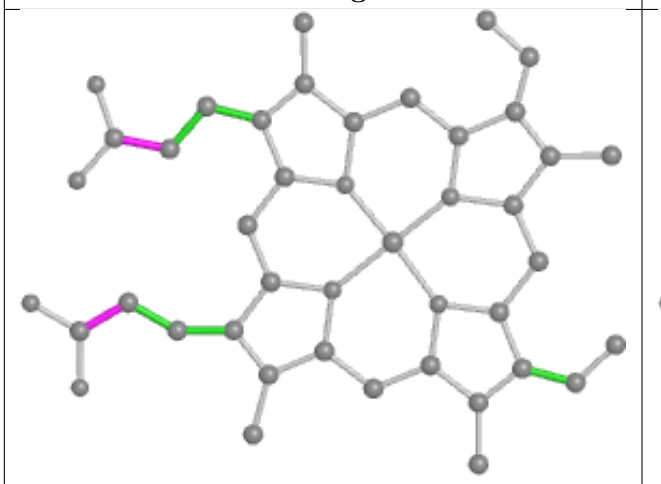


Bond angles



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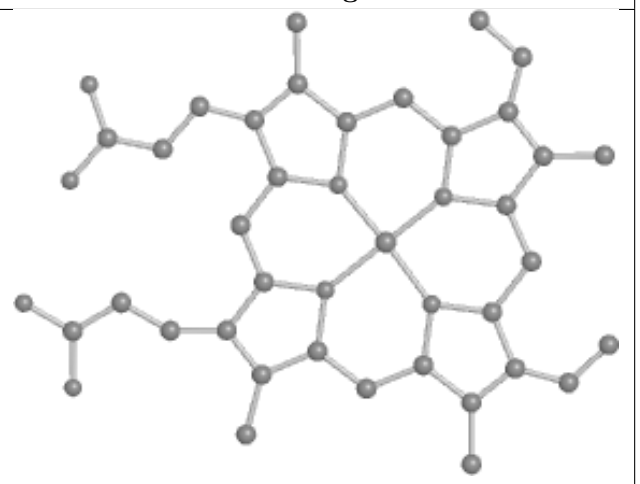
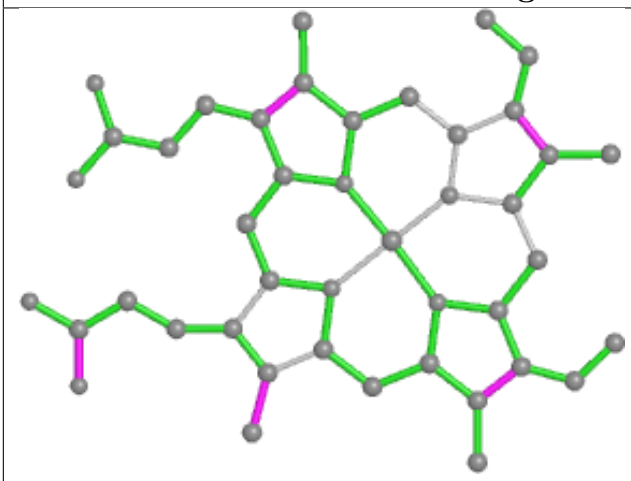


Rings

Ligand HEM H 162



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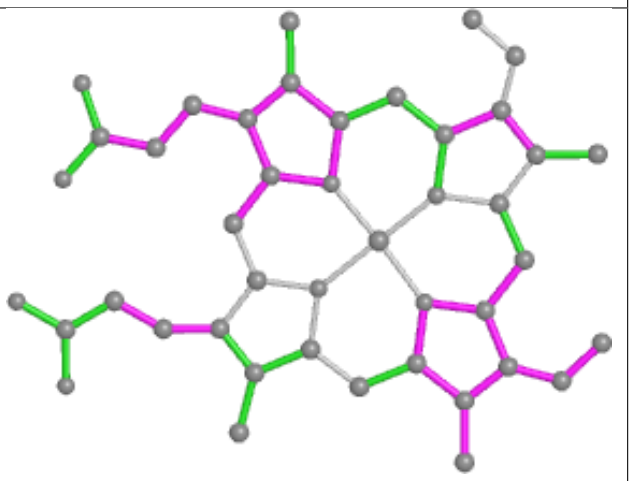
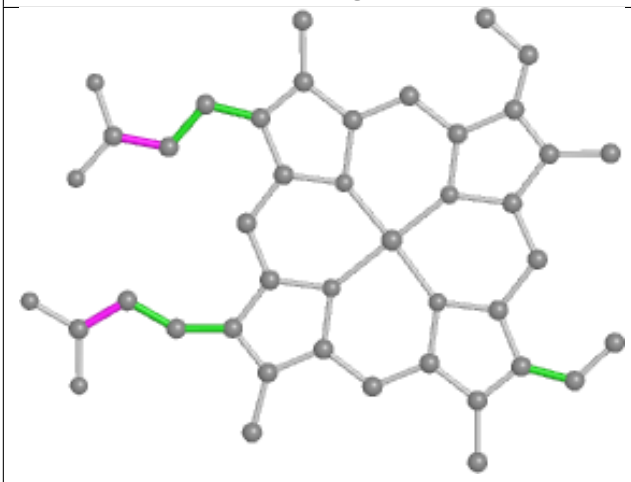


Bond angles



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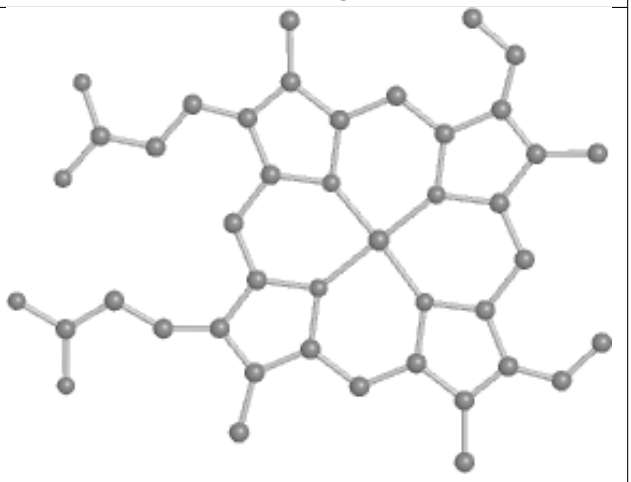
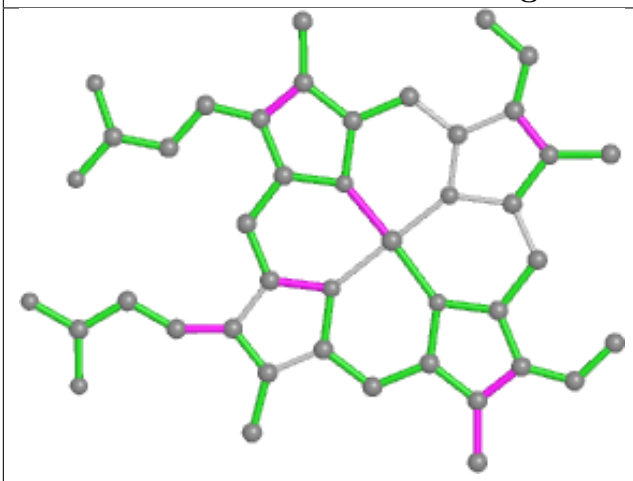


Rings

Ligand HEM F 163



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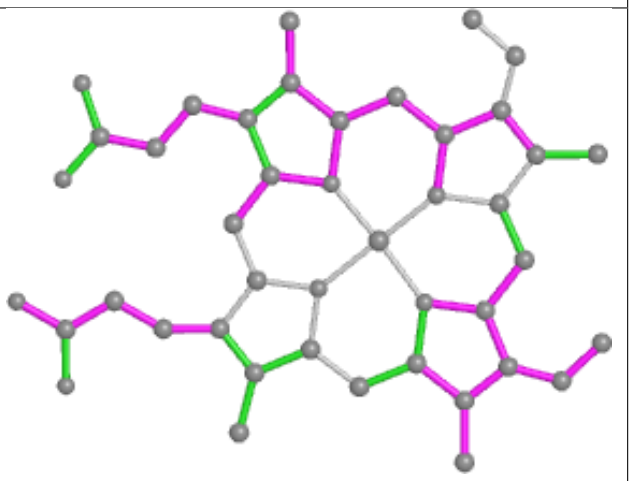
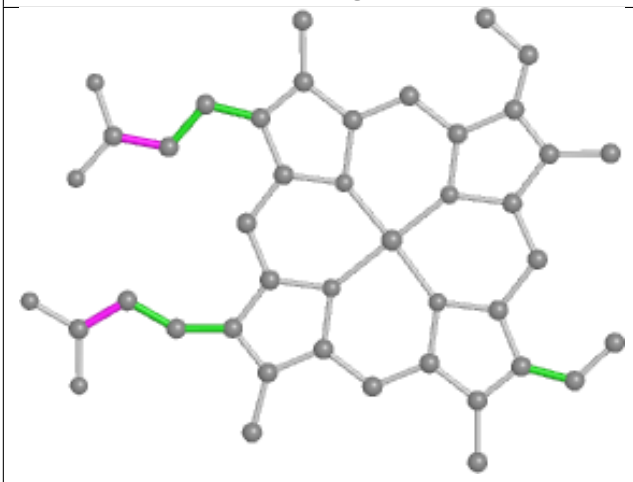


Bond angles



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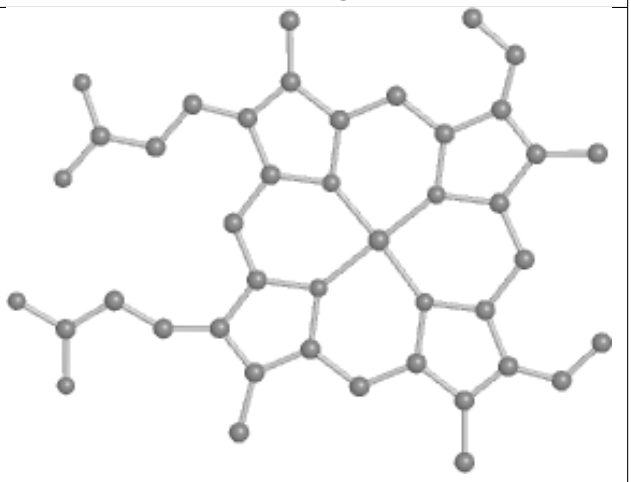
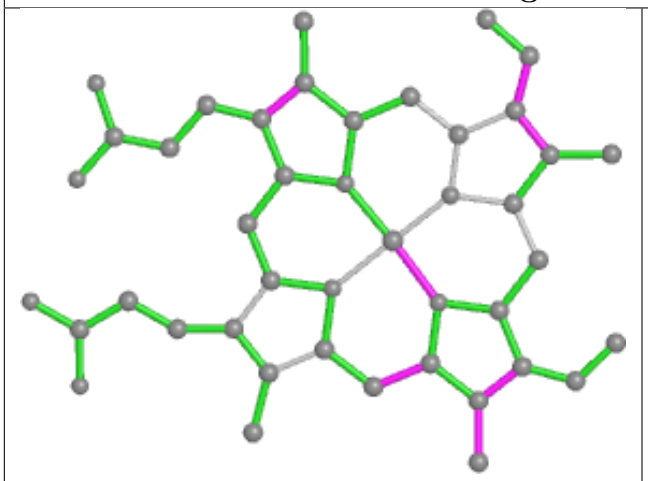


Rings

Ligand HEM P 163



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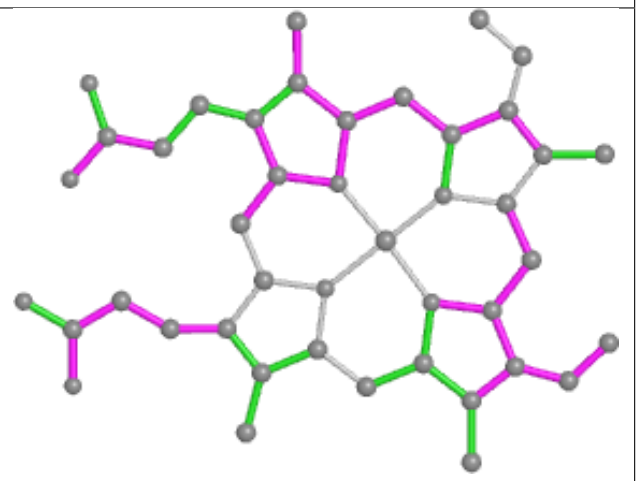
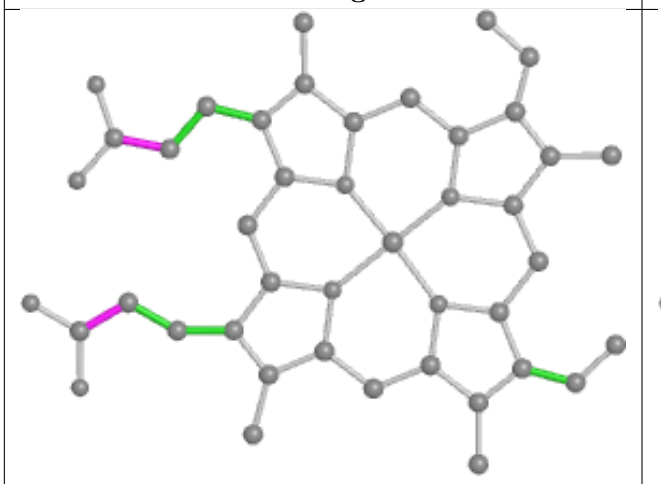
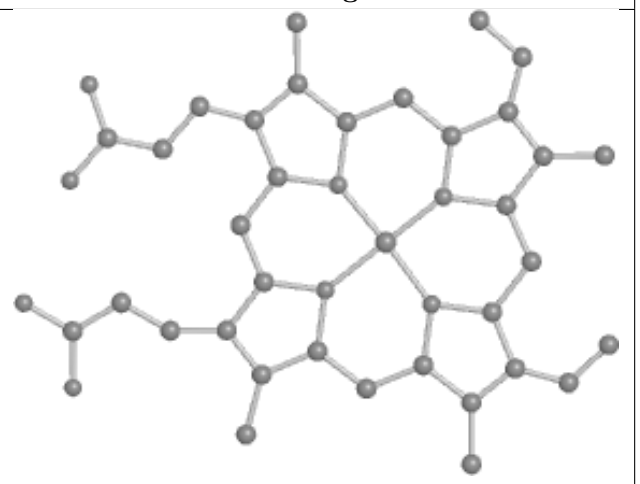


Bond angles

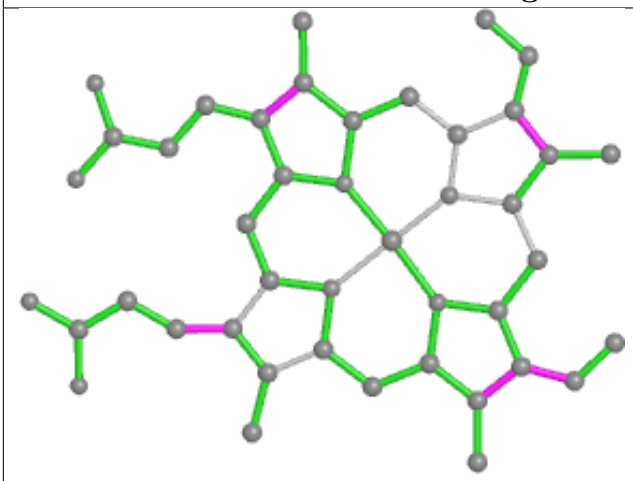


Torsions

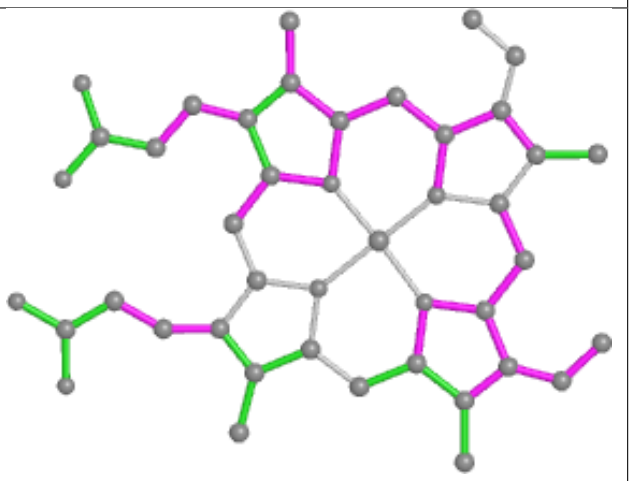


Rings

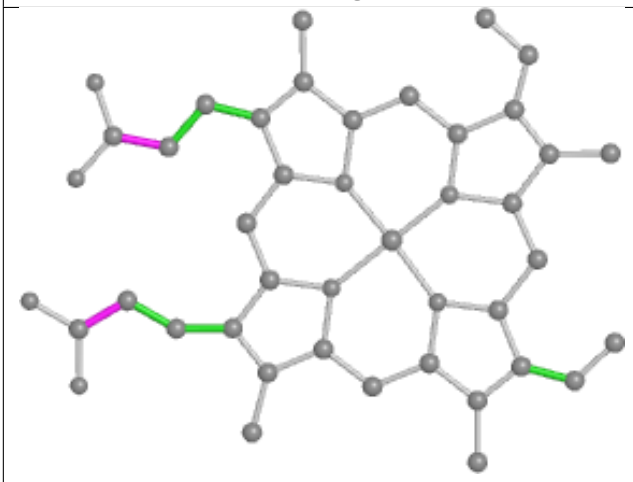
Ligand HEM L 163



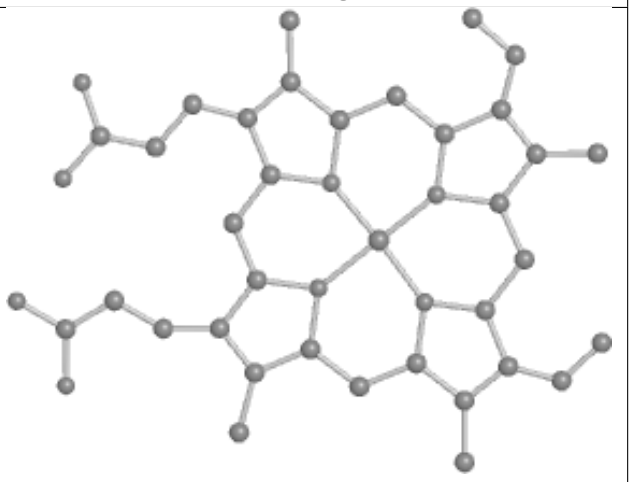
Bond lengths



Bond angles

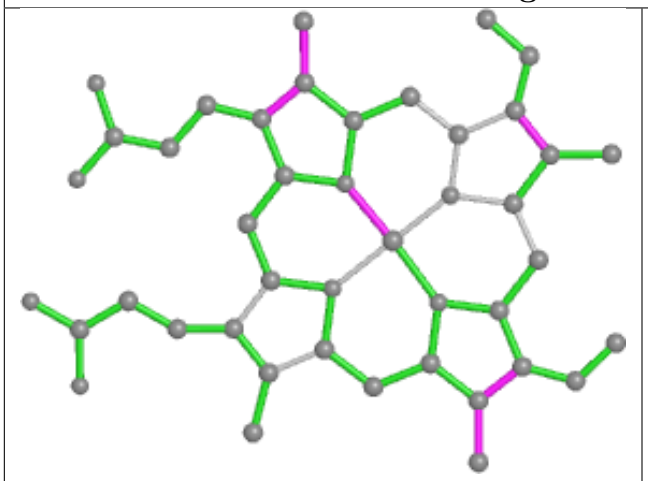


Torsions

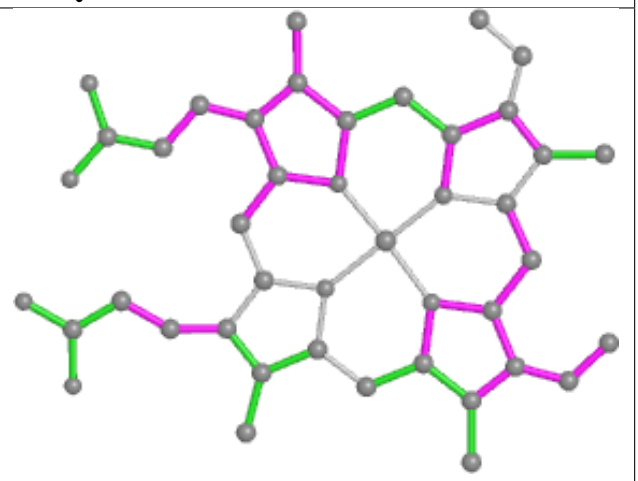


Rings

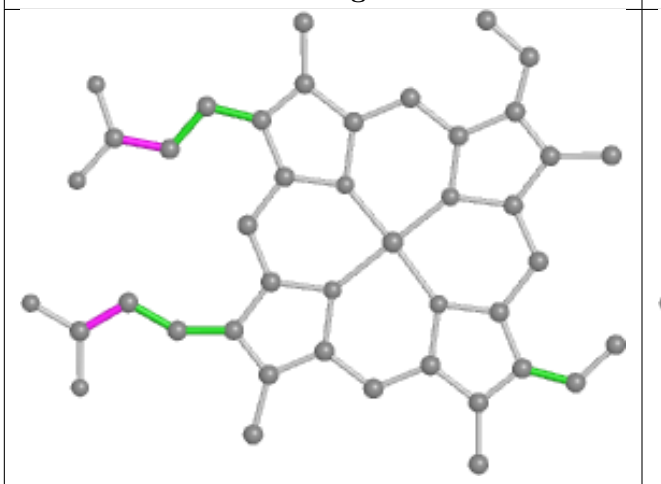
Ligand HEM Q 163



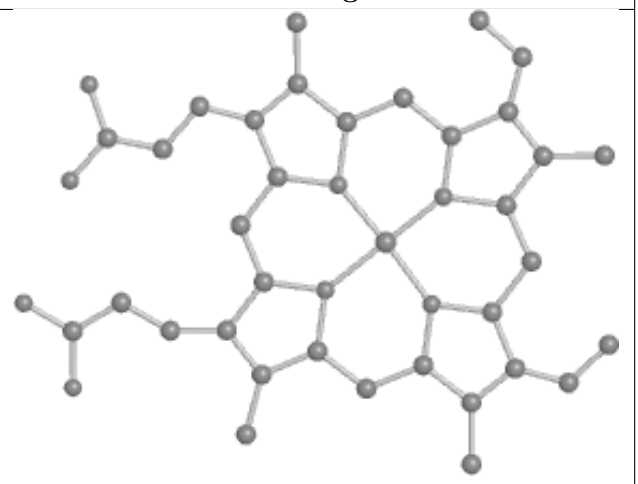
Bond lengths



Bond angles

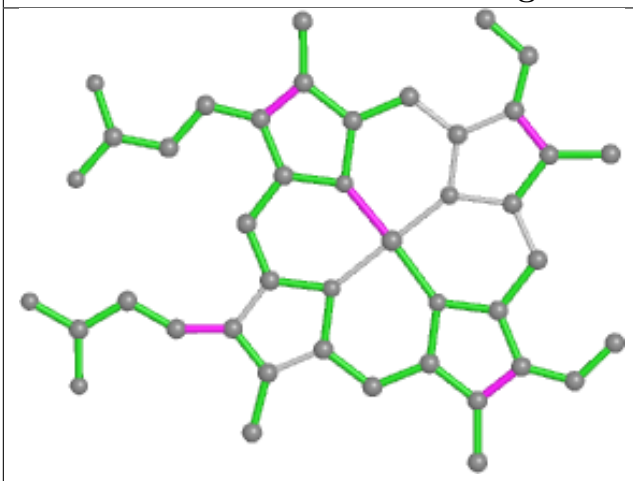


Torsions

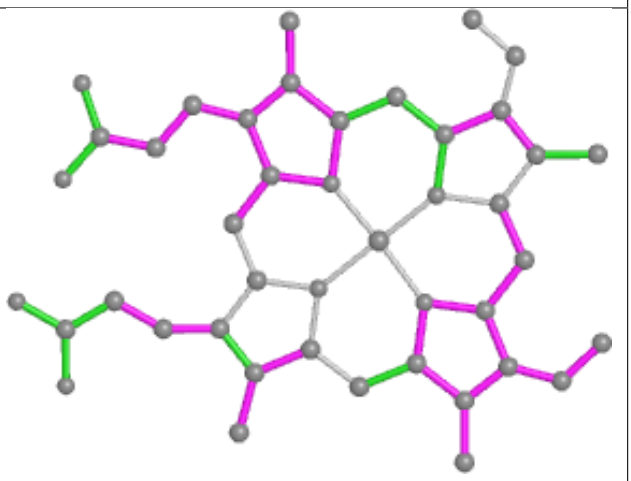


Rings

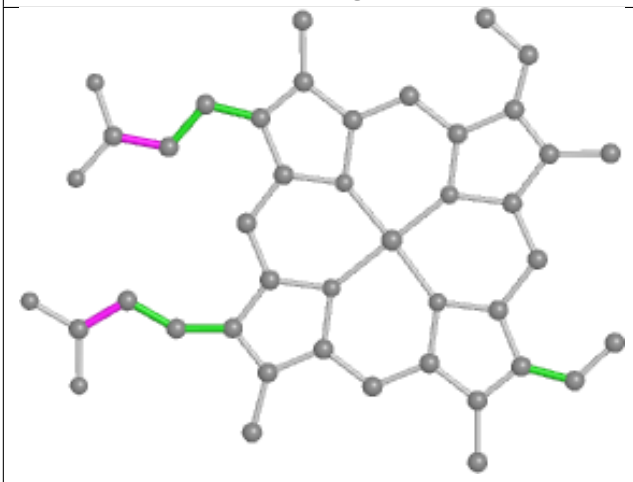
Ligand HEM X 162



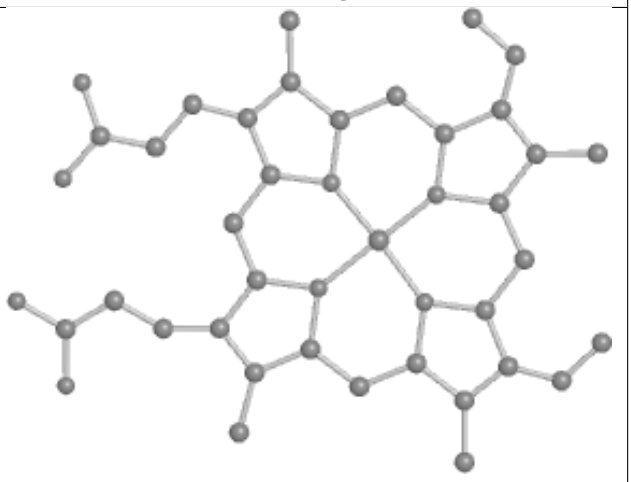
Bond lengths



Bond angles

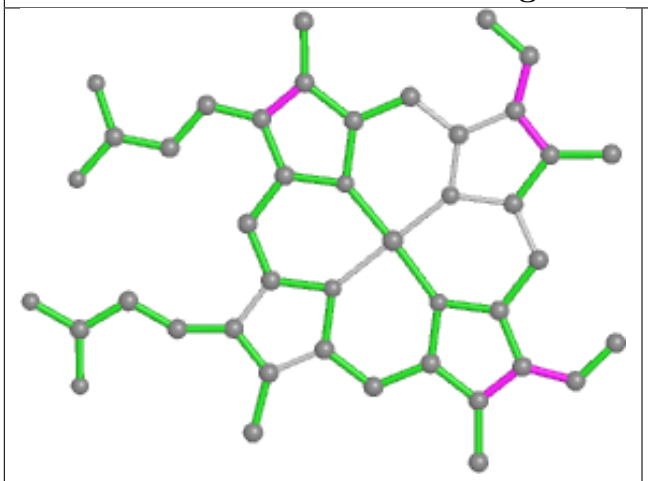


Torsions

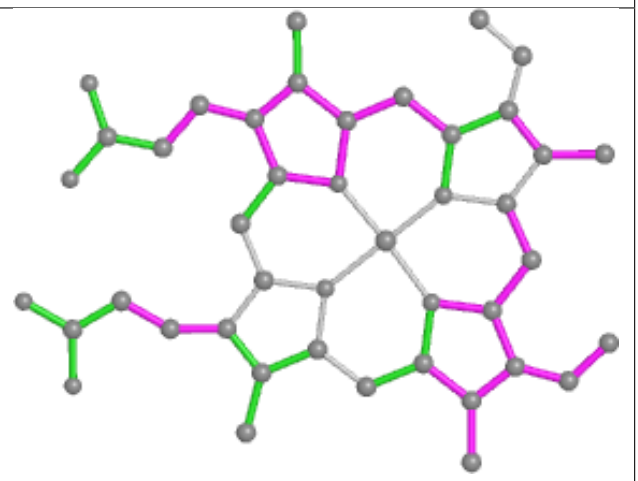


Rings

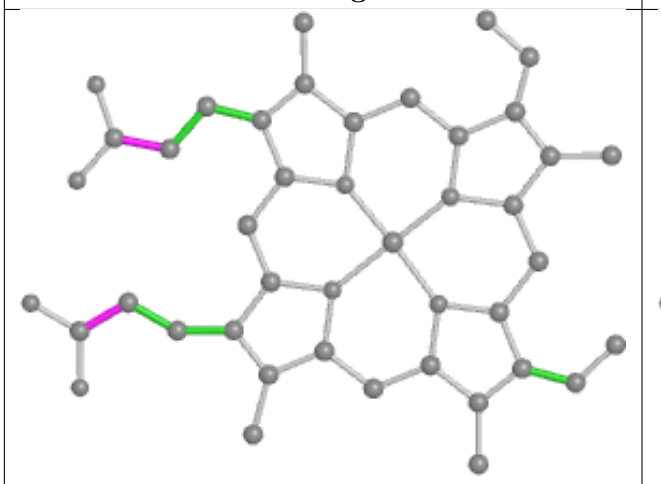
Ligand HEM A 165



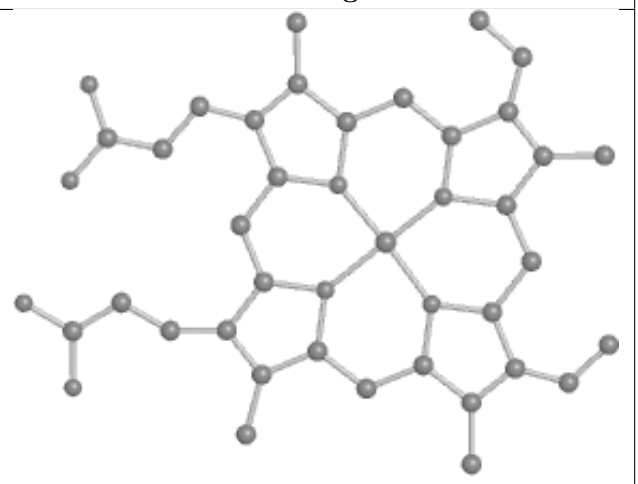
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	155/158 (98%)	-0.51	0	100	100	18, 24, 33, 46	0
1	B	155/158 (98%)	-0.43	0	100	100	17, 23, 35, 46	0
1	C	155/158 (98%)	-0.44	0	100	100	16, 22, 33, 49	0
1	D	154/158 (97%)	-0.39	2 (1%)	77	79	16, 22, 32, 50	0
1	E	155/158 (98%)	-0.49	0	100	100	15, 22, 34, 50	0
1	F	155/158 (98%)	-0.48	0	100	100	16, 22, 32, 43	0
1	G	155/158 (98%)	-0.53	0	100	100	15, 22, 34, 44	0
1	H	154/158 (97%)	-0.43	1 (0%)	89	89	17, 23, 35, 42	0
1	I	154/158 (97%)	-0.45	0	100	100	17, 23, 33, 42	0
1	J	155/158 (98%)	-0.47	0	100	100	17, 22, 32, 44	0
1	K	155/158 (98%)	-0.48	0	100	100	16, 23, 34, 49	0
1	L	155/158 (98%)	-0.44	0	100	100	16, 23, 34, 44	0
1	M	155/158 (98%)	-0.44	0	100	100	19, 25, 35, 47	0
1	N	155/158 (98%)	-0.37	0	100	100	20, 27, 38, 51	0
1	O	155/158 (98%)	-0.46	0	100	100	20, 27, 37, 50	0
1	P	155/158 (98%)	-0.47	0	100	100	20, 25, 36, 47	0
1	Q	155/158 (98%)	-0.43	0	100	100	16, 23, 32, 47	0
1	R	155/158 (98%)	-0.45	0	100	100	16, 23, 33, 48	0
1	S	155/158 (98%)	-0.50	0	100	100	15, 22, 32, 45	0
1	T	155/158 (98%)	-0.47	0	100	100	17, 24, 34, 44	0
1	U	154/158 (97%)	-0.46	0	100	100	15, 21, 30, 38	0
1	V	155/158 (98%)	-0.49	0	100	100	16, 22, 32, 41	0
1	W	155/158 (98%)	-0.40	1 (0%)	89	89	17, 24, 35, 48	0
1	X	155/158 (98%)	-0.40	0	100	100	19, 27, 37, 50	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3716/3792 (97%)	-0.45	4 (0%) 95 96	15, 24, 34, 51	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	GLY	2.8
1	W	4	ASP	2.7
1	D	4	ASP	2.2
1	H	3	GLY	2.2

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
5	SO4	D	163	5/5	0.93	0.22	51,53,53,56	0
5	SO4	M	163	5/5	0.93	0.16	55,55,57,58	0
5	SO4	O	163	5/5	0.93	0.16	56,58,58,59	0
4	HEM	Q	163	43/43	0.94	0.14	23,27,36,39	0
5	SO4	I	164	5/5	0.94	0.19	55,55,57,58	0
4	HEM	S	163	43/43	0.95	0.13	23,27,34,38	0
4	HEM	X	162	43/43	0.95	0.12	25,28,38,44	0
5	SO4	B	165	5/5	0.95	0.19	51,52,55,55	0
2	FE2	N	163	1/1	0.95	0.04	39,39,39,39	0
4	HEM	L	163	43/43	0.95	0.14	21,26,34,40	0
4	HEM	N	165	43/43	0.95	0.14	25,30,37,40	0
2	FE2	M	162	1/1	0.95	0.04	42,42,42,42	0
5	SO4	R	163	5/5	0.95	0.15	47,48,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HEM	C	165	43/43	0.96	0.13	20,24,34,39	0
4	HEM	U	162	43/43	0.96	0.13	21,24,35,37	0
4	HEM	F	163	43/43	0.96	0.13	21,27,37,41	0
4	HEM	H	162	43/43	0.96	0.12	21,25,35,38	0
4	HEM	I	163	43/43	0.96	0.13	21,27,34,38	0
5	SO4	F	164	5/5	0.96	0.15	48,50,52,52	0
2	FE2	G	163	1/1	0.96	0.07	37,37,37,37	0
2	FE2	X	161	1/1	0.96	0.04	42,42,42,42	0
4	HEM	P	163	43/43	0.96	0.15	25,31,37,44	0
4	HEM	A	165	43/43	0.96	0.13	22,27,34,37	0
5	SO4	A	166	5/5	0.97	0.17	49,49,51,51	0
2	FE2	H	161	1/1	0.97	0.06	39,39,39,39	0
3	K	N	164	1/1	0.98	0.06	31,31,31,31	0
2	FE2	D	161	1/1	0.98	0.06	37,37,37,37	0
2	FE2	N	160	1/1	0.98	0.08	27,27,27,27	0
2	FE2	E	163	1/1	0.98	0.05	36,36,36,36	0
2	FE2	O	162	1/1	0.98	0.04	45,45,45,45	0
2	FE2	R	162	1/1	0.98	0.05	32,32,32,32	0
2	FE2	L	161	1/1	0.98	0.04	34,34,34,34	0
2	FE2	M	160	1/1	0.99	0.07	27,27,27,27	0
2	FE2	M	161	1/1	0.99	0.04	34,34,34,34	0
2	FE2	C	163	1/1	0.99	0.05	32,32,32,32	0
2	FE2	D	159	1/1	0.99	0.09	26,26,26,26	0
2	FE2	N	162	1/1	0.99	0.04	39,39,39,39	0
2	FE2	A	160	1/1	0.99	0.07	24,24,24,24	0
2	FE2	O	160	1/1	0.99	0.05	30,30,30,30	0
2	FE2	O	161	1/1	0.99	0.03	39,39,39,39	0
2	FE2	D	162	1/1	0.99	0.04	35,35,35,35	0
2	FE2	P	159	1/1	0.99	0.06	29,29,29,29	0
2	FE2	P	160	1/1	0.99	0.06	28,28,28,28	0
2	FE2	P	162	1/1	0.99	0.03	40,40,40,40	0
2	FE2	Q	159	1/1	0.99	0.05	24,24,24,24	0
2	FE2	Q	161	1/1	0.99	0.08	25,25,25,25	0
2	FE2	Q	162	1/1	0.99	0.05	31,31,31,31	0
2	FE2	R	161	1/1	0.99	0.04	29,29,29,29	0
2	FE2	E	160	1/1	0.99	0.07	24,24,24,24	0
2	FE2	S	159	1/1	0.99	0.08	22,22,22,22	0
2	FE2	S	162	1/1	0.99	0.04	32,32,32,32	0
2	FE2	T	159	1/1	0.99	0.08	23,23,23,23	0
2	FE2	T	160	1/1	0.99	0.05	36,36,36,36	0
2	FE2	U	161	1/1	0.99	0.04	35,35,35,35	0
2	FE2	V	160	1/1	0.99	0.04	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	V	161	1/1	0.99	0.04	32,32,32,32	0
2	FE2	W	159	1/1	0.99	0.06	26,26,26,26	0
2	FE2	W	160	1/1	0.99	0.03	35,35,35,35	0
2	FE2	X	159	1/1	0.99	0.08	28,28,28,28	0
2	FE2	X	160	1/1	0.99	0.04	38,38,38,38	0
2	FE2	E	162	1/1	0.99	0.04	35,35,35,35	0
3	K	A	164	1/1	0.99	0.08	32,32,32,32	0
3	K	B	164	1/1	0.99	0.05	27,27,27,27	0
3	K	C	164	1/1	0.99	0.09	24,24,24,24	0
3	K	G	164	1/1	0.99	0.07	33,33,33,33	0
2	FE2	A	161	1/1	0.99	0.08	24,24,24,24	0
2	FE2	F	160	1/1	0.99	0.09	26,26,26,26	0
2	FE2	F	162	1/1	0.99	0.04	31,31,31,31	0
2	FE2	G	159	1/1	0.99	0.07	24,24,24,24	0
2	FE2	G	160	1/1	0.99	0.09	24,24,24,24	0
2	FE2	G	161	1/1	0.99	0.07	22,22,22,22	0
2	FE2	G	162	1/1	0.99	0.06	35,35,35,35	0
2	FE2	A	162	1/1	0.99	0.05	26,26,26,26	0
2	FE2	H	159	1/1	0.99	0.07	27,27,27,27	0
2	FE2	H	160	1/1	0.99	0.05	36,36,36,36	0
2	FE2	B	160	1/1	0.99	0.06	25,25,25,25	0
2	FE2	I	159	1/1	0.99	0.07	27,27,27,27	0
2	FE2	I	161	1/1	0.99	0.04	35,35,35,35	0
2	FE2	J	159	1/1	0.99	0.06	24,24,24,24	0
2	FE2	J	161	1/1	0.99	0.08	43,43,43,43	0
2	FE2	J	162	1/1	0.99	0.04	36,36,36,36	0
2	FE2	K	159	1/1	0.99	0.07	24,24,24,24	0
2	FE2	K	161	1/1	0.99	0.05	31,31,31,31	0
2	FE2	L	159	1/1	0.99	0.08	24,24,24,24	0
2	FE2	B	163	1/1	0.99	0.04	33,33,33,33	0
2	FE2	L	162	1/1	0.99	0.05	32,32,32,32	0
2	FE2	B	162	1/1	1.00	0.03	35,35,35,35	0
2	FE2	V	159	1/1	1.00	0.07	23,23,23,23	0
2	FE2	E	159	1/1	1.00	0.06	21,21,21,21	0
2	FE2	A	163	1/1	1.00	0.04	37,37,37,37	0
2	FE2	N	159	1/1	1.00	0.06	29,29,29,29	0
2	FE2	E	161	1/1	1.00	0.06	21,21,21,21	0
2	FE2	W	161	1/1	1.00	0.05	33,33,33,33	0
2	FE2	N	161	1/1	1.00	0.06	28,28,28,28	0
2	FE2	C	159	1/1	1.00	0.10	19,19,19,19	0
2	FE2	I	160	1/1	1.00	0.05	25,25,25,25	0
2	FE2	O	159	1/1	1.00	0.07	23,23,23,23	0

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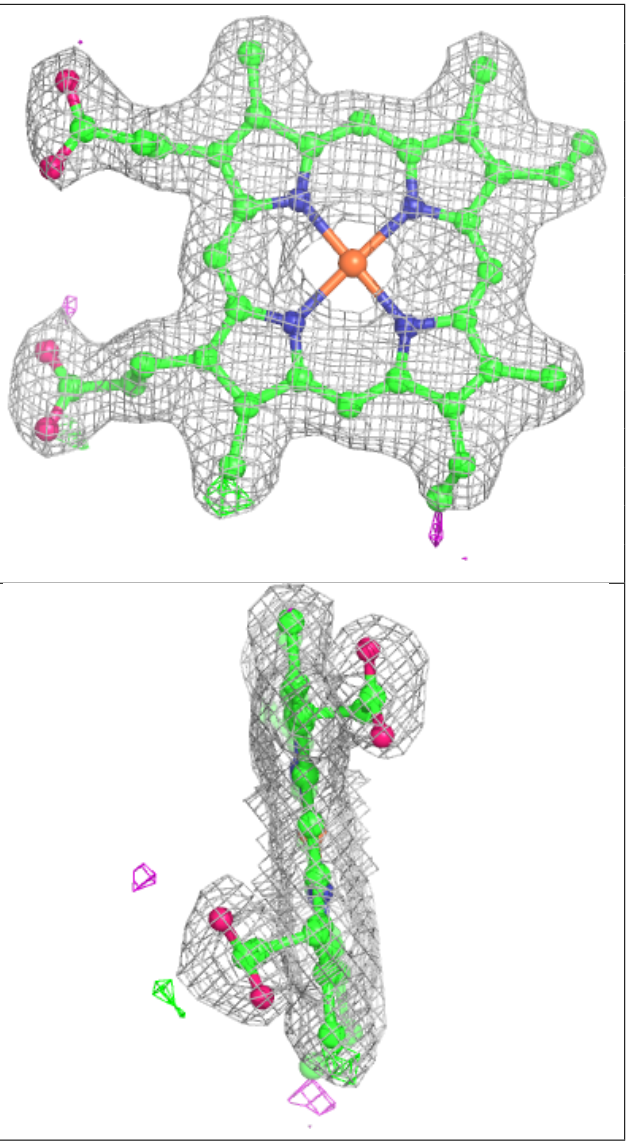
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	C	160	1/1	1.00	0.09	21,21,21,21	0
2	FE2	I	162	1/1	1.00	0.04	37,37,37,37	0
3	K	E	164	1/1	1.00	0.06	26,26,26,26	0
2	FE2	F	159	1/1	1.00	0.07	24,24,24,24	0
2	FE2	J	160	1/1	1.00	0.07	24,24,24,24	0
2	FE2	C	161	1/1	1.00	0.07	23,23,23,23	0
2	FE2	P	161	1/1	1.00	0.03	35,35,35,35	0
2	FE2	F	161	1/1	1.00	0.04	32,32,32,32	0
2	FE2	C	162	1/1	1.00	0.04	33,33,33,33	0
2	FE2	Q	160	1/1	1.00	0.07	21,21,21,21	0
2	FE2	K	160	1/1	1.00	0.07	24,24,24,24	0
2	FE2	B	159	1/1	1.00	0.05	25,25,25,25	0
2	FE2	R	159	1/1	1.00	0.07	25,25,25,25	0
2	FE2	R	160	1/1	1.00	0.09	23,23,23,23	0
2	FE2	K	162	1/1	1.00	0.03	31,31,31,31	0
2	FE2	A	159	1/1	1.00	0.05	25,25,25,25	0
2	FE2	L	160	1/1	1.00	0.09	26,26,26,26	0
2	FE2	S	160	1/1	1.00	0.09	25,25,25,25	0
2	FE2	S	161	1/1	1.00	0.04	33,33,33,33	0
2	FE2	D	160	1/1	1.00	0.09	24,24,24,24	0
2	FE2	B	161	1/1	1.00	0.08	25,25,25,25	0
2	FE2	M	159	1/1	1.00	0.06	28,28,28,28	0
2	FE2	T	161	1/1	1.00	0.03	33,33,33,33	0
2	FE2	U	159	1/1	1.00	0.06	25,25,25,25	0
2	FE2	U	160	1/1	1.00	0.03	32,32,32,32	0

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

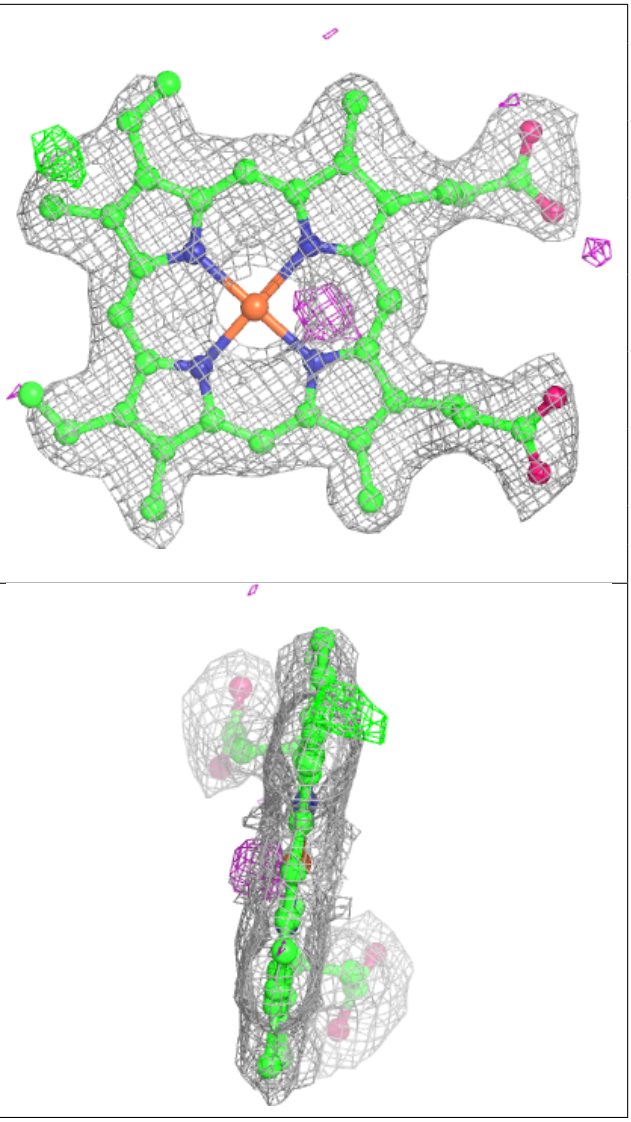
Electron density around HEM Q 163:

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



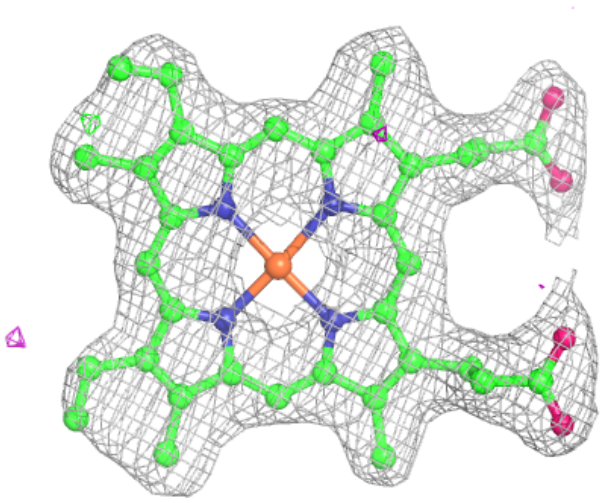
Electron density around HEM S 163:

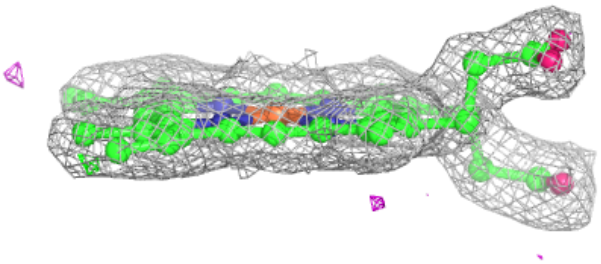
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

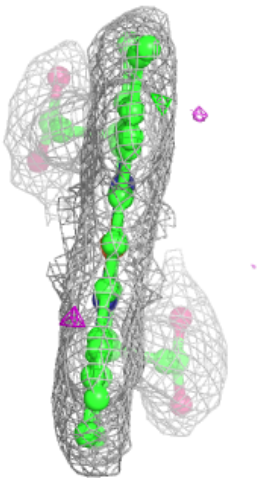


Electron density around HEM X 162:

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

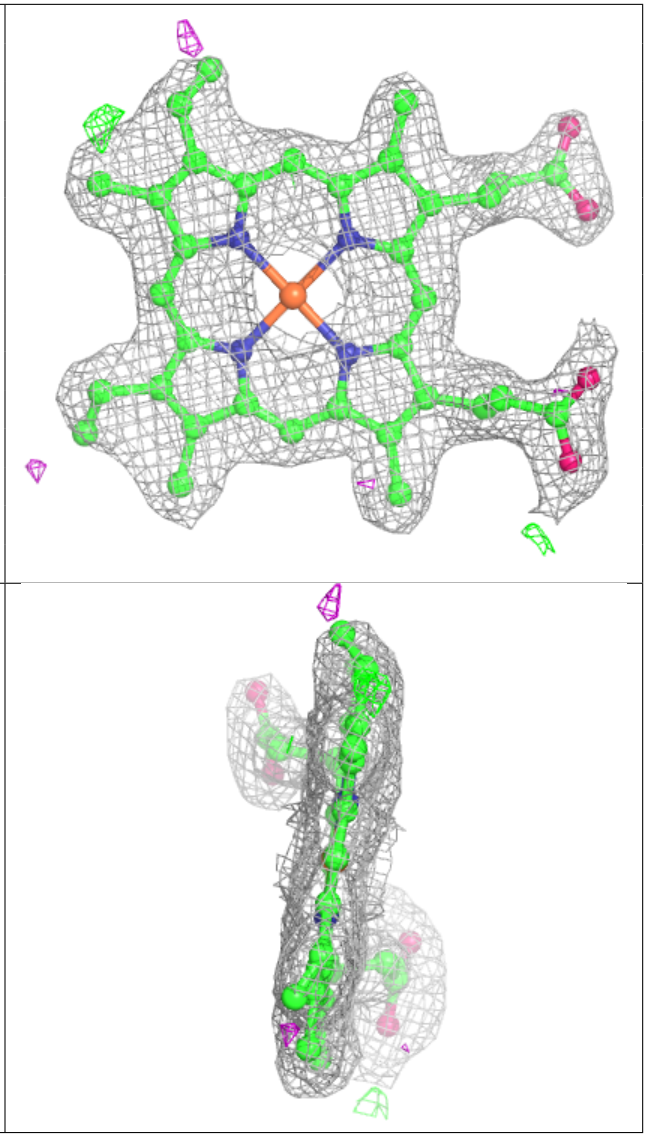






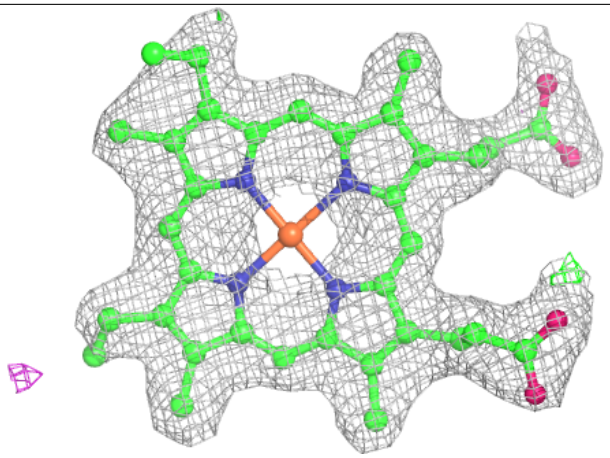
Electron density around HEM L 163:

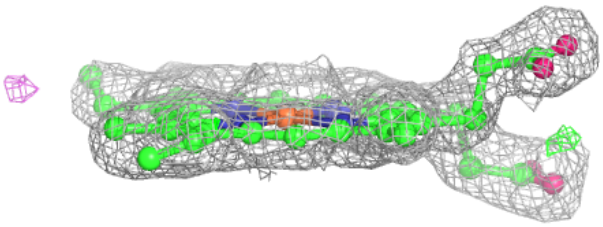
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

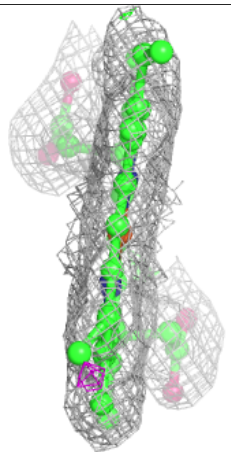


Electron density around HEM N 165:

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

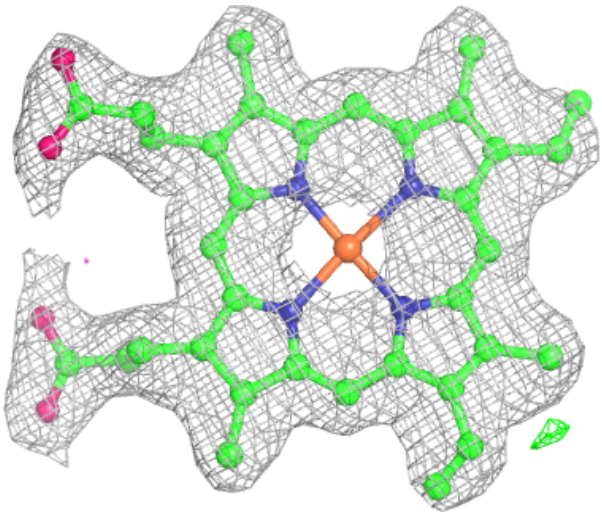


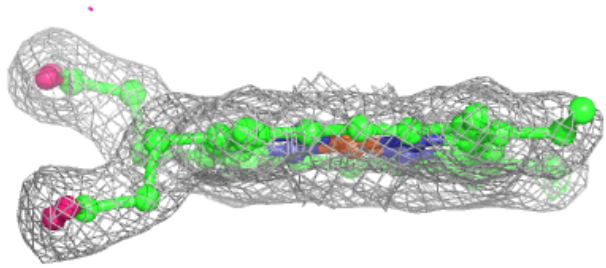


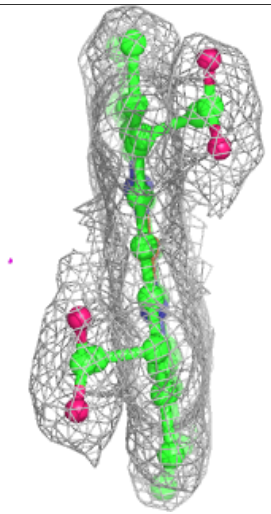


Electron density around HEM C 165:

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

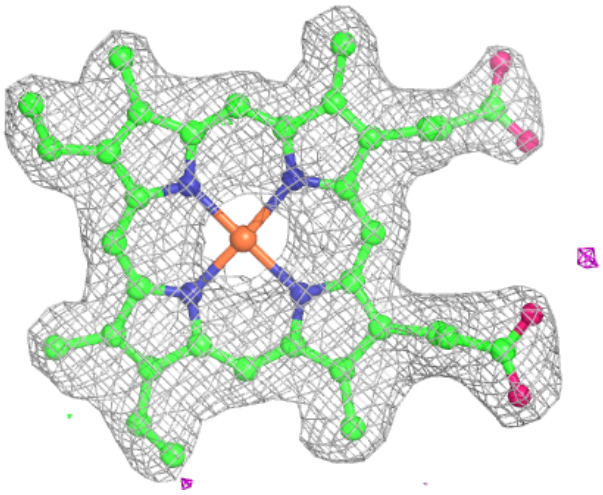


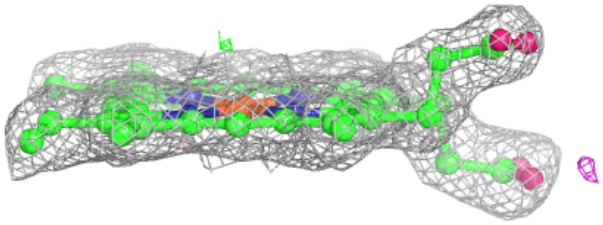


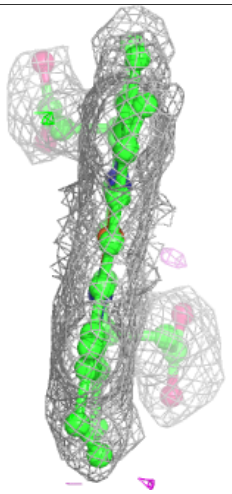


Electron density around HEM U 162:

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

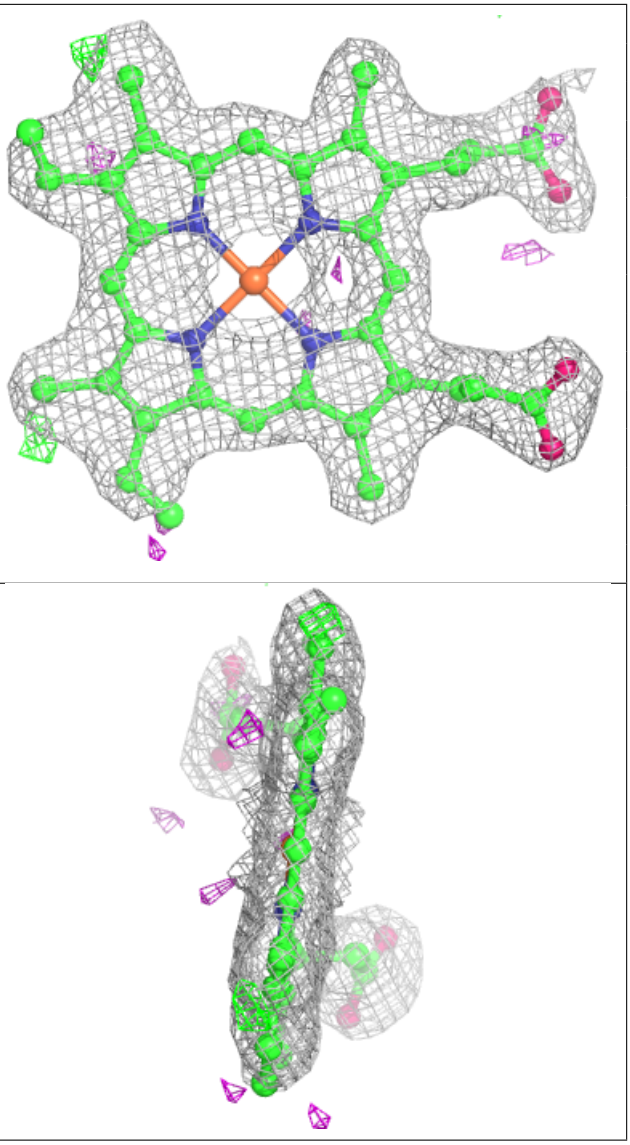






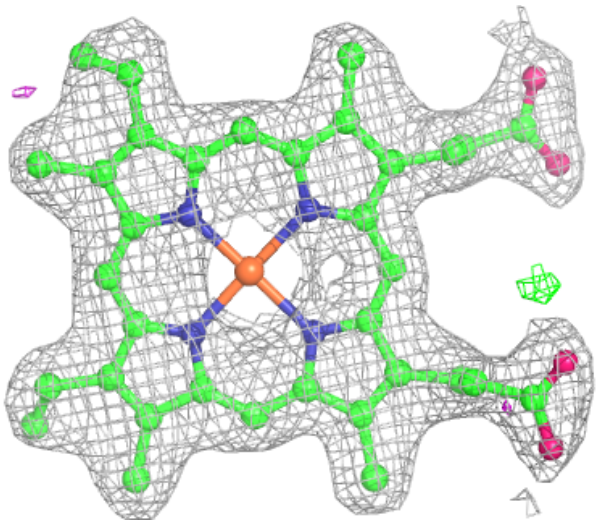
Electron density around HEM F 163:

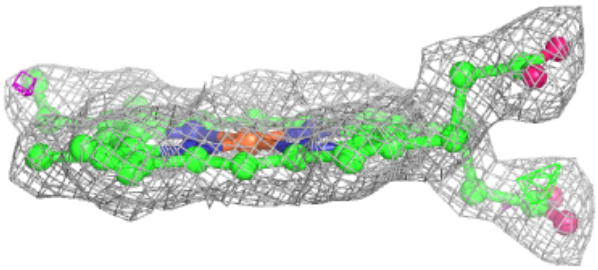
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

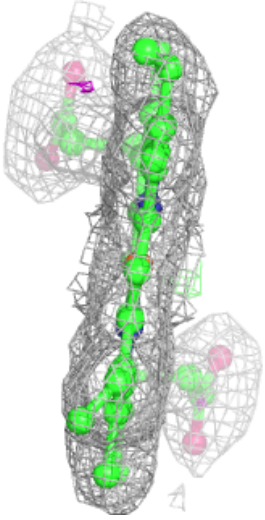


Electron density around HEM H 162:

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

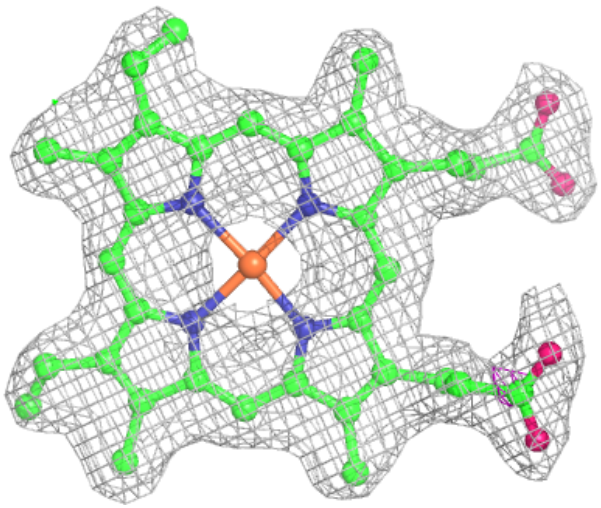


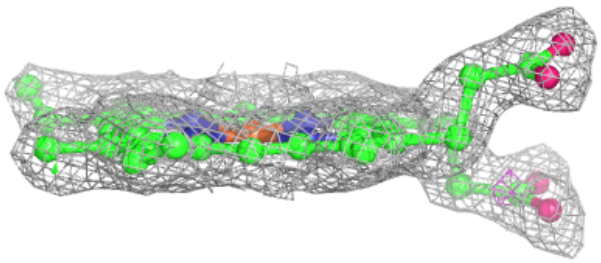


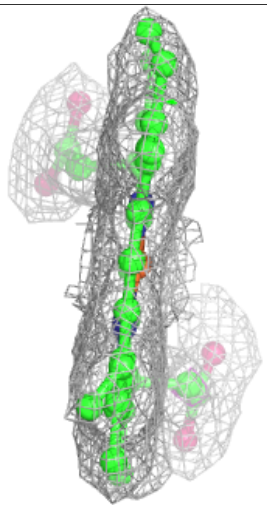


Electron density around HEM I 163:

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

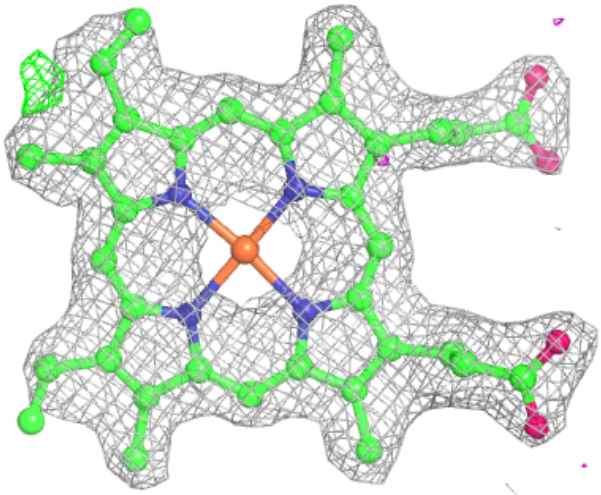


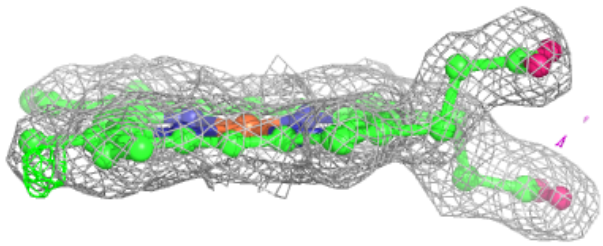




Electron density around HEM P 163:

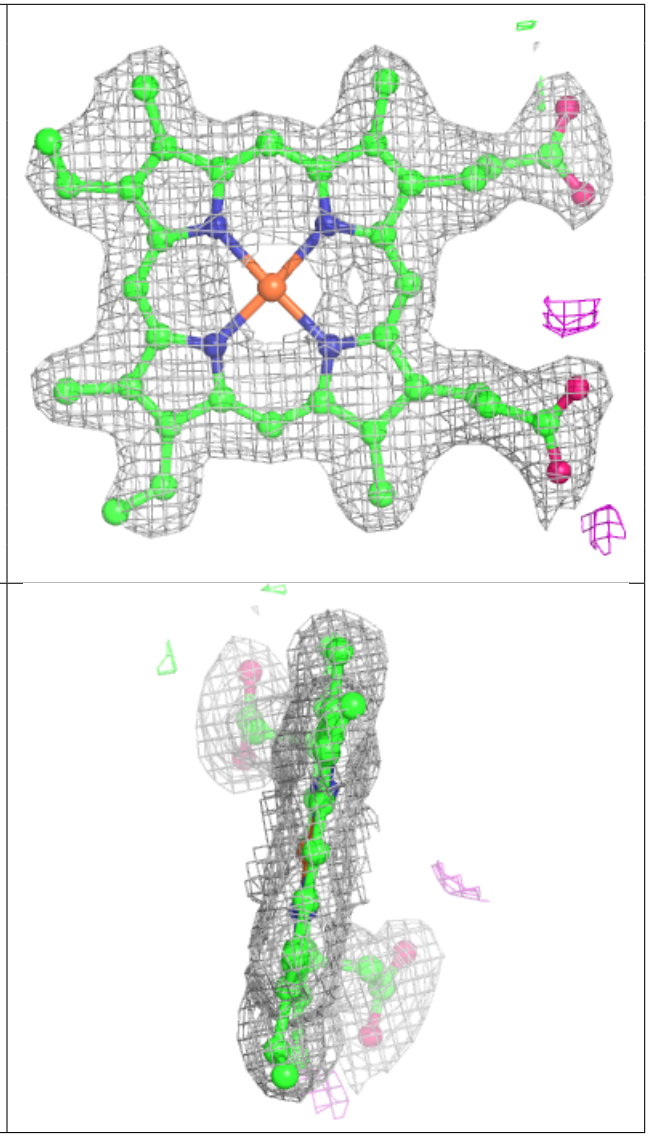
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEM A 165:

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



6.5 Other polymers (i)

There are no such residues in this entry.